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MATPRO

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

EB

PREPARED BY AEROJET NUCLEAR COMPANY FOR

U. S. NUCLEAR REGULATORY COMMISSION

AND

ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION

IDAHO OPERATIONS OFFICE UNDER CONTRACT E(10-1) -1375

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~~Water Reactor Safety Research-~~
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MATPRO

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) developed for use with various LWR fuel rod behavior analytical programs at the Idaho National Engineering Laboratory. Documentation and formulations that are generally semiempirical in nature are presented for uranium dioxide and mixed uranium-plutonium dioxide fuel, zircaloy cladding, gas mixture, and LWR fuel rod material properties.

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

I. INTRODUCTION

Understanding the performance of light water reactor (LWR) fuel under accident conditions is a major objective of the Reactor Safety Research Program being conducted by the U.S. Nuclear Regulatory Commission (NRC, formerly the Atomic Energy Commission). An extensive program has been defined — centered upon out-of-pile and in-pile experiments and their analysis — with the goal of verifying analytical models. These models are expected to be capable of predicting fuel transient performance during a wide range of accident types and conditions, and at any time during the normal useful life of a fuel rod.

The foundation of these codes is the materials properties correlations which define the physical condition of LWR fuel and cladding under changing thermal, nuclear, and physical load conditions. The NRC and the nuclear industry have accumulated a large amount of data on these properties. This handbook describes the materials properties correlations and computer subcodes developed for use with various LWR fuel rod behavior analytical models at the Idaho National Engineering Laboratory.

II. DESCRIPTION OF MATPRO

MATPRO is a computer library of uranium dioxide and mixed uranium-plutonium dioxide fuel, zircaloy cladding, gas mixture, and LWR fuel rod material properties. This handbook describes the 26 subcodes which constitute MATPRO Version 06. Each property is programmed in MATPRO as a separate unit, either as a function or as a subroutine, so that individual correlations may be altered without changes being made elsewhere in the program. This modular format is consistent with the structure of other INEL light water reactor safety analysis programs.

Table I lists the specific materials properties included in MATPRO Version 06 and documented in this handbook. Appendix A presents the uranium dioxide and mixed uranium-plutonium dioxide fuel material properties correlations and subcodes. Appendix B presents the zircaloy cladding thermal and mechanical material properties subcodes. Appendix C presents the gas and LWR fuel rod material properties subcodes; and Appendix D presents various supporting material including a description of the linear interpolation routine used by a number of the subcodes described in Appendixes A and B, a list of the basic SI units and derived units used in MATPRO, and a list of the MATPRO arguments by subcode.

Appendixes A, B, and C contain a separate section for each material property listed in Table I. In each section, the results of a review and evaluation of the data in the literature are presented; the development of a mathematical model based upon theory and experiment is documented; a FORTRAN subcode and comparisons of predictions using that subcode with data are presented; and the limitations of the model are explained. References are provided for each subcode.

The properties described in this handbook have at this time been researched through different degrees of thoroughness. In addition, the amount of data available varies widely among properties. Therefore, deficiencies are present.

Each correlation has been programmed in double precision FORTRAN-IV. In general, the principal variables are expressed as functions rather than as subroutine arguments. In all cases, however, the output quantities are given in the International System (SI) of units^[1,2]. The FORTRAN names of the principal variables have also been standardized to aid the reader.

TABLE I
 PROPERTIES INCLUDED IN MATPRO

<u>Property</u>	<u>Subcode</u>
<u>Fuel Material Properties (Appendix A)</u>	
1. Specific Heat Capacity	FCP
2. Thermal Conductivity	FTHCON
3. Emissivity	FEMISS
4. Thermal Expansion	FTHEXP
5. Elastic Modulus	FELMOD
6. Poisson's Ratio	FPOIR
7. Creep Rate	FCREEP
8. Densification	FUDENS
<u>Cladding Material Properties (Appendix B)</u>	
1. Specific Heat Capacity	CCP
2. Thermal Conductivity	CTHCON
3. Zr-Oxide Emissivity	ZOEMIS
4. Zr-Oxide Thermal Conductivity	ZOTCON
5. Axial Thermal Expansion	CATHEX
6. Diametral Thermal Expansion	CDTHEX
7. Elastic Modulus	CELMOD
8. Strain versus Stress	CSTRAN
9. Stress versus Strain	CSTRES
10. Ultimate Strength	CULTST
11. Creep Rate	CCRPR
12. Poisson's Ratio	CPOIR
13. Shear Modulus	CSHEAR
14. Meyer Hardness	CMHARD

TABLE I (contd.)

PROPERTIES INCLUDED IN MATPRO

<u>Gas and Fuel Rod Material Properties (Appendix C)</u>		<u>Subcode</u>
1.	Gas Thermal Conductivity	GTHCON
2.	Gas Viscosity	GVISCO
3.	Gap Heat Transfer	GAPHTR
4.	Physical Properties	PHYPRO

III. FUTURE VERSIONS OF MATPRO

In order to describe the behavior of LWR fuel rods, the properties of the materials used to fabricate the fuel rods must be known for the entire life of the fuel rods. The material property data for cladding included in this version of MATPRO are generally for unirradiated, cold-worked zircaloy. Anisotropic effects and the effects of irradiation and oxidation during operation or during the course of an accident have in many cases not yet been modeled. Provisions have been made in some of the material subcodes for adding these effects.

Experimental and theoretical investigations of material properties are underway at a number of laboratories. As new information becomes available, the correlations representing those material properties can and will be improved in MATPRO, and revisions of this handbook will be issued.

IV. REFERENCES

1. American Society for Testing and Materials, "Standard Metric Practice Guide", *ASTM Designation E 380-72*.
2. E. A. Mechtly, *The International System of Units: Physical Constants and Conversion Factors*, 2nd revision, NASA SP-7012 (1973).

APPENDIX A
FUEL MATERIAL PROPERTIES

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APPENDIX A

FUEL MATERIAL PROPERTIES

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

Seven properties are given as functions of temperature in the following subcodes. (The fuel densification is considered to be temperature independent.) In addition, four properties are modeled as a function of pellet density, and six have correlations for mixed oxide ($\text{UO}_2\text{-PuO}_2$) fuel. Those having density as an argument are thermal conductivity, elastic modulus, creep rate, and densification. The fuel creep is also modeled as a function of fission rate, stress, and grain size and the fuel densification is modeled as a function of burnup and initial sintering temperature. Mixed oxide correlations are included for each of the eight properties except emissivity and densification. Two additional properties, melting temperature and heat of fusion, are included in a physical properties subcode (PHYPRO, Appendix C, Section 4). The melting temperature is modeled as a function of burnup and, for mixed oxides, as a function of plutonium content.

1. FUEL SPECIFIC HEAT CAPACITY (FCP)

The specific heat capacity of nuclear fuel is needed for temperature calculations in time-dependent fuel behavior problems. Enthalpy data, from which the heat capacity correlations are taken, are employed in stored energy calculations. The subcode FCP presents correlations for the specific heat capacity of UO_2 and of $\text{UO}_2\text{-PuO}_2$ fuel. The correlations are shown in Figure A-1.1.

1.1 UO_2 Specific Heat Capacity

Kerrisk and Clifton^[A-1.1] have fit unirradiated UO_2 enthalpy data from five different investigators, covering the temperature range of 298 to 3,100 K, to one equation and differentiated to obtain the specific heat capacity over that temperature range. The uncertainty of their enthalpy data, for a 95% confidence level, was reported to be less than 1%. The uncertainty of their heat capacity relation was reported to range from 2 to 6% between 500 and 3,000 K. The Bureau of Mines Bulletin #605^[A-1.2] also provides a specific heat capacity relationship for the temperature range 298 to 1,500 K. This relationship agrees very well with that of Kerrisk and Clifton, suggesting that the specific heat capacity of unirradiated UO_2 is adequately characterized.

Fig. A-1.1 Temperature dependence of mixed oxide specific heat capacity calculated by FCP for UO_2 and $\text{UO}_2 - \text{PuO}_2$.

