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for U.S. Nuclear Regulatory Commission

A HANDBOOK OF MATERIALS PROPERTIES FOR USE IN THE ANALYSIS OF LIGHT WATER REACTOR FUEL ROD BEHAVIOR

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To

August 1981



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NUREG/CR-0479 TREE-1280, Rev. 2 R3 and R4

MATPRO-VERSION 11 (REVISION 2) A HANDBOOK OF MATERIALS PROPERTIES FOR USE IN THE ANALYSIS OF LIGHT WATER REACTOR FUEL ROD BEHAVIOR

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ABSTRACT

This handbook describes the materials properties correlations and computer subcodes, MATPRO-Version 11 (Revision 2) developed for use with various LWR fuel rod behavior analytical programs at the Idaho National Engineering Laboratory. Formulations of fuel rod material properties, which are generally semiemph.¹ d in nature, are presented for uranium dioxide and mixed uranium-plutonium dioxide fuel, zirr sloy cladding, and fill gas mixtures.



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APPENDIX A FUEL MATERIAL PROPERTIES

Fifteen materials properties of light water reactor fuel have been modeled for inclusion in MATPRO-Version 11. The apsoaches range from (a) a least-squares fit to available data using a polynomial or other function having little or no theoretical basis to (b) a semiempirical correlation employing an analytical expression suggested by theory with constants determined by comparison with data. The intent of current and future work is to take the second approach whenever possible.

Each material property description includes a listing of a FORTRAN subcode which may be used to calculate the value of the property for various input conditions. All 15 MATPRO fuel subcodes have temperature as an argument. In addition, many are functions of burnup, plutonia content, density, time, and other variables.

Several of the subcodes use a physical properties subcode (PHYPRO, Appendix D, Section 1) to get fuel melting temperatures and heats of fusion. These and other commonly used material parameters are placed in a common block by this separate routine and are thus available to all other subprograms in MATPRO.

1. FUEL SPECIFIC HEAT CAPACITY (FCP) AND FUEL ENTHALPY (FENTHL) (G. A. Revmann)

The specific heat capacity of nuclear fuel is needed for time-dependent temperature calculations. The stored energy, or enthalpy, is calculated from the specific heat capacity. Stored energy is important in reactor transient analysis because the severity of the transient is greatly affected by the initial stored energy of the fuel.

1.1 Summary

The specific heat capacity and enthalpy of nuclear fuel are modeled empirically as functions of four parameters: temperature, composition, molten fraction, and oxygen-to-metal ratio. Since UO2 and PuO2 are the principal LWR fuels, they are the constituents considered. The correlations for fuel specific heat and enthalpy are valid for temperatures from 300 K to more than 4000 K.

Equations for the specific heat and enthalpy of solid UO₂ and PuO₂ are assumed to have the same form, but with afferent constants. The basic equations are

FCP =
$$\frac{K_1 \theta^2 \exp(\theta/T)}{T^2 \left[\exp(\theta/T) - 1\right]^2} + K_2 T + \frac{Y K_3 E_D}{2 R T^2} \exp(-E_D/RT)$$
 (A-1.1a)

and

FENTHL =
$$\frac{K_1^{\theta}}{\exp(\theta/T) - 1} + \frac{K_2^{T^2}}{2} + \frac{Y}{2}K_3^{exp(-E_D/RT)}$$
 (A-1.1b)

9

where

FCP specific heat capacity (J/kg•K)

FENTHL = fuel enthalpy (J/kg)





Т	=	temperature (K)
Y	=	oxygen-to-metal ratio
R	=	8.3143 (J/mol•K)
θ		the Einstein temperature (K

and the constants are given in Table A-1.1.

TABLE A-1.1

Contraction and strate in second of second data	and the second		
Constant	UO ₂	PuO2	Units
K1	296.7	347.4	J/kg*K
Kg	2.43×10^{-2}	3.95 x 10 ⁻⁴	J/kg*K ²
K3	8.745 x 10 ⁷	2.860×10^{7}	J/kg
θ	535.285	571.000	K
ED	1.577×10^{5}	1.967×10^{5}	J/mol

CONSTANTS USED IN UO2 AND PuO2 HEAT CAPACITY AND ENTHALPY CORRELATIONS

The specific heat capacities of UO2 and PuO2 in the liquid state are given by

$FCP = 503 J/kg \cdot K$.

For a mixture of UO₂ and PuO₂, the specific heat capacity of the solid is determined by combining the contribution from each constituent in proportion to its weight fraction. When the material is partially molten, the heat capacity is determined similarly with a seighted sum. The standard error of the UO₂ specific heat capacity correlation is $\pm 3 \text{ J/kg} \cdot \text{K}$; and for the mixed oxide specific heat capacity correlation, it is 6 to 10 J/kg \cdot K, depending on the fraction of PuO₂. For nonstoichiometric fuels, these uncertainties are approximately doubled.

Inspection of Equations (A-1.1a) and (A-1.b) shows that the fuel enthalpy correlation is simply the integral of fuel specific heat correlation from zero kelvin to T kelvin. Because the specific heat correlation is only valid above a fuel temperature of about 300 K, the fuel enthalpy correlation is also not valid below a temperature of about 300 K. Therefore, it is necessary to calculate fuel enthalpy with respect to a reference temperature \geq 300 K. Thus, the fuel enthalpy at any desired temperature, T, is calculated by evaluating Equation (A-1.1b) at T and at any desired reference temperature, T_{REF}, and taking the difference FENTHL(T) - FENTHL(T_{REF}). For temperatures greater than 2 K below melting, the molten fraction and heat of fusion are used to interpolate between the enthalpy of unmelted fuel and just melted fuel at the melting temperature.

Section 1.2 is a review of the surveyed literature. The model development is presented in Section 1.3. Model predictions are compared with data in Section 1.4. An uncertainty analysis is given in Section 1.5. The FORTRAN subcode listings are in Section 1.6, and the references are given in Section 1.7. A bibliography is given in Section 1.8.

10



(A-1.2)

1.2 Review of Literature

An important source for fuel specific heat capacity data is the extensive review by Kerrisk and Clifton.^{A-1.1} Additional data from Kruger and Savage^{A-1.2} are used to find the parameters for PuO_2 in Equation (A-1.1a). The heat capacity of liquid fuel is taken from Leibowitz.^{A-1.3}

1.2.1 Limitations of the Data Source. The data used by Kerrisk and Clifton cover a wide range of temperatures (483 to 3107 K), but these data are restricted to nearly stoichiometric material (oxygen-to-metal ratio between about 2.00 and 2.015). The data of Kruger and Savage are limited in that the highest temperature was only 1400 K, which is well below the melting point of about 2600 K for PuO₂. Their data are also restricted to approximately stoichiometric PuO₂. The oxygen-to-metal ratio has been shown to be significant by Gronvold^{A-1.4} and by Affortit and Marcon. A-1.5

The specific heat capacity of liquid fuel taken from Leibowitz is applicable to UO_2 only. The assumption is made that the liquid UO_2 value is also valid for liquid PuO_2 . Although departures from stoichiometry were found to be significant for solid fuel, no experimental effort has been made to assess the importance of this parameter in the liquid state.

1.2.2 Other Data Sources. Several other data sources are used to estimate the uncertainty of the model, but not in its development. These sources are cited in Section 1.5 where the uncertainty is analyzed.

1.3 Development of the Model

The most common technique of determining specific heat capacity is to measure the enthalpy of a sample by drop calorimetry and deduce the heat capacity by finding the rate of enthalpy change with temperature. Generally, the enthalpy data are fitted with an empirical function, often a simple polynomial equation. Whereas the accuracy of this approach is good, a function based on first principles is preferable because it allows the identification of the physical processes involved and could be extrapolated beyond its temperature base with some degree of confidence. This approach was used by Kerrisk and Clifton and is adopted here.

1.3.1 Specific Heat Capacity of a Typical Solid. The lattice specific heat capacity of solids at constant volume can be characterized theoretically quite well using the Debye model of specific heat. Except at low temperatures, a similar but simpler theory developed earlier by Einstein is also adequate. These theories are described in the most basic solid state textbooks such as Kittel.^{A-1.6} The Einstein formulation is used here because of its simplicity. This formulation is

$$C_{v} = \frac{K_{1}\theta^{2} \exp(\theta/T)}{T^{2} [e^{\gamma} p(\theta/T) - 1]^{2}}$$

where

 C_v = specific heat capacity (J/kg·K)

 K_1 = constant to be determined (J/kg·K).

Equation (A-1.3) gives the specific heat capacity at constant volume. In most reactor situations, the specific heat capacity at constant pressure, C_p , is more appropriate. The relationship between the two is A-1.7

$$C_p = C_v + \left(\frac{\alpha^2 v}{\beta}\right) T$$

(A-1.4)

(A-1.3)



where

- α = coefficient of thermal expansion (K⁻¹)
- β = coefficient of compressibility (Pa⁻¹)

V = i x r lume (m³).

Temperature-dependence of $\alpha^2 V/\beta$ in Equation (A-1.4) is complicated. The compressibility of a liquid or a solid is nearly constant with temperature, but the molar volume and the coefficient of thermal expansion change with temperature. However, expressing the quantity ($C_p - C_v$) as a function of a constant times temperature, yields results well within the scatter of the data. Therefore, C_p is expressed as

$$C_{p} = C_{v} + K_{2}T \tag{A-1.5}$$

where C_v is given by Equation (A-1.3) and K_2 is a constant to be determined by comparison with data.

1.3.2 Defect Energy Contribution to the Specific Heat Capacity. At temperatures >1500 K, the specific heat capacity data show a rapid increase not described by Equation (A-1.5). This increase is generally attributed to the energy necessary to form Frenkel defects. A-1.7, A-1.8, A-1.9 Some investigators A-1 4, A-1.8 have suggested that Schottky defects may also contribute to this rapid increase. However, the assumption used in this model is that the rapid increase in specific heat capacity >1500 K is due to formation of Frenkel defects. The functional form of the extra term that should be added to Equation (A-1.5) may be found from the defect energy contribution to the enthalpy given by A-1.6

$$H_{D} = K_{3} \exp(-E_{-j}/RT)$$
(A-1.6)

where

 H_D = defect energy contribution to enthalpy (J)

 E_D = activation energy for Frenkel defects (J. nol)

 $K_3 = constant$ to be determined (J)

and R and T were previously defined in Equation (A-1.1). To determine the defect contribution to the specific heat capacity, the derivative of H_D with respect to '...mperature, C_D , is used. C_D is given by

$$C_{\rm D} = \frac{K_3 E_{\rm D}}{RT^2} \exp(-E_{\rm D}/RT)$$
 (A-1.7)

Combining Equations (A-1.3), (A-1.5), and (A-1.7) gives the general expression for specific heat capacity

$$C_{p} = \frac{K_{1}\theta^{2} \exp(\theta/T)}{T^{2} [\exp(\theta/T) - 1]^{2}} + K_{2}T + \frac{K_{3}E_{D}}{RT^{2}} \exp(-E_{D}/RT) .$$
(A-1.8)

1.3.3 Determination of the Constants in the Model. For UO₂, the values of the five constants K_1 , K_2 , K_3 , θ , and E_D are taken from Kerrisk and Clifton. For PuO₂, the constants are determined by fitting the data of Kruger and Savage. In both cases, the fuel was nearly stoichiometric. Data sources for pure PuO₂ are scarce. One potential source is the work of Affortit and Marcon. However, they give only correlations fit to data and not the actual data. Also, they do not present an uncertainty analysis. Without

knowing the number or accuracy of the data on which their correlations are based, it is not possible to estimate what weight to give to their results. Therefore, their correlations were not used to determine the constants of Equation (A-1.8). However, their work was useful for the assessment of the effects of departure from stoichiometry.

It should be noted that the constants determined for Equation (A-1.8) are only valid at fuel temperatures >300 K. Data <300 K were not used to determine the constants of Table A-1.1, and the Einstein formulation assumes temperatures above the Einstein temperature, θ .

1.3.4 Effect of Nonstoichiometry. Several investigators have found the oxygen-to-metal ratio of fuel to influence the specific heat capacity, A-1.1, A-1.5, A-1.8, A-1.10 At temperatures >1300 K, departures from stoichiometry typical of those found in light water reactor (LWR) fuel have caused changes in the specific heat capacity greater than the data scatter. The most complete analysis of this effect has been done by Affortit and Marcon. Even though their results are quantitatively different (see Figures A-1.1 and A-1.2, made from their correlations) from sources used to develop this model, they illustrate well the qualitative aspects of this effect. Figure A-1.1 is for UO2 and Figure A-1.2 is for mixed oxide fuels. These figures show that the specific heat capacity increases as the oxygen-to-metal ratio becomes larger than 2.

Very hyperstoichiometric materials, such as U4O9 and U3O8, have specific heat capacities considerably larger than that of UO2. A-1.4, A-1.11 In addition, these materials exhibit peaks in specific heat capacity at temperatures associated with phase transitions. However, the incidence of these states in light water reactor fuel is infrequent, and their influence is neglected in this model.

In reactor fuel, nonstoichiometry is believed to be due to oxygen interstitials for hyperstoichiometric fuel, and oxygen vacancies for hypostoichiometric fuel.A-1.8 Excess oxygen tends to increase and an oxygen deficiency to decrease, the probability of formation of Frenkel and 5 ky defects, thereby, changing the specific heat capacity. Thus, the logical adjustment to Equation (A s) to account for the oxygen-to-metal ratio effect is in its last term, which includes the effect of defect formation. By multiplying the term by the oxygen-to-metal ratio divided by 2.0, the following desirable features are produced.

- 1.1 The correlation is unaffected for stoichiometric fuel.
- 2. The proper temperature dependence is obtained.
- The specific heat capacity is increased for hyperstoichiometry and decreased for 3. hypostoichiometry, in accordance with the data.

Therefore, this correction has been made to Equation (A-1.8) giving Equation (A-1.1a). This is the model used for the specific heat capacity of solid UO2 and PuO2.

If the fuel consists of mixed oxide (MO₂) with a weight fraction of PuO₂ equal to FCOMP, then the specific heat capacit e mixed oxide fuel is calculated by the expression

$$FCP_{MO_2} = FCP_{UO_2}(1 - FCOMP) + FCP_{PuO_2} \cdot FCOMP .$$
(A-1.9)

If the fuel temperature is greater than the fuel melting temperature, FTMELT, plus the liquid-solid coexistence temperature, then the fuel specific heat capacity is not calculated using Equation (A-1.1a) but set equal to the specific heat of liquid fuel, 503 J/kg·K for both UO2 and PuO2 fuel. If the fuel temperature is equal to the fuel melting temperature, TMELT, then the specific heat capacity is calculated by the expression

$$FCP = (1.0 - R) FCP(T - TMELT) + R \cdot FCPMOL$$
(A-1.10)









Specific heat papacity as a function of temperature and oxygen-to-metal ratio for UO2.









where

R = fraction of fuel which is molten

FCPMOL = specific heat capacity of liquid fuel (503 J/kg+K).

Fuel enthalpy, FENTHL, for solid fuel is found by integrating Equation (A-1.1a) with respect to temperature over the interval zero kelvin to T kelvin. The result of the integration is the expression

FENTHL =
$$\frac{K_1 \theta}{\exp(\theta/T) - 1} + \frac{K_2 T_2}{2} + \frac{Y}{2} K_3 \exp(-E_D/RT)$$
 (A-1.11)

Figure A-1.3 shows the enthalpy of UO₂ versus temperature calculated using Equation (A-1.11).

If the fuel consists of a mixed oxide with a weight fraction of PuO₂ equal to FCOMP, then the enthalpy of the mixed oxide fuel is calculated by the expression

$$FENTHL_{MO_2} = FENTHL_{UO_2}(1 - FCOMP) + FENTHL_{PuO_2} * FCOMP .$$
(A-1.12)

If the fuel temperature is equal to the fuel melting temperature, FTMELT, then the fuel enthalpy is calculated by the expression

$$FENTHL = FENTHL(T = FTMELT) + FHEFUS \cdot FACMOT$$
(A-1.13)

where

FHEFUS = heat of fusion of the fuel (J/kg)

FACMOT = fraction of the fuel that is molten (unitless).

If the fuel ten.perature, FTEMPT, is greater than the fuel melting temperature, then the fuel enthalpy is calculated by the expression

FENTHL = FENTHL(T = FTMELT) + FHEFUS + (FTEMP · FTMELT) · FCPMOL (A-1.14)

where

FCPMOL = specific heat capacity of molten fuel $(J/kg \cdot K)$.

1.4 Comparisons of the Model with Data

Figure A-1.4 shows the specific heat capacity correlation, FCP, for UO₂ compared with data from three sources. A-1.4, A-1.12, A-1.13 These data were taken from stoichiometric UO₂. At the high end of the temperature interval (a few hundred kelvin below the melting temperature), the data fall below the model calculations. (Probably the result of partial melting due to a nonuniform temperature distribution within the sample.) For example, the measured specific heat capacity would be smaller because the specific heat capacity in a liquid is considerably lower than in a solid. A similar comparison is shown in Figure A-1.5 for PuO₂. In this instance, the correlation is compared with its own data base. This was necessary due to the lack of a broad data base for PuO₂ fuel. A better test of the accuracy of the model is found by comparing its predictions with mixed oxide data, A-1.5, A-1.10, A-1.14 as shown in Figure A-1.6. None of the data shown in this figure were used in the development of the model. The agreement is relatively good except for the low values repo. ted by Affortit and Marcon. Other experimenters A-1.3, A-1.10 have pointed out that





Figure A-1.3. Enthalpy of UO₂ as a function of temperature to 4000 K.







Specific heat capacity of UO_2 from three experimenters compared with the FCP correlation (solid line) for UO_2 .
FCP/FENTHL





Specific heat capacity of PuO_2 from Kruger and Savage compared with the FCP correlation (solid line) for PuO_2 .





Figure A-1.6. Specific heat capacity of (U_{0.8}Pu_{0.2})0₂ from three experimenters compared with the FCP correlation (solid line) for mixed oxides.

the results of Affortit and Marcon are generally low when compared with their data and have excluded the Affortit and Marcon measurements from their data base. No one has proposed an adequate explanation for the discrepancy. On the other hand, at least one investigator A-1.9 has given considerable weight to the work done by Affortit and Marcon. Herein, the Affortit and Marcon results are used only in the analysis of the effect of departure from stoichiometry on the specific heat capacity.

1.5 Uncertainty of the Model

As would be expected, the accuracy of the FCP model when compared with its own data base is quite good. A better test was found by comparing the correlations with data not used during their development. The UO_2 and mixed oxide fuel correlations are analyzed separately in this section.

1.5.1 Uncertainty in UO₂ Model. Kerrisk and Clifton report an accuracy of $\pm 3\%$ for their correlation over the temperature range 300 to 3000 K, with an approximately uniform distribution relative to temperature. When the calculations of the correlation are compared with the data of Gronvold for stoichiometric oxide, the agreement is even better, having a standard error of only 2.0 J/kg·K. This is a good test of the model since these data were not used to develop the correlation. The paper by Affortit and Marcon gives correlations fit to their data. Arbitrarily taking 200 K intervals over their temperature range from 600 to 3000 K and using their correlations, the standard error is 46 J/kg·K. Affortit and Marcon's predictions are smaller at all temperatures and the residuals increase with temperature.

1.5.2 Uncertainty in the Mixed Oxide Model. Because of the limited number of data for PuO₂, the accuracy of the correlation for mixed oxide fuel was used as a test for this correlation. Data were taken from Leibowitz, A-1.14 Gibby, A-1.10 and Affortit and Marcon. The model presented in this paper, using a



weighted sum of the UO₂ and PuO₂ results, calculates s_1 differences are negligible; At the highest and lowest applicable temperatures (3000 and 300 K), the differences are negligible; <1.0 J/kg·K. At intermediate temperatures, around 1600 K, the residuals are approximately 10.0 J/kg·K, falling off smoothly from this temperature. The standard error of the model relative to these three data sets is 5.6 J/kg·K. This is equivalent to a maximum percentage error of <2.5%. Since these residuals are smaller than the scatter in the data, the model represents these data its adequately. When the model is compared with that of Affortit and Marcon, again taking 200-K steps from 1600 K to melting, the standard error is 46 J/kg·K. Affortit and Marcon always have the smaller value and the residuals increase with increasing temperature, as with the UO₂ results. Because of the lack of actual data, the results of Affortit and Marcon are not included in the standard error estimate.

1.6 Fuel Specific Heat Capacity Subcode FCP and Fuel Enthalpy Subcode FENTHL

A listing of the FCP subcode is given in Table A-1.11, and the FENTHL subcode in Table A-1.111. The function, EMFCP, is the evaluation model fuel specific heat (which is not part of the best estimate materials properties package), and the subroutine DIALOT is part of the uncertainty analysis package.

1.7 References

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- A-1.6. C. Kittel, Introduction to Solid State Physics, 3rd Edition, New York: John Wiley and Sons Inc., 1966.
- A-1.7. D. R. Olander, Fundamental Aspects of Nuclear Reactor Fuel Elements, Technical Information Center, Energy Research and Development Administration, TID-26711-P1 (1976).
- A-1.8. R. Szwarc, "The Defect Contribution to the Excess Enthalpy of Uranium Dioxide-Calculation of the Frenkel Energy," *Journal of Chemistry and Physics of Solids*, 30, (1969) pp. 705-711.
- A-1.9. E. A. Fischer, P. R. Kinsman, R. W. Ohse, "Critical Assessment of Equations of State for UO₂," Journal of Nuclear Materials, 59 (1976) pp. 125-136.
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TABLE A-1.II

LISTING OF THE FCP SUBCODE

FUNCTION FCP (FTEMP, FACMOT, FOTMTL, FRADEN) THE FUNCTION SCP IS USED TO CALCULATE THE SPECIFIC HEAT CAPACITY OF UD2, PUD2: AND (U,PU)O2 FUELS AS A FUNCTION OF TEMPERATURE, FRACTION OF FULL WHICH IS MULTEN, PUD2 CONTENT, AND DXYGEN-TO-METAL RATIC. = DUTPUT FUE: SPECIFIC HEAT CAPACITY (J/(KG*K)) FCP FTEMP = INPUT FUEL MESHPOINT TEMPERATURE (K) FACMOT = INPUT FUEL FRACTION MOLTEN (UNITLESS) FACMOT = 1.0 - FUEL IS ALL MOLTEN FACMOT = 0.0 - FUEL IS ALL SOLID FOTMTL = INPUT DXYGEN TO METAL RATIO (UNITLESS) FOTMTL = (ATOMS OXYGEN)/(ATOMS METAL) IF NOT KNOWN, FRADEN - INPUT FUEL DENSITY (RATIO OF ACTUAL DENSITY TO THEORETICAL DENSITY) * ESTIMATED STANDARD ERROR FOR UD2 (J/(KG*K)) UFCP (NOT CURRENTLY RETURNED) * ESTIMATED STANDARD ERROR FOR PUD2 (J/(KG*K)) PUFCP (NOT CURRENTLY RETURNED) THE EQUATIONS USED IN THIS FUNCTION ARE BASED ON DATA FROM; (1) J.KERRISK AND D.CLIFTON, NUCLEAR TECHNOLOGY, 16 (1972). (2) O.KRUGER AND H.SAVAGE, JOURNAL OF CHEMICAL PHYSICS, 45 (1968). THE EFFECT OF DXYGEN-TO-METAL RATIO WAS ESTIMATED FROM EQUATIONS PUBLISHED BY; (3) C. AFFORTIT AND J. MARCON, REVUE INTERNATIONALE DES HAUTES THE SPECIFIC HEAT CAPACITY OF MOLTEN UO2 WAS TAKEN FROM (4) L.LEIBOWITZ ET AL, JOURNAL OF NUCLEAR MATERIALS, 39 (1970) FCP WAS DRIGINALLY CODED BY V.F. BASTON IN MARCH 1974. LAST MODIFIED BY G.A. REYMANN IN MAY 1978. COMMON / PHYPRO / FIMELT, FHEFUS, CIMELT, CHEFUS, CIRANB, CTRANE, CTRANZ, FDELTA, BU, COMP, DELOXY THE PHYPRO COMMON BLOCK IS SET BY CALL TO THE SUBROUTINE PHYPRO WHICH IS PART OF THE MATERIALS PROPERTIES PACKAGE USED AT THE INEL.

22

CCC

c

CCCCC

CCCC

CCC

FCP/FENTHL

TABLE A-1.II (continued) QUANTITIES CONTAINED IN IT USED IN THIS SUBCODE ARE; FTMELT = FUEL MELTING TEMPERATURE (K) FDELTA = LIQUID-SOLID COEXISTENCE TEMPERATURE (K) COMP = PUO2 CONTENT (WT.2) WHEN THE FUNCTION FCP IS USED ALONE, NOT AS PART OF THE C CCC INEL CODE, VALUES FOR FIMELT, FOFLIA, AND COMP MUST BE 000 INPUT. cc LICENSING ASSISTANCE COMMON BLOCK. CCMMON /LACMDL/ MAXIDX, EMFLAG(21) C 1 2HON DATA ON 1, OFF 1, . # LOCIDX 1 8 C 296.7 , 2.43E-02, 8.745E07, 535.285, 1.577E05 / 347.4 , 3.95E-04, 3.860E07, 571.0 , 1.967E05 / DATA CIU , CZU , C3U , THU , EDU / * 347.4 DATA CIPU, C2PU, C3PU, THPU, EDPU/ 23 CP(C1,C2,C3,TH,ED,T,FOTMTL) = C1*(TH**2)*EXP(TH/T)/((T**2)*((EXP(TH/T)-1.)**2)) + C2*T * + (FOTMTL/2.)*(C3*ED/(8.314*(T**2)))*EXP(-ED/(8.314*T)) # Revised C IF (EMFLAG(LOCIDX) .EQ. JN) FCP = EMFCP(FTEMP, FACMOT, FTMELT, FRADEN) IF (EMFLAG(LUCIDX) .EQ. DN) GO TO 100 8/81 C FTEMP T FACMOT 2 TM FCCMP - COMP/100.0 = 503.0 FCPMOL C FCPMOL = SPECIFIC HEAT CAPACITY OF MOLIEN FUEL (J/(KG*K)) IF (T .GT. (TM+FDELTA)) GO TO 50 С = CP(Clu, C2U, C3U, THU, EDU, T, FOTMTL)*(1.0 - FCOMP) + CP(C1PU, C2PU, C3PU, THPU, EDPU, T, FOTMTL)*FCOMP FCP FCP/FENTHL * C IF (T .LT. (TM-0.1)) GD TO 100 FCP = (1.0 - R)*FCP + R*FCPMOL FCP GO TO 100 C

TABLE A-1.II (continued)

50 FCP FCPMOL UFCP 2.0 PUFCP 5.6 C 100 CONTINUE RETURN END

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TABLE A-1. III LISTING OF THE FENTHL SUBCODE , FCOMP , FACMOT , FOIMTL , FTMELT FUNCTION FENTHL (TEMP , FHEFUS IMPLICIT REAL # 8 (A-H, 0-Z) THIS FUNCTION IS CALLED BY SUBROUTINE ENERGY AND COMPUTES THE ENTHALPY OF FUEL AT A POINT RELATIVE TO ZERO DEGREES ABSOLUTE TEMPERATURE INPUT ARGUMENTS FACMOT - FRACTION OF MULTEN FUEL - PUD2 FRACTION OF THE FUEL FCOMP FHEFUS - HEAT OF FUSSION OF THE FUEL (J/KG) 24a FOTMTL - FUEL OXYGEN TO METAL RATIO FTMELT - FUEL MELTING TEMPERATURE (K) - LUCAL TEMPERATURE (K) TEMP Revised * ** ** ** * * * * * * OUTPUT ********* ********** 8/81 FENTHL - LOCAL FUEL ENTHALPY RELATIVE TO ZERO DEGREES-K (J/KG) FENTHL WAS DRIGINALLY CODED BY G.A. BERNA IN NOVEMBER 1979 IT WAS UPDATED BY L.J. SIEFKEN IN DECEMBER 1979 FURTHER UPDATED BY G.A. REYMANN IN FEBRUARY 1980 FCPMOL = SPECIFIC HEAT CAPACITY OF MOLTEN FUEL (J/(KG*K)) DATA FCPMOL / 503.EO / THE FOLLOWING DATA STATEMENTS CONTAIN CONSTANTS FROM MATPRO-11 FCP C 296.7 , 2.43E-02, 8.745E07, 535.285, 1.577E05 / DATA CIU, CZU, C3U, THU, EDU 1 * C1PU, C2PU, C3PU, THPU, EDPU / 347.4 , 3.95E-04, 3.860E07, DATA 571.0 \$ 1.967E05 / C

FCP/FENTHI

TABLE A-1.III (continued)

```
THE FOLLOWING EQUATION IS THE INTEGRAL OF THE FUEL SPECIFIC HEAT WITH RESPECT TO TEMPERATURE
CC
C
        CPDT(C1, TH, C2, DTM, ED, T, C3) .
                                         C1*TH * ( 1. / (EXP(TH/T)-1.))

* C2 * T * T / 2.E0

* C3 * DTM * EXP(-ED /(T * 8.314E0) )/2.E0
       2
C
        TX=TEMP
        IF (TX, GT. FTMELT) TX .FTMELT
C
                                                     1 C2U FOTMTL
        FENTHL . CPDT (C1U
                                        . THU
                                                                                  ,EDU
      .
                                        .C3U
                          OTX
C
      IF( FCOMP .GT. O.EO )FENTHL = FENTHL + CPDT(C1PU
* ,C2PU ,FOTMTL ,EDPU ,TX
                                                                                  ,THPU
                                                                                  .C3PU J*FCOMP
C
        IFI TEMP .LE. FIMELT - 2.EO ) GO TO 100
č
C
        FENTHL = FENTHL + FHE IS + FACMOT
IF (TEMP.LE. (FTMELT+2. 30 TO 100
CC
        FENTHL = FENTHL + (TEMP-F, MELT) *FCPMOL
  1CO CONTINUE
C
        RETURN
        END
```

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- A-1.11. H. Inaba, H. Shimizu, K. Naito, "Lambda-Type Heat Capacity Anomalies in U₃O₈," Journal of Nuclear Materials, 64 (1977) pp. 66-70.
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- A-1.14. L. Leibowitz, D. F. Fischer, M. G. Chasanov, "Enthalpy of Uranium-Plutonium Oxides (U0.8, Pu0.2) 01.07 from 2350 to 3000 K," Journal of Nuclear Materials, 42 (1972) pp. 113-116.

1.8 Bibliography

The following data sources were used in previous EG&G Idaho Inc., reports dealing with fuel specific heat models, but are not quoted in this version. They are included here for completeness.

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- (4) R. L. Gibby, Enthalpy and Heat Capacity of $U_{0.75}Pu_{0.25}O_{2-x}$ (25–1490C), HEDL-TIME-73-19 (1973).
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2. FUEL THERMAL CONDUCTIVITY (FTHCON) (D. L. Hagrman)

In this section, a correlation is presented for the thermal conductivity of uncracked UO_2 and $(U,Pu)O_2$ fuels. This property and the closely associated models for the effect of fuel cracking on temperature distributions within the fuel are critical to accurate predictions of fuel rod behavior in both steady state operation and in off-normal transients because fuel rod behavior is strongly dependent on temperature.

2.1 Summary

The FTHCON subcode determines the fuel thermal conductivity and its derivative with respect to temperature as a function of temperature, density, oxygen-to-metal (O/M) ratio and plutonium content of the fuel. Burnup is also required input but is used only to calculate the melt temperature.

The data base shows no significant effect , porosity at temperatures above about 1600 K, probably because of the effects of radiation and gas conductivity which increase pore conductivity at high temperature. The thermal conductivity of liquid fuel has been estimated from physical considerations because no data for the conductivity of molten fuel have been found.

With the exception of minor modifications made to eliminate discontinuities in slope in the temperature range 1364 to 2300 K, the expression used to model thermal conductivity of solid fuel is





FTHCON

$$k = \left[\frac{D}{1 + (6.5 - 0.00469T^{-1}(1 - D))}\right] \left[\frac{C_v}{(A + BT^{-1})(1 + 3e_{th})}\right] + 5.2997 \times 10^{-3} T \left[exp\left(\frac{-13358}{T}\right)\right] \left\{1 + \left[0.169\left(\frac{13358}{T}\right) + 2\right]^2\right\}$$
(A-2.1)

where

K = thermal conductivity (W/m·K)

- C_v = phonon contribution to the specific heat at constant volume (J/kg•K). The first term of the MATPRO correlation for fuel specific heat capacity is used for this factor^a
- e_{th} = linear strain caused by thermal expansion when temperature is >300 K (unitless). The MATPRO correlation for fuel thermal expansion is used for this factor

T = fuel temperature (K)

$$T' =$$
 fuel temperature if <1364 K. For temperatures >1834 K, the porosity factor,

$$\frac{D}{1 + (6.5 - 0.00469T')(1 - D)}$$

is equal to 1 and for temperatures in the range 1364 to 1834 K, the factor is found by interpolation as explained in subsection 2.3

T" = fuel temperature if <1800 K. For temperatures >2300 K, T" is equal to 2050 K and for temperatures in the range 1800 to 2300 K, T" is found by interpolation as explained in subsection 2.3

A = a factor proportional to the point defect contribution to the phonon mean free path (m•s/kg). The correlation used for this factor is 0.339 + 11.1 x absolute value (2.0-O/M ratio)

B = a factor proportional to the phonon-phonon scattering contribution to the phonon mean free path $(m \cdot s/kg \cdot K)$. The correlation used for this factor is $J.06867 \times (1 + 0.6238 \times plutonium content of fuel)$.

The first term of Equation (A-2.1) represents the phonon contribution to specific heat, and the second term represents the electronic (electron-hole) contribution. The expression is valid only in the range 90 to 100% of theoretical density. When the fuel is molten, the first term is neglected.

The expected error of the thermal conductivity model has been estimated by computing the standard error of the model with respect to its data base. For stoichiometric UO_2 samples, the standard error was 0.2 (W/m•K) and for stoichiometric (U,Pu)O₂ with 2% Pu, the standard error was 0.3 (W/m•K). On the basis of these results, the following expression is used to calculate the expected standard error of the thermal conductivity of the solid fuel

$$UK = [0.2(1 - COMP) + 0.7 COMP] \times (1.0 + |2 - OTM| 10) .$$
 (A-2.2)

a. The analytical expression for $C_{\rm V}$ as a function of temperature, T, and plutonium content, COMP, is

$$C_{v} = \frac{296.7 (\frac{35.285}{T})^{2}}{T^{2} \left[exp \left(\frac{35.285}{T} \right)^{2} \right]} \left[exp \left(\frac{535.285}{T} \right) \right] \left[(1 - COMP) \right] + \frac{347.4(571)^{2}}{T^{2} \left[exp \left(\frac{571}{T} \right)^{2} \right]^{2}} \left[exp \left(\frac{571}{T} \right) \right] COMP$$

TABLE A-4.I

PARAMETERS USED IN UC2 AND PuC2 SOLID PHASE THERMAL EXPANSION CORRELATIONS

Constant	U02	Pu02	Units
к1	1.0×10^{-5}	9.0×10^{-6}	K-1
K2	3.0×10^{-3}	2.7 x ¹⁰⁻³	Unitless
Кз	4.0×10^{-2}	7.0×10^{-2}	Unitless
ED	6.9 x 10 ⁻²⁰	7.0×10^{-20}	J

where

 $\frac{\Delta L}{L_o}(T_m)$ = thermal expansion strain of solid fuel from Equation (A-4.1) with T = T_m

 T_m = melting temperature of the fuel (K)

FACMOT = fraction of the fuel which is molten (unitless)FACMOT = 0.0—fuel all solidFACMOT = 1.0—fuel all molten.

The correlation used to describe the expansion of entirely molten fuel is

$$\frac{\Delta L}{L_o} = \frac{\Delta L}{L_o} (T_m) + 0.043 + 3.6 \times 10^{-5} [T - (T_m + \Delta T_m)] .$$
 (A-4.3)

The solid to liquid phase transition is isothermal only for pure UO₂ or pure PuO₂. For (U,Pu)O₂, the transition occurs over a finite temperature range, denoted in Equation (A-4.3) by ΔT_m .

The uncertainty of the pooled data was found to be temperature-dependent, increasing approximately linearly with temperature. Therefore, a percentage error is given rather than a fixed number. The $\pm \sigma$ limits were found to be within $\pm 10\%$ of the calculated value.

Section 4.2 contains a discussion and evaluation of the sources used. Section 4.3 presents the development of the model. In Section 4.4, the model predictions are compared with data and an uncertainty estimate is given. Sections 4.5 and 4.6 give listings of the FORTRAN subcode, FTHEXP, and the references, respectively.

4.2 Review of Literature

Data were taken from nine sources for UO_2 , A-4.1—A-4.9 and two sources for PuO_2 . A-4.3, A-4.12 For UO_2 , the data cover a temperature range from 300 to 3400 K; and for PuO_2 , from 300 to 1700 K.

In four of the UO₂ experiments, A-4.1, A-4.2, A-4.8, A-4.9 X-ray measuring techniques were used. This type of measurement gives the change in the lattice parameter rather than the bulk thermal expansion. Several investigators A-4.2, A-4.10, A-4.11 have noted that the change in the lattice parameter is







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appreciably smaller than the bulk thermal expansion measured using dilatometric or interferometric methods, especially at high (>1000 K) temperature. In general, the difference is attributed to the creation of Schottky defects, A-4.2, A-4.10, A-4.11 Hoch and MominA-4.9 obtained results where there was no discrepancy between their X-ray results and bulk results. However, the bulk of the data support the Schottky defect idea since the X-ray data consistently fall below the others at high temperatures, where defects begin to appear in large numbers. Therefore, X-ray data were used in the data base only at low temperatures (< 800 K).

4.3 Model Development

While most authors simply fit their data with a polynomial, in this report correlations based on more physical grounds are used.

4.3.1 Low Temperature Thermal Expansion. The simplest theory of the linear expansion of a solid near room temperature is found in most elementary physics texts such as Sears and Zemansky, A-4.13

$$\Delta L = L_0 K_1 (T - T_0) \tag{A-4.4a}$$

or

$$\frac{\Delta L}{L_0} = K_1 T - K_1 T_0 \tag{A-4.4b}$$

where

the average coefficient of linear expansion (K-1) Κ, Ta a reference temperature (K)

length at reference temperature (m)

at the reference temperature $\Delta L = 0$ or equivalently $L = L_0$.

The low temperature (< 800 K) data were fit by the method of least-squares to a generalized form of Equation (A-4.4b).

$$\frac{\Delta L}{L_0} = K_1 T \cdot K_2$$

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This fit was done separately for UO2 and PuO2 and the coefficients K1 and K2 for each material are listed in Table A-4.1. The numbers in the table have been rounded off to two significant figures. Comparison of Equations (A-4.4b) and (A-4.4c) shows that $T_0 = K_2/K_1$, which for both fuels is 300 K, a temperature typical of the reference temperatures where $\Delta L = 0$ in the data bases. These correlations describe low temperature thermal expansion within the data scatter.

4.3.2 High Temperature Thermal Expansion. For both UO2 and PuO2 Equation (A-4.4c) was inadequate at higher temperatures (T > 1000 K), most likely due to the formation of Schottky defects. Frenkel lefects will also be present, but should have no measurable effect on the thermal expansion, A-4.2, A-4.9 The contribution from Schottky defects should be directly proportional to their concentration A-4.2 which s given by A-4.2, A-4.14

$$\frac{M}{N_0} = K_3 \exp\left(-E_0/kT\right)$$

(A-4.4c)





(A-4.5)

(A-6.1)

6.1 Summary

The FCREEP model calculates creep deformation of UO_2 or mixed oxide fuels. The model includes a time-dependent creep rate for UO_2 , valid for both steady state and transient reactor conditions. Fuel creep is modeled as a function of time, temperature, grain size, density, fission rate, oxygen-to-metal ratio, and external stress.

At a transition stress (a_t) , the creep rate changes from a linear stress dependence to a creep rate proportional to stress to a power n. The transition stress is defined by

$$\sigma_{\rm r} = 1.6547 \times 10^7 / {\rm G}^{0.5714}$$

where

 $\sigma_{\rm t}$ = transition stress (Pa)

 $G = fuel grain size (\mu).$

The creep function is dependent on an Arrhenius type activation energy. This energy is found to be a function of the fuel oxygen-to-metal ratio (O/M). Increasing the O/M ratio increases the creep rate, all other things being constant. The activation energy below the transition stress is given by

$$Q_1 = 17884.8 \left\{ exp\left[\frac{-20}{\ln(x-2)} - 8\right] + 1 \right\}^{-1} + 72124.23$$
 (A-6.2)

where

 Q_1 = activation energy (cal/mol)

= oxygen-to-metal ratio.

The activation energy of UO2 above the transition stress is

$$Q_2 = 19872 \left\{ \exp\left[\frac{-20}{\log(x-2)} - 8\right] + 1 \right\}^{-1} + 111543.5$$
 (A-6.3)

where

 Q_2 = activation energy (cal/mol).



The steady state creep rate of UO_2 is determined using

$$\dot{e}_{s} = \frac{(A_{1} + A_{2} F) \sigma \exp(-0_{1}/RT)}{(A_{3} + D) G^{2}} + \frac{(A_{4} + A_{8} F) - \frac{4 \cdot 5}{2} \exp(-0_{2}/RT)}{A_{6} + D} + A_{7} \sigma F \exp(0_{3}/RT)$$
(A-6.4)

where

es		steady state creep rate (S ⁻¹)
A ₁	π	0.3919
A ₂		1.3100 x 10 ⁻¹⁹
A ₃	-	-87.7
A4		2.0391 x 10 ⁻²⁵
A ₆		-90.5
A ₇		3.72264 x 10 ⁻³⁵
A ₈	5	0.0
Ė		fission rate (fissions/m ³)/s
σ	=	stress (Pa)
Т	н	temperature (K)
D	л	density (percent of theoretical density
G	-	grain size (µm)
Q3	=	2.6167 x 10 ³ (J/mol)
R		universal gas constant (J/mol·K).





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9. FUEL PRESSURE SINTERING (FHOTPS) (R. E. Mason)

Urania or mixed oxide fuel pellets densify when exposed to sufficiently hig: hydrostatic pressures (pressure sintering), high temperatures (thermal sintering), and irradiation. This report discusses a densification model based on published out-of-pile fuel pressure sintering data. The pressure sintering model complements the irradiation-dependent densification model described in Section A-7 of this handbook.

A summary of the pressure sintering model, FHOTPS, is contained in Section 9.1. Section 9.2 describes pressure sintering theories and examines their applicability to model urania and mixed oxide pressure sintering data. Section 9.3 describes the development of the FHOTPS model, provides standard error estimates, and compares FHOTPS calculated results with experimental data. Section 9.4 gives the FORTRAN computer program listing of the FHOTPS model, and the references are given in Section 9.5.