Kerrisk and Clifton's data correlation is used in FCP for the specific heat capacity of the solid phase and extrapolated from 3,100 K to the melting temperature. The specific heat capacity for the liquid phase is based on the data of Leibowitz et al^[A-1.3] (3,173 to 3,523 K). The UO_2 correlations used in FCP are as follows:

UO_2 Solid Phase:

$$C_P = 15.496 \left[\frac{K_1 \theta^2 \exp(\theta/T)}{T^2 [\exp(\theta/T) - 1]^2} + 2 K_2 T + \frac{K_3 E_D}{RT^2} \exp(-E_D/RT) \right] \quad (\text{A-1.1})$$

where

$$\begin{aligned}C_p &= \text{specific heat capacity (J/kg-K)} \\K_1 &= 19.145 \text{ (cal/mol-K)} \\K_2 &= 7.8473 \times 10^{-4} \text{ (cal/mol-K}^2\text{)} \\K_3 &= 5.6437 \times 10^6 \text{ (cal/mol)} \\\theta &= 535.285 \text{ (K)} \\E_D &= 37694.6 \text{ (cal/mol)} \\T &= \text{temperature (K)} \\R &= 1.987 \text{ (cal/mol-K)}.\end{aligned}$$

UO₂ Liquid Phase:

$$C_p = 502.95 \text{ J/kg-K.} \quad (\text{A-1.2})$$

No specific heat capacity measurements are available for irradiated fuel but Bleiberg et al^[A-1.4] have suggested that irradiation will not directly affect UO₂ specific heat capacity.

1.2 UO₂ - PuO₂ Specific Heat Capacity

R. L. Gibby et al^[A-1.5] correlated enthalpy data from Ogard and Leary^[A-1.6] and Leibowitz et al^[A-1.7] for 20 wt% PuO₂ fuel and from Gibby^[A-1.8] for solid 25 wt% PuO₂ mixed oxide fuel. However, they restricted their correlation to samples with oxygen-metal ratios of 1.97 and 1.98 because the enthalpy of the mixed oxide was observed to be a function of stoichiometry above 1,000 C, and oxygen-to-metal ratios of 1.97 to 1.98 are characteristic of commercial mixed oxide fuels. These data were fitted over the temperature range 298 to 3,000 K to the theoretical equation proposed by Kerrisk and Clifton^[A-1.1] for UO₂. The equation was then differentiated to obtain the specific heat capacity as a function of temperature for the solid phase.

The one-standard deviation uncertainty in specific heat capacity was reported to range from 2 to 14% for temperatures from 500 to 3,000 K, respectively. This uncertainty in specific heat capacity corresponds to uncertainties in enthalpy of 0.6 to 1.5%. The enthalpy relation for mixed oxides [the integral of Equation (A-1.1) with use of the mixed oxide constants] is compared in Figure A-1.2 with the enthalpy data for mixed oxides from Leibowitz et al^[A-1.7] and Gibby^[A-1.8].

Leibowitz et al^[A-1.9] also determined a value of 37 cal/mol-K for the specific heat capacity of liquid mixed oxide (as compared with 32.5 cal/mol-K for UO₂). The 12% difference between the specific heats of liquid UO₂ and liquid PuO₂-UO₂ is relatively small

Fig. A-1.2 Comparison of calculated and experimental enthalpy values from Leibowitz et al^[A-1.7] and Gibby^[A-1.8].

and suggests that until more data become available, the UO_2 value can be used for the heat capacity of liquid $\text{PuO}_2\text{-UO}_2$ mixtures. Similar values are theoretically expected for $\text{PuO}_2\text{-UO}_2$ and UO_2 liquid specific heat capacities because of the similarity in structure and atomic bonding.

The $\text{UO}_2\text{-PuO}_2$ correlations employed in FCP, depicted in Figure A-1.1, and coded in Table A-1.I are then:

$\text{UO}_2\text{-PuO}_2$ Solid Phase:

Equation (A-1.1), with

$$\begin{aligned} K_1 &= 19.53 \text{ (cal/mol-K)} \\ K_2 &= 9.25 \times 10^{-4} \text{ (cal/mol-K}^2\text{)} \\ K_3 &= 6.02 \times 10^6 \text{ (cal/mol)} \\ \theta &= 539 \text{ (K)} \\ E_D &= 40,100 \text{ (cal/mol)}. \end{aligned}$$

$\text{UO}_2\text{-PuO}_2$ Liquid Phase:

$$C_p = 502.95 \text{ J/kg-K.} \quad (\text{A-1.3})$$

TABLE A-1.I

LISTING OF FCP SUBCODE

C	FUNCTION FCP(FTEMP,FACMOT,BU,COMP)	FCP 0010
C	IMPLICIT REAL*8(A-H,O-Z)	FCP 0030
C		FCP 0050
C		FCP 0070
C	FCP CALCULATES FUEL HEAT CAPACITY FOR SOLID AND LIQUID PHASES AS	FCP 0090
C	A FUNCTION OF TEMPERATURE AND LIQUID FRACTION.	FCP 0110
C		FCP 0130
C		FCP 0150
C	FTEMP=INPUT FUEL TEMPERATURE(K)	FCP 0170
C	FACMOT=INPUT FUEL FRACTION MOLTEN. FACMOT=1=FUEL ALL MOLTEN AND	FCP 0190
C	FACMOT=0=FUEL ALL SOLID.	FCP 0210
C	BU=INPUT BURNUP, MEGAWATT-SECONDS/KG URANIUM	FCP 0230
C	COMP= PUO2 CONTENT, WEIGHT PERCENT	FCP 0250
C	FCP=OUTPUT FUEL HEAT CAPACITY(JOULES/KG-K)	FCP 0270
C		FCP 0290
C		FCP 0310
C	THE HEAT CAPACITY RELATIONSHIPS USED FOR UO2 IN THIS SUBROUTINE	FCP 0330
C	ARE (1) SOLID IS BASED ON DATA OF KERRISK ET AL (298K TO 3100K),	FCP 0350
C	REFERENCE=NUC.TECH.VOL16 DEC.1972;(2)MOLTEN IS BASED ON DATA OF	FCP 0370
C	LEIBOWITZ ET AL (3173K TO 3523K), REFERENCE=J.NUC.MAT.VOL39(1971).	FCP 0390
C		FCP 0410
C	FCP WAS ORIGINALLY CODED FOR UO2 BY V.F. BASTON IN MARCH 1974.	FCP 0430
C		FCP 0450
C	FCP WAS MODIFIED BY C. S. OLSEN IN JANUARY 1975 TO INCLUDE MIXED	FCP 0470
C	OXIDE HEAT CAPACITY. MODIFIED BY B.W.BURNHAM, JUNE 1975	FCP 0490
C		FCP 0510

TABLE A-1.I (contd.)

LISTING OF FCP SUBCODE

C	THE HEAT CAPACITY RELATIONSHIP USED FOR MIXED OXIDES IN THIS	FCP 0530
C	SUBROUTINE IS BASED UPON GIBBY ET AL (298 TO 3000 K), REFERENCE =	FCP 0550
C	J NUCL MAT VOL 50 (1974) PG 155.	FCP 0570
C		FCP 0590
	DATA UK1,UK2,UK3,UK4,UK5/19.145,535.285,7.8473D-4,5.6437D06,	FCP 0610
	1 3.76946D04/	FCP 0630
	DATA PK1,PK2,PK3,PK4,PK5/19.53,539.0,9.25D-04,6.02D06,4.1004/	FCP 0650
	FHCAP(A,B,C,D,E,T) = A*B**2*DEXP(B/T)/(T**2*(DEXP(B/T) - 1.))**2) +	FCP 0670
	1 2.0*C*T + D*E*DEXP(-E/(1.987*T))/(1.987*T*T)	FCP 0690
	T1 = FTEMP	FCP 0710
	R=FACDOT	FCP 0730
	C1 = COMP/100.0	FCP 0750
	CALL PHYPRO(FTMELT,FHEFUS,CTMELT,CHEFUS,CTRANB,CTRANE,CTRANZ,	FCP 0770
	1 FDELTA,BU,COMP)	FCP 0790
	TM=FTMELT	FCP 0810
	IF (T1 .LT. (TM-1.D-10)) GO TO 10	FCP 0830
	IF ((TM-1.D-10) .LE. T1 .AND. T1 .LE. (TM+FDELTA)) GO TO 30	FCP 0850
	IF (T1 .GT. (TM+FDELTA)) GO TO 50	FCP 0870
10	IF (COMP .LE. 0.0) FCP = 15.496*FHCAP(UK1,UK2,UK3,UK4,UK5,T1)	FCP 0890
	IF (COMP .GT. 0.0) FCP = 15.509*FHCAP(PK1,PK2,PK3,PK4,PK5,T1)	FCP 0910
	GO TO 100	FCP 0930
30	IF (COMP .LE. 0.0) FCP = 15.496*((1.-R)*FHCAP(UK1,UK2,UK3,UK4,UK5,	FCP 0950
1	TM) + R*(32.457))	FCP 0970
	IF (COMP .GT. 0.0) FCP = 15.509*((1.-R)*FHCAP(PK1,PK2,PK3,PK4,PK5,	FCP 0990
1	TM) + R*(32.457))	FCP 1010
	GO TO 100	FCP 1030
50	FCP=32.457*15.496	FCP 1050
	GO TO 100	FCP 1070
100	RETURN	FCP 1090
	END	FCP 1110

1.3 References

- A-1.1. J. F. Kerrisk and D. G. Clifton, "Smoothed Values of the Enthalpy and Heat Capacity of UO_2 ", *Nuclear Technology*, 16 (December 1972).
- A-1.2. C. E. Wicks and F. E. Block, *Thermodynamic Properties of 65 Elements - Their Oxides, Halides, Carbides, and Nitrides*, Bureau of Mines Bulletin #605 (1963).
- A-1.3. L. Leibowitz, M. G. Chasanov, L. W. Mishler, D. F. Fischer, "Enthalpy of Liquid Uranium Dioxide to 3,500°K", *Journ. Nucl. Mat.*, 39 (1971) p 115.
- A-1.4. M. L. Bleiberg, R. M. Berman, B. Lustman, *Effects of High Burnup on Oxide Ceramic Fuels*, WAPD-T-1455 (March 1962).
- A-1.5. R. L. Gibby et al, "Analytical Expressions for Enthalpy and Heat Capacity for Uranium-Plutonium Oxide", *Journ. Nucl. Mat.*, 50, 155 (1974).
- A-1.6. A. E. Ogard and J. A. Leary, in *Thermodynamics of Nuclear Materials*, IAEA, Vienna (1968) p 651.

- A-1.7. L. Leibowitz, D. F. Fischer, M. G. Chasanov, "Enthalpy of Uranium-Plutonium Oxides (U.8 Pu.2)O_{1.97} from 2,350 to 3,000°K", *Journ. Nucl. Mat.*, 42, 113 (1972).
- A-1.8. R. L. Gibby, *Enthalpy and Heat Capacity of U.75 Pu.25 O₂ x (25-1,490°C)*, HEDL-TME-73 19, Hanford Engineering Development Laboratory (January 1973).
- A-1.9. L. Leibowitz, D. F. Fischer, M. G. Chasanov, *Enthalpy of Molten Uranium-Plutonium Oxides*, ANL-8042, Argonne National Laboratory (February 1974).

2. FUEL THERMAL CONDUCTIVITY (FTHCON)

FTHCON calculates UO₂ and UO₂-PuO₂ thermal conductivities (k), the integral of thermal conductivity over temperature, and temperature as a function of the conductivity integral. Fuel behavior codes may employ either the thermal conductivity function directly for temperature calculations, or the conductivity integral ($\int k dT$) and its inverse (temperature as a function of $\int k dT$) for these calculations.

2.1 UO₂ Thermal Conductivity

The thermal conductivity of UO₂ has been the subject of numerous publications [A-2.1 - A-2.12] with fair agreement being exhibited for temperatures up to about 1,400 C. For temperatures above 1,400 C considerable uncertainty exists in the thermal conductivity of irradiated fuel. The effects of irradiation and fuel cracking on thermal conductivity are not clearly established; however, corrections for porosity (density) variation have been established [A-2.13 - A-2.15] and employed. The routine FTHCON uses the thermal conductivity represented by Equation (A-2.1) for 95% TD UO₂ along with the temperature dependent, modified Loeb porosity correction [A-2.13 - A-2.15].

For temperatures between 0 and 1,650 C:

$$k = 100 \left(\frac{1-\beta (1-D)}{1-0.05\beta} \right) \left(\frac{40.4}{464 + T} + 5.86 \times 10^{-5} e^{2.14 \times 10^{-3} T} \right) \quad (A-2.1a)$$

For temperatures between 1,650 C and fuel melting:

$$k = 100 \left(\frac{1-\beta (1-D)}{1-0.05\beta} \right) (0.02 + 5.86 \times 10^{-5} e^{2.14 \times 10^{-3} T}) \quad (A-2.1b)$$

where

k = thermal conductivity (W/cm-C)

D = fraction of theoretical density

β = porosity coefficient = $2.58 - 0.58 \times 10^{-3} T$

T = temperature (C).

Figure A-2.1 contrasts calculated UO_2 thermal conductivities as a function of temperature with experimental data corrected to 95% TD.

Fig. A-2.1 Comparison of measured and predicted [Equation (A-2.1)] UO_2 thermal conductivity for 95% theoretical density material.

The integral of the UO_2 thermal conductivity with respect to temperature is given by Equation (A-2.2). This equation, integrated from 0 C to the UO_2 melting point (2,840 C), results in a value of 97 W/cm, a value consistent with work at AECL, BNW, and GE-APED and with the conclusions of Reference (A-2.10):

For temperatures between 0 and 1,650 C:

$$\int_0^T k dT = 40.4 \ln (464 + T) + 0.027366 e^{2.14 \times 10^{-3} T} - 248.02 \quad (\text{A-2.2a})$$

For temperatures between 1,650 C and fuel melting:

$$\int_{1650}^T k dT = 0.02 (T - 1650) + 0.027366 e^{2.14 \times 10^{-3} T} - 0.93477 \quad (\text{A-2.2b})$$

where

T = temperature (C)

$\int k dT$ = integral of the UO_2 thermal conductivity (W/cm).

The inverse of Equation (A-2.2), where temperature is expressed as a function of the conductivity integral, was obtained by first ignoring the electronic contribution expressed by the exponential function and determining temperature as an analytical solution of the integral and then adding a second order polynomial to represent the effect of the electronic contribution. The constants were determined from a least-squares regression analysis of calculated integral conductivities from Equation (A-2.2) for given temperatures. The result is expressed by Equation (A-2.3):

For temperatures between 0 and 1,650 C:

$$T = 325.903e^{INT/40.4} - 323.403 + 2.6606INT + 0.07540INT^2 \quad (A-2.3a)$$

For temperatures between 1,650 C and fuel melting:

$$T = -2717.39 + 93.1019INT - 0.36928INT^2 \quad (A-2.3b)$$

where

T = temperature (C)

$INT = \int_0^T k dT$ (W/cm).

2.2 UO_2 - PuO_2 Thermal Conductivity

The thermal conductivity of mixed oxides has also been measured and the effects of stoichiometry [A-2.15 - A-2.23], plutonia content [A-2.24 - A-2.26], and porosity [A-2.13] have been evaluated. The highest temperature used in these measurements was 1,825 C.

The thermal conductivity for a given porosity and stoichiometry was correlated with the general expression:

$$\frac{1}{k} = A + BT \quad (A-2.4)$$

where

k = thermal conductivity

T = temperature

A and B are constants.