9.1 Summary

Fuel densification in a reactor environment is a function of temperature, stress, and irradiation. Temperature and stress densification mechanisms are driven by a stress, P, expressed by

$$P = P_e - P_i + \frac{2\gamma}{a}$$

where

Pe = external hydrostatic stress (Pa)

 P_i = internal pore pressure (Pa)







FHOTPS

 γ = surface energy per unit area (J/m²)

a = grain size (m).

Pressure sintering is the dominant densification process if the stress ($P_e - P_i$) is much larger than the surface energy stress, $2\gamma/a$. Densification of in-pile fuel will be dominated by an external hydrostatic stress, P_e , when present, because the internal pore pressure, P_i , and the surface energy stress, $2\gamma/a$, are generally much smaller than the externally applied stress. Over an extended irradiation period and at zero P_e , the internal pore pressure, P_i , could cause fuel swelling and the surface energy stress could cause some fuel densification. However, these changes in fuel volume are small compared with densification caused by applied stress and are not considered in the development of the PHOTPS model.

Equation (A-9.1) does not include an irradiation related driving stress. It is assumed that the irradiation densification driving stress would be added to the right side of Equation (A-9.1). Since the irradiation densification driving stress is a linear term, it is treated independently as a separate model (the FUDENS model of MATPRO 11, Revision 1). The values calculated with the FUDENS model should, therefore, be added to the FHOTPS model described in this section. The reader should, however, be cautioned that data used to develop the FUDENS model were in-pile data that may include some pressure sintering effects so that combining the two model outputs may be conservative. There are no in-pile data available that will allow separation of these effects.

A lattice diffusion creep equation was fit to the data of Solomon^{A-9,1} to give the equation used for urania in the FHOTPS model

$$\frac{1}{\rho}\frac{d\rho}{dt} = 48939 \left(\frac{1-\rho}{\rho}\right)^{2.7} \frac{P}{TG^2} \exp(Q_u/RT)$$

where

here

t = time(s)

T = temperature (K)

 $G = grain size (\mu m)$

 $R = 8.314 (J/mole \cdot K)$

 $Q_{\rm u}$ = activation energy (J/mole)

= fraction of theoretical density (unitless)

P = hydrostatic pressure (Pa).

The activation energy of urania pressure sintering for Equation (A-9.2) is calculated with the oxygen-tometal dependent equation

$$Q_{\rm u} = R \left\{ 9000 \exp\left[\frac{20 - 8 \left|\log(x - 1.999)\right|}{\left|\log(x - 1.999)\right|} + 1.0\right]^{-1} + 36294.4 \right\}$$
(A-9.3)

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x = oxygen-to-metal ratio.

(A-9.2)

The lattice diffusion creep equation was fit to the mixed oxide data of RoutbortA-9.2 to give the mixed oxide fuel pressure sintering equation

$$\frac{1}{\rho}\frac{d\rho}{dt} = 1.8 \times 10^7 \left(\frac{1-\rho}{\rho}\right)^{2.25} \frac{P}{TG^2} \exp \frac{-450000}{RT} .$$
(A-9.4)

The standard error of estimate for both equations is $\pm 0.5\%$ of the calculated density.

Care must be exercised when using these models out of the 1600- to 1700-K and 2- to 6-MPa data base range. Pressure sintering not represented in the data base may be controlled by a different creep densification mechanism, as discussed below. Pressure sintering rates would then be much different than those calculated by Equations (A-9.2) or (A-9.4).

9.2 Pressure Sintering Process and Data

Pressure sintering or volume creep consists of several modes of creep. One of these modes or creep mechanisms can dominate the others, depending on the fuel temperature, pressure, porosity, and grain size conditions as will be discussed below. Equations representing each creep mechanism combined with the theoretical constants of UO₂ were used by Routbort^{A-9.2} to determine the most probable dominating (contributes the highest densification rate) mechanism under reactor operating conditions. These equations, their use, and the published experimental data used to develop the FHOTPS model are described in this section.

9.2.1 Creep Densification. Several distinct mechanisms are observed that contribute to fuel densification. These are lattice diffusion (Narbarro-Herring creep), or rate-independent plasticity (yielding or dislocation glide). A-9.3 Each mechanism imposes specific stress-porosity-temperature-dependent functions. One or any combination of these creep mechanisms can dominate densification, depending on the grain size stress-porosity-temperature conditions. There is no single mechanism that will always dominate the densification process. Therefore, an equation representing each mechanism is presented to indicate the densification parameter dependencies possible.

Pressure sintering by grain boundary diffusion creep (grain boundary acting as a diffusion path) is usually dominant at temperatures less than one half the melting temperature. A-9.3, A-9.4 The densification rate by grain boundary creep is expressed by

$$\frac{d\rho}{dt} = \frac{4.5 \ \delta \ D_b \Omega}{kT \ b^3} \frac{P}{1 - (1 - \rho)^{1/3}}$$
(A-9.5)

where

- δ = grain boundary thickness
- D_{b} = grain boundary diffusion coefficient
- Ω = atomic volume
- ρ = fraction of theoretical density

= time

T = temperature





- P = applied stress
- k = Boltzman's constant
- $b = grain size.^a$

Pressure sintering by grain boundary diffusion creep can dominate only if the grain sizes remain small, so that the diffusion paths along the grain boundaries are small.

Pressure sintering by lattice diffusion creep often dominates at temperatures greater than half the melting temperature and before significant grain growth has occurred. Densification by lattice diffusion creep is expressed by

$$\frac{d\rho}{dt} = \frac{3D_v \Omega P}{kT b^2}$$
(A-9.6)

where

 D_v = lattice diffusion coefficient.

This equation is used to calculate densification by vacancy flow from the surface of a pore to sinks on nearby grain boundaries. A-9.3

Pressure sintering by power law creep can dominate at high fuel temperatures or pressures. Densification by power law creep (dislocation creep) has been derived by Wilkinson and AshbyA-9.4 and by Wolfe and Kaufman. A-9.5 The densification rate equation is

$$\frac{d\rho}{dt} = \frac{SA}{T} \exp\left(\frac{Q}{kT}\right) \left\{ \frac{\rho(1-\rho)}{\left[1-(1-\rho)^{1/n}\right]^n} \right\} \left(\frac{3|\rho|}{2n}\right)^n$$
(A-9.7)

where

S = sign of pressure

n = stress and porosity exponent

A = constant

Q = power law activation energy (J/mole).

Equation (A-9.7) assumes steady state creep and densification independent of the grain size, and is valid even after extensive grain growth.

The fourth pressure sintering mechanism, plastic flow, operates at low temperatures or very high strain rates, and is defined by the expression



a. It was assumed here and in the following equations that the effective particle radius is the grain size. This is consistent with the model that is based on the assumption of about one pore to every grain in the compact.

FHOTPS

(A-9.8)

$$\frac{d\rho}{dt} = \begin{cases} 0 \text{ if } \rho \ge 1 - \exp\left(\frac{-3}{2}\frac{P}{\sigma_y}\right) \\\\ \infty \text{ if } \rho < 1 - \exp\left(\frac{-3}{2}\frac{P}{\sigma_y}\right) \end{cases}$$

where

 ρ = fraction of theoretical fuel density

 $\sigma_{\rm v}$ = yield stress.

Densification by the plastic flow mechanism is assumed to occur instantaneously. A-9.3

The stress dependency of the above equations have been shown by Rossi and Fulrath, A-9.6 McCelland, A-9.7 Fryer, A-9.8 and Wolf A-9.5 to be dependent on the applied stress and the fuel porosity. Porosity in fuel increases stress in the vicinity of the pores, and results in a vacancy concentration difference between the pore surfaces and the grain boundaries. Various porosity-dependent functions have been proposed by the above authors, but the porosity-dependent function of Fryer A-9.8 is the most generally accepted effective stress-porosity-dependent function. The form of Fryer's expression is

$$P = \left(\frac{1-\rho}{\rho}\right)^n \tag{A-9.9}$$

where

P = effective stress

 ρ = fractional density

$$n = 1.0.$$

Routbort^{A-9.2} found that the porosity exponent, n, of Equation (A-9.9) was not constant for mixed oxides but varied with the pressure sintering temperature. Routbort mapped pressure sintering of mixed oxides (determined the most dominant mechanism using theoretical material properties) but used predominately urania material constants. It was found that the lattice diffusion mechanism dominates under light water reactor conditions (fuel temperatures between 1100 and 3136 K, pressures <100 MPa, and fuel densities >0.90% of theoretical density). This conclusion, however, must be exercised with caution because the densification rate equations also depend on the grain size and the oxygen-to-metal ratio and neither were included in the pressure sintering map analysis. The oxygen-to-metal ratio has been shown by Seltzer^{A-9.9}, A-9.10, A-9.11 to strongly influence the activation energy and thereby drastically alter the densification rates predicted by Equations (A-9.5), (A-9.6), and (A-9.7).

The final pressure sintering mechanism is lattice diffusion modified to include an effective applied stress. The expression describing this mechanism is

$$\frac{1}{\rho}\frac{d\rho}{dt} = A\left(\frac{1-\rho}{\rho}\right)^n \frac{P}{TG^2} \exp(Q/RT)$$

(A-9.10)

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where

- A = constant
- Q = activation energy.

9.2.2 Pressure Sintering Data. The model presented in Section 9.1 is based on data published in the open literature that deals with final stage sintering of urania and mixed oxide fuels. The models are based on the urania pressure sintering data of Solomon $^{A-9.1}$ and the mixed oxide pressure sintering data of Routbort, $^{A-9.2}$ Other data are used as comparison data, but fuel resintering data or final stage sintering data are used because these data most closely resemble what is occurring in a reactor. Measurement techniques and urania and mixed oxide data published in the open literature are presented in this section.

9.2.2.1 Measurement Techniques – Immersion density and specimen length changes are used to obtain densification data. Immersion density is the more accurate technique, but only the initial and final densities are obtained. Densities from specimen length changes provide time-density data and are calculated by

$$\frac{\rho}{\rho_{\rm f}} = \left(\frac{\ell_{\rm f}}{\ell}\right)^3 \tag{A-9.11}$$

where

 ρ = initial fraction of theoretical density (unitless)

 ρ_{f} = final fraction of theoretical density (unitless)

 $\ell_{\rm f}$ = final length (mm)

 ℓ = initial length (mm).

Density charges determined from length change measurements have, however, several inherent sources of error. The most critical error is the apparent length change caused by the test sample seating and changing alignment during the initial densification. This strain error is highly variable and only affects the initial 1 to 2% of sample densification. Creep (nonvolumetric strain) of the sample and loading column is also a source of error. Routbort, however, measured final sample immersion densities and final densities from length change calculations and found only about 5% difference between the two techniques.

9.2.2.2 Urania Densification Data-Pressure sintering data of UO₂ fuel have been published by Solomon, A-9.1 Kaufman, A-9.12 Amato, A-9.13 Hart, A-9.14 Fryer, A-9.8 and Warren and Chalklader. A-9.15 The data of Solomon and Kaufman are resintering data, whereas the data of Amato are fabrication sintering data.

Solomon measured pressure sintering rates of UO₂ fuel pellet that were thermally sintered at 1783 K for 3 h to obtain pretest sample densities between 92 and 94% of theoretical density. Pressure sintering tests were performed at 1673 K for up to 136 h. Since the urania samples were presintered at 100 K above the pressure sintering temperature, there should be only a small thermal sintering contribution to the pressure sintering rates. Immersion densities of pretest samples were obtained with an accuracy of $\pm 0.5\%$. Sample integrity was maintained by slowly ramping to the test temperature (1673 K), and then cycling through various temperature-pressure test combinations. Experimental temperatures are reported to be accurate to within ± 1 K and pressures are accurate to within 0.1%. A summary of experimental conditions is provided in Table A-9.1. The pressure sintering tests of Solomon indicate that (a) significant densification occurred prior to application of pressure, (b) internal pore pressures were possibly influencing the densification rate, (c) pressure sintering rates are approximately linear with applied stress ($\sigma^{1.03}$ to $\sigma^{1.2}$), and





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TABLE A-9.1. PRESSURE SINTERING DATA

			Pressure Sintering												
		Presint	ering							Initial					
Reference	Oxygen-to- Metal Ratio	Temperature (K)	Time (h)	Density (2)	Temperature (K)	Time (s)	Pressure (MPa)	Stress Exponent	Porosity Exponent	Size (nm)					
Urania Data															
Solomon ^{A-9,1}	2.004 + 0.001	1783 <u>+</u> 1		92 20 98	1673 <u>*</u> 1	$0 \le t \le 5 \times 10^5$		1.03 < n < 1.2	2.7	3.354					
Kaufman ^{A-9,12}		2023	12 to 24	80 to 92	2123		3.86 to 3.96.x 10 ⁷			10 to 40					
Amato ^{A-9} .13	2.00			68 to 96	1373 to 1473	900 < t < 3660	2.76 to 5.52 x 10^7			19 M.					
Mixed Oxide Data															
Routbort A-9.2	1.98 + 0.01 ⁸			90 to 99	1598 < T < 1823	이 가슴 안 듯	7.6 to 76	1.33	2.25	8.0					

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(d) activation energy for specimens at different temperatures and constant density was 0.290 MJ/g•mole. Solomon, however, determined that an activation energy of 0.480 MJ/g•mole obtained from two isothermal tests to be more accurate. Pressure cycling tests also showed that the specimens swelled after the applied pressure was removed and that the applied pressure-densification and released pressure-swelling rates were essentially reversible.

Kaufman² > 12 reported urania pressuring data of fuel at initial densities of between 80.7 and 83.7% theoretical density. Immersion densities were taken before and after pressure sintering with a $\pm 0.2\%$ accuracy. The data are intermediate sintering data and can only be used to check the FHOTPS model densification rates. The pellets used by Kaufman were sintered at a temperature 100 K less than the test temperature, but were sintered for a relatively long time. Thermal sintering contributions should, therefore, be very similar to the Solomon data. Pressure sintering was performed in a single-action graphite die, lined with a tungsten foil to minimize the reaction of uranium with the carbon. The uranium reaction was also minimized by pressing in a 10^{-3} -Torr atmosphere. Reaction of the urania with the tungsten foil and the graphite die may have occurred, but the extent of influence is undetermined. Temperature control was within $\pm 1\%$. Kaufman observed no densification from heating prior to the application of the load. Kaufman found stress exponent values for Equation (A-9.9) between 1 and 4.5.

AmatoA-9.13 also used a graphite die plunger lined with alumina to obtain hot pressing data. Pressure sintering tests were performed using a vacuum of 10⁻⁵ Torr. Test conditions are listed in Table A-9.1. The Amato data are also intermediate sintering data plus final stage sintering data. Therefore, the data can only be used to check the densification rates, and not as part of the FHOTPS data base. A mato indicated that trapped gases were affecting the densification rate, but data backing this conclusion were not reported.

Fabrication pressure sintering data were reported by HartA-9.14 and Fryer. A-9.8 These data include initial, intermediate, and final stage densification. Since densification rate equations will change for each stage, these data are not useful in the MATPRO modeling effort. Reaction sintering (sintering while the components are chemically reacting) data were reported by Warren and Chalklader. A-9.15 These data are not appropriate for use in the MATPRO modeling effort for the reasons listed above plus the fact that the chemical reaction affects the sintering process.

9.2.2.3 Mixed Oxide Densification Data – The results of Routbort^{A-9.2} and Voglewede^{A-9.16,A-9.17} mixed oxide pressure sintering data are the only data published in the open literature. Their mixed oxide samples consisted of 15 wt% PuO₂ and 75 wt% UO₂. Tests consisted of presintering each sample to an equilibrium density of approximately 90% theoretical density in a double action punch and tangsten die, and then applying additional temperature and pressure to evaluate pressure sintering rates. Immersion densities were obtained before and after each test, and specimen length changes were measured during the test. Pressure sintering data were found to be reproducible to within $\pm 20\%$. Detailed test conditions for Routbort data are provided in Table A-9.1. Routbort found the porosity exponent ranged from 1.5 at 1673 K to 2.25 at 1823 K. Tressure sintering was also shown to be a nonlinear function of stress with a stress exponent of 1.33.

9.3 Model Development at d Uncertainties

The pressure sintering model, FHOTPS, calculates the volume reduction rate of cael under hydrostatic pressures and elevated temperatures. The model is based on the urania and plutonia data described above and the semiempirical equation suggested by Solomon, Routbort, and Voglewede. The model simulates the removal of closed porosity developed during fuel pellet fabrication and porosity created by released fission gases.

The appropriate pressure sintering mechanism to model reactor fuel behavior is best determined by comparing the densification rates calculated with the theoretical equations of Section 9.2. The equation indicating the largest densification rate at expected reactor pressures and temperatures is the best model for in-reactor pressure sintering. Routbort performed this analysis for mixed oxides but used mostly UO2 physical constants. Lattice diffusion was determined to be the controlling mechanism. A similar conclusion was reached by Solomon for the analysis of urania densification rates. The lattice diffusion equation is therefore used as the framework equation for the final FHOTPS equations.

The constants of Equation (A-9.2) were obtained from the general equation for lattice diffusion, Equation (A-9.10), and the data of Solomon. Determining the constant A of Equation (A-9.10) constituted equation fitting to the data. Trial and error adjustments of A were made until the standard error of estimate from Equation (A-9.10) and the data converged to the smallest error possible. The porosity exponent, n, for urania was obtained by using the average slope value of $1/\rho(d\rho/dt)$ plotted versus $\ln [(1 - \rho)/\rho]$. The average slope value was determined to be 2.7.

Equation (A-9.10) was fit to the Solomon data using a porosity exponent of 2.7, an initial grain size of 3.5 µm, an assumed activation energy of 0.48 MJ/mole, the reported hydrostatic pressure, and isothermal temperature. This fitted equation calculates a greater densification rate than indicated by the intermediate stage sintering data of Amato. This is opposite to the expected results because intermediate sintering is usually faster than final stage sintering. The lattice diffusion equation was therefore refit to the Solomon data using an apparent activation energy closer to the 0.290 MJ/mole (apparent activation energy obtained by Solomon from specimen data taken at different temperatures). The activation energy used in the urania pressure sintering model is calculated with Equation (A-9.3). This equation and resulting calculated activation energy were used to be consistent with the FCREEP model of the MATPRO package. With the oxygen-to-metal ratio of 2.004, an apparent activation energy of 0.332 M. (mole is calculated with Equation (A-9.3). This is relatively close to the lowe. Solomon activation energy, Using this activation energy, Equation (A-9.10) was fit by trial and error adjustments of constants to fit the Solomon data with a final error estimation of ±0.48%. Calculations using Equation (A-9.2) compared with data of its data base are shown in Figure A-9.1.

The mixed oxide pressure sintering rate equation suggested by Routbort was used as the FHOTPS mixed oxide model except that the grain size dependence of the theoretical lattice diffusion equation was included to be consistent with the urania model. The 0.4-MJ/mole activation energy for mixed oxides suggested by Routbort, with an oxygen-to-metal ratio of 1.98, was used in the model. This activation energy is assumed not to vary with the oxygen-to-metal ratio because of a lack of data. The porosity exponent is also assumed constant at 2.25, the value determined by Routbort for samples tested at 1823 K. Although Routbort observed a temperature dependence of the porosity exponent, a model for the dependence was not developed because the data on which this conclusion is based was not included in the published report.

Equation (A-9.10) was fit to the Routbort data using an activation energy of 0.4 MJ/g mole, a porosity exponent of 2.25, and an initial grain size of 9 µm. Constants were adjusted until the smallest standard error estimate was obtained. The final standard error of estimation is 0.5%. Figure A-9.2 shows a comparison of the mixed oxide densification rates calculated with the FHOTPS model that correspond with the Routbort data.

The FHOTPS model calculates a density change rate. These calculations are easily modified to obtain strain rate by multiplying calculational results by -1/3. This is a result of the following analysis. Using a fuel mass, g, a change in density can be expressed

$$\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{\frac{g}{\nabla} \cdot \frac{g}{\nabla_{\mathrm{o}}}}{\frac{g}{\nabla_{\mathrm{T}}}}\frac{1}{\Delta t}$$

final volume

fuel mass









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- V_0 = initial volume V_T = volume of the mass, g, at theoretical density
- $\Delta t = time step.$

Eliminating g and multiplying denominator and numerator by VT gives

$$\frac{1}{\rho}\frac{d\rho}{dt} = V_{\rm T} \left(\frac{V_{\rm o} - V}{V_{\rm o}} \right) \frac{1}{\Delta t} \qquad (A-9.13)$$

Assuming that $V_T \cong V$, then Equation (A-9.13) relates a densification strain rate to a volume strain rate of

$$\frac{1}{\rho}\frac{d\rho}{d\lambda} = \left(\frac{V - V_0}{V_0}\right)\frac{1}{\Delta t} .$$
(A-9.14)

This can be reduced to a linear strain rate by the usual assumption that

$$\frac{1}{3}\frac{\Delta V}{V_0 \Delta t} = \frac{\Delta L}{L_0 \Delta t} \frac{1}{\Delta t} \quad . \tag{A-9.15}$$

Equations (A-9.2) and (A-9.4) must be used with caution because the models are based on very limited data. Both equations are based on one data set, and these data cover only a small portion of the temperatures, pressures, oxygen-to-metal ratios, and grain sizes possible in a reactor environment. An additional concern is that a significant change in any one of these parameters could result in a different creep mechanism.

9.4 Subroutine FHOTPS FORTRAN Listing

Table A-9.11 is a listing of the FHOTPS model described above.

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TABLE A-9.II

LISTING OF THE FHOTPS SUBCODE

	FUNCTI	UN	FH	IO T	PS	(C	OM	Ρ,	F	T	EM	1P,		HS	TR	E	s,	(GRI	NS	1	.,	ł	0	м,	-	20)					
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	CUMP FTEMP HSTRES GRNSIZ FUM RC		INITI			PLEYN	UT MPRIL			UTGGA	REL	INT	I E	RESIM	HESETEDE	A P		GHEI	HR	PKENDIN	FL	IE .UL	EN I ES	P	EL	LI	ET S)		P				
	THE DEL DATA FI (1)J. FIN NUC (2)A. HOT	AL-PR	RUST	CA HE JT AG MA	TIFO ETEMO	DEL RINO	LO NSALK	AL IF S,	LUNCON ICON	-	REVICOU	EF OD ICR	RL 7RG	WINEEUF)ANC	THEOMPA	SULPE	TH	15 48 48 90		FU AI	-01 01	S 54	FU			S	A INJ ER	AS 50	R)F .ING	
	FHOTPS FHOTPS	WA	S	DE RE 19	VE VI 81		PE	D BY R-	ANR	0	PEOI	R (M	RA	MM ON	E	D Ta	81		R.	U	Ē	2.2	I A IE	so W	N.	A T	UG	us	T	19	77.	
	STANDAR CALCUL EXTERN	RD	ER	RODE	NSHI		F	S T NC		A	TE	STRO	SAU	ND	ARNE	s 0	0 E	RR	M	N	MI	is	r.	5 B	ŧ		F p	T I	E)			
	RTPG	::	BFHSR	31 EM TR	43 ES	2																											
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	FHOTPS GC TO 3	30	48	93	9.	₩((1	•	-	2))	18	0	•	*2	•	7*	P	*	EX	PI	-	au	11	1)	1	T	* (* (5)			
20	CENTIN	JE																															

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TABLE A-9.11 (continued)

30 CENTINUE 1.80E7*((1.-R0)/R0)**2.25*P*EXP(-450000./(R*T))/(T*6*6) RE TURN END 0

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1

0

. .

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10. FUEL RESTRUCTURING (FRESTR) (R. E. Mason)

The morphology and structural integrity of oxide fuel changes while power is being produced in water reactors. These changes are a function of time, temperature, burnup, and energy density. These structural changes affect the effective fuel thermal conductivity, fuel swelling, fission gas release, and fuel creep. The structure of irradiated fuel can be grouped into four categories: as-fabricated unrestructured fuel, equiaxed grains which are enlarged fuel grains with all sides approximately the same length, columnar grains which have their long axes parallel to the radial temperature gradient, and shattered or desintered grains consisting of fuel grains which are fractured free of bonds to other grains during high power transients. The physical processes which create restructured fuel and models to predict the modified fuel structures are discussed in the following sections.

10.1 Summary

The FRESTR subroutine is used to calculate equiaxed grain size, columnar grain size, and regions of fuel shattering during normal or transient reactor operation. Grain growth is driven by a potential difference across a curved grain boundary or by a temperature gradient but the growth rate is controlled by the motion of impurities at the grain boundaries. Since impurities and migration mechanisms are probably the same in UO_2 and $(U,Pu)O_2$, the model described in the following paragraphs is assumed to apply for both fuel types.

The growth rate of equiaxed fuel grains is calculated with the expression

$$g = \left\{ \frac{1.0269 \text{ x } 10^{-13} \text{ t } \exp \left(-35873.2/T\right)}{(1.0 - 5.746 \text{ x } 10^{-6}\text{B})^2 \text{ T}} + g_0^4 \right\}^{1/4}$$
(A-10.1)

where

g = grain size at the end of a time interval (m) g₀ = grain size at beginning of the time interval (m) t = time interval (s) T = temperature (K) B = burnup (MWs/kg).

The standard error of Equation (A-10.1) with respect to its data base is $\pm 8.4 \times 10^{-6}$ m.

Columnar grains form behind lenticular pores (large lens shaped pores) which move up the temperature gradient in the fuel at a rate given by the equation

v -	49.22 VT exp (-44980/T)	(1.10.2)
v =	T ²	(A-10.2)

where

V = rate of pore movement (m/s) ∇T = temperature gradient (K/m)

T = temperature(K).

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- D = diffusion coefficient for the isotope in fuel (cm²/s), this constant is calculated by the subroutine from the input maximum temperature
 - = diffusion distance for gas release (cm), this constant is estimated by the subroutine from the input fuel density
 - = time since the beginning of irradiation (s).

For the short-lived iodine and cesium isotopes produced in quantity in light water reactor fuels (I-131, I-132, I-133, I-134, I-135, and Cs-138), the expression used to predict the quantity of the isotope available in the steady state condition is

$$R_{i} = \frac{\Delta B}{\Delta t} \left(\frac{1}{1.732 \times 10^{10}} \right) Y_{i} M_{i} \frac{\frac{3}{a} \sqrt{D\lambda_{i}}}{\left(\frac{3}{a} \sqrt{D\lambda_{i}} + \lambda_{i} \right) \lambda_{i}}$$
(A-13.2)

where the symbols not defined in conjunction with Equation (A-13.1) are

 ΔB = burnup during the step considered (MWs/kg fuel)

 Δt = duration of the burnup step considered (s)

 Y_i = fission yield of isotope i (atoms of ith isotope/fission)

 M_i = mole weight of the isotope (kg/mol)

 λ_i = the decay constant of the isotope (s⁻¹).

The diffusion coefficient in Equations (A-13.1) and (A-13.2) is calculated with an exponential expression which is truncated at low temperatures

$$D = 6.6 \times 10^{-6} \exp\left(\frac{-36086}{T}\right)$$
 for T > 1134.054 K

$$D = 10^{-19}$$
 for $T \le 1134.054$ K

where

T = the maximum fuel temperature (K) when D is used in Equation (A-13.1) or

T = the current fuel temperature when D is used in Equation (A-13.2).

The diffusion distance, a, in Equations (A-13.1) and (A-13.2) is obtained from an empirical fit to measured values of effective open surface areas per volume of fuel as determined from gas absorption experiments. The correlation is presented in Section 13.2.1.







a

(A-13.3)

CESIOD

The basis for the model is discussed in Section A-13.2. Section A-13.3 is a review of the predictions of the model. A listing of the CESIOD subcode is provided in Section A-13.4.

13.2 Development of the Model

At fuel temperatures above 1000 K, gaseous fission products become sufficiently mobile to migrate out of the UO₂ lattice in a complex series of processes [A-13.2, A-13.3]. In the simplest useful approach to model this process the fuel is treated as a collection of spheres, Fick's law is used to describe the diffusion of fission gases from the UO₂ lattice, and the surface area per fuel volume (or, the effective radius of the spheres) is estimated from gas absorption measurements. This simple approach has been adopted to model the release of cesium and iodine to the fuel rod gap because a more sophisticated treatment of the diffusion process is not justified without including complex chemical effects. Exact models for the amounts of cesium and iodine in the rod gap would require consideration of the chemical interactions of cesium, iodine, zirconium, and oxygen as well as the details of the diffusion and gas release mechanism.

13.2.1 Derivation of the Mathematical Expressions. The equation which describes the release of stable or long-lived isotopes by diffusion is[A-13.3, A-13.4]

$$\frac{\partial \eta}{\partial t} = -D\nabla^2 \eta + Y \frac{df}{dt}$$
(A-13.4)

where

η	=	number	of	atoms	of	an	isotope	per	unit	volume	of	fuel	
		(atoms/r	$n^3)$										

t = time(s)

D = diffusion coefficient for the isotope (m²/s)

Y = fiss on yield of the isotope (atoms of isotope/fission)

 $\underline{df} = fic...on rate of the fue [(atoms fissioned/m³)/s], deter$ dt ...nined from the burnup rate.

Since $Y \frac{df}{dt}$ is the production rate of the isotopes, the fraction of the isotopes released from a sphere of radius "a" (a = diffusion distance for gas release) is [A-13.3]

 $R = \frac{4\pi a^2}{\frac{4}{3}\pi a^3} \int_{0}^{t} \frac{df}{dt'} \frac{df}{dt'} dt'$ (A-13.5)

The quantity of interest for finding the escape rate coefficient (ν) is the ratio, F, of the isotope release rate to the isotope production rate. This ratio for a sphere of radius a is

$$F = \frac{4\pi a^2 (-D \frac{\partial n}{\partial r})_a}{\frac{4}{3}\pi a^3 Y \frac{df}{dt}}.$$
 (A-13.12)

Equations (A-13.11) and (A-13.12) can be combined to find an expression for F. The resultant expression is [A-13.3]

$$F = \frac{3D}{\lambda a^2} \left[\left(\frac{\lambda a^2}{D} \right)^{1/2} \cos^2 \ln \left(\frac{\lambda a^2}{D} \right)^{1/2} - 1 \right].$$
 (A-13.13)

For $\frac{\lambda a^2}{D} >> 1.0$. Equation (A-13.10) reduces to the form used in the model described here:

$$\vec{r} = \frac{3}{a} \sqrt{\frac{D}{\lambda}}$$
 (A-13.14)

The ratio, F, of the isotope release rate to the isotope production rate may also be written in terms of the escape rate coefficient

$$F = \frac{v N}{\gamma \frac{df}{dt} v} .$$
 (A-13.15)

If the steady state form of Equation (A-13-9) is used to find an approximate expression for N when $\lambda \gg \nu$, and if the resultant expression for N is substituted into Equation (A-13.15) one finds

$$F \sim \frac{v}{\lambda}$$
 (A-13.16)

Finally, from Equations (A-13.14) and (A-13.16)

$$v \approx \frac{3}{a} \sqrt{D\lambda}$$
 (A-13.17)

which is the result obtained by Belle[A-13.4]

Substitution of the approximate value of ν from Equation (A-13.7) into Equation (A-13.10), conversion of the fission rate $\frac{df}{dt}$ to a burnup rate, and conversion of M to kilograms of isotope per m³ of fuel results in Equation (A-13.2). This equation is the one used in the model for the release of the short-lived isotopes of cesium and iodine.

13.2.2 Correlations for Material Constants Used in the Model. The correlations used to obtain the diffusion coefficient for isotopes in the fuel, the diffusion radius for gas release, and the fission yields of the isotopes modeled are discussed in this section.

CESIOD

The correlation for the diffusion coefficient used with the model [Equation (A-13.3)] is the empirical expression recommended by Belle on page 512 of his review A-13.4 Recent results have not seen used because improved values for the diffusion coefficient are simply not relevant until the improved techniques developed for the modeling of Xe and Kr can be adopted to provide significant improvement of the basic expressions for the release of cesium and iodine.

The correlation used for the diffusion radius in cm is

 $a = 3(TD) 10^{[20.61 - TD(67.9 - 46TD)]}$

where

TD = fractional fuel density (ratio of actual density to theoretical density).

The expression is taken from the correlation for free surface area per unit volume recommended in Figure 9.18 of Belle's review. A-13.4 Belle's figure is reproduced as Figure A-13.1 of this report. The data are estimates based on gas absorption measurements







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(A-13.18)
Kiukkola^{A-14.37} used emf measurements from galvanic cells to obtain diatomic vapor pressures over urania. Vapor pressure measurements of urania at compositions of $UO_{2.01}$ to $UO_{2.67}$ were obtained at temperatures between 1073 and 1473 K. Here again, only those data points with urania O/M ratios less than $UO_{2.0}$ were considered.

Markin and Bones^{A-14.38} used emf measurements of urania with O/M ratios between 2.00 and 2.003 in a high temperature galvanic cell. Diatomic oxygen pressures of urania between the temperatures of 973 and 1673 K were investigated. The O/M ratios were controlled and determined by coulormetric titration of oxygen ions using NiO as a source of oxygen. The main purpose of their investigations was to obtain thermodynamic functions and not oxygen vapor pressures so there is very little discussion of the vapor pressure data. Their data indicate a steep slope (decrease in vapor pressure) as the composition of the urania approaches stoichiometry. This is consistent with other data in this composition range. These data are therefore useful in the modeling effort.

AukrustA-14.39 determined equilibrium oxygen pressures over hyperstoichiometric urania. The O/M ratios were determined by a thermogravimetric method and oxygen pressures were determined from known CO₂/CO or O₂/Ar gas mixtures and O/M ratio measurements. Data were obtained at temperatures between 1373 and 1673 K. They report O/M ratios accurate to within ± 0.0002 and the log₁₀ P_{O2} accurate to ± 0.02 .

The data discussed in this section must be divided into two groups; hyperstoichiometric and hypostoichiometric. For hypostoichiometric fuel the data of Tetenbaum and Hunt, Markin, Wheeler, and Alexander are the best available. The data of Javed and Atkins were probably measured under nonequilibrium conditions and should not be used. For hyperstoichiometric fuel and oxygen pressure data of Hagemark and Broli are the most extensive and are the best. The rest are within an order of magnitude of this data and have been used.

14.3 Development of the FVAPRS Code

The equations used in FVAPRS are based on thermodynamic equations fitted to the data. The following section is a discussion of thermodynamic and chemical theory and the technique used to develop the FVAPRS correlations.

14.3.1 Review of Basic Theory. Evaporation is a change in chemical state obeying the !aw of conservation of mass. Equations can therefore be used to show which elements or compounds could be expected to be present in the vapor phase above a fuel substrate. Possible reactions of urania are A-14.12

$$UO_{2(\beta)} \longrightarrow UO_{(g)} + (\frac{1-\alpha}{2}) O_{2(g)} + \alpha O_{(g)}$$
 (A-14.8a)

$$UO_{2(\beta)} \longrightarrow \frac{1}{2} UO_{2(g)} + (\frac{2 \cdot 3\alpha}{4}) O_{2(g)} + \frac{3\alpha}{2} O_{(g)} + \frac{1}{2} U_{(\beta)}$$
(A-14.8b)

$$UO_{2(\beta)} \longrightarrow \frac{1}{2} UO_{(g)} + \frac{1}{2} UO_{3(g)}$$
 (A-14.8c)

$$UO_{2(\beta)} \longrightarrow \frac{1}{3}U_{(g)} + \frac{2}{3}UO_{3(g)}$$
 (A-14.8d)

$$UO_{2(\beta)} \longrightarrow UO_{2(g)}^{+} + e_{(g)}^{-}$$
 (A-14.8e)

 $UO_{(\beta)} \longrightarrow UO_{(g)}$ (A-14.8f)

 $2UO_{2(\beta)}$ (UO₂)_{2(g)} (A-14.8g)





where the subscript, β , denotes the material is in the solid or liquid phase, and g denotes the gas phase. These equations apply only in the oxygen solid solution regions of solid and liquid urania. Of these possible compounds, one is usually much more prominent than the others. Analysis of the data indicates that for substrate temperatures <2000 K, the magnitude of the actinide oxide vapors follow the order, $P_{UO} > F_{UO_2} > P_U > P_{UO_3}$, where P is the vapor pressure. At about 3000 K, the order of partial pressures is $P_{UO_2} = P_{UO} > P_{UO_3} = P_U$; and at temperatures >3500 K, the partial pressure order is $P_{UO_2} > P_{UO_3} > P_{UO_3} > P_{UO_3} > P_{UO_3} > P_{UO_3} > P_{UO_3} = P_U$. The oxygen partial pressure at all temperatures is generally much smaller than the combined vapor pressure of the actinide oxides.

For plutonia, the chemical reactions are similar to those of urania

$$PuO_{2(\beta)} \longrightarrow PuO_{(g)} + \left(\frac{1-\alpha}{2}\right)O_{2(g)} + \alpha O_{(g)}$$
(A-14.9a)

$$\operatorname{PuO}_{2(\beta)} \longrightarrow \frac{1}{2} \operatorname{PuO}_{2(\beta)} + \left(\frac{2 - 3\alpha}{4}\right) \operatorname{O}_{2(g)} + \frac{3\alpha}{2} \operatorname{O}_{(g)} + \frac{1}{2} \operatorname{Pu}_{(\beta)}$$
(A-14.9b)

$$PuO_{2(\beta)} \longrightarrow \frac{1}{2}PuO_{(g)} + \frac{1}{2}PuO_{3(g)}$$
(A-14.9c)

$$PuO_{2(\beta)} \rightarrow \frac{1}{3}Pu_{(g)} + \frac{2}{3}PuO_{3(g)}$$
 (A-14.9d)

$$PuO_{2(\beta)} \rightarrow PuO_{2(g)}^{+} + e_{(g)}^{-}$$
(A-14.9e)

$$PuO_{(\beta)} \rightarrow PuO_{(g)}$$
 (A-14.9f

$$(A-14.9g) \longrightarrow (PuO_2)_{2(b)}$$

It is experimentally determined that PuO is the prominent species of plutonia up to an O/M ratio of approximately 1.99, where PuO_2 becomes more prominent.

Evaporation can be described by simple thermodynamic considerations of a first-order phase transition of a pure substance, solid to vapor or liquid to vapor, at constant temperature and pressure. At the phase transition

$$dG_{\beta} = dG_{\rho}$$
(A-14.10)

where

 dG_{β} = change in Gibbs free energy for the solid or liquid

 $dG_g =$ change in Gibbs free energy for the gas.

Since the process is reversible for a first-order phase transition at constant temperature and pressure

$$dG_{\beta} = V_{\beta}dp - S_{\beta}dT$$
(A-14.11)
$$dG_{\rho} = V_{\rho}dp - S_{\rho}dT$$
(A-14.12)



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15. FUEL VISCOSITY (FVISCO) (C. S. Watson and D. L. Hagrman)

The function FVISCO calculates the dynamic viscosity of uranium dioxide. The viscosity is one of the parameters needed to model the motion of fuel during severe core damage.

The model is preliminary because the effects of departure from stoichiometry and the range of temperatures where liquid and solid UO_2 can coexist are not modeled. Also, the model does not consider any possible contamination of the molten uranium dioxide. Uncertainty estimates are provided based on the data used in the model.

15.1 Summary

Viscosity of uranium dioxide is modeled as a function of temperature, melting temperature (solidus), and the fraction of the fuel that has liquified. Input arguments describing the oxygen-to-metal ratio and plutonium dioxide content are not used in the current correlations for viscosity.

Viscosity is calculated by one of three equations, depending on whether the temperature is below the melting point for uranium dioxide, in the range of temperatures where liquid and solid uranium dioxide can coexist, or above this range.





The equation used to model the viscosity of completely liquified fuels is

$$\eta_{\rho} = 1.23 \times 10^{-2} - 2.09 \times 10^{-6} \text{ T}$$
(A-15.1)

where

 η_{ℓ} = dynamic viscosity of the liquid (Pa+s)

T = temperature(K)

For solid uranium dioxide, the viscosity is modeled with the expression

$$\eta_{\perp} = 1.38 \exp(4.942 \times 10^4 / T) \tag{A-15.2}$$

where

 η_s = dynamic viscosity of the uranium dioxide for temperatures below melting (Pa+s).

In the temperature range where liquid and solid uranium dioxide phases can both exist, the viscosity is modeled with the expression

 $\eta = \eta_{g}(1 - f) + \eta_{f} f$ (A-15.3)

where

 η = dynamic viscosity of the liquid-solid mixture (Pa • s)

f = fuel fraction that is liquid (unitless).

The estimated uncertainty of the values computed with Equations (A-15.1) to (A-15.3) is computed with the FVISCO subcode but not returned as an output argument. The expressions used for this uncertainty are

$$U = \eta A(1 + |Y - 2|)$$

where

U = estimated uncertainty (Pa • s)

- A = 0.33 for temperatures above melting 0.67 for temperatures below melting
- Y = oxygen-to-metal ratio of the fuel (unitless).

Details of the development of the fuel viscosity model used in the FVISCO function are presented in the following sections. Section 15.2 is a review of the data and Section 15.3 is a discussion of the model development. The subcode is listed in Section 15.4 and references are provided in Section 15.5.

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(A-15.4)



(A-15.5)

15.2 Fuel Viscosity Data

Viscosities for solid UO₂, UO_{2.05}, and UO_{2.16} have been reported by Scott, Hall, and Williams.^{A-15.1} Viscosities for the nonstoichiometric oxides are lower than the viscosity of UO₂ at corresponding temperatures and could be measured over a sufficient range to establish the following relation for nonstoichiometric UO₂

$$\eta_{e} = A \exp(-B/T) .$$

where A and B are material constants. The viscosity of UO₂ was determined to be 2 x 10^{11} Pa·s at 1923 K and to be in excess of 10^{17} Pa·s at 1273 K.

Viscosity data at much higner temperatures were obtained by Nelson. A-15.2, A-15.3 An early measurement (0.145•Pa s at a temperature of 3028 K) was reported to correspond to incomplete melting of the sample. Subsequent data (0.045•Pa s at 3028 K and 0.036 at 3068 K) represent a viscous fluid at temperatures below the melt temperature used in the MATPRO Handbook.^a These data are not suitable for use in the viscosity model because all three measurements have indicated viscosities well above the more extensive measurements at temperatures where the uranium dioxide is known to be completely liquified.

Two useful sources of data with completely molten uranium dioxide are available. Tsai and OlanderA-15.4 published data from two samples, and WoodleyA-15.5 published more extensive data from a single sample. The data are tabulated in Tables A-15.1 and A-15.11 and plotted in Figure A-15.1. The

TABLE A-15.I

	Temperature (K)	Viscosity (Pa*s)
Sample 1	3153 3153	0.00583
	3153 2333	0.00594 0.00514
	3113 3113 3173	0.00628 0.00686 0.00762
Sample 2	3083 3188 3188 3188 3138	0.00921 0.00869 0.00771 0.00781
	3328 3328 3328 3248 3248	0.00602 0.00602 0.00765 0.00808 0.00682

UO2 VISCOSITY DATA FROM TSAI AND ULANDERA-15.4



a. The melt temperature for UO2 is given as 3113 K in the PHYPRP subcode of the MATPRO package.

TABLE A-15.11

Viscosity Temperature (K) (Pa*s) 3113 0.00425 3148 0.00365 3148 0.00326 0.00441 3193 3193 0.00434 0.00444 3193 3258 0.00420 3258 0.00417 3258 0.00415 3213 0.00426 3213 0.00428 3218 0.00427 3178 0.00432 3183 0.00436 3183 0.00434 3163 0.00424 3163 0.00420 3163 0.00423 3158 0.00418 3158 0.00428 3163 0.00425 3198 0.00417 3208 0.00418 3198 0.00419 3263 0.00399 3263 0.00405 3263 0.06402 3293 0.00398 0.00395 3298 3303 0.00394 3273 0.00399 3273 0.00398 3273 0.00397 3218 0.00409 3213 0.00406 3218 0.00404 3178 0.00412 3178 0.00406

3178

UO2 VISCOSITY DATA FROM WOODLEYA-15.5



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0.00413





Figure A-15.1. Uranium dioxide viscosities measured as a function of temperature.

precision of the data by Woodley is noticeably higher than the precision of the other data, but there is a larger difference between the two experiments than can be explained by random measurement error. This difference is discussed by Woodley but no definite reason for it was found. The model developed in the next section therefore contains the assumption that the difference between the data of Tsai and Olander and the data of Woodley is caused by some material parameter that has not been considered (oxygen-to-metal ratio, for instance).

15.3 Model Development and Uncertainty

The correlation for the viscosity of UO_2 below the melt temperature was obtained by solving Equation (A-15.5) for the values of the two material constants that reproduce viscosity measured by Scott, Hall, and Williams at 1273 K and the minimum viscosity reported by these authors for uranium dioxide at 1273 K. The fact that this procedure produces only a crude engineering estimate of viscosity is expressed by assigning a large fractional uncertainty, two thirds, to the predicted viscosity of solid uranium dioxide.

Equation (A-15.1), the correlation for viscosity of liquid uranium dioxide, was obtained from the data of Tsai and Olander and the data of Woodley. The less precise data of Tsai and Olander wer, sed because Woodley used only one sample and the viscosities measured by Tsai and Olander with their samples differ from Woodley's data by more than the scatter of their measurements.

The traditional Arrhenius relation (Equation A-15.5) was not used to correlate the liquid viscosities because a simpler linear expression fits the data as well as the exponential form. A linear least-squares fit to the data of Woodley (with the two anomolously low viscosities at 3148 K omitted) produced the equation



•

$$\eta_{f} = 1.09 \times 10^{-2} - 2.09 \times 10^{-6} \text{ T}$$
 (A-15.6)

The data of Tsai and Olander yielded the following correlation

$$\eta_{\ell} = 1.60 \times 10^{-2} - 2.77 \times 10^{-6} \text{ T}$$
 (A-15.7)

The viscosities predicted by Equations (A-15.6) and (A-15.7) are compared with the data in Figure A-15.2. By inspection of this figure, it was concluded that the best mathematical description of the difference in the viscosities measured for the different lots of uranium dioxide is to assume that the viscosities of the two different lots differ by an additive constant.^a

In order to recognize the more precise measurements of Woodley, yet account for the probable lot-to-lot variation indicated by the data of both authors, the least-squares fit to the data of Tsai and Olander was repeated with the added constraint that the slope of the correlation match the slope obtained from the data Woodley. The resultant correlation for the data of Tsai and Olander is





a. The interpretation corresponds to the assumption mentioned at the end of Section 15.2; the difference in viscosities is caused by some unknown material parameter of the uranium dioxide.



The final step in the derivation of Equation (A-15.1) was to average Equations (A-15.8) and (A-15.6). This step assumes that each lot of UO_2 is equally probable.

The estimated uncertainty of the values of viscosity computed with Equation (A-15.8) was determined using the assumption that the important difference in the measurements of the two references is the unknown difference in the two lots of uranium dioxide. The resultant standard deviation is

$$\sigma = \sqrt{\left(1.09 \times 10^{-2} - 1.23 \times 10^{-2}\right)^2 + \left(1.38 \times 10^{-2} - 1.23 \times 10^{-2}\right)^2} \approx 2 \times 10^{-3} \text{ Pa} \cdot \text{s}$$
(A-15.9)

which is approximately one-third the predicted value of the viscosity. The increased uncertainty for nonstoichiometric uranium dioxides shown in Equation (A-15.4) is simply an estimate that has been included to indicate that the model contains no dependence on the oxygen-to-metal ratio of the fuel.

Figure A-15.3 illustrates the viscosities calculated with Equation (A-15.1) for liquid uranium dioxide. The dashed lines are the upper and lower uncertainty limits obtained by adding $\pm 1/3$ of the predicted viscosity and an assumed melt temperature of 3113 K.

Equation (A-15.3), which is employed only in the temperature range where liquid and solid can both exist (for temperatures between the fuel melting temperature and the melt temperature plus the liquid-solid coexistence temperature range), is obtained from the assumption that the viscosity is the volume-weighted average of the solid and liquid viscosities in this temperature range.



Figure A-15.3.

 Viscosities calculated with Equation (A-15.1) (solid line) and upper and lower uncertainty estimates (dashed lines) compared with data.

15.4 Fuel Viscosity Subcode FVISCO Listing

Table A-15.III is a listing of the FViSCO subcode.

15.5 References

- A-15.1. R. Scott, A. R. Hall, J. Williams, "The Plastic Deformation of Uranium Oxides Above 800 K," Journal of Nuclear Materials, i (1959) pp. 39-48.
- A-15.2. W. F. Sheely (ed), Quarterly Progress Report, July, August, September, 1969, Reactor Fuels and Materials Development Programs for Fuels and Materials Branch of USAEC Division of Reactor Development and Technology, BNWL-1223 (November 1969).
- A-15.3. W. F. Sheely (ed), Quarterly Progress Report, October, November December, 1969, Reactor Fuels and Materials Development Programs for Fuels and Materials Branch of USAEC Division of Reactor Development and Technology, BNWL-1279 (February 1970).
- A-15.4. H. C. Tsai and D. R. Olander, "The Viscosity of Molten Uranium Dioxide," Journal of Nuclear Materials, 44 (1972) pp. 83-86.
- A-15.5. R. E. Woodley, "The Viscosity of Molten Uranium Dioxide," Journal of Nuclear Materials, 50 (1974) pp. 103-106.







TABLE A-15.III

LISTING OF THE FVISCO SUBCODE

FUNCTION FVISCO(FTEMP.FOTMTL.FACMOT) EVISCO CALCULATES THE DYNAMIC VISCOSITY OF U02 FUEL. FVISCO . OUTPUT DYNAMIC VISCOSITY (PA+S) UVISCO - ESTIMATED STANDARDD ERROR OF FVISCO (PA+S) (NOT CURRENTLY RETURNED) FTEMP . INPUT FUEL TEMPERATURE (K) INPUT DXYGEN TO METAL RATIO (UNITLESS) INPUT FUEL FRACTION MOLTEN (UNITLESS) FOTMTL . FACMOT . FACMOT = 1.0 MEANS FUEL IS ALL MOLTEN FACMOT = 0.0 MEANS FUEL IS ALL SOLID COMMON / PHY PRO/ FIMELT . FHEFUS .CTMELT .CHEFUS , CTRANB , CTRANE .CTRANZ FDELTA ,COMP 2 . BU . DELOXY THE PHYPRO COMMON BLOCK IS SET BY A CALL TO THE SUBROUTINE PHYPRP WHICH IS PART OF THE MATERIALS PROPERTIES PACKAGE USED AT THE INEL. QUANTITIES CONTAINED IN PHYPRO USED IN THIS SUBROUTINE ARE: FTMELT = FUEL MELTING TEMPERATURE (K) FDELTA = FUEL LIQUID-SOLID COEXISTENCE TEMPERATURE RANGE (K) THE EQUATIONS USED IN THIS FUNCTION ARE BASED ON DATA FROM: (1) R. E. WOODLEY, THE VISCOSITY OF MOLTEN URANIUM DIDXIDE, JOURNAL OF NUCLEAR MATERIALS, 50, (1974), PP 103-105. R. SCOTT, A. R. HALL, AND J. WILLIAMS, THE PLASTIC DEFERMATION OF URANIUM OXIDES ABOVE 800 C, JOURNAL OF NUCLEAR MATERIALS, 1, (1:59), PP 39-48. (2) H. C. TSAI AND D. R. OLANDER, THE VISCOSITY OF MOLTEN URANIUM DIOXIDE, JOURNAL OF NUCLEAR MATERIALS, 44, (1972), (3) PP 83-86. CODED BY C. S. WATSON AND D. L. HAGRMAN OCTOBER 1980 FVISCO = 1.38 * EXP(4.942E+04/FTEMP) IF (FTEMP .LE. FTMELT) GO TO 120 FVISCO = FVISCO * (1. - FACMOT) + (1.23E-02 - 2.09E-06 * FTEMP) * FACMOT

CCCCC

FVISCO



ZOEMIS

TABLE B-3.V

LISTING OF THE ZOEMIS SUBCODE

g SUBROUTINE ZOEMIS(CTMAX, ZROXID, EMISSY) THE EMISSIVITY OF THE CLADDING SURFACE AXIMUM CLADDING TEMPERATURE AND EXPECTED STANDARD ERROR OF THE LIX COMPARED TO IN-REACTOR ZOEMIS CALCULATES THE EMISSIVIT AS A FUNCTION OF MAXIMUM CLADDID OXIDE THICKNESS. EXPECTED STAN CALCULATED EMISSIVITY COMPAKED DATA IS ALSU RETORNED PUENIS - DUTPUT CLADDING SURFACE EMISSIVITY (UNITLESS) PUENIS - DUTPUT POSITIVE STANDARD ERROR EXPECTED IN EMISSV WHEN COMPARED TO IN-REACTOR DATA (NOT CURRENTLY RETURNED) UUEMIS - DUTPUT NEGATIVE STANDARD ERROR EXPECTED IN EMISSY WHEN COMPARED TO IN-REACTOR DATA (NOT CURRENTLY RETURNED) ZREAT - INPUT MAXIMUM CLADENING TEMPERATURE (K) THE EQUATIONS USED IN THIS SUBROUTINE ARE BASED ON DATA FROM (1) AEC FUELS AND MATERIALS DEVELOPMENT PROGRAM PROGRESS REPORT NO. 76, USAEC REPORT GEMP - 1008 (1968). SECTION BY (2) T. B. BURGDYNE AND A. GARLICK, PAPER PRESENTED AT SPECIALISTS MEETING ON THE BEHAVILYR DE WATER REACTOR FUEL ELEMENTS UNDER ACCIDENT CONDITIONS, SPATINO NORWAY (SEPTEMBER 1976) (3) E V. MURPHY ALLOYS IN AIR IN J. NUC. MAT., 60 ENISSIVITY OF ZIRCONIUM IN THE TEMPERA 60 (1976) PP 1 RATURE R 167-176 ZDEMIS CODED BY R. L. MILLER SEPT 1974 MCCIFIEC BY D. L. HAGRMAN OCTOBER 1976 MDCEL FOR IF (ZROXID EMISSV 2 GD ISSV 2 CENISSV 2 CENISSV 2 UUECCEAN TEMPERATURES BELOW 1500K FOLLOWS .GE. 3.88E-06) GO TO 10 3.25E-01+1.246E05*ZROXID 8.C8642E-01-5.00E01*ZROXID 0.1 0.1 .LE. 1500.1 GC 14 80 10 CC MOCIFICAT EMISSY . IF (EMISSY PUEMIS . UUEMIS . ĉ STANCARC ERROR CUT OFF AT MOOSSIBLE VALUES FOLLOWS F (PUEMIS .GI. (1.00-EMISSV); UEMIS = 1.00 - EMISSV IF (UUEMIS .GT. EMISSV) UUEMIS - FHISSV C SO RETURN

- B-3.4. J. V. Cathcart, Quarterly Progress Report on the Zirconium Metal-Water Oxidation Kinetics Program Sponsored by the NRC Division of Reactor Safety Research for April – June 1976. ORNL/NUREG-TM-41 (August 1976).
- B-3.5. Quarterly Technical Progress Report on Water Reactor Safety Programs Sponsored by the Nuclear Pegulatory Commission's Division of Reactor Safety Research, October – December 1975, ANCR-NUREG-1301 (May 1976) p 67.

4. CLADDING THERMAL EXPANSION AND ITS **RELATION TO TEXTURE (CTHEXP) (G. A. Reymann)**

The model described herein calculates components of the thermal expansion strain for single crystal zircaloy. By use of pole figures to ascertain the average orientation of single crystals in a multicrystalline sample, such as zircaloy fuel rod cladding, these single crystal values may be applied to find the thermal expansion strain of any sample.

Thermal expansion strain, especially in the diametral direction, is important in safety analyses because it is a major factor in determining the pellet-cladding gap, and thus the pellet temperature and its stored energy. Since zircaloy is an anisotropic solid, strain parallel and perpendicular to the basal pole direction of single crystal grains are needed to find the diametral strain in a multicrystalline sample. The treatment of this strain as a tensor and the use of pole figures are the primary changes in this version of CTHEXP.

4.1 Summary

A total of six correlations that are functions of temperature only are used to find the single crystal thermal strains. In addition, basal plane symmetry ($\epsilon_{11} = \epsilon_{22}$) is assumed. The model was developed for as-fabricated zircaloy-4, but comparisons with zircaloy-2 and zirconium data also show good agreement for these materials.

The correlations for single crystal thermal strains are

$$\epsilon_{11} = 4.95 \times 10^6 \text{ T} - 1.485 \times 10^3$$

$$\epsilon_{33} = 1.26 \times 10^5 \text{ T} - 3.78 \times 10^3$$

where

circumferential thermal expansion (m/m)

axial thermal expansion (m/m) 622

temperature (K). T

For $1083 \le T \le 1244$ K

$$\epsilon_{11} = \left[2.77763 + 1.09822 \cos\left(\frac{T - 1083}{161} \right) \right] \times 10^{-3}$$

$$\epsilon_{33} = \left[8.76758 + 1.09822 \cos\left(\frac{T - 1083}{161} \pi\right) \right] \times 10^{-3}$$
(B-4.4)

where the arguments of the cosines are in radians.

For T > 1244 K

$$e_{11} = 9.7 \times 10^{-6} \text{ T} - 1.04 \times 10^{-2}$$
(B-4.5)



(B-4.1)

(B-4.2)





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$$\epsilon_{33} = 9.7 \times 10^{-6} \text{ T} - 4.4 \times 10^{-3} . \tag{B-4.6}$$

To obtain cladding strains from these single crystal strains, it is necessary to do a volume-weighted averaging over the entire cladding section. Such an averaging requires a pole figure and is described in Section B-10. The results are

$$\langle \epsilon_{11}^{'} \rangle = \langle \sin^2 \phi \rangle \epsilon_{11}^{'} + \langle \cos^2 \theta \cos \phi \rangle \epsilon_{22}^{'} + \langle \sin^2 \theta \cos^2 \phi \rangle \epsilon_{33}^{'}$$
(B-4.7)

$$\langle \epsilon_{22}^{'} \rangle = \langle \cos^2 \phi \rangle \epsilon_{11}^{'} + \langle \cos^2 \theta \sin^2 \phi \rangle \epsilon_{22}^{'} + \langle \sin^2 \theta \sin^2 \phi \rangle \epsilon_{33}^{'}$$
(B-4.8)

$$\langle \epsilon_{33}^{'} \rangle = \langle \sin^2 \theta \rangle \epsilon_{22} + \langle \cos^2 \theta \rangle \epsilon_{33}$$
 (B-4.9)

where primed strains refer to the laboratory system (cladding and unprimed strains to the single crystals)

- θ = angle between the radial direction of the cladding and e c-axis of the single crystals
- φ = angle between the circumferential direction of the cladding and the projection of the c-axis at a grain onto the circumferential—axial plane at the cladding
- $\langle a \rangle$ = volume-weighted average of a.

As an example, the strains for a typical light water reactor (LWR) cladding tube (zircaloy-4) are, for T < 1083 K

$$<\epsilon_{11}> = 7.09 \times 10^{-6} \text{ T} - 2.13 \times 10^{-3}$$
 (B-4.10a)

$$\langle \epsilon_{22} \rangle = 5.41 \times 10^{-6} \text{ T} \cdot 1.62 \times 10^{-3}$$
 (B-4.10b)

$$<\epsilon_{33}> = 10^{-5} \text{ T} - 3.00 \text{ x } 10^{-3}$$
 (B-4.10c)

Section 4.2 contains a review of the literature consulted. The model development is given in Section 4.3, and Section 4.4 contains a model-data comparison with an uncertainty analysis. The CTHEXP listing is given in Section 4.5 and Section 4.6 contains the references.

4.2 Review of Literature

The most important source is the model on cladding plastic deformation, Section B-8, where the volume-weighted averages of the direction cosines for typical LWR cladding are given. These averages were used with thermal expansion data from a recent EPRI report by Bunnell^{B-4,1} to make the basic model. Since Bunnell does not report data in the beta phase (T > 1244 K) for circumferential expansion, the data can be used only for an alpha phase model. The EPRI data do not show ϵ_{11} or ϵ_{22} equal to zero at 300 K, and therefore each point was shifted by an amount such that this requirement was met. To determine the validity of the resulting data, they were checked against the older data sources of Douglass, B-4.2 Mehan and Wiesinger, B-4.3 Scott, B-4.4 and Kearns. B-4.5 The correlations given here compare well with those of Douglass and Kearns as shown in Figures B-4.1 through B-4.4. The Mehan and Wiesinger data are for plates. To be compared with Equations (B-4.1) and (B-4.2), these equations must be converted from single crystal form to plate form. Since Mehan and Wiesinger give no detailed texture information, typical values for texture coefficients from Hann^{B-4.6} were used. The results are shown in Table B-4.1.



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Figure B-4.1. Comparison of CTHEXP prediction with Douglass' data in the axial direction.

The differences shown in Table B-4.1 can be easily explained by the unknown texture differences between the samples from which the data sets were derived.

All data sets had to be adjusted to give $\Delta L = 0$ at 300 K. This was done by adding or subtracting the strain at 300 K. This technique is not exact for engineering strains but results in negligible error when the strains are small, as in the case here.

These comparisons show that in the alpha phase, the Bunnell data are adequate. Therefore, this data set is used as the data base in the low temperature (T < 1083 K) range.

In the transition region between the alpha and beta phases (1083 \leq T \leq 1244 K), the volume strain was found using lattice constants for alpha zirconium from Douglass and for beta zirconium from Kittel.^{B-4.7} This strain was divided by 3.0 to find an approximate linear strain, which was assumed to be equal in all three directions. A cosine function was fit to their strain to match the values at the end of the alpha phase and the beginning of the beta phase. For the beta phase, the coefficient of expansion for zirconium from Skinner and Johnston^{B-4.8} was used.

The correlations for $T > 10^{83}$ K are approximate. However, at these temperatures, the cladding is so soft that typical in-reactor stresses cause a significantly greater strain than the strain due to thermal expansion.

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Figure B-4.2. Comparison of CTHEXP prediction with Douglass' data in the circumferential direction.

4.3 Model Development

The model development is divided into three sections, depending on the temperature: an alpha phase model, a transition phase region, and a beta phase region.

4.3.1 Thermal Expansion in the Alpha Phase. The basic equations used to model thermal expansion in the alpha phase are tensor transformation equations relating cladding strain components to single crystal strain components, and parameters that describe the distribution of grain orientations in the cladding. The model is based on measured thermal strains in two directions for cladding with known texture. The inverse of the transformation is used to deduce single crystal thermal expansions from data.

Since strain is a second rank tensor, it is necessary to do a formal rotation of axes to describe single crystal strains viewed from a laboratory system. The rotation is shown schematically in Figure B-4.5, which was taken from Section B-5. To derive the various tensors, first consider the transformation necessary to obtain the laboratory unit vectors expressed in terms of the single crystal unit vectors. Since the single crystal is isotropic in planes perpendicular to the C-axis, assume for this transformation that the Y-axis (single crystal) is in the same plane as the C-axis and the radial direction of the tube. Primed coordinates refer to those fixed in the laboratory system, and unprimed coordinates to those fixed in the single crystals. The resulting transformation is

x'	-	$\sin\phi \hat{x} + \cos\theta\cos\phi \hat{y} + \sin\theta\cos\phi \hat{z}$	(B-4.11)
ŷ'	11	$-\cos\theta \hat{x} + \cos\theta\sin\phi \hat{y} + \sin\theta\sin\phi \hat{z}$	(B-4.12)
î'	=	$-\sin\theta \hat{y} + \sin\theta\cos\theta \hat{z}$	(B-4.13)



Figure B-4.3. Comparison of CTHEXP predictions with Kearns' model in the axial direction.

where θ and ϕ are defined in Figure B-4.5.

Equations (B-4.11) through (B-4.13) show a first rank tensor transformation.

$$\hat{\mathbf{x}}_{\mathbf{j}}^{\mathbf{j}} = c_{\mathbf{j}\mathbf{j}}\hat{\mathbf{x}}_{\mathbf{j}}$$
(B-4.14)

where cii is the transformation coefficient.

The corresponding transformations for strains (2nd rank tensors) are

$$\epsilon_{ij} = \sum_{s=1}^{3} \sum_{t=1}^{3} C_{is} C_{jt} \epsilon_{st}$$
(B-4.15)

where

 C_{1S} = coefficient from the first order tensor transform [Equations (B-4.11) to (B-4.13)]. For example, $C_{11} = \sin\phi C_{12} = \cos\theta\cos\phi$, and $C_{13} = \sin\theta\cos\phi$.

Applying Equation (B.4.15) to find e_{11} gives

$$\epsilon_{11} = (C_{11} C_{11} \epsilon_{11} + C_{12} C_{11} \epsilon_{21} + C_{13} C_{11} \epsilon_{31}) + (C_{11} C_{12} \epsilon_{12} + C_{12} C_{12} \epsilon_{22} + C_{13} C_{12} \epsilon_{32}) + (C_{11} C_{13} \epsilon_{13} + C_{12} C_{13} \epsilon_{23} + C_{13} C_{13} \epsilon_{33}) .$$

(B-4.16)

CTHEXP



TABLE B-4.1

COMPARISON OF MEHAN AND WIESINGER PLATE EXPANSION WITH MATPRO MODEL

Direction	Mehan and Wiesinger	MATPRO Model	Difference (%)
Longitudinal	4.62 x 10 ⁻⁶	5.41 x 10 ⁻⁶	-14.60
Transverse	6.58 x 10 ⁻⁶	7.10×10^{-6}	-7.32

Substituting the appropriate C_{ij}s into Equation (B-4.16) gives

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$$\epsilon_{11} = \sin^{2} \phi \epsilon_{11} + \cos\theta \cos\phi \sin\phi \epsilon_{21} + \sin^{2} \theta \cos\phi \epsilon_{31}$$

$$+ \sin\phi \cos\theta \cos\phi \epsilon_{12} + \cos^{2} \theta \cos^{2} \phi \epsilon_{12} + \sin\theta \cos^{2} \phi \cos\theta \epsilon_{32}$$

$$+ \sin\phi \cos\phi \sin\theta \epsilon_{13} + \cos\theta \cos\phi \sin\theta \epsilon_{23} + \sin^{2} \theta \cos^{2} \phi \epsilon_{33} . \qquad (B-4.17)$$

The volume-weighted averages of the strain tensors are needed. These are given by

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$$<\epsilon_{ij}> = \int_{0}^{2\pi} \int_{0}^{\pi} \epsilon_{ij}(\theta,\phi) \ \rho(\theta,\phi) \sin\theta \ d\theta \ d\phi$$

frame of reference.

where

Figure B-4.5.

volume fraction weighted average of $\epsilon_{ij}~({\rm m/m})$ $<\epsilon_{ij}>$ 22 $\epsilon_{ij}^{}(\theta,\phi)$ thermal expansion strain (m/m) - $\rho(\theta,\phi)$ volume fraction of grains with their C-axes oriented in the region $\sin\theta \ d\theta \ d\phi$ about θ and ϕ .

Putting Equation (B-4.17) into Equation (B-4.18) gives

$$<\epsilon_{11}'> = \epsilon_{11} \int_0^{2\pi} \int_0^{\pi} \sin^2 \phi \rho(\theta, \phi) \sin\theta d\theta d\phi$$
$$+ \epsilon_{21} \int_0^{2\pi} \int_0^{\pi} \cos\theta \cos\phi \sin\phi \rho(\theta, \phi) \sin\theta d\theta d\phi$$

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(P 4.18)

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$$+ \epsilon_{31} \int_0^{2\pi} \int_0^{\pi} \sin^2 \theta \cos\phi \rho(\theta, \phi) \sin\theta d\theta d\phi + \dots$$
(B-4.19)

The integral $\int_{0} \int_{0} \sin^{2}\phi \rho(\theta,\phi) \sin\theta d\theta d\phi = \langle \sin^{2}\phi \rangle$, the volume-weighted average of $\sin^{2}\phi$. Similarly, the integral

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$$\int_{0}^{2\pi} \int_{0}^{\pi} \sin^{2}\theta \cos\phi\rho(\theta,\phi) \sin\theta d\theta d\phi = \langle \sin^{2}\theta \cos\phi \rangle = \langle \sin^{2}\theta \rangle \langle \cos\phi \rangle = 0.0$$
(B-4.20)

because averaged over the 0 to 2π interval, $\cos\phi$ equals 0. In the same way $\sin\phi$, $\sin\theta$, and $\cos\theta$ are zero. Only a squared function has a nonzero average. These averages may be found with the CTXTUR subcode of Section B-10 using a pole figure for input texture information.

All nine of tensor elements $\langle \epsilon_{..} \rangle$ may be found using Equations (B-4.15) and (B-4.18). The only nonzero ones are listed in Equations (B-4.21) through (B-4.23).

$$<\epsilon_{11}^{'}> = <\sin^{2}\phi > \epsilon_{11} + <\cos^{2}\theta \cos^{2}\phi > \epsilon_{22} + <\sin^{2}\theta \cos^{2}\phi > \epsilon_{33}$$
 (B-4.21)

$$\triangle \epsilon_{22}^{'2} > = \langle \cos^2 \phi \rangle \epsilon_{11} + \langle \cos^2 \theta \sin^2 \phi \rangle \epsilon_{22} + \langle \sin^2 \theta \sin^2 \phi \rangle \epsilon_{33}$$
(B-4.22)

$$\langle \epsilon_{33} \rangle = \langle \sin^2 \theta \rangle \epsilon_{22} + \langle \cos^2 \theta \rangle \epsilon_{33}$$
 (B-4.23)

From Section B-8, the coefficients of the strains in Equations (B-4.21) to (B-4-23) may be foun ϕ for the cladding used by Bunnell. Substituting these values into Equations (B-4.21) to (B-4.23), Equations (B-4.24) to (B-4.26) are obtained.

$$<\epsilon_{11}> = 0.18 \epsilon_{11} + 0.54 \epsilon_{22} + 0.28 \epsilon_{33}$$
 (B-4.24)

$$<\epsilon_{22}> = 0.82 \epsilon_{11} + 0.12 \epsilon_{22} + 0.06 \epsilon_{33}$$
 (B-4.25)

$$<\epsilon_{33}> = 0.34 \epsilon_{22} + 0.66 \epsilon_{33}$$
 (B-4.26)

In a single crystal, the circumferential strain, ϵ_{11} , is equal to the diametral strain, ϵ_{22} , so Equations (B-4.24) to (B-4.26) reduce to

$$\epsilon_{11} > = 0.72 \epsilon_{11} + 0.28 \epsilon_{22} \tag{B-4.27}$$

$$\langle \epsilon_{22} \rangle = 0.94 \epsilon_{11} + 0.06 \epsilon_{33}$$
 (B-4.28)

$$<\epsilon_{33}^{'}> = 0.34 \epsilon_{11}^{'} + 0.66 \epsilon_{33}^{'}$$
 (B-4.29)

CTHEXP

Bunnell's data were taken in the laboratory frame. Therefore, Equations (B-4.27) to (B-4.29) must be inverted to find the single crystal strains in terms of the cladding strains

$$\epsilon_{11} = -0.27 < \epsilon_{11} > + 1.27 < \epsilon_{22} > \tag{B-4.30}$$

$$\epsilon_{33} = 4.27 < \epsilon_{11} > -3.27 < \epsilon_{22} > \tag{B-4.31}$$

$$\epsilon_{22} = \epsilon_{11} \quad . \tag{B-4.32}$$

Bunnell's data, adjusted so the strain is zero at 300 K, are given in Tables B-4.11 and B-4.111 for circumferential and axial thermal expansion, respectively.

Using the data listed in these tables, the next step is to find the single crystal strains as a function of temperature. Since temperature in the two tables do not always correspond, it was necessary to use Bunnell's correlations, which he used to fit those data, again adjusting them so the strains are zero at 300 K. A least-squares fit was done, with the constraint that the strains are zero at 300 K. The results are

$$\epsilon_{11} = 4.95 \times 10^{-6} \text{ T} - 1.485 \times 10^{-3}$$
 (B-4.33)

$$\epsilon_{33} = 1.26 \times 10^{-5} \text{ T} - 3.78 \times 10^{-3}$$
 (B-4.34)

where T = temperature (K).

Equations (B-4.33) and (B-4.34) are the model for the alpha phase of zircaloy single crystals. If one has a pole figure for cladding, Equations (B-4.18) to (B-4.20) may be used to find the cladding thermal expansion, remembering that $\epsilon_{22} = \epsilon_{11}$.

4.3.2 Thermal Expansion in the Transition Region. To obtain single crystal thermal expansion, both the axial and circumferential cladding thermal expansions are necessary. While axial data in the transition region are available, circumferential data are not. Due to this lack of data and the insignificance of chermal strain at these temperatures, an approximation was made.

For zirconium in the alpha phase at 1123 K, the Douglass^{B-4.2} correlation gives the lattice constants as $c = 5.193 \times 10^{-10}$ m and $a = 3.245 \times 10^{-10}$ m, giving a volume of 47.356 x 10⁻³⁰ m³. Kittel^{B-4.7} gives the lattice constant for beta zirconium at the same temperature as 3.61 x 10⁻¹⁰ m, implying a unit cell volume of 47.046 x 10⁻³⁰ m³. This decrease in volume as the material changes from the alpha close-packed structure to the generall; more open beta body centered cubic is surprising, although it has been reported by many investigators. B-4.2, B-4.4, B-4.8 The volume strain is ~0.66%, in good agreement with Skinner and Johnston. B-4.8 To model the transition region, it is assumed that each dimension contributes equally to this volume strain

$$\frac{\Delta 1}{1_{0}} = \frac{1}{3} \frac{\Delta V}{V_{0}} = \frac{1}{3} \frac{3.1 \times 10^{-31}}{\left(3.61 \times 10^{-10}\right)^{3}} = 2.196 \times 10^{-3}$$

where

 $\Delta 1 = \text{change in length (m)}$

 $1_0 = reference length (m)$





(B-4.35)

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Temperature (K)	$\epsilon'_{11} \times 10^{-3}$ (unitless)	Temperature (K)	$\epsilon'_{11} \times 10^{-3}$ (unitless)
20/ 15	1 906	616 15	2 326
394.15	1.000	620.15	2.520
398.15	1.130	620.15	2.510
401.15	1.200	623.13	1.910
403.15	0.710	027.10	2.920
439.15	1.336	663.15	2.636
444.15	1.516	667.15	2.826
444.15	2.206	671.15	2.226
447.15	0.926	673.15	3.396
481.15	1.616	708.15	2,986
485.15	1.786	712.15	3,126
488.15	1,196	716.15	2,516
488.15	2.196	718.15	3.736
523,15	1.876	751.15	3,266
528.15	2.016	755.15	3.456
531.15	1.416	759.15	2.856
532.15	2.516	761.15	3.916
568.15	2.096	794.15	3.646
572.15	2.216	797.15	3.756
577.15	1.626	802.15	3,166
579.15	2.770	804.15	4.346
836.15	4 026	964 15	4 806
840.15	4.026	060 15	5.026
844.15	3 476	072 15	1. 376
8/6 15	1 306	075 15	4.576
040.15	4.550	773.13	4.070
878.15	4.086	1008.15	5.006
881.15	4.436	1013.15	5.326
885.15	3.786	1017.15	4.656
888.15	4.506	1019.15	4.616
920.15	4.606	1044.15	4.736
925.15	4.716	1044.15	4.876
929.15	4.136	1044.15	5.646
031.15	4.706	1044.15	5.406

BUNNELL'S CIRCUMFERENTIAL THERMAL EXPANSION DATA



TABLE B-4.111

Temperature (K)	$\epsilon'_{11} \times 10^{-3}$	Temperature	$\epsilon_{11}' \times 10^{-3}$
	<u>Auniciess/</u>	<u> </u>	(GRILELESS /
376.15	0.461	69.15	1.321
380.15	0.421	569.15	1.621
289.15	0.531	578.15	1.311
396.15	0.461	579.15	1.631
396.15	0,611	581.15	1.401
8.15	0.481	588.15	1.731
403.15	0.561	599.15	1.451
406.15	0.481	604.15	1.661
411.15	0.581	604.15	1.811
421.15	0.591	613.15	1,901
424.15	0.661	616.15	1.571
428.15	0.741	620.15	1.841
436.15	2.061	627.15	1.551
441.15	0.681	629.15	1.461
444.15	0.811	630.15	1.921
445.15	0.671	646.15	1.701
449.15	0.691	646.15	2.031
45 5	0.901	651.15	1.851
462.15	0.941	653.15	2,111
466.15	0.801	663.15	1.841
468.15	0.901	663.15	2.031
477.15	1.031	671.15	2.151
482.15	0.901	673.15	1.831
489.15	1.121	675.15	1.871
490,15	0.911	686.15	2+221
496.15	i.201	691.15	1.991
504.15	1.201	694.15	2.271
506.15	1.021	697.15	2.221
511.15	1.181	704.15	2.061
512.15	1.251	707.15	2,111
523.15	1.111	711.15	2.351
524.15	1.351	718.15	2.101
531.15	1.451	721.15	2.111
532.15	1.101	726.15	2.401
\$35.15	1,131	833.15	2.511

BUNNELL'S CIRCUMFERENTIAL THERMAL EXPANSION DATA





ABLE E-4.III (continued)

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Temperature	ε ₁₁ x 10 ⁻³	Temperature	$\epsilon'_{11} \times 10^{-3}$	
(K)	(unitless)	(K)	(unitless)	
540.15	1.431	734.15	2.251	
548.15	1.481	738.15	1.051	
550.15	1.211	740.15	2.481	
557.15	1.441	749.15	2.531	
563.15	1.581	750.15	2.381	
760.15	2.351	930.15	3.281	
763.15	2.321	932.15	3.221	
764.15	2.631	932.15	3.471	
771.15	2,691	946.15	3,431	
776.15	2.481	948.15	3,601	
110.15	2.401	340.13	5.001	
782 15	2.721	955 15	3,661	
790.15	2 751	961 15	2.741	
704 15	2 501	963 15	2 521	
804.15	2.611	064 15	3 601	
804.15	2.011	073 15	2 5/1	
004.15	2.011	973.13	5.541	
806 15	2 601	072 15	2 7/1	
Q12 15	2.001	975.15	2.451	
810 15	2 721	979.19	3 671	
826 15	2.06)	991.15	3.801	
828 15	2.901	99. ()	3 031	
020.13	2.941	370	3.931	
935 15	2 781	1003	3 581	
9/3 15	2.701	1007.15	3.701	
045.15	0.001	1007.15	2.051	
844.15	2.021	1007.15	0.001	
848.15	2.761	1015.15	3.941	
851.15	3.081	1017.15	3.801	
862.15	2.961	1021.15	3.711	
868.15	3.171	1032.15	3.901	
869.15	3.191	1035.15	3.961	
877.15	3.051	1042.15	4.181	
878.15	3.181	1044.15	3.671	
882.15	3.261	1047.15	3.821	
886.15	3.061	1048.15	4.041	
889.15	2.941	1052.15	4.071	
890.15	3,321	1052.15	4,421	
904.15	3.181	1052.15	4.161	





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TABL: B-4.III (continued)

(K)	$\frac{11}{11} \times 10^{-3}$ (unitless)	Temperature (K)	$\epsilon_{11} \times 10^{-3}$ (unitless)
908.15 910.15 919.15	3.401 3.401 3.291	1054.15 1084.15	/ 341
919.15 923.15	3.381 3.461		

 $\Delta V =$ change in volume (m³)

 V_0 = reference volume (m³).

At the start of the transition (T = 1083 K), from Equations (B-4.33) and (B-4.34)

$$\epsilon_1 = 3.88 \times 10^{-3}$$

 $\epsilon_3 = 9.87 \times 10^{-3}$

and at the end of the transition

 $\epsilon_1 = 1.68 \times 10^{-3}$ $\epsilon_{33} = 7.67 \times 10^{-3}$.

A simple pair of correlations fit these numbers

for 1083 \leq T \leq 1244 K

$$\epsilon_{11} = \left[2.77763 + 1.09822 \cos\left(\frac{T - 1083}{161} \pi\right) \right] \times 10^{-3}$$

$$\epsilon_{33} = \left[8.76758 + 1.09822 \cos\left(\frac{T - 1083}{161} \pi\right) \right] \times 10^{-3}$$
(B-4.36)
(B-4.37)

where the arguments of the cosines are in radians. There are more significant constants in Equations (B-4.36) and (B-4.37) than in other parts of the model to avoid discontinuities, not to reflect more accurate data.

4.3.3 Thermal Expansion in the Beta Region. For the transition sigin, there are insufficient data to construct a detailed model for the thermal expansion in the beta region. However, the strain due to thermal expansion is relatively unimportant to the total strain at these high temperatures. The model for T > 1244 K, based on the expansivity for zirconium reported by Skinner and Johnston, B-4.8 is

$$\epsilon_{11} = 9.7 \times 10^{-6} \text{ T} - 1.04 \times 10^{-2}$$
 (B-4.38)

$$\epsilon_{32} = 9.7 \times 10^{-6} \text{ T} - 4.4 \times 10^{-3}$$

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(B-4.39)

4.4 Model-Data Comparison and Uncertainty

The only data to which the model is compared are from Bunnell's correlations in the alpha phase. The predictions of the model using Equations (B-4.33) and (B-4.34) are compared with the data predictions in Tables B-4.IV and B-4.V using Bunnell's correlations and Equations (B-4.30) and (B-4.31). The first table is for circumferential strain and the second is for axial strain; both tables are for a single crystal.

TABLE B-4.IV

COMPARISON OF MODEL PREDICTIONS AND BUNNELL'S ALPHA PHASE DATA IN THE DIAMETRAL DIRECTION

Temperature	$\epsilon_{11} \times 10^{-5}$ (model)	$\epsilon_{11} \times 10^{\circ}$ (Bunnell)	Bunnell-Model
(K)	(unitless)	(unitless)	Moge 1
300	0	0	
400	0.0007	0.0009	0.28
500	0.0014	0.0016	0.14
600	0.0021	0.0022	0.05
700	0,0028	0.0028	0.00
800	0.0035	0.0035	0.00
900	0.0043	0.0043	0.00
1000	0.0050	0.0050	0.00
1100	0.0057	0.0055	-0.04

TABLE B-4.V

COMPARISON OF MODEL PREDICTIONS AND BUNNELL'S ALPHA PHASE DATA IN THE AXIAL DIRECTION

	$\epsilon_{11} \times 10^{-3}$	$\epsilon_{11} \times 10^{-3}$	Bunnell-Model
Temperature (K)	(model) (unitless)	(Bunnell) (unitless)	Mode 1
300	0	0	
400	0.0005	0.0006	0.20
500	0.0011	0.0011	0.00
600	0.0016	0.0016	0.00
700	0.0022	0.0021	-0.05
800	0.0027	0.0027	0.00
900	0.0032	0.0032	0.00
1000	0.0038	0.0038	0.00
1100	0.0042	0.0045	0.07



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From these tables, the standard error of estimate is $\pm 12\%$ for the circumferential direction and $\pm 8\%$ for the axial direction. These uncertainties are somewhat artificial since the model is compared to its own data base.

In the transition region and the beta phase, the uncertainty is expected to be much larger. An uncertainty of $\pm 50\%$ was arbitrarily assigned to these regions until appropriate data are available for a better model.

4.5 Cladding Thermal Expansion Subroutine CTHEXP Listing

A listing of the FORTRAN subroutine CTHEXP is given in Table B-4.VI. The expected uncertainties are computed within the code but not returned. In a future simultaneous revision of this subroutine and codes which use it, all uncertainties will be stored in a separate common block.

4.6 References

- B-4.1. L. R. Bunnell et al., *High Temperature Properties of Zircaloy-Oxygen Alloys*, EPRI NP-524 (March 1977).
- B-4.2. D. L. Douglass, "The Physical Metallurgy of Zirconium," Atomic Energy Review, 1, 4 (December 1963) pp. 73-74.
- B-4.3. R. L. Mehan and F. W. Wiesinger, Mechanical Properties of Zircaloy-2, KAPL-2110 (February 1961).
- B-4.4. P. B. Scott, *Physical and Mechanical Properties of Zircaloy-2 and -4*, WCAP-3269-41 (May 1965).
- B-4.5. J. J. Kearns, Thermal Expansion and Preferred Orientation in Zircaloy, WAPD-TM-472 (November 1965) pp. 17-18.
- B-4.6. C. R. Hann et al., Transient Deformation Properties of Zircaloy for LOCA Simulation, NP-526, Volume 3 (March 1978).
- B-4.7. C. Kittel, Introduction to Solid State Physics, 3rd Edition, New York: John Wiley and Sons, Inc. (1966) p. 29.
- B-4.8. G. B. Skinner and H. L. Johnston, "Thermal Expansion of Zirconium Between 298 and 1600 K," *Journal of Chemical Physics*, 21 (August 1953) pp. 1383-1384.