This equation was reported, by several authors [A-7.19, A-7.22, A-2.24], to be valid over the temperature ranges studied. [However, Craeynest [A-2.18] suggests a 1,000 C upper limit on use of Equation (A-2.4) for stoichiometric mixed oxides.] Equation (A-2.4) results in a continuously decreasing mixed oxide conductivity with temperature; however, mixed oxide thermal conductivities have actually been observed to become constant or to increase at high temperature depending upon stoichiometry. This result is attributed to electronic contributions to the thermal conductivity.

The exact plutonia content was found to have no effect on the lattice conductivity when all of the data for various plutonia contents were considered. Therefore, only one equation was formulated by a least squares analysis of all the data using Equation (A-2.4) with the result that $A = 11.39811$ and $B = 0.0257209$. The data indicate that this equation is valid up to about 1,500 C at which temperature the conductivity approaches a constant value of 0.02 W/cm-C. A term for the electronic contributions given by Equation (A-2.5) was added and the constants C and D were determined with the boundary conditions of a total integral conductivity of 90 W/cm [A-2.27, A-2.28] up to the melting point (2,840 C) and an electronic conductivity, k_e , of 0.002 W/cm-C at 1,500 C.

$$k_e = Ce^{DT} \quad (A-2.5)$$

where C and D are constants and T is temperature.

The thermal conductivity for mixed oxides can then be represented by Equation (A-2.6) using a Eucken-Maxwell porosity correction factor [A-2.13, A-2.23, A-2.29] for fuel densities other than 96% TD.

For temperatures between 0 and 1,550 C:

$$k = \left(\frac{D}{1 + B(1-D)} \right) \left(\frac{1 + 0.04B}{0.96} \right) \left(\frac{38.9}{443 + T} + 1.54 \times 10^{-4} e^{1.71 \times 10^{-3} T} \right) \quad (A-2.6a)$$

For temperatures between 1,550 C and fuel melting:

$$k = \left(\frac{D}{1 + B(1-D)} \right) \left(\frac{1 + 0.04B}{0.96} \right) \left(0.0195 + 1.54 \times 10^{-4} e^{1.71 \times 10^{-3} T} \right) \quad (A-2.6b)$$

where $B = 1.43$, and other symbols have been previously defined. Figure A-2.2 shows a comparison of Equation (A-2.6) with the experimental data normalized to 96% TD using the Eucken-Maxwell relation.

In a similar fashion to that for UO_2 , Equation (A-2.6) is integrated with temperature to obtain the conductivity integral as a function of temperature. Equation (A-2.7) is the result.

Fig. A-2.2 Comparison of measured mixed oxide conductivity with predictions using Equation (A-2.6) for 96% theoretical density UO_2 .

For temperatures between 0 and 1,550 C:

$$\int_0^T k dT = 38.9 \ln (433 + T) + 8.9891 \times 10^{-2} e^{1.71 \times 10^{-3} T - 237.1297}. \quad (\text{A-2.7a})$$

For temperatures between 1,550 C and fuel melting:

$$\int_{1550}^T k dT = 0.0195 (T - 1550) + 8.9891 \times 10^{-2} e^{1.71 \times 10^{-3} T - 1.2730}. \quad (\text{A-2.7b})$$

The inverse function of temperature as a function of the conductivity integral was determined for mixed oxides according to the method previously discussed. The results are expressed by Equation (A-2.8):

For temperatures between 0 and 1,550 C:

$$T = 318.143 \frac{\text{INT}}{38.9} - 315.296 + 2.7276 \text{ INT} + 0.08461 \text{ INT}^2 \quad (\text{A-2.8a})$$

For temperatures between 1,550 C and fuel melting:

$$T = -2386.43 + 86.356 \text{ INT} - 0.32365 \text{ INT}^2 \quad (\text{A-2.8b})$$

where INT and T are defined previously.

2.3 Fuel Conductivity Subcode FTHCON Listing

The listing for the subcode used in MATPRO to calculate fuel conductivity is presented in Table A-2.I.

TABLE A-2.I

LISTING OF FTHCON SUBCODE

```

SUBROUTINE FTHCON(FTEMP,CONINP,FRADEN,COMP,BU,CON,CONINT,CONINV) FT0N0010
IMPLICIT REAL*8(A-H,U-Z) FT0N0020
C FT0N0030
C FTHCON CALCULATES FUEL THERMAL CONDUCTIVITY K, INTEGRAL OF THERMAL FT0N0040
C CONDUCTIVITY WITH TEMPERATURE, AND THE INVERSE OF THE CONDUCTIVITY FT0N0050
C INTEGRAL AS A FUNCTION OF TEMPERATURE, FRACTIONAL DENSITY, AND FT0N0060
C COMPOSITION. FT0N0070
C FT0N0080
C FTEMP=INPUT FUEL TEMPERATURE(K). FT0N0090
C CONINP=INPUT CONDUCTIVITY INTEGRAL, WATTS/M. FT0N0100
C FRADEN=INPUT FRACTIONAL FUEL DENSITY(RATIO OF ACTUAL DENSITY TO FT0N0110
C THEORETICAL DENSITY). FT0N0120
C COMP = PUO2 CONTENT, WEIGHT PERCENT. FT0N0130
C BU=INPUT BURNUP, MEGAWATT-SECONDS/KG URANIUM FT0N0140
C CON=OUTPUT FUEL THERMAL CONDUCTIVITY (WATTS/M-K). FT0N0150
C CONINT=OUTPUT INTEGRAL THERMAL CONDUCTIVITY WITH TEMPERATURE, FT0N0160
C (WATTS/M) FT0N0170
C CONINV=OUTPUT TEMPERATURE AS THE INVERSE OF THE INTEGRAL THERMAL FT0N0180
C CONDUCTIVITY WITH TEMPERATURE, DEG K. FT0N0190
C FT0N0200
C FTHCON WAS DEVELOPED AND PROGRAMMED BY C. S. OLSEN IN FEBRUARY FT0N0210
C 1975 FT0N0220
C FT0N0230
C THE THERMAL CONDUCTIVITY FOR UO2 WAS ADAPTED FROM J.A. CHRISTENSEN FT0N0240
C AND MODIFIED TO REFLECT THE CONDUCTIVITY INTEGRAL OF 97 WATTS/CM. FT0N0250
C FT0N0260
C POROS1(D,B)= (1.00 - B*(1.00 - D))/(1.00 - B*5.0-2) FT0N0270
C UTCON1(T) = 40.4D0/(4.64D2 + T) + 5.86D-5*DEXP(2.14D-3*T) FT0N0280
C UTCON2(T) = 0.02D0 + 5.86D-5*DEXP(2.14D-3*T) FT0N0290
C UTINT1(T) = 40.4*DLOG(4.64D2 + T) + 2.7366D-2*DEXP(2.14D-3*T) - FT0N0300
C 1 2.480239D2 FT0N0310
C UTINT2(T) = 2.0-2*(T-1.65D3) + 2.7366D-2*DEXP(2.14D-3*T) - FT0N0320
C 1 0.93477D0 FT0N0330
C UTINV1(T) = 3.259D2*DEXP(T/4.04D1) - 3.234D2 + 2.660575D0*T + FT0N0340
C 1 7.540202D-2*T*T FT0N0350
C UTINV2(T) = 2.71739D3 + 9.31086D1*T - 3.692756D-1*T*T FT0N0360
C FT0N0370
C THE THERMAL CONDUCTIVITY CORRELATION FOR MIXED OXIDES WAS BASED FT0N0380
C UPON STOICHIOMETRIC MIXED OXIDE DATA CONTAINING 5 TO 30% PUO2. FT0N0390
C FT0N0400
C POROS2(D,B)= D/(1.00 + B*(1.00 - D))*(1.00 + B*4.0-2)/0.96 FT0N0410
C PTCON1(T) = 38.9/(443.D0 + T) + 1.54D-4*DEXP(1.71D-3*T) FT0N0420
C PTCON2(T) = 1.95D-2 + 1.54D-4*DEXP(1.71D-3*T) FT0N0430
C PTINT1(T) = 38.9*DLOG(4.43D2 + T) + 8.9891D-2*DEXP(1.71D-3*T) - FT0N0440
C 1 237.1297D0 FT0N0450
C PTINT2(T) = 1.95D-2*(T - 1.55D3) + 8.9891D-2*DEXP(1.71D-3*T) - FT0N0460
C 1 1.2730 FT0N0470
C PTINV1(T) = 3.181D2*DEXP(T/3.89D1) - 3.153D2 + 2.727559D0*T + FT0N0480
C 1 8.46156D-2*T*T FT0N0490
C PTINV2(T) = -2.38643D3 + 8.63562D1*T - 0.3236527*T*T FT0N0500
C T1 = FTEMP -273.15 FT0N0510
C D1 = FRADEN FT0N0520
C CALL PHYPRO(FTMELT,FHEFUS,CTMELT,CHEFUS,CTRANB,CTRANE,CTRANZ, FT0N0530
C 1 FDELTA,BU,COMP) FT0N0540
C TM1 = FTMELT FT0N0550
C IF (T1 - (TM1 - 273.15))10,10,30 FT0N0560