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TABLE B-4.VI

LISTING OF THE CTHEXP SUBCODE

SUBROUTINE CTHEXP (COST42, COSFI2, CTEMP, STRN11, STRN22, STRN33) CTHEXP CALCULATES THE THERMAL EXPANSION STRAIN FOR A PIECE OF ZIRCALDY CLADDING AS A FUNCTION OF TEMPERATURE AND OF CLADDING TEXTURE. STRN11 = OUTPUT THERMAL EXPANSION STRAIN IN THE CIRCUMFERENTIAL DIRECTION (M/M) STRN22 . OUTPUT THERMAL EXPANSION STRAIN IN THE AXIAL DIRECTION (M/M) STRN33 - DUTPUT THERMAL EXPANSION STRAIN IN THE THICKNESS DIRECTION (M/M) CTEMP . INPUT CLADDING TEMPERATURE (K) COSFIZ - INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE SQUARED SINE OF PHI (UNITLESS) COSTH2 - INPUT VOLUME FRACTION WEIGHTED AVERAGE OF THE SQUARED COSINE OF THETA (UNITLESS) VALUES FUR COSFI2 AND COSTH2 MAY BE OBTAINED THROUGH USE OF THE SUBRUUTINE CTXTUR THESE CALCULATIONS ARE BASED ON DATA AND TECHNIQUES IN THE FOLLOWING SOURCES L.R. BUNNELL ET AL, HIGH TEMPERATURE PROPERTIES OF ZIRCALDY-DXYGEN ALLOYS, EPRI NP-524 (MARCH 1977).
 D.L. DOUGLASS, "THE PHYSICAL METALLURGY OF ZIRCINIUM", ATOMIC ENERGY REVIEW, 1,#4 (DECEMBER 1963). (3) C. KITTEL, INTRODUCTION TO SOLID STATE PHYSICS, 3RD EDITION, (4) G.B. SKINNER, H.L. JOHNSTON, "THERMAL EXPANSION OF ZIRCONIUM BETWEEN 298 AND 1600K", JOURNAL OF CHEMICAL PHYSICS, 21 (1953) CTHEXP WAS CODED BY G. A. REYMANN JANUARY 1980. CALCULATE SINGLE CRYSTAL STRAINS STRE33 " SINGLE CRYSTAL STRAIN PERPENDICULAR TO THE C-AXIS STRE33 " SINGLE CRYSTAL STRAIN ALONG THE C-AXIS IF(I .GI. 1083.0) GC TO 10 IF(T .GT. 1244.0) GD TO 20

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STRS11 = 4.95E-06*T - 1.485E-03 STRS33 = 1.26E-05*T - 3.780E-03 GD TO 30 C₁₀ 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)*3.141593/151.0)) STRS33 = STRS33*1.0E-03 GC TO 30 c20 STRS11 = 9.7E-06*T - 1.04E-02 STRS33 = 9.7E-06*T - 4.40E-03 COC CALCULATE CLADDING STRAINS USING SINGLE CRYSTAL STRAINS °30 STRN11 = (COSFI2 +CUSTH2*(1.0-CUSFI2:)*STRS11 + (1.0-COSTH2)*(1.0-COSFI2)*STRS33 * 6 STRN22 = (1.0-COSFI2 + COSTH2*COSFI2)*STRS11 + (1.0-COSTH2)*COSFI2*STRS33 . 2 STRN33 = (1.0-COSTH2)*STRS11 + COSTH2*STRS33 USTRN1 - UNCERTAINTY IN THE TUBE CIRCUMFERENTIAL THERMAL STRAIN USTRN2 - UNCERTAINTY IN THE TUBE AXIAL THERMAL STRAIN USTRN1 = 0.12*STR N11 USTRN2 = 0.08* STRN22 RETURN END

TABLE B-4.VI (continued)

CELMOD/CSHEAR/CELAST

5. <u>CLADDING ELASTIC MODULI (CFLMOD, CSHEAR, and CELAST)</u> (D. L. Hagrman)

Elastic moduli are required to relate stresses to strains. The elastic moduli are defined by the generalized form of Hooke's law as elements of the fourth rank tensor which relates the second rank stress and strain tensors below the yield point. In practice, cladding is frequently assumed to be an isotropic material. In such a case only two independent elastic moduli are needed to describe the relation between elastic stress and strain. These two constants, the Young's modulus and the shear modulus, are calculated by the functions CELMOD and CSHEAR. Elements of the tensor necessary to describe anisotropic ciadding are calculated by the subroutine CELAST.

5.1 Summary

Cladding elastic moduli are affected primarily by temperature and oxygen content. Fast neutron fluence, cold work and texture effects are also included in the models described herein but they are not as important as temperature and oxygen content for typical light water reactor fuel rod cladding. The models are based primarily on data published by Bunnell et al^[B-5,1], Fisher and Renken^[B-5,2], Armstrong and Brown^[B-5,3], and Padel and Groff^[B-5,4] since these data include the best description of texture for the temperature range in which they were used. Data from several other sources^[B-5,5] to B-5.11] are used to evaluate the expected standard error of the CELMOD and CSHEAR codes and to estimate the effect of fast neutron fluence^[B-5,12].

The expressions used in the CELMOD subcode to calculate the isotropic Young's modulus are:

(1) In the alpha phase

 $Y = (1.088 \times 10^{11} - 5.475 \times 10^7 T + K_1 + K_2)/K_3 \qquad (B-5.1a)$

(2) In the beta phase

$$Y = 9.21 \times 10^{11} - 4.05 \times 10^7 T$$
 (B-5.1b)

(3) In the alpha + beta phase

Y = The value obtained by linear interpolation of values calculated at the alpha to alpha + beta and the alpha + beta to beta boundaries

7. CLADDING CREEP (CCSTRN AND CCSTRS) (D. L. Hagrman)

Cladding creep due to coolant pressure during steady state operation is important in modeling the size of the fuel-cladding gap and initial stored energy at the start of transients. For fuel rods with low internal pressure, the creep may be sufficiently rapid to also affect fuel relocation and effective conductivity of fuel pellets. Subroutines for finding creep strain as a function of stress, and stress required to produce a given creep strain are presented in this section. The model used in these subroutines is based primarily on surface displacement data from the HOBBIE-1 test conducted by the U.S. Nuclear Regulatory Commission and the Energieonderzock Centrum Nederland.

7.1 Summary

The basic equation used in both the CCSTRN and CCSTRS subroutines is

$$\dot{\epsilon}(t) = BA - \int_{0}^{t} B \exp\left[-(t - t')\left(\frac{\phi}{\Psi} + \frac{1}{\tau}\right)\right]\dot{\epsilon}(t') \phi t'$$
(B-7.1)

where

$$\epsilon(t) = tangential component of creep strain rate (s-1)$$

- = time since creep strain was zero (s)
- ϕ = fast neutron flux [neutrons/(m²-s)], E > 1 MeV
- Ψ = correlation fluence, Equation (B-7.4) (neutrons/m²), E > 1 MeV
- τ , = zero flux correlation time, Equation (B-7.5)(s)
- A = ultimate strain for infinite correlation (unitless), Equation (B-7.2)
- $B = rate constant (s^{-1}), Equation (B-7.3).$

Correlations for the parameters A and B were obtained from out-of-pile creep strain versus time data. The expressions are

$$A = 3.83 \times 10^{-19} |\sigma|^{r} \frac{\sigma}{|\sigma|}$$
(B-7.2)

B = 4.69 x $10^{-6} |\sigma|^r \exp\left(\frac{-25100}{T}\right)$, for T ≥ 615 K

1.9519804 x
$$10^{-16} |\sigma|^r \exp\left(\frac{-10400}{T\sigma}\right)$$
, for T < 615 K (B-7.3)

where

 σ = tangential component of stress (Pa)

T = temperature (K) (input temperatures are limited to the range 450 to 750 K)

CCSTRN/CCSTRS

r

- = 2.0 for stress between -0.2 and -0.75 times the strength coefficient of cladding
 - = 0.5 for stress between 0 and -0.2 times the strength coefficient of cladding
 - = 25.0 for stress less than -0.75 times the strength coefficient of cladding. The strength coefficient is approximated by the linear expression $1.5 \times 10^9 1.5 \times 10^6$ T and the constants in Equation (B-7.3) are modified when stress is outside the range -0.2 to -0.75 times the strength coefficient to guarantee continuity at the boundaries of this range.

Preliminary expressions for the correlation fluence, Ψ , and zero flux correlation time, τ , were obtained from the slope of secondary creep rates versus temperature under tensile stress. These expressions are

$$\Psi = 2.9 \times 10^{6} \exp\left(\frac{25100}{T}\right), \text{ for } T \ge 615 \text{ K}$$

$$6.967795 \times 10^{16} \exp\left(\frac{10400}{T}\right), \text{ for } T < 615 \text{ K}$$

$$\tau = 8.6 \times 10^{-11} \exp\left(\frac{25100}{T}\right), \text{ for } T \ge 615 \text{ K}$$

$$2.0663116 \exp\left(\frac{10400}{T}\right), \text{ for } T < 615 \text{ K}$$
(B-7.5)

The CCSTRN subroutine calculates the tangential component of cladding creep strain at the end of a time step with constant cladding temperature, flux, and stress. For time step intervals less than a time to steady state, the infinite-correlation approximation^a is used to integrate Equation (B-7.1). The resultant expression for creep strain is

$$\epsilon_{\text{final}} = [A - \epsilon_{\text{boundary}}] [1 - \exp(-B\Delta t)] + \epsilon_{\text{initial}}$$
(B-7.6)

where

€final	=	tangential component of creep strain at the end of the time step (unitless)
€initial	=	tangential component of creep strain at the start of the time step (unitless)
[¢] boundary	=	a boundary condition parameter used to force the creep rate to be con- tinuous at the time step boundary when temperature and stress do not change (unitless); this parameter is zero for the first time step and is determined by Equation (B-7.26) for subsequent time steps
Δt	100	time step duration (s).

For time step durations longer than the time to steady state, the steady state approximation $[\epsilon (t) \approx 0]$ is used to integrate Equation (B-7.1). The resultant expression for creep strain is

$$\epsilon_{\text{final}} = (\mathbf{A} - \epsilon_{\text{boundary}}) \left[1 - \exp(-\mathbf{B} \Delta t_{\text{ss}})\right] + \frac{\mathbf{B}\mathbf{A} \left(\Delta t - \Delta t_{\text{ss}}\right)}{1 + \frac{\phi}{\Psi} \div \frac{1}{t}} + \epsilon_{\text{initial}}$$
(B-7.7)

a. The exponent in Equation (B-7.1) is approximated by a one.

where

Δt_{ss} = the time to steady state (s).

The time to steady state is defined to be the time when creep strain rate given by Equations (B-7.6) and (B-7.7) are equal

$$\Delta t_{ss} = -\frac{1}{B} \ln \left[\frac{A}{1 + \frac{B}{\frac{\phi}{\Psi} + \frac{1}{\tau}}} \frac{1}{(A - \epsilon_{boundary})} \right] \text{ or }$$

0 if the argument of the log term is outside the range

0 < argument < 1.

(B-7.8)

Subroutine CCSTRS uses an interaction technique and trial assumptions to solve Equation (B-7.6) or (B-7.7) for stress when ϵ_{final} , $\epsilon_{\text{initial}}$, and Δt are known. The procedure begins by solving Equation (B-7.6) with the implied assumption that Δt is $<\Delta t_{\text{SS}}$. In this case, the possible range of stresses is bounded and the function is monotonic. The range is cut in half in each of several iterations by testing stress at the midpoint of the possible range. If substitution of the trial solution into Equation (B-7.8) yields a Δt_{SS} , which is $>\Delta t$, the trial solution is adopted.

A second trial solution is obtained by solving Equation (B-7.7) for $|\sigma|^r$ with the assumption Δt_{ss} is zero. If this trial solution yields $\Delta t_{ss} = 0$ in Equation (B-7.8), it is adopted.

If neither of the two trial solutions are adopted, the technique used in Subroutine CCSTRS employs the observation that the initial trial solution provides a maximum $|\sigma|^{T}$, and the second trial solution provides a minimum initial slope. The implied range of possible stress is then cut in half in each of several iterations by testing in Equations (B-7.8) and (B-7.7) with stress at the midpoint of the range.

Uncertainty stimates for creep strain and stress are provided by Subroutines CCSTRN and CCSTRS. Both estimates are based on the observation that the only creep data with compressive stresses are at a temperature of 644 K and stresses in the range -120 to -140 MPa. The expression used to estimate the uncertainty of the strain calculated in CCSTRN is

$$f_{\epsilon} + = 1 + 0.3 \left(1 + 2 \left| \frac{\sigma}{130 \times 10^6} \right| + 5 \left| \frac{T \cdot 644}{644} \right| \right)$$

$$(B-7.9a)$$

$$f_{\epsilon} - = 0.4 \left(1 + 2 \left| \frac{\sigma + 130 \times 10^6}{130 \times 10^6} \right| + 5 \left| \frac{T \cdot 644}{644} \right| \right)$$

$$(B-7.9b)$$

where $f_{\epsilon} \pm$ are the upper and lower uncertainty estimates of the calculated creep strain increment magnitude expressed as a fraction of the calculated creep strain increment magnitude.

The expression used to estimate the uncertainty of stress calculated in CCSTRS is

$$f_{\sigma} + = 1 + 0.075 \left(1 + 2 \left| \frac{\sigma + 130 \times 10^6}{130 \times 10^6} \right| + 5 \left| \frac{T - 6.64}{644} \right| \right)$$
(B-7.10a)



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$$f_{\sigma} = 0.85 / \left(1 + 2 \left| \frac{\sigma + 130 \times 10^6}{130 \times 10^6} \right| + 5 \left| \frac{T - 644}{644} \right| \right)$$
(B-7.10b)

where $f_{\sigma} \pm$ are the upper and lower uncertainty estimates of the calculated stress magnitude expressed as a function of the calculated stress magnitude.

The following subsections discuss available data and development of the model. Section 7.5 contains a fisting of Subroutines CCSTRN and CCSTRS, and references are provided in Section 7.6.

7.2 Survey of Available Data

Data that measure creep under tensile stress are being supplemented by data for creep with compressive stress in very limited ranges of temperature and stress. The available theories and data for creep under compressive stress are surveyed in this section. A bibliography of extensive literature on tensile creep experiments is provided in Section 7.7.

Currently, there are no theories directed specifically at compressive stress, but Dollin and Nichols, B-7.1 Piercy, B-7.2 MacEwen, B-7.3 and Nichols B-7.4, B-7.5 have discussed similar physical models that explain the general features of in-pile creep of cladding under tensile stress. For the temperature range 523 to 623 K, these authors believe the controlling mechanism for in-pile creep at stresses <70 to 100 MPa are the preferred alignment of irradiation-induced dislocation loops during nucleation. At higher stresses, the effective stress at dislocations is thought to be sufficiently large to allow dislocation glide between the neutron-produced depleted zones. The creep rate would then be controlled by combined rates of dislocation glide between depleted zones and climb out of these zones. Although some of Nichol's ideas have been challenged, B-7.5, B-7.6, B-7.7 the predicted linear stress-dependence of strain rate at low stress is supported by several authors, B-7.8, B-7.9 and his prediction that the strain rate at high stress is proportional to approximately the one-hundreth power of stress in the 523- to 623-K temperature range is consistent with the MATPRO models for cladding plastic deformation at high stress. The dependence of strain rate on stress is expected to vary from the tenth power of stress to the first power, and then to the fourth power as stress increases. The physical model proposed by Nichols has been consulted but not used directly because the cost associated with the use of such a detailed model is not justified until compressive creep data confirms the model.

A similar, but less physically founded stress-dependence is proposed by Fidleris in his review of experimental data.^{B-7.9} He reported that creep rate varies linearly with stress at temperatures around 570 K and stresses less than one-third the yield stress. With increasing stress, the strain rate is reported to be proportional to higher powers of stress, reaching a power of 100 at stresses of 600 MPa. The model for creepdown to be developed will use only the general features of the stress dependence reported by Fidleris, because insufficient creepdown data exist to support detailed modeling at this time.

The data referenced by Fidleris show the in-reactor creep rate depends on material, flux temperature, and direction of testing as well as stress. At temperatures below half the melting temperature (1050 K) and stresses lower than the yeild stress, the in-reactor creep reaches a constant rate, while the out-of-reactor creep rate becomes negligibly small with time. The steady state creep rate is stated to be independent of test history or strain, at least for fast neutron fluences below 3 x 10^{24} neutrons/m² (E > 1 MeV).

Below 450 K, temperature is reported to have little effect and, for stresses below the yield stress, the strain is < 0.001. The out-of-reactor creep data of Fidleris can be described by

a. The MATPRO models for cladding plastic deformation, CSTRES, CSTRAN, and CSTRNI are described in Appendix B, Section 8 of the MATRPO handbook.

CCSTRN/CCSTRS

(B-7.11)

$$\epsilon = A \log t + B$$

where

= strain

= time

A,B = constants.

In the range 450 to 800 K, Fidleris reports that the out-of-reactor creep strain is often represented by equations of the type

$$\epsilon = At^{m} + B \tag{B-7.12}$$

where, ϵ , t, A, and B were defined in conjunction with Equation (B-7.11) and m is a constant between zero and one. Recovery of some of the strain is possible in this temperature range and dynamic strain aging B-7.10 frequently causes anomalously low creep strains and rates.

Equations (B-7.11) and (B-7.12) and other conclusions in Fidleris' review are based on his own extensive data for uniaxial, tensile creep of zirconium alloys, both in- and out-of-reactor. B-7.11 From these data, Fidleris concluded that the in-reactor creep is approximately proportional to the fast neutron flux for all temperatures. Other investigators treat the effect of fast neutron flux on creep in different ways. B-7.12 Although most authors have treated in-reactor creep as the sum of the out-of-reactor creep and an additional irradiation-induced creep proportional to fast neutron flux to some power, a, there is disagreement about the magnitude of the exponent, a. Ross-Ross and Hunt, B-7.8 report that creep rate is directly proportional to the fast flux, WoodB-7.13, B-7.14 uses a = 0.85, KohnB-7.15 uses a = 0.65, and GilbertB-7.16 finds a = 0.5 for yielding creep at moderate stress levels. MacEwenB-7.3 and NicholsB-7.4 have resolved this apparent conflict by suggesting the flux exponent can have values from 0 (Nichols) or 0.5 (MacEwen) to 1.0, depending on the flux and temperature.

The expressions for calculating creepdor in that will be developed in the next section will model the effect of fast neutron flux on creep with an *c* pression that is proportional to fast neutron flux for large fluxes, but less dependent on flux for smaller fluxes. Equation (B-7.12), Fidleris' equation for creep strain versus time with tensile stress, will not be used because it is inconsistent with data obtained from tests with compressive stress.

The effects of grain size annealing and texture are addressed by several authors. Fidleris finds that the zircaloy-2 creep rate increases continuously with grain size at 573 K. However, within the limited range of grain sizes formed in his recrystallized zircaloy-2 (6 to 20 μ m), very little variation is reported. Stehle^{B-7.17} reports creep strains in cold-worked material that are more than twice as large as the creep strains in recrystallized tubes, but that plots of creep strain versus time for stress-relieved and recrystallized cladding intersect at about 6,000 h. Kohn^{B-7.15} reported that the biaxial creep rate of Zr-2.5Nb fuel-cladding is about 10 times higher than that of pressure-tube material under similar conditions. He states that texture differences between the materials and the overaged precipitate structure in the as-manufactured cladding can explain the difference in creep rates. The importance of texture is disputed by Stehle^{B-7.17} who reported that mechanical anisotropy (especially in long-time creep) is surprisingly low compared to the anisotropy in short-time creep at room temperature. The effects of grain size, annealing, and texture will not be considered in the creepdown model developed in the next section because an explicit model for these effects on creepdown would be premature at this time.

Theories surveyed above may be misleading when applied to compressive creep because they are based primarily on tensile stress data. Picklesimer, B-7.18 Lucas and Bement, B-7.19 and Stehle B-7.17 have


pointed out that deformation with compressive stress differs from tensile compression. Stehle has obtained data showing that the magnitude of creep strain of tubes under external pressure can be as small as half the creep strain of tubes under internal pressure.

The biaxial compressive stress data now available include out-of-reactor measurements at three stresses and one temperature. Results from a single in-reactor experiment are also available. All experiments except one were conducted by Hobson using tubes from a shipment of typical pressurized water reactor cladding purchased specifically for use in fuel cladding research programs sponsored by the Division of Reactor Safety Research, Nuclear Regulatory Commission. B-7.20

The only biaxial compressive strain data from a different lot of cladding were reported by Stehle.^{B-7.17} His measurements of the tangential creep as a function of time for standard stress-relieved tubing Abricated according to KwU (Kraftwerke Union) specifications are reproduced in Figure B-7.1. The tangential stress in this test was 140 MPa and the temperature was 643 K. The magnitude of the measured creep strains are somewhat smaller than the out-of-pile strains computed in the next section from Hobson's out-of-pile data at the same temperature, but within the range of the scatter reported by Stehle for cladding with varying cold-work and stress-relief annealing histories. Since the details of the stress-relief anneal on the lot of cladding used by Stehle are not reported, the data will be used only to assess the uncertainty of the creepdown model.

The data reported by Hobson^{B-7.21—B-7.24} are radial displacements of the cladding surface at various azimuthal angles and axial positions (6.34 mm apart). The 20 probes used to measure the displacement were arranged in a double helix pattern over a 50.8-mm length of cladding, as shown by probe number in Table B-7.1. This table is arranged so that the location of the probes may be visualized by thinking of the cladding surface as split along the cylinder axis and rolled out in the plane of the page. Hobson has pointed out^{B-7.23} that the exact shape of the cladding surface cannot be determined with point-by-point data from







TABLE B-7.1

				Azimu (de	thal Ang grees)	le		
Axial Position (mm)	0	45	90	135	180	225	270	315
0.00	1				13			
6.35		4				16		
12.70			7				19	
19.05				10				22
25,40	2		8		14		20	
31.75		5				17		
38.10	-		9				21	
44.45		~-		11				23
50.80	3				15			

SURFACE COORDINATES OF PROBES WHICH MEASURE RADIAL DISPLACEMENT

a few radial probes and that the exact stress state at any point in the sample is related to the geometry of the sample. In spite of these complications, the data can be analyzed to obtain the average tangential strain as discussed in the next section of this report. Hobson data plays a dominant role in the development of the creepdown model because the cladding is typical of light water reactor cladding, the stress is compressive, the cladding displacement is reported as a function of time at 2-h intervals, and the temperature is typical of the cladding temperatures predicted by the FRAPCON-2 code. The only atypical feature of the data is the magnitude of the stresses employed by Hobson, 125 and 135 MPa. These stresses are characteristic of low pressure rods so extrapolation to smaller stress magnitudes is decessary to model current fuel rod prepressurization levels.

7.3 Development of the Model

It has been concluded that the most relevant data for modeling cladding creepdown under the compressive stress of steady state LWR reactor conditions are the data of Hobson. Extensive theory and tensile creep data are useful only to provide a tentative extension of the model to stresses and temperatures where no creepdown data are available.

The first step in the analysis of Hobson's data was to estimate the average tangential strain from radial displacements measured by probes at the locations shown in Table B-7.1. This was done by inspecting plots of the radial displacement measured for each test. Table B-7.11 and Figure B-7.2 are examples of the results. The table was constructed from Hobson's data for Test 269-4 (14.48 MPa pressure) at 200 h and the figure is a polar plot of the radial displacement as a function of the azimuthal angle of the probe. The



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				Azimu (de	thal Ang grees)	le		
Axial Position (mm)	0	<u>45</u>	90	135	180	225	270	315
0.00	4				12			
6.35		6				12		
12.70			48				12	
19.05				-19				-29
25.40	31		-63		40		-58	
31.75		3				31		
38.10			-77				-60	
44.45				-36				-38
50.80	31				32			

TABLE B-7.II

RADIAL DISPLACEMENTS AT 200 HOURS IN HOBSON'STEST 269-4ª (10⁻³ mm)

a. 14.48-MPa pressure differential and 0.127-mm pellet-cladding gap.B-7.23

plot exaggerates the radial displacement by a factor of ten compared to the scale of the circle, which represents zero displacement. From an inspection of the figure, it can be seen that the radial displacements at 200 h in Test 269-4 are consistent with the assumption that the cladding surface was an ellipse with major axis between 0 and 45 degrees, and the center of the ellipse displaced slightly toward the 180- to 270-degree quadrant. There is some variation with axial position, as shown by the scatter in the displacements with common azimuthal angles and different axial positions.

The elliptical shape and gradual axial variations are also consistent with general descriptions of cladding surfaces after creepdown given by Stehle^{B-7.25} and Bauer.^{B-7.26} On the basis of several plots like Figure B-7.2 and the general descriptions just mentioned, the author has concluded (a) an ellipse is a reasonable approximation for the cladding surface at any given height prior to extensive fuel-cladding interaction and (b) the major and minor axis (length or orientation, or both) vary slowly with axial position.

The assumption that the cladding surface at any axial position is an ellipse allows calculation of the average tangential strain as outlined in the six steps below.

 The circumference of the elliptical surface was related to the major and minor semi-axis lengths with the approximate expression







$$= 2\pi \sqrt{\frac{a^2 + b^2}{2}}$$
(B-7.13)

where

¢

c = circumference (m)

a,b = semi-axis lengths (m).

2. The average tangential strain was defined as

$$\epsilon_{\theta} = \int_{\text{circumference}}^{\underline{\text{ds}}} \simeq \frac{c_{\text{final}} - c_{\text{initial}}}{c_{\text{initial}}}$$
 (B-7.14)

where

s = arc length (m) ϵ_{θ} = average tangential strain (unitless) c_{initial} = initial circumference (m) c_{final} = final circumference (m).



3. Equations (B-7.13) and (B-7.14) were coorbined to obtain

$$\epsilon_{\theta} \simeq \sqrt{\frac{a_{\text{final}}^2 + b_{\text{final}}^2}{a_{\text{initial}}^2 + b_{\text{initial}}^2}} -1$$

- ainitial and binitial were assumed equal to r_o, and a_{final} and b_{final} were set equal to the initial values plus Δa and Δb.
- 5. A Taylor series expansion to order $\Delta a/r_0$ and $\Delta b/r_0$ was u 2 with Equation (B-7.15) and Step 4 above to find

$$\theta_{\theta} \approx \frac{1}{2} \left(\frac{\Delta a + \Delta b}{r_{o}} \right)$$

where

r_o

 initial radius of the outside (circular) surface of the cladding (m)

$$\Delta a, \Delta b$$
 = change of the major and minor semi-axes lengths (m).

6. Measurements of the radial displacements at one axial position (25.4 mm) and azimuthal weights of 0, 90, 180, and 270 degrees are available from Hobson's data. If these four measurements happen to occur along the major and minor axes of the ellipse, Equation (B-7.16) is sufficient to convert the data to an expression for the average circumferential component of the strain. When the radial displacements at 25.4 mm are not measured along the major and minor axes of the ellipse, the derivation is more complex but the result (to order $\Delta a/r_0$ and $\Delta b/r_0$ in the Taylor series expansion) is an equation of the same form as Equation (B-7.16), with Δa and Δb replaced by the average radial displacements along any two axes at right angles to each other and at any angle to the major and minor axes of the ellipse. The expression then becomes

$$\epsilon_{\theta} \approx \frac{1}{2} \left(\frac{\Delta a' + \Delta b'}{r_{o}} \right) \tag{B-7.17}$$

where

 $\Delta a', \Delta b' =$ change of the cladding radius measured alo g any mutually perpendicular axes at one axial position (m).

The second part of the analysis of Hobson's data was to describe the average tangential strains obtained from the data and Equation (B-7.17). Figure B-7.3 displays the calculated average tangential strain from two out-of-pile tests at 15.86 MPa differential pressure. During the first 600 h, the strains are remarkably consistent. During the last 400 h of the tests, the strain in Test 269-27 was noticeably larger than that of Test 269-8. Test 269-27 had a large simulated axial gap centered about the axial position of the four probes used to determine the strain. Test 269-8 had only a small axial gap. The difference in strain at long times is probably due to the effect of the different contact times with the simulated fuel.

Figure B-7.4 illustrates the strain versus time results obtained from the 14.48-MPa out-of-pile test. The magnitude of the strain at any time is significantly smaller than the strains obtained with the 15.86-MPa tests.

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(B-7.15)

... 7.16)









Figure 8-7.4. Average tangential strain as a function of time at 14.48 MPa differential pressure.

In an effort to describe the strain versus time data shown in Figures B-7.3 and B-7.4, the constants in Equations (B-7.11) and (B-7.12) for tensile creep were fit to selected strain-time pairs. Each equation was then tested by extrapolating to longer or shorter times and comparing the predicted strains to strain-time pairs not used in determining the constants A and B. Neither equation passed this test. Equation (B-7.11) consistently had too much curvature^a and Equation (B-7.12) had too little curvature.

The equation finally adopted for short-time out-of-pile tests was

$$a = A \left[1 - \exp(-Bt)\right]$$

where

ŧ.

 ϵ_{θ} = average tangential strain (m/m)

= time (s)

A,B = functions of stress and temperature.

For the 14.48-MPa test

 $A = -5.32 \times 10^{-3}$ and $B = 7.64 \times 10^{-7}$ s.

For the 15.86-MPa tests

 $A = -6.32 \times 10^{-3}$ and $B = 9.17 \times 10^{-7} s$.

The values of A and B for each stress were determined with a two-step process:

1. A value of B was guessed and one strain-time pair (ϵ_0, t_0) was selected as a reference. Other strain-time pairs (ϵ_j, t_j) were then used to find an improved guess for B according to the relation

$$B_{j} = in \left\{ 1 - \frac{\epsilon_{j} [1 - \exp(-B_{guessed} t_{o})]}{\epsilon_{o}} \right\}.$$
(B-7.19)

 Once a single value of B that worked for several strain-time pairs was determined, a leastsquares fit was carried out to determine A.

The two sets of values for A and B were used to estimate the effect of change in stress. A and B were assumed to be dependent on stress to some power, n, and n was calculated from A and B at the two stresses where they are knc wn

n =
$$\frac{\ln\left(\frac{A \text{ at } 15.86 \text{ Mira}}{A \text{ at } 14.48 \text{ MPa}}\right)}{\ln\left(\frac{15.86}{14.48}\right)} = 1.89$$

a. $\left(\frac{d^2 e_{\theta}}{dt^2}\right)$ too large.

(B-7.20a)



(B-7.18)

n =
$$\frac{\ln\left(\frac{B \text{ at } 15.86 \text{ MPa}}{B \text{ at } 14.48 \text{ MPa}}\right)}{\ln\left(\frac{15.86}{14.48}\right)} = 2.01.$$
 (B-7.20b)

In view of the limited number of tests, both values of n were assumed to be 2. This result implies a strain rate proportional to the fourth power of stress,^a a conclusion that agrees with one of the intermediate stress regions suggested by Dollins and Nichols in Section 7.2.

The resultant expressions for the stress-dependence of A and B near 125 MPa and at a temperature of 644 K are

A = (-5.32 x 10⁻³)
$$\frac{\sigma^2}{(1.245 x 10^8)^2}$$
 (B-7.21)

$$B = (7.64 \times 10^{-7}) \frac{\sigma^2}{(1.245 \times 10^8)^2}$$
(B-7.22)

where

0

= tangential component of stress.

The data from Hobson's in-reactor experiment were converted to average tangential strains with the same technique used for the out-of-reactor experiment. Figure B-7.5 displays the resultant average tangential strains as a function of time, along with the predicted out-of-reactor average strain from Equations (B-7.18), (B-7.21), and (B-7.22). The temperature during the in-reactor experiment was approximately the same as the temperature of Hobson's out-of-reactor experiments, but pressure varied from 13 to 13.5 MPa, so the tangential stress (-116 MPa) was smaller in magnitude than stresses of the out-of-pile experiments.

Interpretation of the in-reactor data is complicated by absence of data for the first 80 h, by reactor shutdown from 540 h to 610 h, and by the apparent positive average tangential strains from 80 to 200 h. Hobson^{B-7.24} has discussed the apparent positive average strains during the early part of the experiment and suggests that the positive readings come from the effects of a reactor scram at 50 h on the experiment clectronics.

The in-reactor strains shown in Figure B-7.5 are consistent with a simple relation between the out-of-reactor strains and the in-reactor strains [for fast neutron flux $\approx 5.4 \times 10^{17}$ neutrons/(m²s)]. The dashed line of the figure is the strain predicted by assuming that the initial out-of-reactor strain rate, AB, is maintained throughout the in-reactor experiment. The strains are described to within the experimental uncertainty by this line.

If this simple relation between initial out-of-reactor creep rates and in-reactor creep is confirmed by subsequent experiments with compressive stress, the implications for model development are significant. The result implies that irradiation-induced creep for compressive stress is not an independent additional creep (as virtually all the models based on tensile deformation data have assumed), but simply the result of destruction of some effect associated with prior creep strain that impedes further creep strain. In the absence of any data other than those from Hobson's experiments, the assumption must be made that either (a) the in-reactor creep rate is related to the initial out-of-reactor creep rate for compressive stress at



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a. The time derivative of Equation (B-7.18) is proportional to A x E.



Figure B-7.5. Average tangential strain as a function of time from Hobson's in-reactor experiment at 13-13.5 MPa differential pressure and 5.4 x 10¹⁷ fast neutrons/(m²/s).

temperatures near 644 K, or (b) that the fast neutron flux, stress magnitude, and temperature are coincidentally at values that make the independent irradiation-induced creep rate equal to the initial out-ofreactor creep rate. The author has selected assumption (a) and has proceeded to develop a model for cladding creepdown that is consistent with this assumption.

To be consistent with the assumption that some effect associated with prior creep strain impedes further creep strain, the independent variable in Equation (B-7.18) was changed from time to prior strain. The equation was then differentiated with respect to time and the differentiated expression used with Equation (B-7.18) to eliminate time, resulted in the expression

$$\epsilon_{\theta} = \mathbf{B}(\mathbf{A} \cdot \epsilon_{\theta})$$

where ϵ_{θ} is the time derivative of the tangential strain (s⁻¹).

If fast neutron flux destroys some effect associated with prior creep strain, the appropriate modification of Equation (B-7.23) to describe in-reactor creep will reduce or eliminate the term, $-B\epsilon_{\theta}$, when a fast neutron flux is present. This was accomplished by adapting the idea of an auto-correlation function from statistical mechanics.^{B-7.27} The total strain in Equation (B-7.23) is replaced by the integral of the strain increment at a prior time, t', times a correlation function that approximates the rate of destruction of the effect of prior strain on the current strain rate. In the absence of detailed information, the correlation function is represented by an exponential. The resultant generalization of Equation (B-7.23) is





(B-7.23)

(B-7.24)

$$e_{\theta} = \mathbf{B} \left\{ \mathbf{A} - \int_{\mathbf{O}}^{\mathbf{t}} \exp\left[-(\mathbf{t} - \mathbf{t}')\left(\frac{\phi}{\Psi} + \frac{1}{-1}\right)\right] d\epsilon(\mathbf{t}') \right\}$$



where

\$

= fast neutron flux [neu*rons/(m^2 s)]

 Ψ = correlation fluence (neutrons/m²)

 τ = zero flux correlation time (s)

and other symbols have been previously defined.

New parameters introduced in Equation (B-7.24) can be given a physical interpretation without defining a detailed mechanistic model. The correlation fluence, Ψ , is the amount of radiation damage required to destroy most of the effect of prior strain on current strain rate, and the zero flux correlation time, τ , is the time at temperature required to anneal most of the effect of prior strain in zero flux. Since Equation (B-7.1) is an alternate form of Equation (B-7.24), the same interpretation can be applied to Equation (B-7.1).

CCSTRN Equations (B-7.6) and (B-7.7) are approximations derived from Equation (B-7.1). Equation (B-7.6) is obtained from Equation (B-7.1) by assuming

$$t\left(\frac{\phi}{\Psi} + \frac{1}{\tau}\right) < < 1 \tag{B-7.25}$$

and integrating Equation (B-7.1) from an initial to a final time, t. Equation (B-7.7) uses the steady state approximation to Equation (B-7.1), derived by setting the time derivative of Equation (B-7.1) equal to zero and solving for the steady state creep rate. If the creep rate at the given final time of a time step interval is greater than or equal to the steady state creep rate, Equation (B-7.6) is employed for the entire time interval. If the creep rate at the given final time of a time step interval is less than the steady state creep rate, the time to steady state is calculated with Equation (B-7.8), and Equation (B-7.7) is used to calculate the final strain from the assumption that the creep rate after the time interval given by Equation (B-7.8) has passed. The time interval to steady state is found by solving the time derivative of Equation (B-7.6) for the time when the creep rate is equal to the steady state creep rate.

Equations (B-7.6) and (B-7.7) contain a term, $\epsilon_{\text{boundary}}$, which is the initial creep strain for any time step in which the temperature and stress are the same as the previous time step. For time steps in which the temperature, stress, or fast neutron flux has changed, Equation (B-7.1) implies that the creep rate should respond immediately to changes in the product AB (a function of stress and temperature) but the response of the creep rate to changes in the factor, $\phi/\Psi + 1/\tau$ (a function of flux and temperature), should be more gradual. A boundary condition is therefore required to make the initial creep rate of Equation (L-7.6) equal to the creep rate at the end of the prior step. The appropriate condition is

for prior steps not in steady state

 $\epsilon_{\text{boundary}} = AP \exp(-BP \Delta tp) + \epsilon P_{\text{boundary}}[1 - \exp(-BP \Delta tp)]$

for prior steps in steady state

$$e_{\text{boundary}} = \frac{AP BP}{\frac{\phi P}{\Psi P} + \frac{1}{\tau P} + BP}$$

(B-7.26)

where

Ĵ.

Land

3 8 **3**

1.

1 S

8 8 AP, BP, Δtp , $\epsilon P_{\text{boundary}}$, ϕP , ΨP , and $\tau P = A$, B, Δt , $\epsilon_{\text{boundary}}$, ϕ , Ψ , and τ during the previous time step

Values for the parameters A and B at 644 K and stresses near 125 MPa have been determined from Hobson's out-of-reactor data. These data can also be used in conjunction with the modeling ideas just developed to find a minimum value for the zero flux correlation time, τ , at 644 K. The strains shown in Figure B-7.3 show that a steady state creep rate (a straight line plot for strain versus time) did not occur prior to 600 \pm in either of the out-of-reactor experiments represented in the figure. Equation (B-7.8), with $\phi = 0$ and Δt_{ss} at least as large as 600 h, implies a τ of at least 6.8 x 10⁶ s. This value was adopted as an interim estimate for τ at 644 K, since the strains calculated from Test 269-27 (test that simulated an axial gap in the fuel pellets) are consistent with steady state creep after 600 h.

The temperature-dependent factors in Equations (B-7.3), (B-7.4), and (B-7.5) are interim estimates because they are based on the temperature-dependence of tensile creep data. The data from Fidleris' tests, R-6 and Rx-14, B-7.11 were selected to estimate the temperature-dependence of B, τ , and Ψ because these tests were carried out at a stress magnitude that closely approximates the magnitude of the stress in Hobson's experiments.

Figure B-7.6 illustrates the steady state creep rates reported by Fidleris for a stress of 138 MPa at several temperatures. The in-reactor data are at fast neutron fluxes of 6.8 x 10¹⁶ or 6.0 x 10¹⁶ neutrons/(m²·s). The range of steady state creep rates predicted by the model for creepdown at 644 K is also represented. A solid square is used to represent the steady state creep rate seen in Hobson's experiment at a fast neutron flux of 5.4×10^{17} neutrons/(m²·s). The slope of the tensile stress data at temperatures >614 K (1/T < 1.626 x 10⁻³) corresponds to a temperature-dependent factor of the form, exp(-25,100/T). The



Figure B-7.6.

Steady state creep rates reported by Fidleris for Tests R 6 and Rx-14 compared to model predictions for steady state creepdown rates derived from these data. in-reactor data <615 K correspond to a temperature-dependent factor of the form, exp(-10,400/T). The temperature-dependent factors in Equations (B-7.3), (B-7.4), and (B-7.5) are the most convenient way of forcing the steady state creep rate implied by Equation (B-7.7) to correspond to the temperature-dependence shown by the Fidleris equation.

The constants, 2.9 x 10^6 and 6.967795 x 10^{16} in Equation (B-7.4), are the result of a least-squares fit to the steady state creep rate data of Fidleris. As expected from the previous discussion, the resultant prediction of the steady state creep rate for Hobsons in-reactor creep rate at 5.4 x 10^{17} neutrons/(m²·s) with a compressive stress is slightly too high. The predicted rate, s⁻¹, is shown in Figure B-7.6 by the dashed line.

7.4 Uncertainty of the Model

Lack of an extensive data base for creep under compressive stress makes the assignment of uncertainty limits very tentative. The data of Stehle (illustrated in Figure B-7.1) are the only other compressive stress data available. These data show creep strains of about half the magnitude of the model predicted strains. Since these are the only appropriate data not used in developing the model, they were used to estimate fractional error of -0.6 and +0.3 in strain at 644 K and -130 MPa stress. The remaining terms of the uncertainty estimate for the strain predicted by CCSTRN [Equation (B-7.9)] are simply engineering judgments that estimate 100% error when the stress differs from -136 MPa by more than 65 MPa, or the temperature differs from 644 K by more than 60 K.

Equation (B-7.10), the expression for the uncertainty of the stress calculated by CCSTRS, was derived from Equation (B-7.9) and the observation that the predicted strain is usually proportional to the fourth power of stress. The resultant uncertainty in stress expressed as a fraction of stress is one-fourth the fractional uncertainty in strain.

7.5 Cladding Creepdown Subroutines (CCSTRN and CCSTRS) Listings

Listings of the FORTRAN subroutines CCSTRN for creep strain as a function of stress and CCSTRS for stress as a function of creep strain increment are given in Tables B-7.111 and B-7.1V. Uncertainty estimates are computed within the subcodes, but are not returned.

7.6 References

- B-7.1. C. C. Dollins and F. A. Nichols, "Mechanisms of Irradiation Creep in Zirconium-Base Alloys," Zirconium in Nuclear Applications, ASTM-STP-551 (1974) pp. 229-248.
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- B-7.6. D. O. Northwood, "Comments on In-Pile Dimensional Changes in Neutron Irradiated Zirconium Base Alloys," Journal of Nuclear Materials, 64 (1977) pp. 316-319.
- B-7.25. H. Stehle et al., "Uranium Dioxide Properties for LWR Fuel Rods," Nuclear Engineering and Design, 33 (1975) pp. 230-260.

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TABLE B-7.III

LISTING OF THE COSTRN SUBCODE

TABLE B-7.III (continued)

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CCSTRN/CCSTRS

TABLE B-7.III (continued)

```
C

If (CTEMP .GT. 750.) I = 750.

IF (CTEMP .LT. 450.) T = 450.

S = ABS(CHSTRS)

C

APPROXIMATE STRESS EXPONENT BY COMPARISON TO STRENGTH

CDEFFICIENT APPROXIMATION

AK = 1.5E+09 = 1.5E+06 * T

A = 3.83E-19 * (S**3) /CHSTRS

IF (S .LT. (C.20 * AK)) A = A * ((0.20 * AK / S )**1.5)

IF (S .GT. (0.75 * AK)) A = A * ((S/(0.75 * AK))**23)

C

IF (T .LT. 615.) GO TO 10

B = 4.669E-06 * (S**2) * EXP(-2.51E+04/T)

TAU = 8.6E-11 * EXP(2.51E+04/T)

GO TO 20

10 B = 1.9519804E-10 * (S**2) * EXP(-1.04E+04/T)

TAU = 2.0663116 * EXP(1.04E+04/T)

TAU = 2.0663116 * EXP(1.04E+04/T)

20 IF (S .LT. (0.20 * AK)) B = B * ((S/(0.75 * AK))**23)

IF (S .GT. (0.75 * AK)) B = B * ((S/(0.75 * AK))**23)

A = 1.9519804E-10 * (S**2) * EXP(1.04E+04/T)

A = 0.0663116 * EXP(1.04E+04/T)

A = 0.0663116 * EXP(1.04E+04/T)

A = 0.075 * AK)) B = B * ((S/(0.75 * AK))**23)

A = 0.075 * AK) B = B * ((S/(0.75 * AK))**23)

A = 0.075 * AK) B = B * ((S/(0.75 * AK))**23)

A = 0.075 * AK) B = B * ((S/(0.75 * AK))**23)

A = 0.075 * AK) B = B * ((S/(0.75 * AK))**23)

A = 0.075 * AK) B = B * ((S/(0.75 * AK))**23)
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TABLE B-7.IV

LISTING OF THE COSTRS SUBCODE

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TABLE B-7.IV (continued)

```
CC
        X = AC + (ABS(STRESS) ++ 0.5 2.0 DR 25.)
        Y . X/AC
C
        CALL CTP(CTEMP, BC, TAU, PSI, AK)
        AC = 3.83E-19
RCT = CFLUX/PSI + 1.0/TAU
DELSTN = CCSTNF - CCSTNI
C
        BRANCH FOR POSITIVE OR NEGATIVE STRAIN INCREMENT
C
        IF (DELSIN . EQ. 0.) GO 13 800
IF (DELSIN .GT. 0.) GO 10 300
        BRANCH FOR SUBCASES OF NEGATIVE STRAIN INCREMENT
£
        IF((CSTNB + DELSTN) .GT. 0.1 GC TO 110
CC
       SUBCASE ONE CSTN8 + DELSTN IS NEGATIVE
ARG = BC + DELT + (CSTN8 + DELSTN) / AC
IF(ARG .LT. -C30.) GO TO 260
XL = - ( CSTN8 + DELSTN )
        CXP . EXP(ARG)
        DELTA = AC * DELSTN /(-AC*(1. - CXP) + DELSTN * BC * DELT * CXP)
        60 10 210
        SUBCASE THO CSTNB + DELSTN IS POSITIVE
Ĉ
   116 XL = 0.
        DELTA = -AC * DELSTN / (CSTNB * BC * DELT)
C
   210 N = 0
        M = 0
   215 XH * XL + DELTA
        STN *(-XH- CSTNB) * (1. - EXP(-BC * DELT * XH/AC))
IF(STN .GE. DELSTN) GO TO 220
DELTA * DELTA / 5.
        M = M + ]
        IF (" .LT. 5) GO TO 215
   226 XH XL + DELTA
        STN = (-XH- CSTNB) * (1. - EXP(-8C * DELT * XH/AC))
IF(STN .LT. DELSTN) GU TO 230
DELTA * DELTA * 2.
        N = N +
        IF (N .LT. 5) GO TO 220
   230 CONTINUE
        N = 0
        XM = (XL + XH) * 0.5
STNM = (-XM- CSTNB) * (1. - EXP(-BC * DELT * XM/AC))
```

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TABLE B-7.IV (continued) 240 IF (STNM .LT. DELSTN) XH = XM IF (STNM .GE. DELSTN) XL = XM XM = (XL + XH) * 0.5 *(-XH- CSTNB) * (1. - EXP(-8C * DELT * XM/AC)) STNM FE . ABS(STNM/DELSTN - 1.0) IF (FE .LT. 0.01) GO TO 250 N = N + 1 IF(N .LT. 11) GO TO 240 250 A = - XM GO TO 500 260 XM = -DELSTN - CSINB L = -XM GO TO 500 LCC POSITIVE STRAIN INCREMENT Ĉ BRANCH FOR SUBCASES OF POSITIVE STRAIN INCREMENT 300 IF((CSTNB + DELSTN) .LT. 0.) GO TO 310 C SUBCASE DNE CSTNB + DELSTN IS POSITIVE ARG =-BC + DELT + (CSTNB + DELSTN) / AC C 140 120 IF (ARG .LT. -030.) GO TO 460 XL = CSTNB + DELSTN CXP = EXP(ARG) DELTA = AC * DELSTN / (AC*(1. - CXP) + DELSTN * BC * DELT * CXP) Revised GO TO 410 C SUBCASE TWO CSTNB + DELSTN IS NEGATIVE ∞ 310 XL . 0. DELTA = -AC + DELSTN / (CSTNB + BC + DELT) 00 410 N = 0 M = 0 415 XH = XL + DELTA STN = (XH- CSTNB) * (1. - EXP(-BC * DELT * XH/AC)) IF (STN .LE. DELSTN) GD TD 420 DELTA = DELTA / 5. M = M + 1 IF(M . LT. 5) GD TO 415 420 XH = XL + DELTA STN = (XH- CSTNB) * (1. - EXP(-BC * DELT * XH/AC)) IF(STN .GT. DELSTN) GD TO 430 DELTA = DELTA + 2. N = N + 1 IF(N .LT. 5) GD TO 420

CCSTRIN CCSTRS

TABLE E-7.1 (ontinued)

```
430 CONTINUE
      N = 0
       XM = (XL + XH) * 0.5
  STNM = (XM- CSTNB) * (1. - EXP(-BC * DELT * XM/AC))
440 IF(STNM .LT. DELSTN) XL = XM
       IF(STNM .GE. DELSTN) XH . XM
      XM = (XL + XH) # 0.5
       STNM = (XM- CSTNB) * (1. - EXP(-BC * DELT * XM/AC))
      FE = ABSISTNM/DELSTN - 1.0)
      IF (FE .LT. 0.01) GO TO 450
      N = N + 1
       IF (N .LT. 11) GO TO 440
  450 A * XM
      GO TO 500
  460 XM . DELSTN + CSTNB
       A = XM
č
      BRANCH FOR PRE OR POST STEADY STATE
  500 B * BC * XM/ AC
Z * A / ((A - CSTNB) * (1. + B/RCT))
       # # 1.
      IF (DELSTN LT. 0.) W = -1.
IF (Z .GE. 1.) GO TO 510
OTSS = -(_____ALOG(Z))/B
       Y = XM/ AC
       ARG = -B + DELT
       IF (ARG .GE. -030.) CSTNBN = -( EXP(ARG)) * (A - CSTNB) + A
IF (ARG .LT. -030.) CSTNBN = A
       IF(DELT .LE. DISS) GO TO 700
000
      TREAT THE CASE WHERE THE WHOLE STEP IS STEADY STATE AND
      FIND UPPER LIMITS OF ABS(STRESS' FOR TRANSITION CASE
       STRESS FOR PURE STEADY STATE
  SLO EDAV = ABS (DELSTN) /DELT
      Y = (EDAV/(2. * RCT * AC)) * (1.0 + (1.0 + 4. * AC * RCT * RCT /
     # (BC * EDAV) 1**0.51
      CHECK TO SEE IF PURE STEADY STATE IS CONSISTENT
C
       Z = W * Y * AC /((W * Y * AC - CST'B)*(1. + BC*Y /RCT))
      CSINBN = -AC * BC * (Y**2) / RCT
      IF(Z .LE. O. .OR. Z .GE. 1.) 60 TO 700
      TREAT THE CASE WHERE ONLY PART OF THE STEP IS STEADY STATE
      XH IS UPPER LIMIT ON ABS STRESS. PURE PRIMARY CASE IS THIS LIMIT
č
      XH = XM
```

1.40

TABLE B-7. IV (continued) C XLL IS LOWER LIMIT ON ABS STRESS. PURE SS CASE SLOPE IS THIS LIMIT XLL = (W * CSTNB + 'CSTNB**2 + 4.*((AC*Y)**2)/(1.+(BC*Y/RCT))) # ##0.51/2. DELTA = (XH - (LL)/10. IF (DEL TA .LE. O.) DELTA . XH/10. XL = XH N . 0

```
610 XL = XL - DELTA
BL = BC = XL / AC
         * # * XL /((#* XL - CSTNB) * (1. + BL /RCT))
      DISS - ( ALOG(ZL) BL)
     STIL = -CSTNB + BL + + * XL + ((1./RCT) + DELT - DTSS)
+ /(1. + (BL/RCT))
      IF ((# * STNL) .LT. (# * DELSTN)) GD TO 620
       XH = XL
      N = N + 1
      IF(N .LT. 9) GO TO 610
       XL = XLL
  620 N . 0
  630 XM = (XL + XH) * 0.5
       BM . BC . XM / AC
       ZM = W * XM /((W * XM - CSTNB) * (1. + BM / RCT) )
      DTSS = -( ALOG(ZM) / 8M )
       STNL = -CSTN8 + 8M + W + XM + ((1./RCT) + DELT - DTSS)
     # /(1. + (BM/RCT))
      FE . ABS((STNL/DELSTN) - 1.0)
      IF(FE .1T. 0.01) GO TO 640
      IF((W * STNL) .LT. (W * DELSTN)) XL . XM
       IF((W * STNL) .GE. (W * DELSTN)) XH = XM
      N = N +
       IF(N .LT. 15) GO TO 630
  640 Y = XM/AC
      CSTNBM * W * XM * BM /RCT
C
  70C ALIMH = (0.75 * AK)**2
       ALIML = (0.20*AK)**2
      CHSTRS = # * (Y**0.5)
      IF (Y .GT. ALIMH) CHSTRS = W*(Y**0.04) * ((0.75*AK)**0.92)
       IF (Y .LT. ALIMLI CHSTRS . W . (Y**2) / ((0.20* A()**3)
      GO TO 810
  800 CHSTRS . 0.0
  810 CONTINUE
CC
      ESTIMATE UNCERTAINTY IN STRESS
UCTR = 2. * ABS( (CHSTRS + 1.3E+08)/1.3E+08)
+ 5. * ABS( (CTEMP = 644.)/644.)
```

CSTRN/CCSTRS

0

TABLE B-7. IV (continued)

```
USTRU = (1. + 0.075 * (1. + UCTR)) * CHSTRS
USTRL = (0.85/(1. + UCTR)) * CHSTRS
C
        RETURN
        END
         SUBRUUTINE CTP(CTEMP,82,TAU, PSI,AK)
C
        CTP CALCULATES PARAMETERS FOR THE CLADDING CREEP DOWN SUBROUTINE COSTRS
0000
         BC
                   OUTPUT STRESS COEFFICIENT OF RATE CONSTANT
                   . OUTPUT ZERD FLUX CORRELATION TIME (S).
0000
         TAU
         CTEMP . INPUT CLADDING TEMPERATURE (K)
         T = CTEMP
        IF (CTEMP .GT. 750.) T = 750.
IF (CTEMP .LT. 450.) T=450.
AK = 1.5E+09 - 1.5E+06 * T
C
        IF(T .LT. 615.) GO TO 10
BC = 4.69E-06 * EXP(-2.51E+04/T)
TAU = 8.6E-11 * EXP(2.51E+04/T)
PSI = 2.9E+06 * EXP(2.51E+04/T)
GO TO 20
    10 BC = 1.9519804E-16 * EXP(-1.04E+04/T)
        TAU = 2.0063116 * EXP(1.04E+04/T)
    20 CONTINUE * 6.967795E+16 * EXP(1.04E+04/T)
         RETURN
         END
```

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$$d\epsilon_{1} = \frac{d\epsilon}{\sigma} \left[\sigma_{1} (A1E + A3E) - \sigma_{2} A1E - \sigma_{3} A3E \right]$$

$$d\epsilon_{2} = \frac{d\epsilon}{\sigma} \left[-\sigma_{1} A1E + \sigma_{2} (A2E + A1E) - \sigma_{3} A2E \right]$$
(B-8.5b)

$$d\epsilon_3 = \frac{d\epsilon}{\sigma} \left[-\sigma_1 A3E - \sigma_2 A2E + \sigma_3 (A3E + A2E) \right]$$
(B-8.5c)

where all the terms have been previously defined.

As mentioned in conjunction with Equations (B-8.3) and (B-8.4), coefficients of anisotropy are provided by the CANISO subroutine. The information required by this subroutine is the temperature, the three principal components of plastic strain during a time interval, three constants related to the cladding basal pole distribution at the start of the time interval, and three constants related to the deformation history of the cladding prior to the time interval. For each time step, the subroutine updates the six constants required and provides the six coefficients of anisotropy required by Equations (B-8.3) through (B-8.5a—c). Initial (no plastic deformation) values of the pole figure and deformation history constants will be discussed in conjunction with the following summary of the equations used in the CANISO subcode.

For undeformed cladding, with σ_1 , σ_2 , σ_3 of Equation (B-8.3) defined to be the axial, circumferential, and radial components of stress, the expressions used to find the stress anisotropy constants are

$A1S = (1.5f_2 - 0.5) g(T) + 0.5$	(B-8.6a)
$A2S = (1.5f_2 - 0.5) g(T) + 0.5$	(B-8.6b)
$A3S = (1.5f_{0} - 0.5) g(T) + 0.5$	(B-8.6c)

where

- g(T)
- a function which is 1.0 for temperatures <1090 K, 0 for temperatures >1255 K, and found by linear interpolation for temperatures between 1090 and 1255 K
- f_r, f_z, f_θ = average of the squared cosine between the c axis of grains in the cladding and the radial, axial, and tangential reference directions, respectively, weighted by the volume fraction of grains at each orientation. These averages can be obtained from a pole figure and the CTXTUR subroutine described in Section 10.10 ($f_r = COSTH2$, $f_z = COSF12 - CT2CF2$, and $f_\theta = 1$ - COSTH2 - COSF12 + CT2CF2 in the notation of the CTXTUR subroutine). Values of f_r , f_z , and f_θ for typical cladding textures are $f_r \ge 0.06$, $f_z = 0.06$, and $f_\theta = 0.28$. B-8.2

The change of the factors, f_f , f_θ , and f_Z , of Equations (B-8.6a—c) due to deformation — odeled with the following correlations

 $\Delta f_{r} = -d\epsilon_{3}(-1.505 + T \cdot 0.00895)$ $\Delta f_{r} = -d\epsilon_{1}(-1.505 + T \cdot 0.00895)$ (B-8.7b) $\Delta f_{r} = -d\epsilon_{2}(-1.505 + T \cdot 0.00895)$ (B-8.7c)

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where

$$\Delta f_{r}^{\prime}, \Delta f_{Z}^{\prime}, \Delta f_{\theta}^{\prime} = \text{change in } f_{r}, f_{Z}, \text{ and } f_{\theta} \text{ due to deformation}$$

$$T = 644 \text{ K}, \text{ for temperature } < 644 \text{ K}, \text{ the temperature for } \leq 644 \text{ K}, \text{ the temperature for } \leq 644 \text{ K}, \text{ the temperature } \leq 1090 \text{ K}, 1090 \text{ K} \text{ for temperature } > 1090 \text{ K}$$

The strain anisotropy coefficients A1E, A2E, and A3E are given by Equations (B-8.6) and (B-8.7a-c) with A1S, A2S, and A3S replaced by A1E, A2E, and A3E when the cladding temperature is below 650 K. However, limited data at temperatures above 800 K suggest initial strain anisotropy coefficients of 0.5 (the isotropic values). The description of high temperature strain anisotropy thus requires a separate set of f-values, set initially at the isotropic values and changed during each time step by an amount given by Equ. tions (B-8.7a-c). The expressions for A1E, A2E, and A3E which are used to model this rather complex switching from texture dependent to deformation dependent strain anisotropy are

$$A1E = \frac{A1S + [(1.5f_{f}^{*} - 0.5) g(T) + 0.5] \exp\left[\frac{T - 725}{18}\right]}{\exp\left(\frac{T - 725}{18}\right) + 1}$$

$$A2E = \frac{A2S + [(1.5f_{Z}^{*} - 0.5) g(T) + 0.5] \exp\left[\frac{T - 725}{18}\right]}{\exp\left(\frac{T - 725}{18}\right) + 1}$$

$$A3E = \frac{A3S + [(1.5f_{\theta}^{*} - 0.5) g(T) + 0.5] \exp\left[\frac{T - 725}{18}\right]}{\exp\left(\frac{T - 725}{18}\right) + 1}$$

$$(B-8.8b)$$

 $f'_{r}, f'_{3}, f'_{\theta} =$ deformation dependent parameters set equal to 1/3 at zero deformation and changed like the parameters, f_{r}, f_{z} , and f_{θ} in Equation (B-8.7)

Effects of cladding temperature, cold-work, irradiation, in-reactor annealing, and oxidation on mechanical properties are expressed as changes in the strength coefficient, K; the strain hardening exponent, n; and the strain rate sensitivity exponent, m; of Equations (B-8.1) and (B-8.2). For fully annealed isotropic zircaloy-2 or zircaloy-4 cladding, the temperature and strain rate dependent values of m, n, and K as shown below.

(1) Values of the Strain Rate Sensitivity Exponent, m^a

For temperature, T, less than 730 K

 $\exp\left(\frac{T-725}{18}\right) + 1$

m = 0.02

For temperature between 730 and 900 K

$$m = 2.063172161 \times 10^{1} + T \left[-7.704552983 \times 10^{-2} + T \left(9.504843067 \times 10^{-5} + T \left(-3.860960716 \times 10^{-8} \right) \right) \right]$$
(B-8.9b)

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(B-8.9a)



(B-8,8c)

a. Eight to ten significant figures are used in these expressions to minimize discontinuities

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(B-8.9d)

For temperature between 900 and 1090 K

m :

m

$$= -6.47 \times 10^{-2} + T2.203 \times 10^{-4} . \tag{B-8.9c}$$

For temperature between 1090 and 1172.5 K

$$= -6.47 \times 10^{-2} + T2.203 \times 10^{-4}$$

$$= -6.47 \times 10^{-2} + T2.203 \times 10^{-4}$$
or
$$= -6.78 \times 10^{-2} \left(\frac{T - 1090}{82.6}\right) \ln \left(\frac{6.34 \times 10^{-3}}{\epsilon}\right)$$
for $\epsilon < 6.34 \times 10^{-3}/s$

For temperature between 1172.5 and 1255 K

m = -6.47 x 10⁻² + T 2.203 x 10⁻⁴

$$\begin{bmatrix}
0 \text{ for } \epsilon \ge 6.34 \text{ x } 10^{-3} / \text{s} \\
\text{or} \\
+ \\
6.78 \text{ x } 10 \quad \left(\frac{1255 \cdot \text{T}}{82.5}\right) \ln \left(\frac{6.34 \text{ x } 10^{-3}}{\frac{\epsilon}{\epsilon}}\right) \\
\text{for } \epsilon < 6.34 \text{ x } 10^{-3} / \text{s}
\end{bmatrix}$$
(B-8.9e)

For temperature between 1255 and 2100 K

$$m = -6.47 \times 10^{-2} + T2.203 \times 10^{-4} . \tag{B-8.9f}$$

(2) Values of the Strain Hardening Exponent, n

For temperature, T, <1099.0772 K

$$n = -9.490 \times 10^{-2} + T[1.165 \times 10^{-3} + T(-1.992 \times 10^{-6} + T9.588 \times 10^{-10})] .$$
 (B-8.10a)

For temperature between 1099.0722 and 1600 K

$$n = -0.22655119 + 2.5 \times 10^{-4} T . (B-8.10b)$$

For temperatures >1600 K

$$n = 0.17344880$$
 (B-8.10c)

When the strain is < n/(1 + m), the strain hardening exponent is modified^a to a larger value than the one given by Equations (B-8.10a-c). The expression used to modify n for strains < n/(1 + m) is

$$n' = \text{the smaller of} \left\{ \begin{array}{l} ANL & \text{or} \\ n^2 / [(1 + m).\epsilon] \end{array} \right\}$$
 (B-8.10d)

where

n

ANL =
$$0.17 \text{ fer T} \le 730 \text{ K}$$

 $0.056 \cdot T - 11.218$ for temperatures in the range 730 to 780 K; or 0.95 for T \ge 780 K

= the number given by Equations (B-8.10a-c)

n' = the revised number to be used with Equation (B-8.1) or (B-8.2) in place of n.

(3) Values of the Strength Coefficient, K

For temperature, T < 750 K

$$K = 1.17628 \times 10^9 + T[4.54859 \times 10^9]$$

$$+ T(-3.28185 \times 10^3 + T 1.72752)$$
] (B-8.11a)

For temperature between 750 and 1090 K

$$K = 2.522488 \times 10^{6} \exp\left(\frac{2.8500027 \times 10^{6}}{T^{2}}\right).$$
(B-8.11b)

For temperature between 1090 and 1255 K

$$K = 1.8413760^{39} \times 10^8 - T \ 1.4345448 \times 10^5 . \tag{B-8.11c}$$

For temperature between 1255 and 2100 K

 $K = 4.330 \times 10^7 + T[-6.685 \times 10^4 + T(3.7579 \times 10^1 - T7.33 \times 10^{-3})] . \qquad (B-8.11d)$

The changes in form of Equations (B-8.9a and b) through (B-8.11a—d) in various temperature ranges are caused by changes in the physical mechanism of the plastic deformation. At 700 to 900 K, the deformation becomes significantly strain-rate-dependent, the strength of the material begins to decrease rapidly with temperature, and strain hardening becomes relatively unimportant. This change is generally attributed to thermal creep at high temperature, but the specific deformation s_3 stem change has not been identified. The 1090- to 1255-K region is the $\alpha + \beta$ phase region for zircaloy and the region above 1255 K is the β phase region for zircaloy and the region above 1255 K is the β phase region for this material.

The change in the strain hardening exponent due to irradiation and cold-working of cladding is described by multiplying the value of p given in Equations (B-8.10a--c) by

 $BIC = [0.847 \exp(-39.2 \text{ COLDW}) + 0.153 + \text{COLDW}(-9.16 \times 10^{-2} + 0.229 \text{ COLDW})]$

$$\exp\left[\frac{-(\Phi)^{1/3}}{3.73 \times 10^7 + 2 \times 10^8 \text{ COLDW}}\right]$$
(B-8)

where

đ

RIC = strain hardening exponent for irradiated and cold-worked material divided by the expression in Equations (B-8.10a-c)

- COLDW = effective cold-work for strain hardening exponent (unitless ratio of areas) changes in the effective cold-work as a function of time and temperature are modeled by the CANEAL subroutine discussed in Section 9)
 - effective fast neutron fluence (neutrons > 1.0 Mev/m²) changes in the effective fast neutron fluence are modeled by the CANEAL subroutine discussed in Section 9).

The change in the strength coefficient due to irradiation and cold-working of the cladding is modeled with the expression

$$DK = 0.546 \text{ COLDW} \cdot K + 5.54 \times 10^{-10} \Phi$$

•

.12)

(B-8.13)



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Figure B-8.4. Base data, MATPRO prediction and uncertainty estimate for strain hardening exponent of annealed tubes.

Equations (B-8.11a-d) for the strength coefficients, K, of fully annealed, isotropic cladding are based on uniaxial tests of cladding, B-8.5 B-8.27, on uniaxial plate tests^{B-8.20} and on two closed tube burst tests. ^{B-8.2} For the low temperature data, the effects of varying amounts of cold-work and stress relief in the tubing tested were removed prior to including the measured values of K in the data base. This was done by using the cladding annealing model discussed in Section B-9 and the models for the effects of irradiation and cold-work which will be described in the next subsection. The effects of different strain rates were similarly removed with the model discussed in previous paragraphs of this Section^a.

The strength coefficients based on uniaxial tests of cladding were modified to apply to isotropic cladding using the empirical anisotropy coefficients discussed in the previous subsection. This was done by substituting values of effective stress from Equation (B-8.3) and values of effective strain from Equation (B-8.5a) into the equation of state, Equation (B-8.1) to obtain

$$\sigma_{z} = \left[\frac{K}{\frac{1+m+n}{(1.5 f_{r} + 1.5 f_{\theta})}}\right] \epsilon_{z}^{n} \left[\frac{\hat{\epsilon}_{z}}{10^{\cdot 3}}\right]^{m}.$$
(B-8.27)

a. Strain rate effects and annealing effects were removed from K as follows: first K^{\dagger} as given in Reference B-8.5 for use in the expression $\sigma = K^{\dagger}$, η was redefined to be equal to

$$\mathbf{K}^{\mathrm{t}} = \mathbf{K} \left[\frac{2}{10^{13}/\mathrm{s}} \right]^{\mathrm{m}}$$

then the fractional change in K expected from varying amounts of cold-work and annealing was removed to give values for the K of annealed tubing consistent with the model adopted by MATPRO for the effects of cold-work and annealing.

CSTRES, CSTRAN, CSTRNI, CANISO

Thus, the isotropic strength coefficient is related to the strength coefficient determined in a uniaxial test by the expression

$$K = K_{axial test} (1.5f_r + 1.5f_{\theta})^{1 + m + n/2}.$$
 (B-8.28)

This aperoach is different than the usual practice of taking the uniaxial test as the equation of state. B-8.43 The new approach restriction the scatter in values of K because the texture of the material being tested is considered.

Unfortune ely, values of f_r and f_θ were not given in Reference B-8.5, so estimated values based on the texture factors were employed. The approximation which worked best to reduce the scatter in values of the strength coefficient was

$$f_r + f_{\theta} \approx 1 - [axial (002) texture coefficient]/4.$$
 (B-8.29)

The factor of 1/4 was determined by requiring the sum of the axial, tangential, and radial (002) texture coefficients of Reference B-8.5 to be approximately 1.5 (f factors sum to 1).

The base data and the values of the strength coefficient predicted by the MATPRO correlation of the strength coefficient Equations (B-8.11a-d) are shown in Figure B-8.5. Discontinuities in the slope of the predicted strength coefficient as a function of temperature occur at 750, 1090, and 1255 K.

Values of the strength coefficient from BMI-NUREG-1961, GEMP-482, and ANL-75-58 were calculated from ultimate tensile strengths (presumed = maximum engineering strength at constant engineering strain rate). In order to estimate $K_{axial test}$, the axial stress and strain rate are converted to their engineering equivalents,^a the true strain at maximum engineering stress is round,^b and this true strain is substituted into Equation (B-8.1) to find



where

Smax = mostimum engineering stress (Pa)

= engineering =: ain rate (s⁻¹).

This approach is not very satisfactory because it neglects possible necking of the test sample. It is used because true-stress/true-strain curves are not available.

The most important strength coefficient data shown in Figure B-8.5 are the two values determined from data in EPRI NP-526 (Vol. 3). These strength coefficients were determined with a least squares regression technique which found the values of K, n, and m of Equation (B-8.1) which best fit the measured values of the stress and plastic strain.^c

b. The true strain at maximum engineering stress with constant engineering strain rate is 1 + m/n.

c. Elastic strains were calculated with the CELAST model and subtracted from the total strain components.





(B-8.30)

a. Engineering stress = true stress x exp($-ru_c$ strain) inside the exp of the first equation, true strain rate = engineering strain rate x exp($-ru_c$ strain).



Figure B-8.6. Data and least-squares fit to strength coefficients as a function of cold-work and irradiation at room temperature.

To estimate the effect of temperature on this correlation, values of the strength coefficient determined from the limited data from References B-8.12 and B-8.10 at temperatures of 553 and 573 kelvins were also fit to a straight line with the resultant correlation

$$K' = 373 + 238 CWK = 373 (1 + 0.64 CWK)$$
. (B-8.32)

Comparison of the two results shows that they are consistent with a temperature dependent expression of the form

$$\mathbf{K}' = \mathbf{K} \quad (\mathbf{T}) \left[\mathbf{I} + \text{constant CWK} \right] \tag{B-8.33}$$

where

K (T) = the temperature dependent function describing the behavior of the strength coefficient of annealed zircaloy (juations (B-8.11a) to (B-8.11c)).

The form of Equation (B-8.33) has therefore been assumed. The constant coefficient of the cold-work is taken to be 0.546 as determined at room temperature because the room temperature data exhibit much less scatter then the high temperature data taken from several different sources.



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CSTRES, CSTRAN, CSTRNI, CANISO

Figure B-8.7 illustrates the effect of cold-work and irradiation on the strain hardening exponent, n as determined at room temperature in Reference B-8.8. The strain hardening exponent of unirradiated material shown in Figure B-8.7 can be described by the empirical relation

$$n = 0.11 \exp \left(-39.2 \text{ CWN}\right) + 0.03(\text{CWN})^2 - 0.12(\text{CWN}) + 0.021$$
(B-8.34)

where

CWN = effective cold-work for strain hardening exponent.

This expression is essentially a decreasing exponential function for small values of cold-work and a slowly increasing parabola for large values of cold-work.

At higher temperatures, trends exhibited by the limited and scattered values of n (which have been obtained at 553 kelvins^{B-8,12} and 573 kelvins^{B-8,10} are consistent with the assumption that the fractional changes in n with cold-work are similar to the fractional changes in n at room temperature. The following functional relationship is assumed in the present model

n (T, cold-work) = n (T) $\frac{n(cold-work)}{n(at \ 0 \ cold-work)}$



Figure B-8.7. Data and analytical functions for strain hardening coefficient as a function of cold-work and irradation at room temperature.



(B-8.35)

TABLE B-8.I

Temperature (K)	Oxygen Content (weight fraction)	Ultimate Tensile Strength (MPa)	Calculated K (MPa)	<u>K/K</u> o
297	0.0009	524	781	1.00
297	0.0018	616	918	1.18
297	0.0034	785	1170	1.50
297	0.0063	949	1414	1.81
422	0.0009	354	527	1.00
422	0.0034	544	811	1.54
422	0.0063	680	1013	1.92
533	0.0009	266	396	1.00
533	0.0018	298	444	1.12
533	0.0034	361	538	1.36
533	0.0063	462	688	1.74
644	0.0009	227	338	1.00
644	0.0018	241	359	1.06
644	0.0034	283	422	1.25
644	0.0063	373	556	1.64

STRENGTH COEFFICIENT CALCULATED WITH DATA OF L. S. RUBENSTEIN

and reported only the parameters K, n, and σ_0 for many different strain intervals and oxygen concentrations. The additional variable, σ_0 , will cause the stress, σ , resulting from Equation (B-8.40) for a given ϵ to differ from that of Equation (B-8.3) for the same K and n.

The Argonne curves generally start at strains of 0.0004 and their data are fit accurately to the Ludwik equation by dividing the flow curve into two or three strain intervals with different values of K, n, and σ_0 for each interval. There are scattered examples in the Argonne results indicating that this approach may be inappropriate for small strains. In several of these cases, $\sigma_0 < 0$. Since σ_0 can be interpreted as the yield strass, \mathbf{R} -8.43 a negative value indicates a physical inconsistency. To avoid these problems, the Argonne correlations were use only for strains greater than an arbitrarily chosen minimum of 0.002.

To get a base for a model, "data" were generated using Equation (B-8.40) and fit to Equation (B-8.3) (the Holloman equation). The strain interval (from 0.002 to the maximum reported strain) was divided into 20 equally-speced intervals for each temperature-oxygen content combination. The Ludwik equations were then used to find a stress associated with each strain, and the resulting stress-strain pairs were fit by the method of least-squares to the Holloman equation. Only those tests where $\epsilon = 10^{-3}/s$ were used. This included 82 equations describing 60 different samples. The fluctuations in the resulting strength coefficient and the strain hardening exponent were much smaller for the Holloman equation than they were for the Ludwik equation.

For these derived data, the ratio (K/K_0) was calculated, as was done with the low temperature data. As with the Rubenstein data, (K/K_0) increases with oxygen concentration for all temperatures.

(3) Correlation for the Effect of Oxygen Concentration on the Strength Coefficient—Because little is known about the physical mechanism causing the strength coefficient of zircaloy to change with oxygen concentration, a model based on theory is not possible at this time. An empirical fit to the data is therefore the approach chosen. In addition to fitting the data, the correlation should satisfy the obvious condition that $(K/K_0) = 1$ when $C = C_0$. A quite simple correlation which does this is

$$\frac{K}{K_0} = 1 + a(C - C_0)$$

C

where

= oxygen concentration (weight fraction)

C₀ = oxygen concentration of as-received zir, aloy (weight fraction)

= a function of temperature to be determined (weight fraction)⁻¹.

An equation of the form of Equation (B-8.41) for each temperature was generated by a least-squares-fit technique using the data. The results are presented in Table B-8.11.

The ratio (K/K₀) derived from Equation (B-8.41) is plotted as a function of oxygen concentra ion for all temperatures used in Figure B-8.8. The data from Table B-8.11 are shown in the same figure. The six lowest temperatures are represented by a single line with a = 130 because they are too close together to be distinguishable.

The general characteristics of the temperature dependence of a are that it is relatively constant until about 1200 kelvins, rises rapidly between 1200 and 1400 kelvins, and then begins to level off. The leveling off is based on only the data point at the highest temperature. However, there are too few data to justify a sophisticated correlation. A single function can be found which fits the data with acceptable accuracy over the entire temperature range, thus having the advantages of automatically avoiding discontinuities and fitting compactly into a computer routine. For 300 < T < 1673 kelvins, the function is

TABLE B-8.II

Temperature (kelvins)	a	
297	160	
422	178	
533	137	
644	115	
1123	89	
1173	95	
1223	343	
1273	541	
1323	676	
1373	891	
1673	1116	

RATE OF CHANGE OF K/K, WITH OXYGEN CONTENT

(B-8.41)

9



It is somewhat surprising that a model based on uniaxial decormation and empirical texture coefficients stays within about 25 K of these biaxial data. Apparently the temperature dependence of the strength coefficient for the "second mode" of deformation discuised in Section B-8.9.3 is similar to the temperature dependence of the mode observed with uniaxial tests. Inspection of the predicted strain curves and Hardy's data seems to confirm the different (large) strain hardening exponent found with the biaxial test by Hann. Strains are systematically underpredicted when they are small and tend to be overpredicted when they are large. It is also possible that the relatively large initial strain is caused by an as yet unmodeled anealistic deformation.

A more sensitive test is provided by a stress rupture experiment reported by H. M. ChungB-8.24 In this test, temperature and pressure were set at 1023 K and 5.2 MPa. Chung's data and the MATPRO model predictions for 1023 and 1048 K are shown in Figure B-8.19. The model overpredicts cladding strength at 1023 K but the prediction at 1048 K approximates Chung's data fairly well out to strains of 0.2 where ballooning becomes important.

8.5 Uncertainties

Equations (B-8.17 to B-8.19) for the expected error of the constants K, n, and m obtained by comparing values predicted by Equation (B-8.9) to (B-8.11) with their own data base. Two points should be emphasized for users of these expressions (a) they are not standard errors and (b) they do not apply to irradiated or oxidized material. Standard error was not used as a measure of uncertainty because the scatter in the data is a function of temperature. Use of a single standard error would lead to nonphysical predictions such as negative strengths at high temperatures and there is not enough data to define a more reasonable distribution than the Gaussian distribution of the usual standard error definition. The error estimate of Equation (B-8.11) seems to be consistent with the comparison to burst tests which were discussed in the previous section. That is, the error from Equation (B-8.11) (strength coefficient/3.0) is approximately equivalent to an error of 25 K. The limited burst test data also were found to be in error by 25 K.



Figure B-8.19. Measured diametral strain versus MATPRO predictions for Chung's test at 1023 K and 5.2 MPa.

CSTRES, CSTRAN, CSTRNI, CANISO

8.6 Listing of the Subcodes CSTRES, CSTRAN, CSTRNI and CANISO

Tables B-8.1V to B-8.VII present listings of the CSTRES, CSTRAN, CSTRNI and CANISO subcodes. The subroutine CKMN which is presented in Table B-8.VIII is called by each of the first four subroutines to obtain values for the strength coefficient, strain rate sensitivity exponent, and strain hardening exponent. The expected uncertainties of the strength coefficient strain rate sensitivity exponent and strain hardening exponent are computed within the subroutine CKMN but are not returned.

8.7 References

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TABLE B-8.IV

LISTING OF THE CSTRES SUBCODE

SUBROUTINE CSTRES(CTEMP, DEL DXY, FNCK, FNCN, CWKF, CWNF, RSTRAN, STRANT, STREST) CSTRES CALCULATES CLADDING EFFECTIVE STRESS AS A FUNCTION OF TRUE CLADDING STRAIN, TRUE CLADDING STRAIN RATE, CLADDING TEMPERATURE, AVERAGE DXYGEN CONCENTRATION IN CLADDING, FAST NEUTRON FLUENCE, AND COLD WORK. STREST . DUTPUT EFFECTIVE TRUE STRESS (PA) INPUT EFFECTIVE TRUE PLASTIC STRAIN (UNITLESS) INPUT EFFECTIVE TRUE PLASTIC STRAIN RATE (S**(-1)) INPUT CLADDING MESHPOINT TEMPERATURE (K) INPUT AVERAGE DXYGEN CONCENTRATION EXCLUDING STRANT . RSTRAN . . INPUT AVERAGE DXYGEN CONCENTRATION EXCLUDING DXIDE LAYER - AVERAGE DXYGEN CONCENTRATION OF AS RECEIVED CLADDING (KG DXYGEN/KG ZIRCALDY) INPUT EFFECTIVE FAST FLUENCE FOR STRENGTH CDEFFICIENT (NEUTRONS/(M**2)) INPUT EFFECTIVE FAST FLUENCE FOR STRAIN HARDENING EXPONENT (NEUTRONS/(M**2)) INPUT EFFECTIVE COLD WORK FOR STRENGTH CDEFFICIENT (UNITLESS RATIO OF AREAS) INPUT EFFECTIVE COLD WORK FOR STRAIN HARDENING EXPONENT (UNITLESS RATIO OF AREAS) DELOXY . FNCK FNCN CWKF CWNF THE SUBCODE CKMN IS USED IN THIS SUBROUTINE CONVERSION FROM PA TO PSI IS 1.4505E-04 (PSI/PA) CSTRES WAS ADAPTED FROM CSTRAN (A SUBROUTINE BY P.L. MILLER AND R.R. HOBBINS) BY G.A. BERNA IN APRIL 1975 MODIFIED BY D.L. HAGRMAN OCTOBER 1, 1978 MODIFIED BY D. L. HAGRMAN TO REDUCE YIELD STRENGTH TO MEASURED VALUES JULY 1981. CALL CKMN(CTEMP, DELOXY, FNCK, FNCN, CWKF, CWNF, RSTRAN, AK, AN, AM) REVISE AN FCR SMALL STRAINS IF (STRANT .LT. (AN/(1. + AM))) AN = AN * AN /((1. + AM) * # STRANT) ANL = 0.17 IF (CTEMP .GT. 730.) ANL = 1.56E-02 * CTEMP - 11.218 IF (CTEMP .GE. 780.) ANL = 0.95 IF (AN .GT. ANL) AN = ANL

CSTRES,

CSTRAN,

CSTRNI, CANISC

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TABLE B-8.IV (continued)

ARG * AK * ((RSTRAN/1.0E-3)**AM) STREST * ARG * (STRANT**AN) RETURN END

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С

0

CSTRES, CSTRAN, CSTRNI, CANISO

TABLE B-8.V

LISTING OF THE CSTRAN SUBCODE

	iL	18	R	10	JU	T	I	N	E		¢	S	T	R		N		(CR	s		11		N	DE,S	L	OR	XE	Y	T	F	NC S T	KR	,	FN	N	ŝ	••	c	*	ĸ	F	• (C 1	11	F	,						
	SALADSA			IN IS	NCIATET	LNDWDR	CAGORA	AD INTN	LOTNAH .	CIEGLA	UNM , T	1011	A	TSRAHH	LA SOCIE	SRITAS	EUTUU	CORNESB	LANENDEC	A , JARO		RIAN	IN	NUENRLS	CHAR HAN	NOG LONG	TLUUDTN	RA ENUN	ADONTR	IDXCAAF	NIYEITO	AGE	SNADTI	SEHT	ATCOLEE	RONR	FANC	IN NELSPE	C NOTUD	TRT	IAR MA V	DTAONVE	NETR AR	I LUI				I	s				
5	5 1	R	1	1	T	ţ.	•	í.	0	U	1	F	1	IT		E	F	F	E	C	T	I	VI	E	1	R	U	E		PI	L	15	T	I	C		SI	FR	A	I	N		(1	Jħ	41	1	L	E	\$ 5	5 3			
01400	STE	FIEL		SAP	N				IIII	XZZZX	PPPPI		ITITIE		EECAL	FFLVA	FFAEY	mmonu	CCDAR	TIG	INNE	VE	EE	MXW	FRESCR	RUFEA	EMPNG	OE	SPIC	TLNO	RATNX	STIEG	SHENE	CETZ	PR	PSEAC	RATE		IUNE	ZR Z	E	X XR	A		E	(SN	* GD	* F	: -	•1	,,	
+	h	10	1	ć.					AIC	SNO	P	RU		C		IFF	Arr.C	PER 2	DC	T	I	VI	ALL			NO	GTN	c	F			N	UC2	KE	r ,	GF		2	KS	GT	R	E	N	G	TH	1	.0	Y)				
f	N	10	1	ł			•		LIL	XZC	100	i L	IT	IF	LEZ	FT	LI-	ELL	CN	T	I	VI					T	N	FI	LI		IN	ic	É	'	F	0	2	S	T	R	A	1	N	۲	11	R	0	E	11	N	G	
¢			F				•	i.	IC	NO	PC	L.F	ITF	1	EC	FI	FE	EN	C	Ť	Ĩ	VI	EN	1		E	US	S	W	R	RIAI		F	0	R	F	S		E	NA	G	T	H										
(IN	1 8	-			*		IE	NX	PP		TIN	E	EN	F	F	E	CU	T.N.	I	VETI	E	E	s	S	OR		Ť	I	RHO	0	F	0	RA	R	SI	IS	1	I	11		H	AF	20) 6	N	I	N	3			
T	•	18		S	U	B	C	0	D	E		c			IN	e,	I	s		U	SI	EC	0	1	1	1	r	н	I	s		su	18	R	0	U	1	IN	E														
¢	:0	1	11	16	R	S	I	0	N		F		20	M		P	A	i.		T	0		ş	9 9	51	t		I	s	3	1	. 4	5	0	5	E	-()4	e	(P	S	1	15	2	1							
9	S	1	F	A	ND	1	H	A	Ş	0	ç	2	0	E	D		B	Y		R	•	1	.,	ė	۲	1 3	L	L	E	R	1	IN	D	1	R	•	1	2.	•	H	0	8	8	[]	NS	5							
	10			FFF	Kranat	Dmmo	000	M	BBBE	YYYA	s	TODU	IR	E	LLD	•	۷	HHA	AAL	GIGU	RIRE	M/ S	A !	4			T	OR 1	BEIG	E DI	R	E	1	9 Y	71	8 E	LI	D	S	T	R	Ē	N	GI	r -	,							
000	A	L	A	iN	ç	K	M =	N	"	S	T	E	ME	S	f	01	E(LA	0 K	X	*				RS		FR	NA	CIN	N	í (0	KE	F	.0	c3				RR	Si	Ţ	R	4		1	K .	.0	A !	H .	4	M)	
-	EF	V	1	S	ER	A	AN	NT		F.	G	RE		S	M (AA	LN	Ļ	(51		21	A 1	It	1	5)	,	,		G	0	1	ro	1	1	0	c																

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TABLE B-8.V (continued)

```
II = 0

ANL = 0.17

IF(CTEMP .GT. 730.) ANL = 1.56E-02 * CTEMP - 11.218

IF(CTEMP .GE. 780.) ANL = 0.95

50 II = II + 1

ANA = AN * AN /((1. + AM) * STRANT)

IF(ANA .GT. ANL) ANA = ANL

STRANT = ((STREST/(AK * ((RSTRAN/1.0E-03)**AM)))**(1.0/ANA)