```

TABLE A-2.I (contd.)

LISTING OF FTHCON SUBCODE

10 IF (COMP .GT. 0.0) GO TO 15	FTON0570
B1 = 2.58 - 0.58D-3*T1	FTON0580
CONINP = CONINP/(POROS1(D1,B1)*100.0)	FTON0590
IF (T1 .GT. 1650.0 .OR. CONINP .GT. 62.2269) GO TO 11	FTON0600
CON = UTCN1(T1) * POROS1(D1,B1) * 100.0	FTON0610
CONINT = UTINT1(T1) * POROS1(D1,B1) * 100.0	FTON0620
CONINV = UTINV1(CONINP) + 2.7315D2	FTON0630
GO TO 100	FTON0640
11 CON = UTCN2(T1) * POROS1(D1,B1) * 100.0	FTON0650
CONINT = (UTINT1(1.65D3) + UTINT2(T1)) * POROS1(D1,B1) * 100.0	FTON0660
CONINV = UTINV2(CONINP) + 2.7315D2	FTON0670
GO TO 100	FTON0680
15 B1 = 1.43	FTON0690
CONINP = CONINP/(POROS2(D1,B1)*100.0)	FTON0700
IF (T1 .GT. 1550.0 .OR. CONINP .GT. 59.6806) GO TO 16	FTON0710
CON = PTCN1(T1) * POROS2(D1,B1) * 100.0	FTON0720
CONINT = PTINT1(T1) * POROS2(D1,B1) * 100.0	FTON0730
CONINV = PTINV1(CONINP) + 2.7315D2	FTON0740
GO TO 100	FTON0750
16 CON = PTCN2(T1) * POROS2(D1,B1) * 100.0	FTON0760
CONINT = (PTINT1(1.55D3) + PTINT2(T1)) * POROS2(D1,B1) * 100.0	FTON0770
CONINV = PTINV2(CONINP) + 273.15D0	FTON0780
GO TO 100	FTON0790
30 A2 = TM1 - 273.15	FTON0800
IF (COMP .GE. 0.0) GO TO 31	FTON0810
B1 = 2.4153D0	FTON0820
CONINP = CONINP/(POROS1(9.124D-1,B1)*100.0)	FTON0830
CON = UTCN2(A2) * POROS1(9.124D-1,B1) * 100.0	FTON0840
CONINV = (CONINP - 97.0D0)/UTCN2(A2) + TM1	FTON0850
GO TO 100	FTON0860
31 B1 = 1.43	FTON0870
CONINP = CONINP/(POROS2(9.124D-1,B1)*100.0)	FTON0880
CON = PTCN2(A2) * POROS2(9.124D-1,B1) * 100.0	FTON0890
CONINT = (PTCN2(A2) * (T1 - A2) + 90.0) * POROS2(9.124D-1,B1) *	FTON0900
1 100.0	FTON0910
CONINV = (CONINP - 90.0D0)/PTCN2(A2) + TM1	FTON0920
100 RETURN	FTON0930
END	FTON0940

2.4 References

- A-2.1. J. C. Hedge, *Measurement of Thermal Conductivity of Uranium Oxide*, AECU-3381, Armour Research Foundation of Illinois Institute of Technology (September 20, 1956).
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- A-2.4. R. D. Reisswig, "Thermal Conductivity of UO₂ to 2,100°C", *Journ. Amer. Ceram. Soc.*, 44, 48 (1961).

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- A-2.8 T. Nishijima, T. Kawada, A. Ishihata, "Thermal Conductivity of Sintered UO_2 and Al_2O_3 at High Temperatures", *Journ. Amer. Ceram. Soc.*, 48, 31 (1965).
- A-2.9 J. Belle, R. M. Berman, W. F. Bourgeois, I. Cohen, R. C. Daniel, *Thermal Conductivity of Bulk Oxide Fuels*, WAPD-TM-586 (Revised), Bettis Atomic Power Laboratory (April 1967).
- A-2.10 J. L. Bates, *High Temperature Thermal Conductivity of "Round Robin" Uranium Dioxide*, BNWL-1431, Battelle Northwest Laboratories (July 1970).
- A-2.11 L. A. Goldsmith and J. A. M. Douglas, *Measurements of the Thermal Conductivity of Uranium Dioxide at 670-1,270°K*, TRG Dept. 2103, Reactor Development Laboratory Windscale (1971).
- A-2.12 G. Fayl and K. Hansen, *In-Reactor Determination of the Thermal Conductivity of UO_2 -Pellets up to 2,200°C*, RISO Dept. 269, Danish Atomic Energy Commission Research Establishment RISO (July 1972).
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- A-2.16 F. J. Hetzler et al, "Thermal Conductivity of 20:80 (Pu:U) O_2 ", *Trans. Amer. Nucl. Soc.*, 8, 36 (1965).
- A-2.17 F. J. Hetzler et al, *The Thermal Conductivity of Uranium and Uranium-Plutonium Oxides*, GEAP-4879, General Electric Company (August 1967).

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- A-2.19 R. L. Gibby, *The Effect of Oxygen Stoichiometry on the Thermal Diffusivity and Conductivity of $U_{.75}Pu_{.25}O_{2-x}$* , BNWL 927, Pacific Northwest Laboratory (January 1969).
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- A-2.28 L. A. Lawrence and J. A. Christensen, "Melting Heat Rating of UO_2 -25 Wt% PuO_2 Fuels", *Nucl. Tech.*, 12, 367 (1971).
- A-2.29 R. L. Gibby, *Fabrication Microstructure and Thermal Conductivity in UO_2 -25 Wt% PuO_2 Sintered Pellets*, HEDL-TME-72-88, Hanford Engineering Development Laboratory (May 1972).

3. FUEL EMISSIVITY (FEMISS)

Emittance is a highly variable property because of its strong dependence on the roughness and reflective properties of the surface. Belle^[A-3.1] presents tabulated values for spectral emissivity of UO_2 at 6,500 Angstrom units for the temperature range 1,000 to 2,400 K. These values are listed in Table A-3.I. A regression analysis of these data was

TABLE A-3.I

SPECTRAL EMISSIVITY OF UO_2

<u>Temperature (C)</u>	<u>Emissivity</u>
727	0.850
1,047	0.789
1,320	0.628
1,482	0.510
1,522	0.515
1,580	0.417
1,647	0.402
1,682	0.484
1,780	0.446
1,947	0.370
1,800 - 2,100 C	0.40

performed to obtain a fifth-order polynomial to be used in the routine FEMISS. The emissivity is assumed to take on constant values outside of the tabulated range: below 900 K, the emissivity is assumed to be 0.83, and above 2,400 K the emissivity is assumed to be 0.40.