* + STRANT ) * 0.5

IF(II .LT. 9) GD TD 50

100 CONTINUE

RETURN

END
```

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TABLE B-8.VI

LISTING OF THE CSTRNI SUBCODE

	SU	BI	20	UI	1	N	E	C	S	Ti	RM	41		(E	R	H	si	1	ES	MI	RI	AN	E	1))	(1	,	FN	1 (K	,	FN	IC	N	, (K	F,	C	-	IF	•	
	CORTICA	MINU	EC	NICST	10AURO	BADPA			/LGZNK	A E		SRC	E ELC	SIA	A.000	D I	DDIN	BANGN	IG T	IE	SAMF	TIL	RATER	IRA	NUTIN		SCE	LAR	A	HODAN N	UIEF	NNRL	GAGUE	ISEN	P c	N RADX	I	FNG	E					
	ST	RI	N	T	•	j		IT	P	UC	UR	ER	FE	FIN	C	T	I			TS	RI	E	E	Pt	L	AS		L	C E	2010	T	R	AI	N		AT		T	HE		EN	D	0	F
	ST	RER	S	Ţ	:		IN	NP NP	U	T	-	HHC	FF	E	I	I	VI	E,	T	RRR		E	SP	TL	RA	EST	SI	CN	()	51	IRU	A	IN		A	T	T	н	E	s	T	R	r	
	DE	LHENL		Y				PP		TTT	104	ILV.	DEALY	EOIR	SIG	TZLI	EG		SEY	ISGO	ZHEA	E P P		UNN DO	TNY		E NA	MTN	PIR	ERAT	AI	5 100		EET	Xo	(K	10	DO	IN	16	6			
	FN	C+			•			PE	RUF	ETF		IFI	-VH H		T	CIL	LIV	ACEL	DFT	IAR.	N SOL	GIN	FI	11	KUN	NA NA	1000	XEI	Y (NR	7	ST	R	Z.U	IRNO	ĊT	AH		Y	5			
	CW	KF			*				U O U F	NITE	ENE	F	F	EIN	E	10.1	Y I	E	NC	ASO-	111	1	N N N	100	RIA		F	0	R		T	R	EN	G	T	н	•	4	A •	(U	En		NG	
	CH	N			•		IN E)	IP (F	U	TN	EN	F	F		T	Ì	VI	E	CS	is	L	R	AT	i I	RIO	(F	0	RAF	21	TA	RS		ÍN		н	R	0	EN	11	N			
	TH	E	S	UE	30	0	DE		С	K	MN	1	4	S	U	S	E	D	I	N	1	T	HI	S	-	si	18	R	01	11	I	N	E											
	co	N	IE	RS	5 1	0	N	F	R	0	٩	P	A		Ţ	۵		P	• 5	I		1	E S	;	1	• 4	5	0	58	-	-0	4	1	P	S	1	P	Ą)					
	C S MO		F	I	N D D	A	SBB	, C	000	DI	ELL		B	Y HA	GGG	RRR	MM	LANAN		HOT	ACO	GI	RE	AED	ZRUS			T7Y	8	BI	ER		1 4	P7	7 E	N	G T	н						
	MO 10	01	F	IEL	DED	AR	51	T P	DI	K		•-	0	H/	GI	LAKZ	M	AL	P	TH	DA	-	+	MB	I	i,	S	R	RI	G		N	RA		E	Y								

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CSTRES, CSTRAN, CSTRNI, CANISO

TABLE B-8.VI (continued)

```
RSTRAN = 1.0E-03
CALL CKMN (CTEMP, DEL DXY, FNCK, FNCN, CWKF, CWNF, RSTRAN, AK, AN, AM)
T = CTEMP
C
        IF (STRANT .LT. 1.08-06) STRANT = 1.0E-06
C
č
        REVISE AN FOR SMALL STRAINS
IF (STRANT .LT. (AN/(1. + AM))) AN = AN * AN /((1. + AM) *
      # STRANT )
        ANL . 0.17
        IF(CTEMP .GT. 730.) ANL . 1.56E-02 * CTEMP - 11.218
        IF (CTEMP .GE. 780.) ANL . 0.95
        IF (AN .GT. ANL) AN . ANL
C
        STRAN4 = STRANT
        II = 0
   10. STRANT = ((AN/AM + 1.0)*(1.0E-3)*((STREST/AK)**(1./AM))*DELH
                     + (STRAN4) ** (AN/AM + 1.0)) ** (AM/(AN+AM))
      #
        RSTRAN = (STRANT - STRAN4)/DELH
CORRECT AM FOR REVISED RSTRAN IF NECESSARY
C
        IF(T .LT. 1090.) GO TO 200
        IF(T .GT. 1255.) GO TO 200
IF(RSTRAN .GI. 6.34E-03) GO TO 200
        IF (RSTRAN .LT. 1.0E-05) RSTRAN . 1.0E-05
        I1 = II + 1
  AM = -6.4E-02 + T*2.203E-04
IF(T - 1172.5) 123,123,124
123 AM = AM + 6.78E-02*ALUG(6.34E-03/RSTRAN)*((T-1090.)/82.5)
        GO TO 125
  124 AM = AM + 6.78E-02*ALOG(6.34E-03/RSTRAN)*((1255.-T)/82.5)
125 AM = AM + EXP(-69. * DELOXY)
        IF(II .LT. 10) GO TO 104
C
  200 CONTINUE
        RETURN
        END
```

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TABLE B-8.VII

LISTING OF THE CANISO SUBCODE

* 5	1	B	R	0	U	T	[]	E		с	A1	II	s	0	1		E A	PD	1,	, ,	E	P	25	,	0	EP A2	35	, (C 1	TE	13	P	, ;	1	FE	, ,	FZ	PE	, ,	A	BE	;		10),	4	20	,	
Oww		NFF	IEEE	SCC		I		AL	coss	UTT	RIR	ATES	ESN	S	TIT		ESS	FIT	FRA		ISA	E	ZUC	TOO	SMM		FNN	E	ANN		IS		TR	30	R	Ě	FLA	P	R	N	;E	L	A	T	IN	G			
4	11	S				•	1		TF	PHO	UC	Ţ	CV	DEG	E	FF	R	CHIC	I	EN	11	U	OZC	FIC	TÍ	AN	ISI	SSS		TF	20	19	Y	F	0	R	0		L		JL		T T		IG				
4	13	35					- more		FTF	E HO H	CUC		SOA5	EDE	E	ST	ACK CK	SHOW	SIS	IS IN	11	U	ZOZ	IFI	TI	LE	SIS	SSSS		TR	10	P	Y	F	:0	R	c	. A	L	C 1.	11	4	T	IN	16				
I	ł	EF	E	FC	P	RI	M a	E	FS	T	R	HES	s	E	-	1	T	IAA		NSC	F.+ 1	0	RU	Se	E	FF	EAA	c	1	1	E	Se	SI		EAA	S	5)	1**	\$	20	15++	s	u	Me	D		to	6	BE
A N	11	ER	RE	ES	s	s		GM	AP	0	1 NI	EN	ST	I	GI	MA		42	3	SAM	10	,	is	SI	G	A	Ā	3	3		E	š	IGPR		A	c	1)	*	*	2	X	*	\$	0.	5				
4	1	E				•	-		TF	PE	U	I.	CV	DE	E	FF	R	CA	I	N	1		0	F	1	AN	I	S	01	r R	10	P	Y	F	0	R	c		L	cı	IL	. A	T	IN	IG				
4	12	E			1	•	0		F	PE	U C	TI	CV	Ē	E	FF	R	CA	I	N	17		0	F	1	AN	I	SI			10	P	Y	F	0	R	0	A	L	C L	JL		r •	[N	IG				
4	13	BE				•	1		F	PE	C		V	E	E	51	R	A	11	N	11		0	۲	1	Ari	1	2	U		(1	14	1	r	u	ĸ	C	A			<i>.</i>	A	1	10	46				
-	F	F	e	FC	P	RI	M V E	E	S	T	R	HEAI	N	E	-	145	I	IM		N	F	E	F	F	E	FF	EI	VI	E	IN		R	SI		-	I	N	R	SE	4	SN	F	S	ME	ED		to.	ł	BE
-			HR	E	TM	E	E NI	rs	C	RO	M		N	E	N	R	E	Mag	E	1	15	;	D	E	FI	EN	E	D	1	IN	4	T	ER		15	1	OF		S	1.		t	N						
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F	:]	LP				-			Ŧ	PWT	UEI	EN	v	8	A	UN SA	ELN	T	PI		GER	HS	T	EAS	NI	ADEP	č	E	R	RI	GE	N	A) S	I	NIA	E I	l S	F	1	TH	E		A !	NG IE	L	EN	D	

CoTRES, CSTRAN, CSTRNI, CANISO

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TABLE B-8.VII (continued)

CSTRES, CSTRAN, CSTRNI, CANISO

E2P		n		P		r i	vi	ii.	i.e	46	1	4F	T	SH	T	ED		AV	FR	4.5	G	F	ci	S	[N	E	01		7 1	46		AN	G	LE			
		B	ET	WI	E	N	CI	A	SIR	AL	T	POT	LI	ES		ANST	D	C	00	R	D	IN	AT	Ē	4	X	IS	2	1	T		TH	E	E	4	D	
F3P	•	0.00	UTET	PWT	UTEE	N	VEL	JR	UISR	MEAL	T	EDT	IL	GHSE	T	EDAN	DE	AVCP	EF	RADR	GED	ĪN	AT	E	I N A	EXI	S	3	T	AT		ANTH	GL	E	N	0	
AlD		0	UI	P	19	Ľ	H)	IC	H	T	E	MP	E	RA	T	UR	E	S	Ţ	4	I	N	AN	1	so	TR		Y		:0	EF	FF	1	: 1	EI	NT	
AZD		0	UT	P	U1	12	H	G	H	UT	E	4P	THU	RA	T	XX	KED	S	ţ	A A	11	N	AN	I		TR	OF	Ŷ			SHO	FF	1(: I	E	T	
A3 D	*	0	UTAT	P		1E TE	H	GN	HD	TO	EF	9P T	EH	RA	T		ER	EN	İ F	A	IN	NE	ANS	I	SOP	TR		YII	TI	E	ELS.	FF	I	I	EI	TN	
CTEMP DEP1	:	I	NP	U	Ţ	CC			0	IN	GG	Tp	EL	MP	EF	RAIC	T	JR	ER	(1	K) N	I	NC	R	EH	EN	T.	A	L	N	G	1		s T			
DE P2		I	NP	U	f	000	LA	1D	0	IN	G	P	E.J	1S	T	KKIC	E	ST	R	AI	N	I	NC	ERE	ĘM	EN	IT	A	L	NC	G	2	1	ND			
DEP3		I	NP	U	Ĭ	Dese		R	0	IN	G	P	L	1S	T	KK	t	ST	RA		N	I	NC	R	EM	EN	IT	A		JN C	200	3	\$	RD	ł,		
F1P	•	100	ANPET		S T E	VN		KU A	Mi	GELL	H H	EI	110-11	HTES	E	RRDAN	LADU	VEC	R	AG	EO	CIN	AT	E	NEA	X	IF	1	HH	AT	A	NG TH	E	Es	T	ART	
FZP	•	UHB0	NPET	UW	TEE	VEN	ăie c		MISO	AL	WE	EI	GIL	HTES	E	DAN	AD	VEC	RA	G	ED	IN	AT	Ē	NEA	x	F	12	H	AT	A!	N G T H	E	s	т	ART	
F3P	*	180	NPET	-UW	TEL	V		BA	KESO	EL	W	EI	GL	HTESHE	ε	DAN	ADE	VEC	RI	GR	ED	IN	AT	E	NEA	x	DF	T 3	H	E T	A !	NG	E	e s	τ	ART	
A10	*	LAC	NP	Ť	TH	H	I	HAT	RP	TETT	MI	PEFT	RTE	ATHE	U	RECU	R	RE	R J N 1		NT	A	NIE	S	TE	RC) P 1	s	CE	DE	FI	FI	c •	IE 5	N	T	
A2D	•	IAL	NP	U	HETH	H	ICST	HAT	RR	TE	Mi	PE	RIF	AT	U	PE	R	STRE	RI	AI	NTI	A	NI	S		P	191	s	E	DE T	FI	F I	C .	5 5	N	T	
A 3D	*	IAF	NP	UT	Ť HE TI	HE	I	GH A	RR	TE ST	MI	PE	RTE	HE	U	RECU	R	RE	RANI	I	NT	IM	NIE	S		P	191	s	E	JE	FI	FIO	c :	I E	N	T	
THE CI	R	RE	LAHACA	TNL	N	DN E	STE	U	SAL	ED 0		A	TIS	TH RA IM	INU	SILA	SI	JB	C C	DE	EFN	DR-	RE MA 52	T	BA	SXX	P	NO	NPE	DR	AT		SA	FR	H	M: 19	78)
CANTS	1		c '	c	0	TE	0		Y	6	Į.	1	J.	14		GP	M	AN	6	10	TO	R	FR		1 9	7											

MODIFIED BY D. L. HAGRMAN IN JUNE 1979

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TABLE 3-8.VII (continued)

MODIFIED BY D. L. HAGRMAN JULY 1981 TO KEEP A10, A2D, A3D, A1P, A2P, AND A3P IN THE RANGE 0 - 1.5 (CDR-MP-04) 00000 CONVERT F FACTORS TO APPROPRIATE ANISOTROPY COEFFECIENTS A3P = 1.5*F2P A2P = 1.5*F1P A1P = 1.5*F3P C SAC = 1.0 IF(CTEMP .GE. 1090.) SAD = 7.6060606 - CTEMP * 6.060606E-03 IF(CTEMP .GE. 1255.) SAD = 0.0 SPD = 1.0/(EXP((CTEMP - 725.)/18.) + 1.0) RAC = -2.757 + CTEMP * 1.343E-02 IF(CTEMP .LE. 644.0) RAC = 0.52762 IF(CTEMP .LE. 644.0) RAC = 0.5176 IF (CTEMP .GE. 1090.) RAC = 6.5174 APN = 1.0 IF(A1P .GT. IF(A2P .GT. IF(A3P .GT. 1.48) APN . O.C 1.481 APN = 0.0 APN = 0.0 1.48) LT. 0.02) IF (AIP APN . 0.0 APN = 0.0 IF(A2P IF (A3P ADN = 1 IF (A1D IF (A2D IF (A3D APN . 0.0 1.48) .GT. ADN = 0.0 .GT. ADN . 0.0 .GT. 1.48) ADN = 0.0 IF (A10 .LT. 0.021 ADN = 0.0 IF (A 2D C.021 ADN . 0.0 .LT. .LT. 0.021 ADN . 0.0 IF (A3D A1P = A1PA2P = A2PRAC + APN+ DE P3 --RAC * APN*DEP1 A3P . A3P RAC*APN*DEP2 -1.50) PRINT 901 1.5) AIP = 1.49 1.50) PRINT 902 1.5) /2P = 1.49 ·GI: IF(ALP IF(ALP C IF (A2P IF (A2P C .GT. .GT. 1.50) PRINT 903 1.5) A3P = 1.49 IF(A3P C .GT. IF(A3P .GT. IFIAIP 0.00) PRINT 904 C .LT. A1P = 0.01 IF(A1P .LT. 0.00) IF(A2P C 0.00) PRINT 905 .LT. IF (A2P A2P = 0.01 .LT. 0.001 C LF (A3P .LT. C.00) PRINT 906 0.00) A3P = 0.01 IF(A3P .LT. A10 = A10 -RAC*ADN*DEP3

TABLE B-8.VII (continued)

420 = A20 -RAC*ADN*DEP1 · A3D RAC * ADN * DEP2 430 -1.501 PRINT 901 .GT. IF (A1D C 1.5) AlD * 1.49 IF(A10 .GT. 1.50) PRINT 02 IF (A2D IF (A2D C .GT. 1.51 A20 = 1.49 .GT. 1.501 PRINT 903 IF (A3D .GT. C A30 = 1.49 PRINT 904 F(A3D 1.5) .GT. IF (ALD .LT. 0.001 A10 = 0.01 IF (A1D .LTe PRINT 905 IF(A2D .LT. IF(A2D .LT. IF(A3D .LT. 0.001 C 0.001 A20 = 0.01 pr. 0.00) PRINT 906 A30 = 0.01 901 FORMAT(94H ERROR IN ANISOTROPIC CLADDING DEFORMATION * A1 TOO LARGE. TRY SMALLER TIME STEFS.) 902 FORMAT(94H ERROR IN ANISOTROPIC CLADDING DEFORMATION * A2 TOO LARGE. TRY SMALLER TIME STEPS.) 903 FORMAT(94H ERROR IN ANISOTROPIC CLADDING DEFORMATION * A3 TOO LARGE. TRY SMALLER TIME STEPS.) 904 FORMAT(94H ERROR IN ANISOTROPIC CLADDING DEFORMATION * A3 TOO LARGE. TRY SMALLER TIME STEPS.) 904 FORMAT(94H ERROR IN ANISOTROPIC CLADDING DEFORMATION * A1 TOO SMALL. TRY SMALLER TIME STEPS.) 0.001 IF(A3D .LT. 905 FORMAT(94H ERROR IN ANISOTROPIC CLADDING DEFORMATION # A2 TOD SMALL. TRY SMALLER TIME STEPS.) 906 FORMAT(94H ERROR IN ANISOTROPIC CLADDING DEFORMATION # A3 TOD SMALL. TRY SMALLER TIME STEPS.) A1E = (A1P*SPO + A1D*(1.0 - SPO)) * SAO +0.5*(1.0 - SPO)) SADI + A2D*(1.0 - SPO)) + SAD +0.5*(1.0 - SAD) + A3D*(1.0 - SPO)) + SAD +0.5*(1.0 - SAD) * (A2P*SPO AZEAJE = (A3P*SP0 + A1S = A1P * SAD +0.5*(1.0 -A2S = A2P * SAD +0.5*(1.0 -A3S = A3P * SAD +0.5*(1.0 -SACI £ CONVERT ANISOTROPY COSFFICIENTS TO F FACTORS F1P = A2P/1.5 F2P = A3P/1.5 C F3P = A1P/1.5 C RETURN END

361c Revised 8/81

CSTRES, CSTRAN, CSTRNI, CANISO

361d Revised 8/81

SUBROUTINE CKMNICTEMP, DELOXY, FNCK, FNCN, CWKF, CWNF, RSTRAN, AK. AN	, AM)
CKMN CALCULATES PARAMETERS FOR THE CLADDING EQUATION OF STATE AS A FUNCTION OF TEMPERATURE, AVERAGE DXYGEN CONCENTRATION, FAST NEUTRON FLUENCE, AND COLD WORK.	
AK = OUTPUT STRENGTH CDEFFICIENT (PA) AN = OUTPUT STRAIN HARDEMING EXPONENT (UNITLESS) AM = OUTPUT STRAIN RATE SENSITIVITY EXPONENT (UNITLESS) UM = ESTIMATED UNCERTAINTY OF AM (NOT CURRENTL' RETURNED) UN = ESTIMATED UNCERTAINTY OF AN (NOT CURRENTLY RETURNED) NOTE AN - UN IS NEGATIVE NEAR 1000K UK = ESTIMATED UNCERTAINTY OF AK (NOT CURRENTLY RETURNED)	
CTEMP = INPUT CLADDING MESHPOINT TEMPERATURE (K) DELDXY = INPUT AVERAGE DXYGEN CONCENTRATION EXCLUDING DXICE LAYER - AVERAGE DXYGEN CONCENTRATION OF AS RECEIVED CLADDING (KG DXYGEN/KG ZIRCALDY) FNCK = INPUT EFFECTIVE FAST FLUENCE FOR STRENGTH CDEFFICIENT (NEUTRONS/(M**2)) FNCN = INPUT EFFECTIVE FAST FLUENCE FOR STRAIN HARDENING EXPONENT (NEUTRONS/(M**2)) CWKF = INPUT EFFECTIVE COLD WORK FOR STRENGTH CDEFFICIENT (UNITLESS RATID OF AREAS) CWNF = INPUT EFFECTIVE COLD WORK FOR STRAIN HARDENING EXPONENT (UNITLESS RATID OF AREAS) CWNF = INPUT EFFECTIVE COLD WORK FOR STRAIN HARDENING EXPONENT (UNITLESS RATID OF AREAS) CWNF = INPUT EFFECTIVE TRUE PLASTIC STRAIN RATE (S**(-1))	
THE EQUATIONS USED IN THIS SUBROUTINE ARE BASED ON DATA FROM (1) C.R. WOODS, PROPERTIES OF ZIRCALOY-4 TUBING, WAPD-TM-585 (1966) (2) ULTIMATE STRENGTH DATA OF H.C. BRASSFIELD, ET AL. GEMP-482(1968) (3) A.L. BEMENT, JR., EFFECTS OF COLD WORK AND NEUTRON IRRADIATION ON THE TENSILE PROPERTIES OF ZIRCALOY-2,	
(4) A. COWAN AND W.J. LANGFORD J.NUCLEAR MATER. 30 (1969) PP 271-231 (5) L.M. HOWE AND W.R. THOMAS, J. NUCLEAR MATER. 1 (1960) P 248	

TABLE B-8.VIII

LISTING OF THE CKMN SUBCODE

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TABLE B-8.VIII

LISTING OF THE CKMN SUBCODE

CSTRES, CSTRAN, CSTRNI, CANISC

(6) A. M. GARDE LIGHT-WATER-REACTOR SAFETY RESEARCH PROGRAM QUARTERLY PROGRESS REPORT APRIL - JUNE 1975 Ć ANL-75-58 (7) A. M. GARDE LIGHT-WATER-REACTOR SAFETY RESEARCH PROGRAM QUARTERLY PROGRESS REPORT JULY - SEPTEMBER 1975 C ANL -75-72 (8) R.L. MEHAN AND F.W. XIESINGER. MECHANICAL PROPERTIES OF ZIRCALOY-2, KAPL-2110 (9) D. LEE AND W.A. BACKOFEN TMS-AIME 239 (1967) PP 1034-1040 (10) P. J. CRESCIMANNO, HIGH STRAIN RATE TENSILE TESTS OF ZIRCALOY AT 550F, WAPD-TM-1263 (FEBRUARY 1976) (11) C. R. HANN ET AL, TRANSIENT DEFORMATION PROPERTIES DF ZIRCALDY FOR LOCA SIMULATION, EPRI NP-526 VOLUME 3 (MARCH 1978) CODED BY D. L. HAGRMAN AUGUST 1977 MODIFIED BY G. A. REYMANN AND M. A. MORGAN MARCH 1978 MODIFIED BY D. L. HAGRMAN JUNE, 1980 C T = CTEMP LIMIT STRAIN RATE TO A MINIMUM OF 1.0E-05 IF(RSTRAN .LT. 1.0E-05) RSTRAN = 1.0E-05 C C C FIND STRAIN RATE EXPONENT, AM IF(T . LE. 730.) AM = 0.02 C Δ . 20.63172161 - 0.07704552983 B C . 9.504843067E-05 D = - 3.860960716E-08 IF (T .GT. 730.) AM . A + T*(B+ T*(C+ T*D)) IF(T .GE. 900.) AM = -5.47E-02 + T + 2.203E-04 C C MODIFY STRAIN RATE EXPONENT, AM, IN ALPHA - BETA REGION IF (RSTRAN .GE. 6.34E-03) GO TO 100 IF (T .LE. 1090.0) GO TO 100 IF (T .GE. 1255.0) GO TO 100 IF(T .GT. 1172.5) GO TO 24 AM = AM + 6.78E-2*ALOG(6.34E-3/RSTRAN)*((T-1090.)/82.5) GO TO 100 24 AM = AM + 6,78E-2*ALUG(6,34E-3/RSTRAN)*((1255,-T)/82.5) C

361e Revised 8/8

TABLE B-8.VIII (continued)

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C

C

C

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C

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FIND UNCERTAINTY
100 IF(T .LE. 700.) UH = 0.01
    IF(T .GT. 700.) UM = -2.97992E-02 + T + 5.6856E-05
     IF(T .GT. 900.) UM . 0.16 * AM
    AM = AM + EXP(-69. +DELOXY)
    FIND STRAIN HARDENING EXPONENT, AN
     AN = -9.490E - 02 + T * (1.165E - 03 + T * (-1.992E - 06 + 1))
            T*9.558E-101)
     IF(1 .GE. 1099.0722) AN = -0.22655119 + 2.5E-04 * T
     IF(T .GE. 1600.000 ) AN . 0.17344880
    FIND UNCERTAINTY
    IF(T. LE. 700.) UN = 0.017
    IF (T .GT. 700.) UN = -2.8405405E-02 + T * 6.4864864E-05
     IF ! T.GT. 1255.1 UN = 0.053
    AN = (8.47E-01 * EXP(-3.92E+01*CWNF) + 1.53E-01 +
CWNF * (-9.16E-02 + CWNF *2.29E-01) *
            EXP(-((FNCN)**0.33)/(3.73E+07 + 2.0E+08*CWNF)) * AN
    AN = AN*(1. + (1250. - (1250./(EXP((T-1380.)/20.) + 1.)))
    *DELOXY)
IF (AN .GT. 0.8) AN . 0.8
   *
     FIND STRENGTH COEFFICIENT, AK
AK = 1.17628E+09 + T*(*.54859E+05 + T*(-3.28185E+03 +
    T*1.72752))
IF(T .GE. 750.0) AK = .5224880E+06 * EXP(2.8500027E+06/(T**2.0))
IF(T .GE. 1090.) AK = 184.1376039E+06 - 1.4345448E+05 * T
   *
    IF(T .GE. 1255.) AK . 4.330E+07 + T+(-6.685E+04 +
                               T*(3.7579E+01 - T*7.33E-031)
   .
     IF(T.GT.2100.)AK=1.0
     FIND UNCERTAINTY
     IF(T .LE. 700.) UK = 77.00E+06
     IF(T .GT. 700.) UK = 110.43693E+06 - T * 4.7767045E+04
IF(T .GT. 800.) UK = AK/3.0
    AK = AK * (1.0 + 5.46E-01*CWKF)
AK = AK + FNCK * 5.54E-18
     AK = AK*(1. + (1120.-(990./(EXP((T-1301.5)/61.) + 1.)))
          *DELOXY)
   #
     RETURN
     END
```

CSTRES, CSTRAN, CSTRNI, CANISC

CSTRES, CSTRAN, CSTRNI, CANISO

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CMLIMT and CBRTTL



Figure B-11.8. Hobson-Rittenhouse and PBF data for fast cooled rods compared with the critical fractional wall thickness as calculated from the 0.65 and 0.70 v % and 90 and 95% filled criteria.

CMLIMT and CBRTTL

Consequently, the model for fast cooled cladding is that the cladding is considered embrittled if the oxygen content of the beta phase exceeds

- (1) 90% of the saturation content, or
- (2) 0.65% of weight.

A third criterion limiting the maximum cladding temperature to < 1700 K is added to fit the highest temperature data.

The data are still too limited to consider this model final. But the accuracy is encouraging, especially considering the differences in the experiments. The Hobson-Ritteniouse samples were oxidized on both sides, out-of-pile, and quenched rapidly; while the PBF samples were oxidized primarily on the outside, in-pile, and quenched slowly.

11.2.5 Model for Slow Cooled Cladding. Designation of this part of the model as being applicable to slow cooled cladding is slightly misleading; it is meant to apply during the pre-quench of a LOCA. As described in Section 11.2.2 of this report, Chung, Garde, and Kassner^{B-11.32,B-11.35,B-11.36} have completed many out-of-pile tests of this sort and developed an embrittlement criterion requiring at least 0.1 mm of cladding thickness with <1 wt% oxygen. When this criterion was checked using COBILD, it was found that at least 0.3 mm with <1 wt% oxygen is required to avoid failure by thermal shock. No reason for the difference between this and the ANL minimum thickness of 0.1 mm has been found. It p ssibly lies in the mechanics of the two codes. When the ANL code is more fully documented, this can be checked. Until then, the criterion established with COBILD will be recommended for use with the MATFRO package.

In Figure B-11.9, this criterion is compared with the data. Only temperatures >1244 K are considered, since this is the lower range of validity for COBILD. Not all of the data are shown in the figure because many are coincident, or nearly so. Of the 146 intact rods, 16 or 11% are predicted to fail; and of the 57 failed rods, 4 or 7% are predicted to remain intact. In the entire data set, <10% of the predictions are incorrect. Given the scatter in the data, this is considered acceptable accuracy.

Since all the tubes tested at ANL has a wall thickness of 0.635 mm, it is impossible to conclude whether the 0.30 mm is the actual minimum thickness required to retain ductility, or if there is some minimum F_W . The former is more reasonable on physical grounds because it seems logical that there should be a minimum thickness of ductile material necessary for ductility.

If the embrittlement criteria for fast cooled rods are compared with the slow cooled data, failure would be predicted in most cases, contrary to experimental observation. Similarly, the criterion used for the slow cooled rods almost never predicts a failure when compared to the fast cooled data. These facts underscore the importance and complexity of cooling rate on the ductility of zircaloy at high temperature, and further emphasize the importance of clearly specifying the cooling rate.

11.2.6 Uncertainty of the Models. A primary pource of uncertainty for both models is in temperature measurement. For the Hobson-Rittenhouse data set, the temperature uncertainty is estimated by comparing the temperature reported for a given layer thickness with that calculated using isothermal oxidation kinetics published by Cathcart^{B-11.42} for the same thickness. From this analysis, the root mean square of the temperature differences is about 50 K. A similar technique was used for the PBF and ANL data. Seiffert and Hobbins^{B-11.31} also arrived at an uncertainty of about 50 K, while Chung^{B-11.35} found an 85-K uncertainty. This technique should give a reasonable estimate because Cathcart's correlations are based on a careful analysis of his own data. This analysis shows the data to have a high degree of consistency, and the major error in measurement should be the temperature; the layer thicknesses being much easier to obtain with accuracy.

TABLE B-11.VII (continued)

C

C

CCCC

C

C

CCCC

C

C C

```
DC 1 J = 2,9
                IF(A4(J) .LT. 1.02-02) GC TO 12
CONTINUE
c : .
               ANUME = 9.0 - FLGAT(K)
BCRIT = BETA THICKNESS AITH LESS THAN 1.0: DXYGEN BY WEIGHT.
BCRIT = ANUMENY2 + ((.01-AN(K))/(AN(K-1)-AN(K)))*Y2
GC TC 25
BCRIT = 5.C*Y2
c15
   64
   25
                9CKIT = S * 3CRIT
1F(BCRIT .LT. 0.03)
CC TO 100
                                                             CBRITL = 1.0
                                                 HIGH COOLING PATE CALCULATION
   50
                IF(CTEMP .GT. 1753.) CBRITL = 1.7
IF(CTEMP .CT. 1755.C) GO TC 100
                          * (BWTFRD + 0.0012) * 100.0

* AVERAGE CONCENTRATION IN THE BETA (WEIGHT PER CENT).

CON . GT. 0.65) CBRITL * 1.0
                BCON =
BCON =
1F(BCON
               SAT = J.12
SAT = SATURATION CONCENTRATION IN THE BETA FOLLOWS.
IF(CTEMP .LT. 1239.C) GO TO 55
SAT = -4.2075-C3 + SORT((CTEMP/392.46) - 3.1417)
IF(CTEMP .LT. 1373.C) GO TO 55
SAT = (CTEMP - 1.31.7)/491.157
c<sup>55</sup>
               BSAT = 1.0304 * (BETER 0+.0012)/SAT
BSAT = PER CENT OF SATURATION CONCENTRATION IN THE BETA.
IF(BSAT .GT. 90.0) CORTTL = 1...
                RETURN
   160
                END
```

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If COBILD does not terminate due to an excess diffusion rate, then at the end of the oxygen redistribution calculation the total oxygen in the beta is calculated using the concentrations at the nine nodes and integrating by Simpson's rule.

14.2.3 Oxygen Weight Fraction in the Beta Zircaloy. As mentioned in the preceding subsection, the total oxygen in the beta region is calculated. This quantity, called BWT, has units of kg/m^2 and is the total mass of oxygen in the full beta thickness for each square meter at the alpha-beta interface. To find the ratio of this mass to the mass of beta-zircaloy, it is divided by the product of the density of zircaloy and the beta thickness. This divisor is the mass of zircaloy per square meter of alpha-beta interface. The weight fraction of oxygen in as-fabricated zircaloy (0.0012) is subtracted from this since BWT includes all the oxygen in the beta region. In SI units the result is given by

$$BWTFRO = \frac{BWT}{6490 BX} - 0.0012$$
(B-14.6)

where

BWTFRO		oxygen weight fraction in beta in excess of the as-fabricated content (dimensionless)
BWT	=	total oxygen in beta (kg/m ²)
6490	=	density of zircaloy (kg/m ³)
BX		thickness of beta layer (m)
0.0012	=	oxygen weight fraction of as-fabricated zircaloy.

14.2.4 Oxygen Weight Fraction in Alpha Zircaloy. This quantity has a nearly constant value: a weight fraction of 0.047, and is therefore only ¹²sted in the code and not calculated.

14.2.5 Linear Power Generation Due to the Metal-Water Reaction. The zirconium metal-water reaction is exothermic. Knowing the mass of zirconium converted to ZrO_2 during a time step and the heat of reaction, the heating rate resulting from this reaction may be found. However, such a calculation will underpredict the heating rate because it neglects the heat of solution of the dissolved oxygen in the material beneath the oxide layer. To get a more realistic heating rate, an "effective" oxide thickness is computed for use in the heating calculation. This effective thickness, found by assuming that all the oxygen uptake goes into forming ZrO_2 , is

$$ox = \frac{W1}{5820 \times 0.26}$$

where

ox = effective oxide thickness (m) W1 = total oxygen uptake (kg/m²) 5820 = density of ZrO_2 (kg/m³) 0.26 = weight fraction of oxygen in ZrO_2 .

During each time step new ZrO_2 will form. This new ZrO_2 will be in the shape of a thin cylindrical shell of volume







(B-14.7)

$$\Delta V' = 2\pi R_{o}(xo_{1} - xo_{2}) L$$

where

 $\Delta V' =$ volume of ZrO₂ formed during time step (m³)

 $R_0 =$ original rod radius (m)

effective oxide thickness at the beginning of the time step (m) xoi 1

 $xo_f =$ effective oxide thickness at the end of the time step (m)

L = length of the fuel rod (m).

Because zircaloy experiences a 50% volume expansion in transforming to ZrO2, only two-thirds of the volume given by Equation (B-14.8) is zirconium. Therefore, the volume of zirconium converted into ZrO2 during a time step is

$$\Delta V = \frac{4L\pi}{3} R_0 (ox_f - ox_i) \quad . \tag{B-14.9}$$

To obtain the heat generation rate per unit length due to the conversion of zirconium to ZrO₂, Equation (B-14.9) is multiplied by the density of zirconium and by the exothermal heat of reaction per kilogram from the conversion, then divided by both the length of the rod and the duration of the time step. The result is

$$P = \frac{[6490(6.45 \times 10^6) \ 4.2R_0(ox_f - ox_i)]}{DT}$$
(B-14)

where

P rate of heat generation per meter (W/m) -6499 density of zirconium (kg/m³) 100 6.45 x 10⁶ 100 heat of reaction per kg of Zr (J/kg) DT duration of time step (5). -

A plot of P versus temperature for a fuel rod with initial radius, $R_{\rm e} = 6.25 \text{ x } 10^{-3} \text{ m}$, is shown in Figure B-14.3 for various initial oxide thicknesses and a time step of 1 s.

Equation (B-14.10) may underpredict the oxidation heating rate because it uses the heat released in the reaction

$$2H_{2}O + Zr - 2H_{2} + ZrO_{2} + Q$$
 (B-14.11)

With $Q = 6.5 \times 10^6 \text{ J/kg}$ of zircaloy reacted, B-14.16 Q is smaller by nearly a factor of 2 than Q₁, the heat released in the following reaction

$$Zr + O_2 - ZrO_2 + Q_1$$
 (B-14 '2)

4.10)

APPENDIX C GAS MATERIAL PROPERTIES

Properties of the internal gas of light water reactor fuel rods have been included in MATPRO-Version 11. The thermal conductivity of ten gases (and their mixture in any combination) is modeled, as is gas viscosity. Gas viscosity and thermal conductivity are modeled as functions of temperature and composition.

1. GAS THERMAL CONDUCTIVITY (GASCON, GTHCON, GJUMP) (D. L. Hagrman)

The heat conductance of gas filled gaps or pores is dependent on the thermal conductivity of the gas mixture when the dimensions of the gas filled regions are large compared to the mean distance between gas molecule collisions (mean free path of the gas molecules). When the mean free path is not smaller than the gap dimension, the conduction component of gas gap heat conductance becomes a function of the number of gas molecules present and the nature of the gas gap interfaces. This section presents data and correlations for the thermal conductivities of 10 gases of interest in fuel rod analysis. The effect of long mean free paths on gap conductance is also discussed.

1.1 Summary

Three functions are provided to meet varying analytical code needs. GASCON calculates gas thermal conductivity as a function of temperature and gas component fractions. GTHCON calculates the conduction part of gas gap heat conductance as a function of the gas conductivity, the gas pressure, and the gap width. The conductance includes a series resistance term that accounts for cases where the mean free path is not smaller than the gap dimensions. GJUMP determines an effective jump distance that is derived from the models used in GASCON and GTHCON.

The correlations used for pure noble or diatomic gases are all of the form

$$k = A T^B$$

where

k = thermal conductivity [W/(mK)]

T = gas temperature (K).

The constants A and B fcr each noble or diatomic gas are given in Table C-i.I.

The following conductivity equations are used for carbon dioxide and steam

$$k_{\text{carbon dioxide}} = 9.460 \times 10^{-6} \text{ T}^{1.312}$$
 (C-1.2)

For T ≤ 973.15

$$k_{\text{steam}} = (-2.8516 \text{ x } 10^{-8} + 9.424 \text{ x } 10^{-10} \text{ T} - 6.005 \text{ x } 10^{-14} \text{ T}^2) \frac{1}{7}$$



(C-1.1)

TABLE C-1.1

CONSTANTS USED IN GAS THERMAL CONDUCTIVITY CORRELATIONS

	Constar	it.
Gas	A	В
He	2.639×10^{-3}	0.7085
Ar	2.986×10^{-4}	0.7224
Kr	8.247 x 10 ⁻⁵	0.8363
Xe	4.351×10^{-5}	0.8616
H ₂	1.097 x 10 ⁻³	0.8785
N ₂	5.314 x 10 ⁻⁴	0.6898
02	1.653 x 10 ⁻⁴	0.8729
со	1.403×10^{-4}	0.9090

+
$$\frac{1.009 \text{ P}^2}{\text{T}^2(\text{T} - 273)^{4.2}}$$
 - 8.4083 x 10⁻³ - 1.19998 x 10⁻⁵

For T > 973.15

$$k_{\text{steam}} = 4.44 \times 10^{-6} \text{ T}^{1.45} + 9.5 \times 10^{-5} \left(\frac{2.1668 \times 10^{-9}}{\text{T}} \text{ P}\right)^{1.3}$$
(C-1.3)

where

 $P = gas pressure (N/m^2).$

The uncertainty of the values predicted by Equations (C-1.1) to (C-1.3) are summarized in Table C-1.II.

The thermal conductivity of gas mixtures is calculated with the expression

$$k_{\min} = \sum_{i=1}^{n} \left(\frac{\frac{k_i x_i}{i i}}{x_i + \sum_{\substack{j=1\\j \neq i}}^{n} \psi_{ij} x_j} \right)$$
(C-1.4)

TABLE C-1.II

UNCERTAINTY OF THE GAS THERMAL CONDUCTIVITY CORRELATIONS

Gas	Uncertainty (W/m*K)
He	8.00 x 10-7 T1.5
Ar	$4.96 \times 10^{-10} T^{2.25}$
Kr	$1.45 \times 10^{-9} T^2$
Xe	2.77 x 10 ⁻⁸ T ^{1.5}
H ₂	2.10 x 10 ⁻⁶ T ^{1.5}
N ₂	2.64 x 10 ⁻⁶ T
02	$2.34 \times 10^{-9} T^2$
со	{for T between 300 and 400 K, 0.02 K; for T > 400 K, 0.02 + 4/3 (T - 400) x 10^{-4} K
co ₂	$8.78 \times 10^{-12} T^3$
H20	0.06 K

where

$$_{j} = \phi_{ij} \left[1 + 2.41 \frac{(M_{i} - M_{j})(M_{i} - 0.142 M_{j})}{(M_{i} + M_{j})^{2}} \right]$$

and

$$j = \frac{\left[1 + \left(\frac{k_{i}}{k_{j}}\right)^{1/2} \left(\frac{M_{i}}{M_{j}}\right)^{1/4}\right]^{2}}{2^{3/2} \left(1 + \frac{M_{i}}{M_{j}}\right)^{1/2}}$$

and

¢

n = number of components in mixture (unitless)

 M_i = molecular weight of component i (kg)

 x_i = mole fraction of the component i (unitless)

 k_i = thermal conductivity of the component i (W/m·K).



The conduction part of the gas gap heat conductance is calculated with the equation

$$\mathbf{h} = \sum_{i=1}^{n} \left(\frac{\frac{\mathbf{k}_{i} \mathbf{x}_{i}}{1}}{\sum_{\substack{i \neq 1 \\ j = i}}^{n} \psi_{ij} \mathbf{x}_{j}} \right) \left[\frac{1}{1 + \frac{\sqrt{M_{i}^{T}}}{18} \left(\frac{\gamma_{i} - i}{\gamma_{i} + 1} \right) \frac{1}{\mathbf{a}_{i} p} \left(\frac{\mathbf{k}_{i}}{\sum_{\substack{i \neq i \\ j \neq i}}^{n} \psi_{ij} \mathbf{x}_{j}} \right)} \right]$$

where

a;

- h = conduction part of t' e gas gap heat conductance $(W/m^2 \cdot K)$
- γ_i = ratio of the specific teats at constant volume and constant pressure for component i (unitless)
 - a constant (provided in Table C-1.III) which describes the nature of the gas gap interfaces (unitless)

= gap width (m).

Detail of the development of the models used in the GTHCON subcode are presented in the following sections. Section 1.2 is a review of the data and Section 1.3 is a discussion of the model development. The subcode is tisted in Section 1.4 and references are provided in Section 1.5. Section 1.6 contains a bibliography.

1.2 Gas Thermal Conductivity and Accommodation Coefficient Data

Most gas thermal conductivity data are for temperatures < 500 K. At higher temperatures of interest in reactor fuel behavior analysis, interpretation of experiment measurements (power transferred across a gas filled gap at known temperatures) is difficult. Significant energy can be transferred by convection or radiation as well as by conduction. Also, the mean free path of the gas molecules can become nonnegligible compared to gap width for some combinations of pressure, temperature, and gap width. When this happens, experiment data measures not only the bulk gas thermal conductivity, but also gap surface effects and numbers of molecules available to transfer energy across the gap.

Experimenters usually correct their data for the effects of long mean free paths and convection by measuring power at several differing gas pressures. Since the mean path is inversely proportional to pressure and the effect of convection is proportional to the square of the gas density (pressure), C-1.1 it is usually possible to find combinations of experiment dimensions and pressures where the reciprocal conductance is independent of pressure or increasing linearly with reciprocal pressure. When the data show no pressure dependence, both mean free path and convection effects can be neglected. When the linear dependences is present, gas conductivity is found by extrapolation to infinite pressure. Groups of data with eval temperature and varying pressure are fit to an equation of the form

$$\frac{1}{h} = \frac{t}{k} + \frac{constant}{P}$$

(C-1.6)

(C-1.5)

Corrections for radiation heat transfer are applied when necessary by using the Stefan-Boltzmann law. In most experiments, the radiation correction is smaller than measurement uncertainty and the correction is neglected.

Data used in the development of the correlations for pure gas thermal conductivities were taken from the references listed in Table C-1.III. The method of correcting for long mean free paths and temperature range investighted are listed in the comment column. With the exception of the two publications by Timrot and Umanskii, C-1.6, C-1.11 the references reported conductivities and temperatures that could be used without further analy. 3. The analysis of high temperature data of Timrot and Umanskii is discussed below.

Data reported by Timrot and Umanskii are reduced power per unit length and temperatures for a coaxial cylindrical cell. The reduced power was defined to be the power per unit length that would be obtained with a small mean free path and it was obtained from measurements of power at several pressures. The technique was similar to the approach of extrapolation to infinite pressure.

In contrast to most authors, Timrot and Umanskii correlated values of reduced power with temperature, and determined their correlation for gas thermal conductivity by taking the derivative of the correlation. The appropriate expression is

$$k = \frac{\ln\left(\frac{R}{r}\right) dW(T)}{2\pi dT}$$

 $a_{sg} = \frac{T_2 - T_1}{T_s - T_1}$

where

W(T) = equation for power per unit length measured in the experiment (W/m)

R = outer wall radius of the cell (m)

r = inside wall radius of the cell (m).

The analysis by Timrot and Umanskii^{C-1.6} is an excellent approach to modeling thermal conductivity with data from a single experiment, but it is inconvenient for use in conjunction with the other literature data. In order to use Timrot and Umanskii's data with data from other references, the reported values of reduced power and temperature have ocen used to find approximate point-by-point conductivities. The derivative of W with respect to temperature at temperature T_i was a proximated with the expression

$$\frac{dW(T_i)}{dT} \approx \frac{1}{2} \left(\frac{W_{i+1} - W_i}{T_{i+1} - T_i} + \frac{W_i - W_{i-1}}{T_i - T_{i-1}} \right)$$
(C-i.8)

where the subscript i refers to the ith measured value in a series of measurements listed in order of increasing temperature. Equations (C-1.7) and (C-1.8) convert the data reported by Timrot and Umanskii to thermal conductivities.

When the mean free path of the gas molecules in a gap is long, compared to the gap dimensions, the transfer of energy from the hot gap surface to the gas and then to the cold gap surface during individual molecular collisions becomes more important to the heat conductance than the bulk gas thermal conductivity. The experiment data of interest in this case are surface accommodation coefficients, defined by the relation



(C-1.9)

(C-1.7)

TABLE C-1.III

PURE GAS CONDUCTIVITY REFERENCES

-	Reference	Comments
Ka	nnuluik and Carman ^{C-1,1}	Extrapolated to infinite pressure temperatures to 580 K
Ga	mbhir, Gandhí, and Saxena ^{C-1.2}	Pressure-independent conductivity temperatures to 370 K
vo	n Ubisch ^{C-1.3}	Extrapolated to infinite pressure at 300 and 790 K
Sa	xena and Saxena ^{C-1.4}	Pressure-independent conductivity temperatures to 1300 K
Τi	mrot and Totskii ^{C-1,5}	Radiation effects correction, but long mean free path correction not discussed
Ti	mrot and Umanskii ^{C-1.6}	Analysis discussed in the text of this report (Section 1.2)
		Temperatures from 800 to 2600 K
Za	itseva ^{C-1} .7	Extrapolated to infinite pressure temperatures from 350 to 800 K
Ch	eung, Bromley, and Wilke ^{C-1.8}	Extrapolated to infinite pressure at 370 and 590 K
Jo	nnston and Grilly ^{C-1.9}	Extrapolated to infinite pressur temperatures to 383 K
Ka	nnuluik and Carman ^{C-1.1}	Extrapolated to infinite pressure temperatures from 370 to 380 K
Ga	mbhir, Gandhi, and Saxena ^{C-1,2}	Pressure-independent conductivity temperatures from 310 to 370 K
vo	n Ubisch ^{C-1.3}	Extrapolated to infinite pressure at 300 and 790 K
Za	itseva ^{C-1.7}	Extrapolated to infinite pressure temperatures from 520 to 790 K
Ch	eung, Bromley, and Wilke ^{C-1.8}	Extrapolated to infinite pressure at 370 and 590 K
Sc	hafer as quoted by Brokaw ^{C-1.9}	At 1370 K

Gas	Reference	Comments
Kr	Kannuluik and Carman ^{C-I.1}	Extrapolated to infinite pressure temperatures from 370 to 580 K
	Gambhir, Gandhi and Saxena ^{C-1.2}	Pressure-independent conductivity temperatures from 310 to 370 K
	von Ubisch ^{C-1.3}	Extrapolated to infinite pressure at 300 and 790 K
	Zaitseva ^{C-1.7}	Extrapolated to infinite pressure temperatures from 310 to 800 K
Xe	Kannuluik and Carman ^{C-1.1}	Extrapolated to infinite pressure temperatures from 370 to 380 K
	Gambhir, Gandhi, and Saxena ^{C-1.2}	Pressure-independent conductivity temperatures from 310 to 370 K
	von UbischC-1.3	Extrapolated to infinite pressure at 300 and 790 K
	Zaitseva ^{C-1.7}	Extrapolated to infinite pressure temperatures from 310 to 790 K
H ₂	Johnston and Grilly ^{C-1.9}	Extrapolated to infinite pressure temperatures to 370 K
	Geier and Schafer as quoted by Brokaw ^{C-1.10}	At 1373 K
	Timrot and Umanskii ^{C-1.11}	Analysis discussed in the text of this report (Section 1.2)
N ₂	Cheung, Bromley, and Wilek ^{C-1.8}	Extrapolated to infinite pressure at 380 and 590 K
	Figure 4, Keys ^{C-1.12}	Temperatures from 320 to 620 K
02	Cheung, Bromley, and Wilek ^{C-1.8}	Extrapolated to infinite pressure at 370 and 590 K
02	Johnston and GrilleyC-1.9	Extrapolated to infinite pressure temperatures to 380 K

TABLE C-1.III (continued)

Johnston and Grilley^{C-1.9} CO

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Extrapolated to infinite pressure

temperatures to 380 K

Gas	Reference	Comments
co ₂	Cheung, bromley, and Wilek ^{C-1.8}	Extrapolated to infinite pressure at 380 and 590 K
	Johnston and Grilley ^{C-1.9}	Extrapolated to infinite pressure temperatures to 380 K
	Figure 4, Keys ^{C-1.12}	Temperatures from 320 to 620 K

TABLE C-1.III (continued)

where

a _{sg}	-	surface accommodation coefficient for a particular gas-surface interface (unitless)
T _S	-	surface temperature of the hot gap surface (K)
T ₁	-	average temperature of the gas molecules impinging on the surface (K)
T2	-	average temperature of the gas molecules after striking and again leaving the surface (K).

Surface accommodation coefficients tend to be large for massive gas molecules, and they are increased when an intermediate gas layer is absorbed on the surface. For example, $White^{C-1.13}$ reports accommodation coefficients of 0.09, 0.041, 0.16, and 0.20 for H₂, He, Ar, and 0₂ on clean tung. on surfaces at 90 K. For heavy polyatomic molecules, accommodation coefficients are reported to be generally in the range 0.8 to 0.9. For He on nickel with and without absorbed gas White reported accommodation coefficients of 0.360 and 0.071 at 273 K. For helium on glass (a ceramic), the accommodation coefficient is 0.34, a value larger than the helium-metal accommodation coefficients mentioned above.

Numerous sources of low temperature data were reviewed but not used in the development of the thermal conductivity model to avoid giving undue emphasis to data that have been replaced by more relevant information. These sources of data and some theoretical discussions are included in a bibliography at the end of this report.

1.3 Model Development and Uncertainty Estimates

Development of analytical models for gas gap conductance will be described in several steps. Initially, the data discussed in Section 1.2 are used to develop models for the thermal conductivity of pure gases. Uncertainties are discussed and analytical expressions for these uncertainties are presented. The conductivity of mixed gases is discussed next, and the conduction contribution to the conductance of narrow gaps (or gas filled fuel regions) is modeled.

An elementry treatment of gas conductivity that considers the gas to be a collection of hard spheres led s to the conclusion that the conductivity of a single-component gas is proportional to the square root of temperature, the square root of the molecular mass, and inversely proportional to the square of the molecule's diameter. The expression that results from the elementary treatment (given in most college statistical mechanics texts and therefore not repeated here) is



$$k_{\text{ideal}} = \frac{3}{2} \frac{\mathrm{m}^{1/2}}{\sigma} \mathrm{K}_{\mathrm{B}}^{3/2} \mathrm{T}^{1/2}$$
(C-1.10)

where

k _{ideal}		thermal conductivity of an idealized gas (W/m+K)
m	=	mass of the molecules (kg)
КВ	=	Boltzmann's constant (J/K)
σ	=	area of the sphere's cross section (m ²).

For real gases where the molecules have structure and distant dependent interactions, Equation (C-1.10) must be replaced by an equation of the form

$$K = A T^{D}$$
(C-1.11)

where A and B are constants for a given gas. Data referenced in Section 1.2 and the least squares method were used to find the values of A and B given in the summary.

Figures C-1.1 to C-1.4 illustrate the correlation predictions and the data base for the monatomic gases He, Ar, Kr, and Xe. The values of B for these four gases (0.7085, 0.7224, 0.8363, and 0.8616) increase with increasing boiling temperatures (4, 87, 120, and 166 K); an indication that the increasing departure from



Figure C-1-1.

Thermal conductivity of helium as a function of temperature.









the idealized gas temperature-dependence is due to increasing intermolecular forces. This regular trend and the fact that a single exponent serves to model the extensive helium data lends confidence to the extrapolations beyond the low temperature data available for krypton and xenon.

Dashed lines in Figures C-1.1 to C-1.4 are the expected standard error of the correlations. Since the data show increasing scatter with increasing temperature, the expected standard error of the thermal conductivity was determined from the standard error of a new variable defined to be the thermal conductivity divided by a power of temperature. Trial values of the power were varied until the residuals of the new variable were temperature-independent. Once the appropriate power was determined, the standard error of the new variable was calculated and the expected standard error of the conductivity was obtained by multiplying the standard error of the new variable by the power of the temperature.

For the diatomic molecules, H_2 , N_2 , O_2 , and CO, the relation between the exponent B in Equation (C-1.1) and boiling temperatures is no longer apparent. The conductivities of these gases cannot be expected to be related in any simple fashion because they transfer energy in complex molecular rotational and vibrational modes, in addition to translational modes. The data base, correlation predictions, and expected standard errors for these gases are shown in Figures C-1.5 to C-1.8.

The analysis of the diatomic gas data followed the procedure of the monatomic gases with the exception of the determination of the expected standard error of the CO conductivity correlation. For carbon monoxide, only four data were available and an arbitrary uncertainty of 0.02 times the thermal conductivity (typical of low temperature measurement scatter) was assigned over the temperature range of the data. The 0.02 was replaced with a linear function of temperature for temperatures >400 K, and the coefficients in this function were determined to predict an expected standard error of 0.10 times the predicted thermal conductivity at 1000 K.





Thermal conductivity of nitrogen as a function of temperature.



Figure C-1-8.

Thermal conductivity of carbon monoxide as a function of temperature.

Figure C-1.9 is a co. son of the data base and correlation predictions for the thermal conductivity of CO_2 . It is possible that the large exponent of temperature in the carbon dioxide correlation (1.3) is due to an extreme departure from the idealized gas approximation at the low temperatures for which data are available. The vapor pressure of solid carbon dioxide is one atmosphere at 195 K^a and the data extend only over a range of two to three times this temperature. If the large exponent of temperature obtained from data in the range 300 to 600 K is due to the fact that all the data are at temperatures where significant intermolecular forces are present, the exponent can be expected to decrease at temperatures >600 K. The temperature-dependence of the uncertainty has been forced higher than the dependence indicated by the limited CO_2 data to reflect this concern. A temperature-cubed dependence for the expected standard error was selected because the cube is the largest exponent of temperature that gives physically reasonable conductivities over the range of solid fuel temperatures.

The low temperature part of the correlation for the thermal conductivity of steam was taken from the ASME steam tables; C-1.14 and the colerance given in this reference, 0.06, times the conductivity, has been adopted as the expected standard deviation.

The high temperature part of the MATPRO correlation was taken from Tsederberg.^{C-1.15} Tsederberg's expression was used for high temperatures because the power law he used does not become negative at high temperatures. No data were found above the 973-K limit of the ASME steam tables.





a. There is no liquid phase of CO2 at atmospheric pressure, so the closest measure of boiling point is the one given here.

When gases are mixed, the thermal conductivity of the mixture is not simply related to the conductivities of the mixture components because the ability of each component to diffuse through the mixture is affected by the presence of all the other components. The relation between pure gas conductivities and gas mixture conductivities, Equation (C-1.4), is taken from the work of Brokaw.^{C-1.10} Figure (C-1.10) is a comparison of the conductivities predicted by Equation (C-1.4) to data reported by Von Ubisch^{C-1.3} for helium-xenon mixtures at 793 K. The measurements show excellent agreement with the conductivities predicted by Equation (C-1.4), although less satisfactory agreement can be expected for mixtures containing diatomic molecules that transport energy in rotational and vibrational modes, Equation (C-1.4) is adequate for fuel rod analysis because the principal gas mixture components are monatomic.

Equation (C-1.5), the expression: for the conduction contribution to the conductance of a gas filled gap, is based on kinetic theory developed by Knudsen, C-1.16 as well as the thermal conductivity correlations which have been developed. Knudsen studied low pressure gases and pointed out that molecules striking a surface do not attain thermal equilibrium with the surface in a single collision. The average speed and





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temperature of molecules that have just colluded with a wall are somewi at less than the values implied by the wall temperature. Knudsen derived an expression for the power per unit area transferred from a hot surface to a cold gas

$$W_{s} = \sqrt{\frac{2R}{\pi MT_{g}}} \frac{1}{4} \left(\frac{\gamma + 1}{\gamma - 1} \right) P(T_{s} - T_{g}) a_{sg}$$
(C)

where

power per unit area transferred across the surface (W/m²) Ws -

- R the gas constant [J/(K-moi)] -
- M molecular weight of the gas (Kg/mol) -
- ratio of the constant volume to the constant pressure specific heats of the gas Y 122 (unitless)
- Tg temperature of the gas (K).

The corresponding expression for the energy transferred from a hot gas to a cold surface is

$$W_{s} = \sqrt{\frac{2R}{\pi MT_{g}}} \frac{1}{4} \left(\frac{\gamma + 1}{\gamma - 1}\right) P(T_{g} - T_{s}) \left(\frac{a_{sg}}{1 - a_{sg}}\right).$$
(C-1.12)

If the mean free path of the gas molecules is long compared to the gap width, the power per unit area transferred across the gap in the steady state can be found by equating the expressions for the power per unit area across the two surfaces. The resultant expression C(1,1) is

$$W_{ss} = \sqrt{\frac{2R}{\pi MT_g}} \frac{!}{4} \left(\frac{\gamma + 1}{\gamma - 1}\right) P(T_h - T_c) \left(\frac{a_{hg}a_{cg}}{a_{hg} + a_{cg} - a_{hg}a_{cg}}\right)$$
(C-1.13)

where

power per unit area transmitted across the gap in the steady state (W/m²) $W_{ss} =$

temperature of the hot gap surface (K) Th -

$$T_c$$
 = temperature of the cold gap surface (K)

surface accommodation coefficient for the hot surface-gas interface (unitless) ahg . 32

surface accommodation coefficient for the cold surface-gas interface (unitless). ace -

Equation (C-1.13) could have been obtained less rigorously by defining a thermal impedance for each surface

$$r_{s} = \frac{\Delta T}{W_{ss}}$$
(C-1.14)





-1.11)
where

$$r_s$$
 = thermal impedance for surface S (Km²/w)

 $\Delta \Gamma$ = temperature difference between the surface and gas (K)

and adding the two series impedances that represent the surfaces to find an effective impedance for the entire gap in the limit of mean free paths that are much longer than gap width. This thermal impedance approach has been adopted to model the conductivity of a fuel rod gap when the gas mean free path is not long compared to gap width.

Single-component gases are considered first. The expression for the power per unit area transferred across tb gas is

$$W_{B} = \frac{k \Delta T_{B}}{t}$$
(C-1.15)

where

 W_B = power per unit area transferred across a region of gas (W/m²)

 ΔT_{B} = temperature change across the gas (K).

The thermal impedance of the gas is

$$r_{\rm B} = \frac{t}{k} \tag{C-1.16}$$

where

 $r_{\mathbf{B}}$ = thermal impedance of gas.

Summation of the series thermal impedances that represent the two surfaces and the gas bulk, produces the following expression for gap impedance

$$r_{\rm eff} = \frac{t}{k} + \sqrt{\frac{\pi MT}{2R}} \frac{g}{4} \left(\frac{\gamma - 1}{\gamma + 1}\right) \frac{1}{aP}$$
(C-1.17)

where

a

 r_{eff} = effective impedance of a gap containing a single-component gas (m²K/W)

$$= \frac{a_{hg}a_{cg}}{a_{hg} + a_{cg} - a_{hg}a_{cg}}$$

The gap conductance is the reciprocal of the effective impedance

$$h = \frac{k}{t + 4\frac{k}{aP}\left(\frac{\gamma - 1}{\gamma + 1}\right)\sqrt{\frac{\pi MT_g}{2R}}}$$
(C-1.18)



where

h = gap conductance for a gap containing a single component gas
$$(W/m^2 \cdot K)$$
.

Equation (C-1.18) illustrates several features of gap conductance. The surface impedance term in the denominator is not important for large gaps. For gaps of a given width, the surface impedance is large at low pressures and high temperatures. Finally, the impedance term is most important for gases with large thermal conductivities.

Equation (C-1.5) is derived with a slight generalization of the arguments just given for a singlecomponent gas. Inspection of Equation (C-1.4), the expression for the thermal conductivity of gas mixtures, shows that the i-sum in the equation represents the combination of parallel impedances due to each component of the mixture (the j-sum represents the modification of the scattering cross section seen by each component due to the presence of all the other components). The arguments just given for a singlecomponent gas can be repeated for impedance due to each component of the gas mixture. The resultant expression for the gap conductance due to the ith component of the gas mixture is

$$h_{i} = \frac{x_{i}}{t + \frac{4x_{i}}{a_{i}P_{i}}\left(\frac{\gamma_{i}}{\gamma_{i}} + \frac{1}{1}\right)\sqrt{\frac{\pi M_{i}T}{2R}}}$$

where

- $h_i = gap$ conductance due to the ith component of the gas mixture (W/m²·K)
- $x_i = i^{\text{th}}$ term in Equation (C-1.4)
- P_i = partial pressure of ith component of mixture
- ai = value of factor a of Equation (C-1.17) for each gas component and the two gap surfaces (unitless).

The partial pressure of the ith gas component is given in terms of the mole fraction of the component and the total pressure by the idealized gas law. The relation is

$$P_i = P X_i$$

Equation (C-1.5) is obtained by substituting Equation (C-1.20) into Equation (C-1.19) and combining the parallel gap conductances due to each component of the mixture.

Values of V_i and M_i are contained in the GTHCON subroutine. The specific heat ratios were taken from ZemanskyC-1.17 and the molecular weights were taken from the Handbook of Chemistry and Physics,C-1.18

The surface accommodation coefficients required to use Equation (C-1.5) were estimated from data and trends mentioned in Section 1.2. The coefficients and values of a_i that result are listed in Table C-1.IV. The accommodation coefficients for helium on zircaloy and fuel were approximated with helium-mckel and helium glass data. Hydrogen accommodation coefficients were assumed to be approximately the same as those of helium because of the similar masses of these molecules. The accommodation coefficient for argon on zircaloy was assumed equal to the argon-tungsten coefficient. An estimate for the argon-fuel coefficient was obtained by using the ratio of argon and helium coefficients on zircaloy to multiply the helium-fuel coefficient. For heavy molecules (krypton, xenon, and carbon dioxide), White's estimate of

(C-1 20)

(C-1.19)

Cas	Factor a of	a gas-zircalov	a gas-fuel
000	infunction (0 1137		
He	0.06	0.071	0.34
Ar	0.15	0.16	0.8
Kr	0.74	0.85	0.85
Xe	0.74	0.85	0.85
H ₂	0.06	0.071	0.34
N ₂	0.19	0.2	0.85
02	0.19	0.2	0.85
CO	0.19	0.2	0.85
co ₂	0.74	0.85	0.85
HaD	0.19	0.2	0.85

TABLE C-1.IV

SURFACE ACCOMMODATION COEFFICIENTS

0.85 is used for the accommodation coefficients of both fuel and zircaloy. The nitrogen-zircaloy coefficient was adopted for nitrogen, oxygen, carbon monoxide, and steam because of the similar masses of these molecules. A heavy molecule estimate of 0.85 was used for the fuel surface accommodation coefficient of the nitrogen-like group because the estimate obtained from scaling up with the zircaloy surface coefficients was greater than one.

The effective jump distance calculated by GJUMP is determined with Equations (C-1.4) and (C-1.5). The mixed gas conductivity is divided by the heat conductance for a gap with zero width and with the twosurface accommodation coefficient replaced by the single-surface accommodation coefficient.

1.4 Gas Thermal Conductivity Functions GASCON, GTHCON, and GJUMP Listings

GASCON, GTHCON, and GJUMP function listings are presented in Tables C-1.V to C-1.VII.

TABLE C-1.V

LISTING OF THE GASCON SUBCODE

GASCON, GTHCON, GJUMP

FUNCTION GASCON(GMIX, GTEMP, GPRES) GASCON CALCULATES GAS THERMAL CONDUCTIVITY AS A FUNCTION OF TEMPERATURE AND GAS COMPONENT FRACTIONS. GAP SURFACE EFFECTS ARE NOT CONSIDERED GASCON = OUTPUT GAS THERMAL CONDUCTIVITY (#/(M*K)) UGASK(I) = OUTPUT STANDARD ERROR EXPECTED FOR THE THERMAL CONDUCTIVITY OF EACH COMPONENT OF THE GAS MIX (W/(M*K)). THIS OUTPUT IS CALCULATED IN GASCON BUT NOT RETURNED GMIX(1) . INPUT MOLE FRACTIONS OF THE GAS COMPONENTS (UNITLESS) 1 IS HELIUM
2 IS ARGON
3 IS KRYPTON KRYPTON * 4 IS * 5 IS XENON HYDROGEN • 6 IS • 7 IS NITROGEN DXYGEN I = 8 IS CARBON MONOXI I = 9 IS CARBON DIDXID I = 10 IS WATER VAPUR I =10 IS WATER VAPUR I NPUT GAS TEMPERATURE (K) INPUT GAS PRESSURE (PA) CARBON MONOXIDE CARBON DIDXIDE GTEMP GPRES THE GAS THERMAL CONDUCTIVITY CALCULATED BY THIS FUNCTION IS BASED ON DATA FROM THE FOLLOWING REFERENCES W. G. KANNULUIK AND E. H. CARMAN, THERMAL CONDUCTIVITY (1) OF RARE GASES, THE PROCEEDINGS OF THE PHYSICAL SOCIETY 65 (1952) PP 701 - 709. R. S. GAMBHIR, J. M. GANDHI AND S. C. SAXENA, THERMAL CONDUCTIVITY OF RAPE GASES, DEUTERIUM AND AIR, INDIAN JOURNAL OF PURE AND APPLIED PHYSICS 5 (1967) PP 457 - 463. H. VON UBISCH, THE THERMAL CONDUCTIVITIES OF MIXTURES (2) (3) OF RARE GASES AR 29C AND AT 520C, ARKIV FOER FYSIK 16 (1959) PP 93 - 100. V. K. SAXENA AND S. C. SAXENA, MEASUREMENT OF THE THERMAL CONDUCTIVITY OF HELIUM USING A HOT-WIRE TYPE OF THERMAL DIFFUSION COLUMN, BRITTISH JOURNAL OF APPLIED PHYSICS 1 (1968) PP 1341 - 1351. (4) (5) D. L. TIMROT AND E. E. TOTSKII, DILATOMETRIC METHOD FOR THE EXPERIMENTAL DETERMINATION OF THE THERMAL CONDUCTIVITY OF CORROSIVE GASES AND VAPORS AT HIGH TEMPERATURE, HIGH TEMPERATURE 3 (1965) PP 685 - 690.

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TABLE C-1.V (continued)

D. L. TIMROT AND A. S. UMANSKII, INVESTIGATION OF THE THERMAL CONDUCTIVITY OF HELIUM IN THE RANGE 400 - 2400 K, HIGH TEMPERATURE 3 (1965) PP 345 - 351. L. S. ZAITSEVA, AN EXPERIMENTAL INVESTIGATION OF THE HEAT CONDUCTIVITY OF MONATIMIC GASES OVER WIDE TEMPERATURE INTERVALS, SOVIET PHYSICS - TECHNICAL (6) (7) PHYSICS 4 (1959) PP 444 - 450. (8) H. CHEUNG, L. A. BRONLEY AND E. R. WILKE, THERMAL CONDUCTIVITY OF GAS MIXTURES, AICHE JOURNAL 8 (1962) PP 221 - 228. (9) R. S. BROKAN, PREDICTING TRANSPORT PROPERTIES OF DILUTE GASES, I AND EC PROCESS DESIGN AND DEVELOPMENT 8 (1969) PP 240 - 253. (10) D. L. TIMROT AND A. S. UMANSKII, THERMAL CONDUCTIVITY OF HYDROGEN AND ARGON, HIGH TEMPERATURE 4 (1966) (11) F. G. KEYES, THE HEAT CONDUCTIVITY, VISCOSITY, SPECIFIC HEAT AND PRANDTL NUMBERS FOR THIRTEEN GASES, NP-4621 (1952). GASCON WAS CODED BY D. L. HAGRMAN DCTOBER 1979 MODIFIED BY D. L. HAGRMAN JULY 1981 TC PREVENT NEGATIVE STEAM CONDUCTIVITY AT HIGH TEMPERATURE (CDR-MP-03) COMMON / LACEMDL / MAXIDX, EMFLAG DIMENSION EMFLAG(1) DIMENSION GMIX(10), A(3), 3(9), C(10), W(10), AU(9), BU(9), UGASK(10) DATA A 12.639E-03,2.986E-04,8.247E-05,4.351E-05, # 1.097E-03, 5.314E-04, 1.853E-04, 1.403E-04, 9.460E-06/ DATA B /0.7085,0.7224,0.8363,0.8616, * 0.8785, 0.6898, 0.8729, 0.9090, 1.312/ DATA AU /8.00E-07,4.96E-10,1.45E-09,2.77E-08 # 2.10E-06, 2.64E-06, 2.34E-09, 1.00E+00, 8.78E-1 / DATA BU /1.50, 2.25, 2.00, 1.50, 1.50, 1.00, 2.00, 1.00, 3.00/ DATA W /4.003, 39.944, 83.800, 131.300, # 2.016,28.020,32.000,28.010,44.010,18.020/ DATA ON 1 2HON /. OFF 1 3HUFF # 13 LOCIDX / * 16 IF (EMFLAG (LOCIDX) .EQ. ON) GASCON - EMGTONIGMIX, GTEMP, GPRES, 0.01 # IF(EMFLAG(LOCIDX) .EQ. ON) GO TO 100 IF(GTEMP .LT. 4000.) GO TO 20 10 WRITE (6,900) GTEMP, GMIX 900 FORMAT(25H1GASCON INPUT BAD. GTEMP=, 1PE12.4, 2H K,/ # 10H0FRACTIONS, (10E12.4))

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GASCON, GTHCON, GJUMP

TABLE C-1.V (continued)

```
STOP
   20 X = 0.0
       DO 30 I · 1,10
   30 X = X + GMIX(I)
       IF (X .LT. 0.9 .OR. X .GT. 1.1) GD TO 10
c
       FIND PURE GAS CONDUCTIVITIES
       DC 40 I . 1,9
       UGASK(I) = AU(I) + (GTEMP**BU(I))
   40 C(I) = A(I) * (GTEMP**B(I))
UGASK(8) = 0.02 * C(8)
       IF (GTEMP .GE. 400.) UGASK(8) = (0.02 + 4.0E-4*(GTEMP - 400.)/
      # 3.) * C(8)
       IC = GTEMP - 273.15
       C(10) * 17.6E-3 + TC*( 5.87E-5 + TC*( 1.04E-7 - 4.51E-11*TC))
USE IDEAL GAS LAW TO FIND DENSITY
IF(GMIX(10) *LE* 1.0E-9) GO TO 50
C
       PS = GPRES * GMIX(10)
       DEN * 2.1668E-6 * PS / GTEMP
C(10) * C(10) + DEN*( 103.51E-3 + TC*(0.4198E-3 - 2.771E-8*TC)
                                      + 2.1482E+11 * DEN/TC **4.2)
      #
       UGASK(10) = 0.06 * C(10)
       IF (GTEMP .LE. 973.15) GO TO 50
       C(10) * 4.44E-06*(GTEMP**1.45) * 9.5E-05 * ((2.16682-09 *
      # GPRES/GTEMP) ##1.3) - 1.283668E-03
       UGASK(10) = 0.05 + C(10)
    50 CONTINUE
       FIND MIXTURE CONDUCTIVITY
C
       GASCON = 0.
DC 70 I = 1,10
       IF (GMIX(I) .LE. 1.0E-9) GO TO 70
       SUM . 0.0
       D0 60 J = 1,10
IF(J .EQ. I) GD TO 60
IF(GMIX(J) .LE. 1.0E-9) GD TO 60
RC = C(I) / C(J)
       RW = W(I) / 4(J)
       RWSR = SQRT(RW)
       GIJ = 1. + 2.41 * (RW-1.) * (RW-0.142) / (1.+RW)**2
       FIJ=((1. + SQRT(RC*RWSR) )**2)/ SQRT(8.*(1.+RW))
       SUM * SUM + GIJ * FIJ * GMIX(J)
   GASCON = GASCON + C(I) + GMIX(I) / (GMIX(I) + SUM)
  100 CONTINUE
       RETURN
       END
```

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GASCON, GTHC MULT



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GASCON, GTHCON, GJUMP

TABLE C-1.VI

LISTING OF THE GTHCON SUBCODE

FUNCTION GTHCON(GMIX. GTE AP. GPRES, GPTHK) GTHCON CALCULATES THE CONDUCTION PART OF GAS GAP HEAT CONDUCTANCE AS A FUN TION OF SEMPERATURE, GAS COMPONENT FRACTIONS, GAP WIDTH AND GAS PRESSURE. GAP SURFACE EFFECTS ARE CONSIDERED . OUTPUT CONDUCTION PART OF GAS GAP HEAT GTHCON CONDUCTANCE (W/((M**2)*K)) INPUT MOLE FRACTIONS OF THE GAS COMPONENTS (UNITLESS) I = 1 IS HELIUM I = 2 IS #RGON GMIX(I) ISIS 3 **ARYPTON** . . 4 XENON HYDROGEN 5 . = 6 1S = 7 IS = 8 IS CARBON MONDXIDE I = 9 IS CARBON DIDXID I = 10 IS WATER VAPOR = INPUT GAS TEMPERATURE (K) = INPUT GAS PRESSURE (PA) CARBON DIDXIDE GTEMP GP RES INPUT GAP WIDTH (M) **GP THK** A LINIMUM GAP WIDTH 25 4.4E-6 IS SUGGESTED TO ACCOUNT FOR TYPICAL FUEL SURFACE ROUGHNESS THE SURFACE EFFECTS CALCULATED BY THIS DUNCTION ARE BASED ON DATA FROM THE REFERENCES LISTED BELOW. THERMAL CONDUCTIVITY DATA REFERENCES ARE LISTED IN THE GASCON FUNCTION. (1) G. K. WHITE, EXPERIMENTAL TECHNIQUES IN LOW TEMPERATURE PHYSICS, DXFORD PRESS (1959) PP 181 - 183. (2) M. W. ZEMANSKY, HEAT AND THERMODYNAMICS, MCGRAW - HILL BOOK COMPANY, INC (1957). C. D. HODGMAN (ED), HANDBOOK OF CHEMISTRY AND PHYSICS. THIRTY - EIGHTH EDITION, CHEMICAL RUBBER PUBLISHING CO. (3) (1956). GTHCON WAS CODED BY R. C. YOUNG MARC' MODIFIED BY D. L. HAGRMAN DETOBER 19 MODIFIED BY D. L. HAGRMAN JULY 1981 10. FNT NEGATIVE STEAM CONDUCTIVITY AT HIGH TEMPERATU. (CDR-MP-03)

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TALLE C-1.VI (continued)

COMMON / LACEMOL DIMENSION EMELAG(1) / MAXIDX. EMFLAG DIMENSION GMIX(10), A(9), B(9), C(10), W(10), AC(10), AR(10), BR(10) DATA A /2.639E-03,2.986E-04,8.247E-05,4.35LE-05, # 1.097E-03, 5.314E-04, 1.853E-04, 1.403E-04, 9.460E-06/ DATA B /0.7085,0.7224,0.8363,0.8616, C.8785,0.6898.0.8729,0.9090,1.312/ DATA # /4.003, 39.944, 83.800, 131.300, 2.01.,28.020, 32.000, 28.010, 44.010, 18.020/ # DATA AC 10.06,0.15,0.74,0.74,0.66,0.19,0.19,0.19,0.74,0.19/ DATA AR /1.6667,1.6667,1.6667,1.6667, # 1.4045,1.4006,1.4006,1.4006,1.2057,1.2857/ DATA BR /-2.E-9,3.53E-8,3.53E-8,3.53E-8, # 2.5E-9,2.21E-8, 2.21E-8, 2.21E-8, 6.29E-8, 6.29E-8/ 1 2HON /, DATA ON OF F 1 3HUFF /. LOCIDX / 16 * IF (EMFLAG (LOCIDX) .EQ. DN) GTHCON = EMGTON (GMIX, GTEMP, GPRES, GPTHK) / GPTHK 2 IF(EMFLAG(LOCIDX) .EQ. ON) GO TO 100 IF(GIEMP .LT. 4000.) GO TO 20 10 WRITE (6,900) GTEMP, GMIX 900 FORMATI25HIGASCON INPUT BAD. GTEMP=, 1PE12.4, 2H K, / 10HOFRACTIONS, (10E12.4)) STOP 20 X = 0.0 DO 30 I = 1,10 30 X - X + GMIX(I) IF(X LT. 0.9 DR. X GT. 1.1) GO TO 10 FIND PURE GAS CONDUCTIVITIES C DD 40 I = 1,9 40 C(I) = A(I) + (GTEMP**B(I)) IC . GTEMP - 273.15 C(10) = 17.6E-3 + TC*(5.87E-5 + TC*(1.04E-7 - 4.51E-11*TC)) JSE IDEAL GAS LAW TO FIND DENSITY C IF(GMIX(10) .LE. 1.0E-3) GO TO 50 PS * GPRES * GMIX(10) DEN = 2.1668E-6 * FS / GTEMP C(10) = C(10) + DEN*(103.51E-3 + TC*(0.4198E-3 - 2.771E-8*TC) + 2.1482E+11 * DEN/TC**4.2) IF (GTEMP .LE. 973.15) GD TO 50 C(10) = 4.44E-06*(GTEMP**1.45) + 9.5E-05 * ((2.1558E-09 * # GPRES/GTEMP) ** 1.3) - 1.283668E-03 50 CONTINUE FIND MIXTURE CONDUCTIVITY Ć GTHCON = 0 DD 70 I = 1,10

GASCON, GTHCON, GJUMP

TABLE C-1.VI (continued) IF (GMIX(I) .LE. 1.0E-9) GO TO 70 SUM = 0.0 D0 60 J = 1,10 IF(J.EQ. I) GD TD 60 IF(GMIX(J) .LE. 1.0E-9) GO TD 60 KC = C(I) / C(J) RW = W(I) / W(J) RWSR = SORT(RW) GIJ = 1. + 2.41 * (RW-1.) * (RW-0.142) / (1.+RW)**2 FIJ=((1. + SQRT(RC*RWSR))**2)/ SQRT(6.*(1.+RW)) SUM = SUM + GIJ * FIJ * GMIX(J) 60 CONTINUE SPHI = AR(1) + BR(1) + GPRES YI = SORT(W(1)* GTEMP)*(SPHI-1.)*C(1)/(10.0 * (SPHI+1.)*AC(1) 496m # # GPRES! GTHCON * GTHCON + C(I) * GMIX(I)/((GMIX(I) + SUM) * GPTHK + YI) 75 CONTINUE 100 CONTINUE Revised 8/81 RETURN END

TABLE C-1.VII

LISTING OF THE GJUMP SUBCODE

GASCON, GTHCON, GJUMP

FUNCTION GJUMP(GMIX,GSTEMP, GPRES, ISURF) GJUMP CALCULATES THE EFFECTIVE JUMP DISTANCE AT GAP SURFACES AS A FUNCTION OF GAS TEMPERATURE AT THE SURFACE, GAS COMPONENT FRACTIONS, GAS PRESSURE, GAP SURFACE MATERIAL AND WHETHER THE SURFACE IS A HEAT SOURCE OR A HEAT SINK. . OUTPUT EFFECTIVE JUMP DISTANCE AT GAP SURFACE (M) GJUMP . INPUT MOLE FRACTIONS OF THE GAS COMPONENTS (UNITLESS) GMIX(I) IS HELIUM . . KRYPTON IS . 3 XENDN . I = 6 IS NITCEN I = 7 IS DXYGEN I = 7 IS DXYGEN I = 9 IS CARBON DIDXIDE I = 9 IS CARBON DIDXIDE I = 10 IS WATER VAPOR INPUT GAS TEMPERATURE AT THE SURFACE (K) INFUT GAS PRESSURE (PA) INFUT GAS PRESSURE (PA) INFUT GAP SURFACE MATERIAL PARAMETER INPUT GAP SURFACE MATERIAL PARAMETER ISURF = 0 FOR ZIRCALDY SURFACE HEAT SINK ISURF = 1 FOR FUEL SURFACE HEAT SOURCE ISURF = 1 FOR FUEL SURFACE HEAT SOURCE ISURF = 1 FOR FUEL SURFACE WITH ACCOMODATION COEFFICIENT OF 1) COEFFICIENT OF 1) IS HYDROGEN GS TEMP GPRES **I**SURF THE FUNCTION GASCON IS CALLED BY GJUMP GJUMP WAS CODED BY D. L. HAGRMAN OCTOBER 1979 / LACEMDL / MAXIDX, EMFLAG COMMON DIMENSION EMFLAG(1) DIMENSION GMIX(10), W(10), ACF(10), ACC(10), AR(10), BR(10) DATA W /4.003, 39.944, 83.800, 131.300, 2.016,28.020, 32.000, 28.010, 44.010, 18.020/ DATA ACF /0.34, 0.80, 0.85, 0.85, 0.85, 0.85, 0.85, 0.85, 0.85, 0.85, 0.85, 0.85, 0.20/ DATA ACC /0.071, 0.16, 0.85, 0.85, 0.071, 0.20, 0.20, 0.20, 0.85, 0.20/ DATA AR /1.6669, 1.6567, 1.6667, 1.6667, 1.2057/ # 1.4045,1.4006,1.4006,1.4006,1.2857,1.2857/ DAIA BR /-2.E-9,3.53E-8,3.53E-8,3.53E-8, # 2.5E-9,2.21E-8,2.21E-8,2.21E-8,6.29E-8,6.29E-8/

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TABLE C-1.VII (continued)

:	DATA ON / 2HON /, OFF / 3HOFF /, LOCIDX / 16 /
	IF (EMFLAG (LCCIDX) . EQ. DN)
	IF (EMFLAG(LOCIDX) .EQ. DN) GO TO 100 IF (GSTEMP .LT. 4000.) GC TO 20
900	FORMAT(26H1GJUMP INPUT BAD. GSTEMP=, 1PE12.4, 2H K, / 10H0FRACTIONS, (10E12.4)
20	STOP X = 0.0
30	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
	IF(X .LT. 0.9 .OR. X .GT. 1.1; GO TO 10 GTHCON = 0.0
	DO 70 I = 1,10 IF(GM1X(I) .LE. 1.0E-9) GO TO 70 SPHI = AR(I) + BR(I) + GPRES
	IF(ISURF .EG. 0) AC - ACC(I)/(1 ACC(I))
	IF (ISURF .EQ. 1) AC = ACF(I) YI = SQRT(W(I)*GSTEMP)*(SPHI-1.)/(18.0 * (SPHI+1.)*AC*GPRES) GTHCON = GTHCON + GMIX(I)/YI
70	CONTINUE A GASCONLOMIX-GSTEMP. GPRESI
100	GJUMP = X/GTHCCN CONTINUE RETURN FND
	10 900 20 30 70

GASCON, GTHCON, GJUMP

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1.2 UO2 and (U,Pu)O2 Heat of Fusion

The two calorimetrically determined values for the heat of fusion of unirradiated UO₂ are in good agreement. Specifically, Hein and Flagella^{D-1.8} found 76 \pm 2 kJ/mol, and Leibowitz^{D-1.9} reported a value of 74 kJ/mol. These results suggest that the heat of fusion of unirradiated UO₂ is adequately known from present analyses. The routine PHYPRP uses Leibowitz's calorimetry value of $\frac{1}{2}$ /4 x 10⁵ J/kg for the heat of fusion of UO₂.

Leibowitz^{D-1,10} determined a heat of fusion for mixed oxides of 67 kJ/mol from three tests. This 10% agreement between UO₂ and mixed oxide values for the heat of fusion is reasonable because of the similarity in crystal structure and atomic bonding. Therefore, unless conflicting data become available, the UO₂ value will be used for the heat of fusion of mixed oxides.

1.3 Zircaloy Melting Point and Transformation Temperatures

The reported melting point of zircaloy is below that reported for unalloyed zirconium. The addition of tin lowers the zirconium melting point, D-1.11 and small amounts of iron, nickel, or chromium decrease the solidus temperatures of a binary mixture about 70 K for each 0.1% addition of solute. D-1.12 'f hese results are for the binary mixtures of zirconium and one solute: tin, iron, chromium, or nickel. In the five-component zircaloy system, the effect of each solute may not be additive, and therefore, a separate determination is required. The zircaloy-2 melting point has been measured to be about 2098 K, and this value is returned by PHYPRP.