Ehlert and Margrave^[A-3.2] have reported the UO_2 spectral emissivity, at 6,500 Angstrom units and at temperatures within 100 C of the melting point, to be 0.416 ± 0.26 . This value agrees closely with Belle's^[A-3.1] value at 2,100 C, suggesting that the assumption of an emissivity of 0.40 from 2,100 C to the melting temperature is reasonable. Spectral emissivity below 1,000 K is difficult to evaluate because the temperature is too low for sufficient brightness. However, requirements for precise emissivity data are of low priority because the uncertainty in fuel surface geometry causes the largest error in calculations requiring the fuel emissivity.

Figure A-3.1 shows the UO_2 emissivity plotted versus temperature using the data from Belle.

3.1 Fuel Emissivity Subcode FEMISS Listing

Table A-3.II is a listing for the subcode FEMISS used in MATPRO to calculate fuel emissivity.

Fig. A-3.1 Emissivity of UO_2 as a function of temperature. Data from Belle, Reference A-3.1.

3.2 References

- A-3.1 J. Belle (ed.), *Uranium Dioxide: Properties and Nuclear Applications*, U.S. Government Printing Office, Washington, D.C. (1961).
- A-3.2 T. C. Ehlert and J. L. Margrave, "Melting Point and Spectral Emissivity of Uranium Dioxide", *Journ. Amer. Ceram. Soc.*, 41, (1958) p 330.

TABLE A-3.II

LISTING OF THE FEMISS SUBCODE

C	FUNCTION FEMISS(FTEMP)	FESS0010
C	IMPLICIT REAL*8(A-H,O-Z)	FESS0020
C		FESS0030
C	FEMISS CALCULATES FUEL EMISSIVITY AS A FUNCTION OF TEMPERATURE.	FESS0040
C		FESS0050
C	FTEMP=INPUT FUEL TEMPERATURE(K)	FESS0060
C	FEMISS=OUTPUT FUEL EMISSIVITY(UNITLESS,RATIO OF RADIANCE)	FESS0070
C		FESS0080
C	THE EMISSIVITY RELATIONSHIP USED IN THIS SUBROUTINE IS A FIFTH	FESS0090
C	ORDER POLYNOMIAL FIT TO THE TABULATED DATA PRESENTED BY J.BELLE	FESS0100
C	(900K<FTEMP<2300K): REFERENCE: UO2 PROPERTIES AND NUCLEAR	FESS0110
C	APPLICATIONS.BY J.BELLE P.197.	FESS0120
C		FESS0130
C	FEMISS WAS CODED BY V.F.BASTON IN MARCH 1974.	FESS0140
C	CODING REVISED BY R.C.YOUNG NOV 74.	FESS0150
C		FESS0160
C	DATA A, B, C, D, E, F/	FESS0170
C	1 19.32400, -6.680-2, 9.3960-5, -6.3970-8, 2.100-11, -2.6670-15/	FESS0180
C	DATA T1, E1, T2, E2 /	FESS0190
C	1 900.. 0.8300, 2300.. 0.4000/	FESS0200
C	T=FTEMP	FESS0210
C	IF (T.LT.T1) GO TO 50	FESS0220
C	IF (T.GT.T2) GO TO 70	FESS0230
C	FEMISS = A + T*(B + T*(C + T*(D + T*(E + T*(F))))	FESS0240
C	GO TO 100	FESS0250
C	50 FEMISS = E1	FESS0260
C	GO TO 100	FESS0270
C	70 FEMISS = E2	FESS0280
C	GO TO 100	FESS0290
C	100 RETURN	FESS0300
C	END	FESS0310
		FESS0320
		FESS0330
		FESS0340
		FESS0350

4. FUEL THERMAL EXPANSION (FTHEXP)

A fuel thermal expansion model is required to predict changes in pellet geometry due to changes in temperature. Linear thermal expansion models have been developed for both UO_2 and $\text{UO}_2\text{-PuO}_2$ fuel. The models used in FTHEXP include three regimes : expansion in the solid phase, expansion due to the phase change at the melting point, and expansion in the liquid phase.

4.1 UO_2 Thermal Expansion

Linear thermal expansion data for unirradiated UO_2 have been published by Burdick and Parker^[A-4.1], Conway et al^[A-4.2, A-4.3], Christensen^[A-4.4], and Hoch and Momin^[A-4.5]. Belle^[A-4.6] also reports data from Lambertson and Handwerk^[A-4.7],

Bell and Makin^[A-4.8], and Murray and Thackray^[A-4.9]. These sets of data are generally consistent although Christensen reported slightly lower values at temperatures below 2,000 C. The effect of irradiation on UO₂ thermal expansion is usually assumed to be negligible. However, no experimental data are available to support this assumption. In-pile fuel thermal expansion is uncertain because accurate descriptions of fuel cracking (resulting from thermal stresses) and healing are not available.

4.1.1 UO₂ Solid Phase. The data between 1,000 and 2,250 C presented by Conway et al^[A-4.2] and the low temperature data of Burdick and Parker^[A-4.1], Lambertson and Handwerk^[A-4.7], Bell and Makin^[A-4.8], and Murray and Thackray^[A-4.9] for the solid phase were fit by regression analysis to a third-order polynomial. The resulting correlation is given by Equation (A-4.1).

$$\frac{\Delta L}{L} = -4.972 \times 10^{-4} + 7.107 \times 10^{-6}T + 2.581 \times 10^{-9}T^2 + 1.140 \times 10^{-13}T^3 \quad (\text{A-4.1})$$

where

$$\frac{\Delta L}{L} = \text{linear thermal expansion}$$

$$T = \text{temperature (C).}$$

4.1.2 UO₂ Phase Change at Melting Point. The data of Christensen^[A-4.4] are used for the thermal expansion due to the phase change at the melting point. Uniform expansion is assumed. The resulting correlation is expressed by Equation (A-4.2) :

$$\frac{\Delta L}{L} = \frac{\Delta L}{L}(T_m) + 3.096 \times 10^{-2} R \quad (\text{A-4.2})$$

where

$$\frac{\Delta L}{L}(T_m) = \text{the thermal expansion given by Equation (A-4.1) with } T_m \text{ equal to the melting temperature}$$

$$R = \text{fraction of molten fuel.}$$

4.1.3 UO₂ Liquid Phase. The coefficient of expansion presented by Christensen^[A-4.4] is used for the liquid phase (above the temperature at which all the fuel is molten). The resulting correlation is given by Equation (A-4.3) :

$$\frac{\Delta L}{L} = \frac{\Delta L}{L}(T_m) + 3.096 \times 10^{-2} + 3.5 \times 10^{-5} (T - T_m) \quad (\text{A-4.3})$$

where

T_m = fuel melting temperature (C)

T = fuel temperature above melting (C).

This correlation and those for the solid and phase change regimes are shown in Figure A-4.1, superimposed upon the data for the solid phase.

4.2 UO₂ - PuO₂ Thermal Expansion

Linear thermal expansion data for solid unirradiated PuO₂ have been published by Tokar et al^[A-4.10] and by Brett and Russell^[A-4.11]. The data of these investigators were fit to a third-order polynomial and programmed in FTHEXP as follows :

$$\frac{\Delta L}{L} = -3.9735 \times 10^{-4} + 8.4955 \times 10^{-6}T + 2.1513 \times 10^{-9}T^2 + 3.7143 \times 10^{-16} T^3 \quad (A-4.4)$$

where T is again the temperature in degrees centigrade. The expansion of solid mixed oxides is calculated from the weighted average of the expansion for UO₂ [Equation (A-4.1)] and the expansion of PuO₂ [Equation (A-4.4)].

The thermal expansion for the phase change and for the liquid phase of mixed oxides is assumed to be the same as that for UO₂ [Equations (A-4.2) and (A-4.3)] because of the similarity in structure of UO₂ and UO₂-PuO₂ mixed oxides.

Figure A-4.2 shows the linear expansion of PuO₂ as a function of temperature as based on the preceding correlations and the data of Tokar et al^[A-4.10] and Brett and Russell^[A-4.11].

4.3 Fuel Thermal Expansion Subcode FTHEXP Listing

Table A-4.I presents a listing of the subcode FTHEXP used for calculation of fuel thermal expansion.

4.4 References

- A-4.1 M. D. Burdick and H. S. Parker, "Effect of Particle Size on Bulk Density and Strength Properties of Uranium Dioxide Specimens", *Journ. Amer. Ceram. Soc.*, 39, (1956) p 181.
- A-4.2 J. B. Conway, R. M. Fincel, Jr., R. A. Hein, "The Thermal Expansion and Heat Capacity of UO₂ to 2,200°C", *Trans. Amer. Nucl. Soc.*, 6, 1 (June 1963).

Fig. A-4.1 Comparison of UO_2 thermal expansion data with that calculated from FHTEXP subcode.

Fig. A-4.2 Comparison of PuO_2 thermal expansion data with that calculated from FHTEXP subcode.

- A-4.3 J. B. Conway, R. M. Fincel, Jr., R. A. Hein, *The Thermal Expansion and Heat Capacity of UO_2 to 2,200°C*, TM 63-6-6, General Electric Company (1963).
- A-4.4 J. A. Christensen, "Thermal Expansion and Change in Volume of Uranium Dioxide on Melting", *Journ. Amer. Ceram. Soc.*, 46, 12 p 607 (1963).
- A-4.5 M. Hoch and A. C. Momin, "High Temperature Thermal Expansion of Uranium Dioxide and Thorium Dioxide", *High Temperatures - High Pressures*, 1, 4 (1969) p 401.

TABLE A-4.I

LISTING OF FTHEXP SUBCODE

	FUNCTION FTHEXP(FTEMP,FACMOT,BU,COMP)	FTXP0010
	IMPLICIT REAL*8(A-H,O-Z)	FTXP0020
C		FTXP0030
C	FTHEXP CALCULATES FUEL LINEAR THERMAL EXPANSION FOR SOLID AND	FTXP0040
C	LIQUID PHASES AS A FUNCTION OF TEMPERATURE AND LIQUID FRACTION.	FTXP0050
C		FTXP0060
C	FTEMP=INPUT FUEL TEMPERATURE (K).	FTXP0070
C	FACMOT=INPUT FUEL FRACTION MOLTEN. FACMOT=1=FUEL ALL MOLTEN AND	FTXP0080
C	FACMOT=0=FUEL ALL SOLID	FTXP0090
C	BU=INPUT BURNUP. MEGAWATT-SECONDS/KG URANIUM	FTXP0100
C	COMP=INPUT PUO2 CONTENT, WEIGHT PERCENT	FTXP0110
C	FTHEXP=OUTPUT FRACTIONAL FUEL THERMAL EXPANSION (UNITLESS,	FTXP0120
C	LT-L298/L298)	FTXP0130
C		FTXP0140
C	THE THERMAL EXPANSION RELATIONSHIPS USED IN THIS SUBROUTINE ARE	FTXP0150
C	(1) SOLID UO2 IS BASED ON DATA OF CONWAY ET AL, TRANS AMER NUCL	FTXP0160
C	SOC, VOL 6 JUNE 1963, BELL AND MAKIN, BURDICK AND PARKER,	FTXP0170
C	LAMBERTSON AND HANDWERK., MURRAY AND THACKRAY. REFERENCE UO2	FTXP0180
C	PROPERTIES EDITED BY J. BELLE.	FTXP0190
C	CHRISTENSEN (MELTING TO 3200C), REFERENCE=J.AM.CER.SOC.VOL46(12)	FTXP0200
C	DEC.1963.	FTXP0210
C		FTXP0220
C	FTHEXP WAS ORIGINALLY CODED BY V. F. BASTON IN MARCH 1974 AND WAS	FTXP0230
C	MODIFIED BY C. S. OLSEN IN FEBRUARY 1975 TO INCLUDE MIXED OXIDE	FTXP0240
C	PROPERTIES AND TO UPDATE UO2 THERMAL EXPANSION.	FTXP0250
C		FTXP0260
C	THE THERMAL EXPANSION FOR SOLID PUO2 IS BASED UPON DATA OF TOKAR	FTXP0270
C	ET AL. REFERENCE IS NUCL TECH VOL 17 147(1973).	FTXP0280
C		FTXP0290
	UEX(T) = -4.972D-4 + 7.107D-6*T + 2.581D-9*T*T + 1.140D-13*T**3	FTXP0300
	PEX(T) = -3.9735D-4 + 8.4955D-6*T + 2.1513D-9*T*T + 3.7143D-16*T**4	FTXP0310
1	3	FTXP0320
	T1 = FTEMP- 273.15	FTXP0330
	R=FACMOT	FTXP0340
	C1 = COMP/100.	FTXP0350
	CALL PHYPRO(FTMELT,FHEFUS,CTMELT,CHEFUS,CTRANB,CTRANE,CTRANZ,	FTXP0360
	1 FDELTA,BU,COMP)	FTXP0370
	TM=FTMELT - 273.15	FTXP0380
	IF (T1 .LT. (TM-1.0-10)) GO TO 10	FTXP0390
	IF (T1 .GE. (TM-1.0-10) .AND. T1 .LE. (TM+FDELTA)) GO TO 30	FTXP0400
	IF (T1 .GE. (TM+FDELTA)) GO TO 50	FTXP0410
10	IF (COMP .GT. 0.0) GO TO 15	FTXP0420
	FTHEXP = UEX(T1)	FTXP0430
	GO TO 100	FTXP0440
15	FTHEXP = (1. - C1)*UEX(T1) + C1*PEX(T1)	FTXP0450
	GO TO 100	FTXP0460
30	IF (COMP .GT. 0.0) GO TO 35	FTXP0470
	FTHEXP = UEX(TM) + R*3.096D-2	FTXP0480
	GO TO 100	FTXP0490
35	FTHEXP = (1. - C1)*UEX(TM) + C1*PEX(TM) + R*3.096D-2	FTXP0500
	GO TO 100	FTXP0510
50	IF (COMP .GT. 0.0) GO TO 55	FTXP0520
	FTHEXP = UEX(TM) + 3.096D-2 + (3.5D-5*(T1 - TM))	FTXP0530
	GO TO 100	FTXP0540
55	FTHEXP = PEX(TM) + 3.096D-2 + (3.5D-5*(T1 - TM))	FTXP0550
	GO TO 100	FTXP0560
100	RETURN	FTXP0570
	END	FTXP0580

- A-4.6 J. Belle (ed.), *Uranium Dioxide: Properties and Nuclear Applications*, USAEC (1961).
- A-4.7 W. A. Lambertson and J. H. Handwerk, *The Fabrication and Physical Properties of Urania Bodies*, ANL-5053, Argonne National Laboratory (1956).
- A-4.8 I. P. Bell and S. M. Makin, "Fast Reactor - Physical Properties of Materials of Construction", *Review of Progress from September 1, 1953 to April 1, 1954*, RDB(C)/TN-70 (1954).
- A-4.9 P. Murray and R. W. Thackray, *The Thermal Expansion of Sintered UO₂*, HERE M/M 22 (no date).
- A-4.10 M. Tokar, A. W. Nutt, T. K. Keenan, "Linear Thermal Expansion of Plutonium Dioxide", *Nucl. Tech.*, 17 (February 1973) p 147.
- A-4.11 N. H. Brett and L. E. Russell, "The Thermal Expansion of PuO₂ and Some Other Actinide Oxides Between Room Temperature and 1,000°C", in *Plutonium 1960*; E. Grison, W. B. H. Lord, and R. D. Fowler (eds.), *Proceedings of the 2nd International Conference on Plutonium Metallurgy, Grenoble, France, April 19-22 1960*, p 397.

5. FUEL ELASTIC MODULUS (FELMOD)

FELMOD calculates the elastic modulus (Young's modulus) for UO₂ and for UO₂-PuO₂ mixed oxides as a function of porosity and temperature. The available data support the assumption of a linear decrease in elastic modulus with both increasing temperature and increasing porosity.