Pure zirconium isothermally transforms from the α phase to the β phase at 1135 K.D-1.13 The routine PHYPRP returns 1135.15 K for the zirconium transformation temperature when the variable, CTRANZ, is called. Zircaloy, however, undergoes the same transformation over a range of temperatures. CTRANB, the temperature of the formation of the first β -phase regions in the α lattice, is a function of the oxygen concentration in the zircaloy.

For oxygen concentrations < 0.025 weight fraction

$$CTRANB = 1094 + W(-1.289 \times 10^{3} + W \times 7.915 \times 10^{3})$$
(D-1.3a)

for oxygen concentrations ≥0.025 weight fraction

$$CTRANB = 1556.4 + 3.8281 \times 10^4 \times (W - 0.025)$$
(D-1.3b)

where W is the total oxygen concentration in the zircaloy in weight fraction.

CTRANE, the highest temperature at which any α phase regions are found in the β lattice, is also a function of the oxygen concentration in the zircaloy.

For oxygen concentrations < 0.00597 weight fraction

$$CTRANE = 3924600(W^2 + 3.1417 \times 10^{-4})$$
(D-1.4a)

for oxygen concentrations ≥ 0.00597

 $CTRANE = 1079.6388 + W \times 49115.7.$

Equations (D-1.3) and (D-1.4) are based on data presented in Reference D-1.14.





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(D-1.4b)

1.4 Zircaloy Heat of Fusion

The heat of fusion of zircaloy depends to some extent on its composition and the extent of oxidation. Brassfield has suggested that the heat of fusion of zircaloy 4 differs little from that of zirconium and lists the heat of fusion of zirconium as 20.5 kJ/mol. However, QuillD-1.15 lists the heat of fusion of zirconium as 23 kJ/mol with uncertainty. The routine PHYPRP returns Brassfield's listed heat of fusion for zirconium of 2.25 x 10^5 J/kg.

1.5 Physical Properties Subcode PHYPRP Listing

The FORTRAN subcode PHYPRP is listed in Table D-1.1.

TABLE D-1.1

LISTING OF PHYPRP SUBCODE

	-		R	R	au	1	1	N	Ē	ş	H	Y	PI	R 1	,																																	
		111	PIN	HHS	PEAT	RTT	UND	TIN		RAFL	N	FP	UU	SIR	2 OF	NU	11	AS	PN .	0	QZ	21	RC	0	ZZ	DI	UM	I	RCAT		L	g	Y P	EC.	E A	LC	Y	NO	i.	PI	11	N	Ţ	S	ß	ē 1	A	
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	FT	PE	14 14	U	IS				U	TP	UL	Ţ	-		22				MM	IX	www.	DO	2	X	I		Line .	FFF	Ų	EL		MH	EL	Ŧ	I			P ()I JS	NI	55		0		ĸ	61		
	CONSCRETE OF	MERRAL	UFAAAL	LUNNNT	SBEZA			000000		PPPPPPPP	101100	TTTTT			AND	CCR HU		000	FZHS	HEZERL	LARSEN	T	ALC	FAPAD	LTLU	FPAPX		IET	OF	NEASI	TATAC	j R	TATT	GASAM	PICIA	****	STISA	EM	E PT R	TURE		R	AJAN	T I E UC	R	1244		()
		PL.	PD	x	Y			ITIO	NNNF	PLOPA	in the second		BIP PICR	LIN C	AND/ON	U	PCNI	1NCD	MTO	WENCL	STEA	N	KGUTA	TAN	URTG	1 11		G	- (X	YG	GEN	N	ĸ	ç	IN I	CE	NC	7 s Al	8 A	T	11	n				
and the second second	TTBRIAR	HKI TIL	410-1-22	UNK71A	2447 .00	RRA	ADDKOUM	NMMCLUS	DAAME	THULLEPI	RUCHALL	-02-0	CFBLGC	LOREAT	ALSHOR	POL BUDO	INFORM	GREE R	SUSTED	PR LPAN	*COMMINM	LETINO	TE BNIA	NELW G2	GN HO .	CGTFH	PEER 24	I *PEOT	N ITO	44	S D 2 LK	A2 F	N F L JAS	-00.00	THNERO	EAL	THE . O	SEAMLE	OT 1 4	FIN	AF IC	U FOXX	SPI LC	I I I I I I I I I I I I I I I I I I I	NTC	TNIMM	R	
a sub-	HALTA	GOUNA	HUHLA	RINA		NIPRE	GIAFI	TAL	L	N32 .8	R LC	DCDOT.	NFOSK	NIN	CAUAC	FLMN .		LOLN	PIPFE	H494×	- IEY	BRO	EZR	A .	•	1	RA RA	NNS	SI		SA	A	RE	IP	EG	RA	TIO	UR F	A FZ	T	A SC	1	Z M	12	15	.,*		
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PHYPRP

TABLE D-1.I (continued)

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3.21063*C - 1.448513E-2*C*C
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1.49-10
        ELTA
TC
               20
                     CIMP
SLEUS(C1) + 273.15 - 32.0*FPU/10000.
LICOUS(C1) - SLOUS(C1)- 32.0*FBU/10000.
    FT
1
     FTMELT
FDELTA
                  .
    EHEFUS
CTMELT
CHEFUS
24
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2.98.15
22.5:+04
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4.73569372-03) GC

* DELLXY + (.12)
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IF(DELDXY

CTFANE

CTFANE

CTFANZ

CTFANZ
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(Y + 0.1242807)
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     RETURN
     END
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1.6 References

C

6

C

C

C

C

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POLATE

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2. LINEAR INTERPOLATION (POLATE (D. L. Hagrman)

A number of the MATPRO subcodes contain tables for a property rather than analytical expressions. POLATE is used when analytical expressions based on theory are not available or are too complex, as in the case of cladding specific heat capacity.

The POLATE function returns the interpolated value of Y(X) using an input value of X for which Y(X) is desired and a table of pairs of numbers $Y_k = Y(X_k)$ and X_k . To increase the efficiency of the POLATE function, an estimate of the expected location of the value of the input X in the table of numbers is als accepted. The number of the pair that was used in a previous interpolation is often used for this estimate.

Beginning with its initial estimated value, the index K is raised or lowered until a pair of X_k and X_{k+1} are found which bound X. $Y(X_k)$ and $Y(X_{k+1})$ are then used to interpolate for Y(X).

If X is outside the range of the set of X_k given as input, the Y_k of the member of the set of X_k closest to X is returned by POLATE.

A listing of the POLATE function is given in Table D-2.1.





TABLE D-2.1

LISTING OF THE POLATE SUBCODE

	FUNCTION POLATE (XY, XX, NN, KK)
	POLATE RETURNS AN INTERPOLATED NUMBER, Y(XX), USING AN INPUT TABLE OF UP TO 13 PAIRS OF NUMBERS.
	POLATE = OUTPUT INTERPOLATED VALUE OF Y AT XX. KK = OUTPUT LOCATION OF XX IN THE TABLE OF Y, X PAIRS (NUMBER OF FIRST PAIR NITH X LESS THAN XX).
	<pre>XY - INPUT TABLE OF UP TO 13 PAIRS OF Y AND X VALUES Y(1),X(1),Y(2),X(2),,Y(NN),X(NN). XX - INPUT VALUE OF INDEPENDENT VARIABLE FOR</pre>
	NN = INPUT NUMBER OF PAIRS IN THE INPUT TABLE. KK = INPUT ESTIMATED LOCATION OF XX IN THE TABLE OF PAIRS (NUMBER OF FIRST PAIR WITH X LESS THAN XX
	POLATE WAS CODED BY D. L. HAGRMAN TO REPLACE AN OLDER MATPRO SUBCODE OF UNKNOWN ORIGIN JULY 1981 (CDR-MP-05).
	DIMENSION XY(26)
901 20	CHECK FOR O OR 1 TABLE ENTRIES IF(NN - 1) 10,20,25 PRINT 901 FORMAT(23H POLATE GIVEN NO DATA) POLATE = 0.0 RETURN POLATE = XY(1) RETURN
25	CHECK SUGGESTED POSITION VERSUS TABLE LIMITS IF(KK .LT. 1) KK = 1 IF(KK .GT. (NN - 1)) KK = NN - 1 K = KK
	FIND TABLE VALUES NEAREST XX BY ADJUSTING INDEX K
30	LOOP TO LOWER INDEX UNTIL XY(2*K) IS LESS THAN OR EQUAL TO XX IF(XY(2*K) .LE. XX) GO TO 00 K = K = 1 IF(K .GT. 0) GC TO 30 POLATE = XY(1)

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CCC

0000000000

c

c

CCCC

POLATE

TABLE D-2.I (continued)

```
C

C

LOOP TO RAISE INDEX UNTIL XY(2*K) IS LARGER THAN XX OR

THE TABLE IS EXHAUSTED

40 IF(XY(2*K+2) .GT. XX) GO TO 50

K * K + 1

IF(X .LT. NN) GO TO 40

POLATE * XY(2*NN - 1)

RETURN

C

C

IF XX IS BOUNDED ABJVE AND BELOW BY TABLE VALUES

DO A LIMEAR INTERPOLATION

50 KK * K

POLATE * XY(2*K-1) *(XX-XY(2*K)) * (XY(2*K+1)-XY(2*K-1))

RETURN

END
```

1.0

3. MELTING TEMPERATURES OF URANIUM-ZIRCONIUM-OXYGEN COMPOUNDS (PSOL AND PLIQ) AND URANIUM DIOXIDE SOLUBILITY IN ZIRCALOY (PSLV) (D. L. Hagrman)

The temperature of the appearance of the first liquid phase (solidus) and the temperature of the melting of the last solid phase (liquidus) of uranium-zirconium-oxygen compounds are needed to model the behavior of light water reactor cores when cladding temperatures exceed 1575 K. The function PSOL computes the solidus temperature for these compounds and the function PLIQ computes the liquidus temperature.

It is also necessary to know the amount of uranium dioxide fuel that can be dissolved by liquid zircaloy as a function of temperature. The function PSLV calculates this quantity. It is included in this section because the solubility and iiquidus represent a single line with independent a d dependent variables interchanged.

3.1 Summary

Solidus and liquidus temperatures for uranium-zirconium-oxygen compounds are calculated from values of the atomic fraction of each element of the compound. A weighted average of the temperatures obtained from binary phase diagrams is employed. The equation used to average the temperatures obtained from binary phase diagrams is

$$T = \left[1 - \left(\frac{Y}{2}\right)^2\right] \left(\frac{Z}{Z + U}TZ + \frac{U}{Z + U}TU\right) + \left(\frac{Y}{2}\right)^2 TD$$
(D-3.1)

where

- T = solidus or liquidus temperature of ternary compound (K)
- Y = oxygen-to-metal ratio of the compound for oxygen-to-metal ratios ≤ 2 . For oxygento-metal ratios > 2, Y is four minus the oxygen-to-metal ratio (unitless)
- Z = atomic fraction zircaloy in the compound (unitless)
- U = atomic fraction uranium in the compound (unitless)
- TZ = solidus or liquidus temperature from binary zirconium—zirconium dioxide phase diagram (K)
- TU = solidus or liquidus temperature from binary uranium—uranium dioxide phase diagram (K)
- TD = solidus or liquidus temperature from binary uranium dioxide—zirconium dioxide phase diagram (K).

The oxygen-to-metal ratio required by Equation (D-3.1) is calculated from the atomic fractions required as input with the relation

PSOL, PLIQ, PSLV

$$Y = \frac{X}{U + Z}$$

where

X = atomic fraction of oxygen in the compound (unitless).

The correlations used to determine TZ, TU, and TD for solidus temperatures are listed in Table D-3.1, and the correlations used to determine TZ, TU, and TD for liquidus temperatures are listed in Table D-3.1I. The parameters, D and F, which are required for the correlations displayed in these tables, are calculated from atomic fractions with the following relations

TABLE D-3.I

CORRELATIONS FOR SOLIDUS TEMPERATURES OF BINARY COMPOUNDS

Zirconie	umZirconium Oxide
X, Atomic Fraction Oxygen	TZ, Solidus Temperature
0.00 - 0.10	2,098 + X 1,150.
0.10 - 0.18	2,213.
0.18 - 0.29	1,389.5317 + x(7,640.0748 - x 17,029.172)
0.29 - 0.63	2,173.
0.63 - 0.667	-11,572.454 + X 21,813.181
>0.667	-11,572,454 + X(1.334 - X) 21,818.181
D, Departure from Stoichigeetry	TU, Solidus Temperature
<u>Urani</u> D, Departure from Stoichignetry	umUranium Oxide TU, Solidus Temperature
All value:	3,119 D (873.7 + D 1,469). If TU is calculated to be <2700, the calculated value is replaced by 1373.
Uranium Dio	xideZirconium Dioxide
F, Zircaloy-to-Metal Ratio	TD, Solidus Temperature
0.00 - 0.55	3,119. + F(-1,130.394 + F 1,007.3297)
0.55 - 0.88	2,773.6667 + F 51.515151
0.88 - 1.00	1,689.6667 + F 1,283.3333

0

TABLE D-3.11

CORRELATIONS FOR LIQUIDUS TEMPERATURES OF BINARY COMPOUNDS

89.3	Provide and a	1	198.1	*			100 1	
1 2 1	1 7 1 1 1	nn1	1177	1 8 0	001	11777	1121	0.0
- 6-F - 2	to the start of	18.8 A.	1819 50	So the New	U114	1.8.111	100	1. 1. A. C.

X, Atomic Fraction Oxygen	TZ, Solidus Temperature
0.00 - 0.19	2,125 + X(1,632.1637 - X 5,321.6374)
0.19 - 0.41	2,111.6553 + X(1,159.0909 - X 2,462.1212)
0.41 - 0.667	895.07792 + X 3,116.8831
>0.667	895.07792 + (1.334 - X) 3,116.8831

Uranium--Uranium Oxide

D, Departure from Stoichiometry

All Values

3,119. - D^2 1,610. If TU is calculated to be <2700, the calculated value is replaced by 1373.

TD, Solidus Temperature

Uranium Dioxide--Zirconium Dioxide

F, Zircaloy-to-Metal Ratio	TD, Solidus Temperature
0.00 - 0.50	3,119. + F(44.4208 - F 1.342302)
0.50 - 0.52	3,119. + F(-1,130.3949 + F 1,007.3297)
0.52 - 0.55	2,224.2377 + F 1114.1132
0.55 - J.93	3,180.9473 + F(-1,116.5869 + F 893.14194)
0.93 - 1.00	2,144.4285 + F 828.57142

$$D = \frac{Y}{U + Z} - 2$$
(D-3.3)
$$F = \frac{Z}{U + Z}$$
(D-3.4)

where

D = departure from stoichiometry (unitless)

F = zircaloy-to-metal ratio (unitless).



PSOL, PLIQ, PSLV

The estimated uncertainty of the solidus and liquidus temperatures is computed in the PSOL and PLIQ functions but not returned. The expression used for this uncertainty is

$$U = 10 + 50(1 - |Z - U|) + 100(Y |Y - 2|).$$
(D-3.5)

The expressions for the solubility of uranium diexide in oxygen-stabilized alpha phase zircaloy are for temperatures ≤ 2103 K

$$FR = 0 \tag{D-3.6a}$$

for temperatures between 2103 and 2673 Ka

$$FR = 1.19143754 + T(-1.2127195 10^{-3} + T 3.1857023 10^{-7})$$
(D-3.6b)

for temperatures in the range 2673 to 3119 K

$$FR = 2.0859332 + T(-1.1311691 10^{-3} + T 2.5104264 10^{-7})$$
(D-3.6c)

for temperatures >3119 K

$$R = 1$$
 (D-3.6d)

where

F

FR = uranium dioxide in melt at saturation (mole fraction of melt)

T = temperature (K).

An estimated uncertainty of 0.025 is defined within the PSLV function for values of FR between zero and one. When FR is zero or one, the uncertainty is assumed to be zero.

Section 3.2 is a review of the melt temperature and solubility data. Section 3.3 is a description of the development of the functions for calculating melt temperatures and solubility. FORTRAN listings of the PSOL, PLIQ, and PSLV subcodes are in Section 3.4, and references are provided in Section 3.5.

3.2 Melt Temperature and Solubility Data

Temperatures of the onset of melting in the ternary uranium-zirconium-oxygen system have been reported by Hofmann and Politis. D-3.1 Their data are reproduced in kelvin in Fig. re D-3.1. Vertices of the triangular coordinate system used in this figure correspond to pure oxygen, uranium, or zirconium. The baseline corresponds to binary mixtures of uranium and zirconium, and the left and right sides of the triangle represent uranium and zirconium oxides. Temperatures increase rapidly as the stable dioxide compounds (two-thirds of the distance from the baseline to the oxygen vertex) are approached. There is a less pronounced decrease in the melt temperatures of the dioxide compounds as equal amounts of zircaloy are approached.

Data shown in Figure D-3.1 were used to estimate model uncertainties but not to construct the models. There are not enough data at oxygen-to-metal ratios near 2 to define correlations.



a. Several significant figures are used to minimize discontinuities.



Figure D-3.1. Onset of melting in kelvin for uranium-zirconium-oxygen compounde according to Hofmann and Politis.

More detailed information for both solidus and liquidus temperatures are available from binary phase diagrams. The remainder of this section is a review of binary phase diagrams that span different parts of the ternary uranium-zirconium-oxygen system.

Laata and Fryxell^{D-3.2} have published both solidus and liquidus temperatures for uranium oxides with oxygen-to-uranium ratios ranging from 1.46 to 2.23. Their data, which correspond to an expanded plot of the region represented on the left side of the triangle of Figure D-3.1, are shown in Figure D-3.2 and listed in Table D-3.111.

Figure D-3.2 illustrates the rapid increase in the solidus temperature as oxygen-to-uranium ratios of 2 are approached. The liquidus temperature also exhibits a maximum for oxygen-to-uranium ratios near 2, but the liquidus maximum is not as sharp as the solidus peak. Both solidus lines are approximately symmetric about oxygen-to-uranium ratios of 2. There is a sharp discontinuity in the solidus data near 2700 K. The discontinuity marks the appearance of a second phase that is liquid and mostly uranium. This second phase melts at 1373 K. A lower solidus line slopes to the right from this discontinuity, separating the two-phase $U_{liq} + UO_2$ region from the single-phase solid UO_{2-x} region to the right.

Table D-3.1II repeats the solidus and liquidus data shown in Figure D-3.2 and adds posttest analysis of the test samples. Inspection of the table shows that the samples tended to be reduced by the tungsten or rhenium capsules that held them. Samples with oxygen-to-metal ratios >2 had several percent metallic impurities in them but, with the exception of sample 156, contamination of the hypostoichiometric samples by the capsule was minimal. The hypostoichiometric data are therefore somewhat more reliable than the hyper-to-induction data.

Solidus and liquidus temperatures of zirconium-oxygen mixtures have been published by Domagala and 'McPherson^{D-3.3} and modified by Ruh and Garrett.^{D-3.4} Figure D-3.3 is part of the phase diagram of the zirconium-oxygen system reported by these references. The solidus curve is made up of several segments above the β , $\alpha + \beta$, $\alpha + ZrO_2$, and cubic ZrO₂ regions. The liquidus curve is composed of the two



Figure D-3.2. Solidus and liquidus temperatures for uranium oxides according to Laata and Fryxell.

segments under the liquid region. The modifications proposed by Ruh and Garrett are shown in dashed lines and labeled parenthetically. Their work suggests a solidus that is virtually identical to the solidus of Domagala and McPherson's data but raises the liquids temperature for oxygen fractions above 0.55. Data for oxygen fractions below 0.55 were not presented.

Solidus and liquidus temperatures of the zircaloy-oxygen system show the same sharp increase near the dioxide that was observed for the uranium-oxygen system. Another similarity is the appearance of a metallic second phase in the oxide when the material is slightly hypostoichiometric (0.63 oxygen fraction in zircaloy). An important difference in the systems is the fact that the α -phase component that appears in zircaloy-oxygen compounds is solid to 2173 K. In uranium-oxides, the metallic phase melts at 1373 K.

Table D-3.1V lists the solidus and liquidus temperatures reported by Domagala and McPherson. Since these points are not sufficient to provide a complete description of the solidus and liquidus lines, additional data were taken from the phase diagrams of this reference.

Another important binary system for the models that will be developed in the next section is the UO_2 - ZrO_2 system. Figure D-3.4 shows the liquidus and solidus temperatures for this system as a function of the mole fraction of zirconium dioxide. The figure was taken from Figure 6 of the UO_2 - ZrO_2 phase equilibrium study by Romberger, Baes, and Stone. D-3.5 The results of Reference D-3.5 were used in preference to a similar diagram published earlier by Cohen and SchanerD-3.6 because the Cohen and Schaner phase diagram shows a melting temperature of 3030 K for pure UO_2 . The fact that this value is 90 K lower than those obtained by numerous other investigators D-3.1 D-3.2, D-3.5 raises doubts about the temperature measurements and the purity of the UO_2 samples used by Cohen and Schaner.

The final system that will be considered in this section is the oxygen-stabilized α -phase zirconiumuranium dioxide phase diagram. This system is important because the two components used to construct



TABLED-3.III

				Posttest Capsule	Melting Points				
Sample Number	Pretest	Posttest	Capsule <u>Material</u>	Material in Sample (% or ppm)	Solidus (K)	Liquidus (K)			
221	2.23		Re	0.67	2837	3031			
217	2.23	10	W	5.56	2851	3013			
188	2.184	2.169	W	5.02	2878	3045			
201	2.13	2.109	Re	1.37	2940	3078			
192	2.12	2.103	Re	2.00	2907	3071			
303	2.095	2.092	W	3.94	3003	3088			
208	2.095	2.050	Re	1.34	3001	3090			
172	2.058	2.058	W	3.32	3067	3109			
204		2.022	Re	26 ppm	3085	3136			
193	2.019	2.009	W	0.26	3109	3125			
212	1.998	1.998	Re	54 ppm	3118	3138			
190	1.997	2.003	V	0.25	3118	3138			
194	1.997	2.000	W	0.24	3120	3135			
209	1.993	1.995	Re	37 ppm	07	3133			
189	1.980	1,990	W	0.15	3105	3133			
146	1.980	1.985	Ŵ	0.148	3106	3133			
153	1.956	1.955	W	0.12	3076	3130			
138	1.943	1.943	W	0.046	3069	3118			
184	1.020	1.930	W	0.060	3043	3113			
150	1.890	1.929	W.	low	3002	3105			
154	1.856	1.861	W	0.02	2970	3083			
177	1.809	1.795	W	0.378	2888	3033			
156	1.803	1.849	W	8.0	2893	3033			
159	1.793	1.809	W	0.014	2874	3031			
129	1.75	1.803	W	0.14	2818	2983			
104	1.790	1.759	W	0.007	2863	3013			
164	1 736	1.736	LT	0.012	2786	2968			
166	1.662	1.689	Ŵ	0.064	2686	2923			
0.00	1.60			방법은 문화가 있다.	2606	2957			
160	1.00		he ca		2090	2007			
168	1.550		W	0 100	2708	2/03			
207	1.50	1.593	W	0.198	2701	2771			

SOLIDUS AND LIQUIDUS TEMPERATURES OF UO2+x ACCORDING TO LATTA AND FRYXELL



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Figure D-3.3. Phase diagram of the zirconium-oxygen system according to Domagala and McPherson as modified by Ruh and Garrett.

the diagram are those components one would expect to find in a reactor core as liquefaction begins. Figure D-3.5 is a reproduction of the equilibrium quasi-bivary phase diagram for α -Zr(O) - UO₂ shown in Figure 29 of an investigation by Politis. D-3.7

The cross-hatched region between zero and 0.05 mole fraction UO₂ and near 2200 K represents the effect of varying oxygen concentrations in the α -Zr(O) and is consistent with the liquidus line of Figure D-3.3. From the three-phase eutectic point at 0.05 mole fraction UO₂ and 2100 K, the temperature of the liquidus line increases with increasing UO₂ content up to the point (0.226, 2673 K). At temperatures >2673 K and UO₂ concentrations >0.226 mole fraction, two liquid phases are formed: L₁, an α -Zr(O)-rich melt, and L₂, a uranium dioxide-rich melt. At about 0.85 mole fraction UO₂ and 2673 K, the three phases, L₁, L₂, and UO_{2-X}, are in equilibrium. From this point, the liquidus line proceeds to the melting point of pure UO₂, approximately 3120 K.

The two-phase region below the liquidus line for concentrations of UO₂ above 0.85 was not labeled by Politis. From Politis' description of the three-phase point at (0.85, 2673) as being like a euteetic, with the exception the L₁ is liquid, and from his comment that the three phases are L₁, L₂, and UO₂, the tentative label L₂ + UO_{2-x} has been assumed. The label for the solid (U, Zr)O_{2-x} region was also not specified by Politis' figure. The region has been tentatively labeled as a solid solution (U, Zr)O_{2-x} by comparing Figure D-3.5 to Figure D-3.4.

Although the liquidus line just discussed is usually plotted as a concentration-dependent temperature, the same line can be interpreted as a temperature-dependent solubility of UO₂ in α -Zr(O). The data will actually be used only in the construction of the expressions for solubility of UO₂ in α -Zr(O) as a function of temperature because their use would make the computation of solidus and liquidus temperatures for ternary compounds unnecessarily complicated.

TABLE D-3.IV

Oxygen Co	ntent		
(wt%)	(at%) ^a	Solidus (K)	Liquidus (K)
0	0	2125	2125
1.25	6.7	2213	
2 to 3.75	10 to 18	2213	
5.5	23	2248	2248
6.75 to 23	29 to 63	2173	
11	41	2173	2173
26	66.7	2973	2943

SOLIDUS AND LIQUIDUS TEMPERATURES OF Zr02-x ACCORDING TO DOMAGALA AND McPHERSOND-4.3

a. Atomic weights of 16 for oxygen and 91.22 zirconium were used to convert weight fractions to atomic fractions. The relationship is

weight fraction oxygen = 16 atomic fraction oxygen + 91.22 (1-atomic fraction oxygen)

atomic fraction oxygen = $\frac{\text{weight fraction oxygen 91.22}}{75.22 \text{ weight fraction oxygen + 16}}$

3.3 Models Development and Uncertainties

Expressions used in the PSOL and PLIQ functions for solidus and liquidus temperatures of melts as a function of component concentrations have been developed by correlating the binary phase diagram information represented in Figures D-3.2 to D-3.4 of the previous section. Compositions not represented by one of the binary phase diagrams are modeled with an interpolation scheme which is based on the trends apparent in the ternary system plot, Figure D-3.1. The solidus temperatures shown in this figure have a sharp maximum for those compounds in which the oxygen-to-metal ratio is 2. This maximum is modeled in the basic Equation (D-3.1) with a weighted average. By trail and error, weighting factors equal to the square of the oxygen-to-metal ratio and one minus this square were found to work well.

The correlations used to represent the solidus or liquidus temperatures of the dioxides, TD in Equation (D-3.1) and Tables D-3.1 or D-3.11, were obtained from the binary $UO_2 + ZrO_2$ -phase diagram of Romberger, Baes, and Stone. D-3.5 Since the solidus and liquidus lines published by these authors are





Figure D-3.4. Solidus and liquidus temperatures for the UO₂-ZrO₂ system according to Romberger, Baes and Stone.





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complex curves, numerous simple polynomial segments were used to represent these curves. The values used to generate functions for the several segments represented in Tables D-3.I and D-3.II are shown in Table D-3.V.

The factor that multiplies one minus the square of the oxygen-to-metal ratio in Equation (D-3.1) is a weighted average. In this factor, the solidus or liquidus temperature obtained from the zirconium-oxygen binary phase diagram, TZ, is averaged with the solidus or liquidus temperature obtained from the uranium-oxygen binary phase diagram, TU. Since these binary phase diagrams describe the solidus or liquidus temperatures at the right or left edge of the ternary plot of Figure D-3.1, the weighting factors multiplying TZ and TU are simply the zircaloy-to-metal and uranium-to-metal ratios, respectively.

The expressions for TZ shown in Tables D-3.1 and D-3.11 were obtained by fitting simple polynomial segments to the data reported by Domagala and McPherson (Table D-3.1V and Figure D-3.3) for the solidus or liquidus lines of the binary zirconium-oxygen system. The corresponding expressions for TU were obtained by least-squares fits to the hypostoichiometric uranium-oxygen binary system data of Laata and Fryxell (Table D-3.1II and Figure D-3.2). The hyperstoichiometric data of this reference were not used because of the larger concentrations of capsule material found after tests with hyperstoichiometric uranium dioxide. Instead of modeling with questionable data, the simple assumption that the expressions for the solidus and liquidus lines are symmetric about oxygen-to-uranium ratios of 2 was made.

Equation (D-3.5), the uncertainty estimate for the solidus and liquidus temperature calculated with Equation (D-3.1), is an estimate constructed to show increasing uncertainty as compositions differ by increasing amounts from the binary phase diagrams used to derive Equation (D-3.1). The factors of 50 and 100 were deduced from comparisons of calculated temperatures to the limited ternary system data reported

TABLE D-3.V

Mole Fraction Zr02	Solidus (K)	Liquidus (K)
0	3119	3119
0.400		2922
0.456	2813	
0.500		Value of T_{sol} correlation at 0.500
0.520		Value of T_{sol} correlation at 0.520
0.550	2802	2837
0.880	2819	2890
0.930		2915
1.000	2973	2973

SOLIDUS AND LIQUIDUS TEMPERATURES OF UO₂ + ZrO₂ USED TO FORMULATE THE MATPRO MODEL

PSOL, PLIQ, PSLV

by Hofmann and Politis. D-3.1 There is, unfortunately, systematic error because the data base is the uranium-zirconium-oxygen system, while the model attempts to predict the behavior of uranium-zircaloy-oxygen systems with fission product impurities.

Equations (D-3.6a) to (D-3.6d), the expressions used in the PSLV function to calculate the solubility of UO₂ in α -Zr(O), are polynomial segments obtained from the liquidus line of the α -Zr(O) - UO₂ quasibinary phase diagram of Politis (Figure D-3.5). The points used to define the polynomial segments are (2.03 K, 0.05 fraction UO₂), (2347 K, 0.10 fraction UO₂), and (2673 K, 0.226 fraction UO₂) for Equation (D-3.6b); and (2673 K, 0.856 fraction UO₂), (2846, 0.900 fraction UO₂), and (3119 K, 1.000 fraction UO₂) for Equation (D-3.6c). A more complete inverse to the PSOL and PLIQ functions, namely a description of all the compositions that could correspond to a given solidus or liquidus temperature, was not produced because the computations would be unnecessarily complicated.

The estimated uncertainty of the PSLV calculation, 0.025, is an estimate of the errors of the value taken from the phase diagram of Politis (Figure D-3.5). A more detailed estimate was not attempted because the phase diagram used to construct the function was the only source of data.

3.4 Subcodes PSOL, PLIQ, and PSLV Listings

Tables D-3.VI and D-3.VII are listings of the PSOL and PLIQ functions for the solidus and liquidus temperatures of uranium-zircaloy-oxygen compounds. A listing of the PSLV function, which calculates the solubility limit of UO₂ in α -Zr(O), is presented in Table D-3.VIII.

3.5 References

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- D-3.3. R. F. Dornagala and D. J. McPherson, "System Zirconium-Oxygen," Journal of Metals, 6, Transactions AIME 200 (1954) pp. 238-246.
- D-3.4. R. Ruh and H. J. Garrett, "Nonstoichiometry of ZrO₂ and its Relation to Tetragonal-Cubic Inversion in ZrO₂," *Journal of the American Ceramic Society*, 50 (1966) pp. 257-261.
- D-3.5. K. A. Romberger, C. F. Baes, Jr., H. H. Stone, "Phase Equilibrium Studies in the UO₂-ZrO₂ System," *Journal of Inorganic and Nuclear Chemistry*, 29 (1966) pp. 1619-1630.
- D-3.6. I. Cohen and B. E. Schaner, "A Metallographic and X-Ray Study of the UO₂-ZrO₂ System," Journal of Nuclear Materials, 9 (1966) pp. 18-52.
- D-3.7. C. Politis, Untersuchungen in Dreistoffsystem Uran-Zirkon-Sauerstoff, KfK 2167 (date unknown).

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TABLE D-3.VI

LISTING OF THE PSOL SUBCODE

FUNCTION PSOL(X,U,Z) PSOL CALCULATES THE SOLIDUS TEMPERATURE OF URANIUM - ZIRCALOY - DXYGEN COMPOUNDS PSOL . OUTPUT SOLIDUS TEMPERATURE (K) INPUT ATOMIC FRACTION OXYGEN IN COMPOUND (UNITLESS)
 INPUT ATOMIC FRACTION URANIUM IN COMPOUND (UNITLESS)
 INPUT ATOMIC FRACTION ZIRCALOY IN COMPOUND (UNITLESS) ¥ U THE SOLIDUS TEMPERATURE CALCULATED BY THIS FUNCTION IS BASED ON DATA FROM THE FOLLOWING REFERENCES (1)R. E. LATTA AND R. E. FRYXELL, DETERMINATION OF SOLIDUS-LIQUIDUS TEMPERATURES IN THE UG2+X SYST5M (-0.50 LESS THAN X LESS THAN 0.20), JOURNAL OF NUCLEAR MATERIALS 35 PP. 195-210 (1970). (2)K. A. ROMBERGER, C. F. BATES JR. AND H. H. STONE, PHASE EQULIBRIUM STUDIES IN THE UG2 - ZRO2 SYSTEM, JOURNAL OF INORGANIC AND NUCLEAR CHEMISTRY 29 PP. 1619-1630 (1966). (3) R. RUH AND H. J. GARRETT, NONSTOICHIDMETRY OF ZRO2 AND ITS RELATION TO TETRAGONAL-CUBIC INVERSION IN ZRO2, JOURNAL OF THE AMERICAN CERAMIC SOCIETY 50 PP 257-261 (1966).
(4) R. F. DOMAGALA AND J. D. MCPHERSON, SYSTEM ZIRCONIUM-GXYG5N, JOURNAL OF METALS 6 TRANSACTIONS AIME 200 PP 238-246 (1954). P SOL WAS CODED BY D. L. HAGRMAN OCTOBER 1980 FIND DXYGEN TO METAL RATIO. ASSUME SYMMERTY ABOUT 2.0 YE = X/(U + Z) IF (YE .GT. 2.23) GD TD 80 IF (YE .GT. 2.) YE = 4. - YE ZIRCALDY - ZIRCALDY OXIDE MODEL IF(Z .LT. 1.0E-06) GO TO 10 X = X CX TZ = 2098. + X0Z * 1150. IF (X0Z LE. 0.10) GO TO 10 TZ = 2213. IF (XDZ .LE. 0.18) GD TD 10 IZ = 1.3895317E+03 + XDZ+(7.6400748E+03 - XDZ+1.7029172E+04) IF (XOZ .LE. 0.29) GO TO 10

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PSOL, PLIQ, PSLV

TABLE D-3.VI (continued)

TZ = 2173. IF(XOZ .LE. 0.63) GD TO 10 TZ = -1.15724545+04 + XJZ*2.1818181816+04 IF (XOZ .LE. 0.667) GO TO 10 XOZ = 1.334 - XOZ TZ = -1.1572454E+04 + X02+2.1818181E+04 ç URANIUM - URANIUM OXIDE MODEL 10 TU = 0.0 IF(U .LT. 1.0E-06) GD TD 20 DSTOC = ABS(X/(U+Z) - 2.) TU = 3119. + DSTOC * (-873.7 - DSTOC*1469.) IF(TU .LT. 2700.) TU = 1373. c URANIUM DIOXIDE - ZIRCALOY DIOXIDE MODEL 20 TD . 0.0 IF (YE .LT. 1.0E-02) GO TO 30 ZOU - Z/(U+Z) TD = 3119. + ZDU*(-1.1303949E+03 + ZDU*1.0073297E+03) IF (ZOU .LE. 0.55) GO TO 30 TD + 2773.6667 + 200+51.515151 IF (ZOU .LE. 0.88) GO TO 30 TD = 1.68966676+03 + ZOU+1.2833333E+03 cc COMBINE BINARY ESTIMATES ASSUMING DXYGEN TO METAL RATIO IS MOST IMPORTANT 30 W = (YE/2.)**2 C PSOL = (1 - W) + ((Z/(Z+U)) + TZ + (U/(Z+U)) + TU) + W + TDc ESTIMATE UNCEPTAINTY UPSOL = 10. + 050. * (1. - ABS(Z - U)) + 100. * YE * ABS(YE - 2.) . GO TO 100 LO WRITE 900.YE 900 FORMAT(29H DXYGEN TO METAL RATIO = ,E16.5,38H OUTSIDE RANGE OF * MATPRO FUNCTION PLIQ) STOP C 100 CONTINUE RETURN END

PSOL, PLIQ, PSLV

C

FUNCTION PLIG(X, U, Z)

PLIQ CALCULATES THE LIQUIDUS TEMPERATURE OF URANIUM - ZIRCALDY - DXYGEN COMPOUNDS OUTPUT LIQUIDUS TEMPERATURE (K) PLIQ INPUT ATOMIC FRACTION DXYGEN IN COMPOUND (UNITLESS'
 INPUT ATOMIC FRACTION URANIUM IN COMPOUND (UNITLESS)
 INPUT ATOMIC FRACTION ZIRCALDY IN COMPOUND (UNITLESS) x U Z THE LIQUIDUS TEMPERATURE CALCULATED BY THIS FUNCTION IS BASED ON DATA FROM THE FOLLOWING REFERENCES (1)R. E. LATTA AND R. E. FRYXELL, DETERMINATION OF SOLIDUS-LIQUIDUS TEMPERATURES IN THE UD2+X SYSTEM (-0.50 LESS THAN X LESS THAN 0.20), JOURNAL 06 54LE -9 MATERIALS 35 PP. 195-210 (1970). (2)K. A. ROMBERGER, C. F. BATES JR. AND H. H. STONE, PHASE EQULIBRIUM STUDIES IN THE UD2 - ZRD2 SYST54# JOURNAL OF INDRGANIC AND NUCLEAR CHEMISTRY 29 PP. 1619-163 (1966). (3)R. RUH AND H. J. GARRETT, NONSTOICHIOMETRY OF ZRO2 AND ITS RELATION TO TETRAGONAL-CUBIC INVERSION IN ZPO2, JOURNAL OF THE AMERICAN CERAMIC SOCIETY 50 PP 257-261 (1966). (4)R. F. DOMAGALA AND J. D. MCPHERSON, SYSTEM ZIRCONIUM-DXYGEN, JOURNAL OF METALS 5 TRANSACTIONS AIME 200 PP 238-246 (1954). PLIQ WAS CODED BY D. L. HAGRMAN OCTOBER 1980 FIND DXYGEN TO METAL RATIO. ASSUME SYMMERTY ABOUT 2.0 YE = X/(U + Z) IF(YE .GT. 2.23) GO TO 80 IF(YE .GT. 2.) YE = 4. - YE ZIRCALOY - ZIRCALOY OXIDE MODEL TZ = 0.0 IF(Z .LT. 1.0E-06) GD TO 10 X02 * X TZ = 2125. + X0Z*(1.6321537E+03 - X0Z*5.3216374E+03) IF(X0Z.LE. 0.19) GO (0 10 TZ = 2.1116553E+03 + X0Z*(1.1590909E+03 - X0Z*2.4621212E+03) IF (XOZ .LE. 0.41) GO TO 10 TZ . 8.9507792E+02 + XOZ . 3.1168831E+03 IF (XOZ .LE. 0.667) GO TO 10 XDZ = 1.334 - XDZ

TABLE D-3.VII

LISTING OF THE PLIQ SUBCODE

TABLE D-3.VII (continued)

```
TZ = 8.9507792E+02 + X3Z * 3.1168831E+03
C
       URANIUM - URANIUM OXIDE MODEL
    10 TU . 0.0
       IF(U .LT. 1.0E-06) GD TO 20
       DS TOC = X/(U+Z) - 2.0
       TU • 3119. - DSTOL DSTOC*1.61E+03
IF(TU -LT. 2700.) TU • 1373.
c
       URANIUM DIOXIDE - ZIRCALOY DIOXIDE MODEL
   20 10 . 0.0
       IF (YE .LT. 1.0E-02) GU TO 30
       ZOU = Z/(U+Z)
       TD = 3119. + 20U*(44.4208 - 20U*1.3423020)
       IF (ZOU .LE. 0.50) GO TO 30
TO = 3119. + ZOU*(-1.1303949E+03 + ZOU * 1.0073297E+03)
       IF(ZOU .LE. 0.52) GO TO 30
TO = 2224.2377 + ZOU + 1114.1132
       IF(ZOU .LE. 0.55) GU TO 30
TD = 3.1809473E+03 + ZOU *(-1.1165869E+03 + ZOU*8.9314194E+02)
       IF (ZOU .LE. 0.93) GO TO 30
TD = 2.1444285E+03 + ZOU * 8.2857142E+02
C
   COMBINE BINARY ESTIMATES ASSUMING DAYGEN TO METAL
RATIO IS MOST IMPORTANT
30 W = (YE/2.) **2
C
       PLIQ = (1 - W) + ((2/(2+U)) + TZ + (U/(2+U)) + TU) + W + TD
CC
       ESTIMATE UNCERTAINTY
       UPLIQ = 10. + 050. + (1. - ABS(Z - U))
                 + 100. * YE + ABS(YE - 2.)
      *
       GD TO 100
   BO WRITE 900, YE
  900 FORMAT (29H
                         DEYGEN TO METAL RATIO . ,E16.6, 38H OUTSIDE RANGE OF
      # MATPRO FUNCTION PSOL)
       STOP
C
  100 CONTINUE
       RETURN
       END
```
CCC

CCCC

CC



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TABLE D-3.VIII

LISTING OF THE PSLV SUBCODE

FUNCTION PSLV(TEMP) PSLV CALCULATES THE SOLUBILITY OF UO2 IN DXYGEN STABLIZED ZIRCALOY PSLV = OUTPUT UD2 IN MELT AT SATURATION (MOLE FRACTION OF MELT) RATIO UO2/ZIRCALOY IS PSLV/(1 - PSLV). THIS RATIO IS INFINITE AT 3119 KELVIN OR HIGHER INPUT TEMPERATURE TEMP THE SOLUBILITY CALCULATED BY THIS FUNCTION IS BASED ON DATA FROM C. POLITIS, UNTERSUCHUNGEN IM DREISTOFFSYSTEM URAN-ZIR KON-SAUER STUFF, KFK 2167 (). PSLV WAS CODED BY D. L. HAGRMAN NOVEMBER 1980 PSLV = 0.0 UPSLV = 0.0 IF(TEMP .LE. 2103.) GJ TO 20 PSLV = 1.19143754 + TEMP*(-1.2127195E-03 + TEMP*3.1857023E-07) IF(TEMP .LT. 2673.) GO TO 10 PSLV = 2.0859332 + TEMP*(-1.1311691E-03 + TEMP*2.5104264E-07) IF (TEMP .GT. 3119.) PSLV = 1.0 10 UPSLV = 0.025 IF(TEMP .GT. 3119.) UPSLV . 0.0 20 CONTINUE RETURN END