5.1 UO₂ Elastic Modulus

Two reviews have been published that include data for the mechanical properties of oxide fuels, one by Wolfe and Kaufman^[A-5.1] and a more recent review by Vollath^[A-5.2]. The data cited in these reviews were obtained from unirradiated samples; much of Wolfe and Kaufman's data are for mixed oxide fuel (PuO₂-UO₂, ThO₂-UO₂, and ZrO₂-UO₂), and some of the data are from samples that were not well characterized. The correlation presented by Vollath is used in the computer routine FELMOD because this correlation expresses the elastic modulus as a function of both temperature and porosity. The temperature range of the 98% TD fuel data used for the correlation is 1,000 to 1,700 C. Consequently, the correlation was extrapolated below 1,000 C and above 1,700 C. The temperature-dependent portion of the correlation was obtained from deformation experi-

ments with a strain rate of 0.097 m/m per hour. The porosity dependent portion of the correlation was obtained from ultrasonic wave propagation experiments. Vollath's equation is as follows:

$$E = (1,671,500 - 924.4T) [1 - 2.28 (1-D)] / 1.02 \times 10^{-5} \quad (\text{A-5.1})$$

where

E = elastic modulus (N/m^2)

T = temperature (C)

D = fractional fuel density.

The elastic modulus of the fuel as calculated from this correlation is plotted as a function of temperature and porosity in Figure A-5.1.

Fig. A-5.1 Young's modulus as a function of temperature and porosity for UO_2 .

Comparison of the elastic modulus calculated using Equation (A-5.1) with the temperature-dependent data of Marlowe^[A-5.3] used in the General Electric Company fuel rod behavior code BEHAVE-2^[A-5.4] indicates an approximate factor of two difference at 1,000 C. Marlowe's value for elastic modulus at 1,000 C is 1.89×10^{11} N/m². This difference suggests either that the mechanical data are not adequately characterized or that a more consistent correlation should be formulated.

5.2 UO₂-PuO₂ Elastic Modulus

Padel and de Novion^[A-5.5] determined the Young's modulus for 95% theoretical density U_{0.8} Pu_{0.2} O_{2+x} between 25 and 1,300 C. A Young's modulus of 1.808×10^{11} N/m² was measured at 25 C for an oxygen-metal ratio of 1.962; for an oxygen-metal ratio of 2.000, a Young's modulus of 2.265×10^{11} N/m² was measured; and for an oxygen-metal ratio of 2.077, a value of 1.620×10^{11} N/m² was measured. Thus, Young's modulus in mixed oxides varies strongly with change in oxygen-metal ratio. Young's modulus for stoichiometric UO₂-PuO₂ was also found to decrease with temperature as follows :

$$E = 2.265 \times 10^{11} (1 - 7.8431 \times 10^{-4} T) \quad (\text{A-5.2})$$

where

E = Young's modulus (N/m²)

T = temperature (C) .

Nutt and Allen^[A-5.6] determined Young's modulus for U_{0.8} Pu_{0.2} O_{1.984} at room temperature as a function of porosity as follows :

$$E = 2.1027 \times 10^{11} (1 - 2.03 \rho) \quad (\text{A-5.3})$$

where

ρ = the volume fraction porosity

Equations (A-5.2) and (A-5.3) were combined to obtain an overall effect of temperature and porosity on Young's modulus for stoichiometric mixed oxides. The resultant expression given by Equation (A-5.4) is shown in Figure A-5.2 as a function of temperature and porosity and used in FELMOD to calculate Young's modulus for mixed oxides :

$$E = 2.265 \times 10^{11} (1 - 2.03 \rho) (1 - 7.8431 \times 10^{-4} T) . \quad (\text{A-5.4})$$

5.3 Fuel Elastic Modulus Subcode FELMOD Listing

Table A-5.I presents a listing of the MATPRO subcode FELMOD used for calculating Young's modulus for UO₂ and UO₂-PuO₂ mixed oxides.

Fig. A-5.2 Young's modulus as a function of temperature and porosity for UO_2 - PuO_2 mixed oxides.

5.4 References

- A-5.1 R. A. Wolfe and S. F. Kaufman, *Mechanical Properties of Oxide Fuels*, WAPD-TM-587 (October 1967).
- A-5.2 D. Vollath, "Mechanical Properties of Unirradiated Oxide Fuels", *Fuel Rod Model Theory*, Karlsruhe Nuclear Research Center, EURFNR-968 (October 1971).
- A-5.3 M. O. Marlowe, "High Temperature Isothermal Elastic Moduli of UO_2 ", *Journ. Nucl. Mat.*, 33, (1969) p 242.

TABLE A-5.I

LISTING OF FELMOD SUBCODE

```

C      FUNCTION FELMOD(FTEMP,FRADEN,COMP)                      FEOD0010
C      IMPLICIT REAL*8(A-H,O-Z)                                FEOD0020
C                                                                FEOD0030
C      FELMOD CALCULATES FUEL ELASTIC MODULUS AS A FUNCTION OF FEOD0040
C      TEMPERATURE, FRACTIONAL DENSITY, AND PUO2 CONTENT.      FEOD0050
C                                                                FEOD0060
C      FTEMP=INPUT FUEL TEMPERATURE(K)                         FEOD0070
C      FRADEN=INPUT FRACTIONAL FUEL DENSITY (RATIO OF ACTUAL DENSITY TO FEOD0080
C      THEORETICAL DENSITY)                                     FEOD0090
C      COMP=INPUT PUO2 CONTENT, WEIGHT PERCENT.                FEOD0100
C      FELMOD=OUTPUT FUEL MODULUS OF ELASTICITY(N/M**2).        FEOD0110
C                                                                FEOD0120
C      THE MODULUS OF ELASTICITY RELATIONSHIP USED IN THIS SUBROUTINE FORFEOD0130
C      UO2 IS BASED UPON THE FOLLOWING DATA FOR POROSITY DEPENDENCE: FEOD0140
C      M. O. MARLOWE AND A. I. KAZNOFF, J. AM. CER. SOC. 53 90(1970)FEOD0150
C      A. R. HALL, J. NUCL. MAT. 37 314(1970) AND AERE-R 5650 (1967)FEOD0160
C      A. PADEL AND C. DE NOVION, J. NUCL. MAT. 33 40(1969).    FEOD0170
C      R. J. FORLAND ET AL, J. AM. CER. SOC. 50 93(1967).      FEOD0180
C      R. SCOTT ET AL, J. NUCL. MAT. 1 39(1959).                FEOD0190
C      THE TEMPERATURE DEPENDENCE WAS DETERMINED FROM THE FOLLOWING DATA:FEOD0200
C      J. B. WACHTMAN ET AL, WADC-TR-59-278 (1959)              FEOD0210
C      A. PADEL AND C. DE NOVION, J. NUCL. MAT. 33 40(1969).    FEOD0220
C      J. BELLE AND B. LUSTMAN, FUEL ELEMENTS CONFERENCE, PARIS. FEOD0230
C      FOR TEMPERATURES ABOVE 2000 C FOR UO2 AND 1275 C FOR UO2-PUO2, FEOD0240
C      THE ROUTINE ASSUMES A CONSTANT VALUE OF 7.0D+8 N/M**2.  FEOD0250
C                                                                FEOD0260
C      YOUNG'S MODULUS FOR MIXED OXIDES IS BASED UPON DATA FROM NUTT AND FEOD0270
C      ALLEN, J AMER CERAM SOC VOL 53 205(1970) AND PADEL AND NOVION, FEOD0280
C      J NUCL MAT VOL 33 40(1969).                              FEOD0290
C                                                                FEOD0300
C      FELMOD WAS ORIGINALLY CODED BY V. F. BASTON IN MARCH 1974 AND WAS FEOD0310
C      MODIFIED BY C. S. OLSEN IN FEBRUARY 1975 TO INCLUDE MIXED OXIDE FEOD0320
C      PROPERTIES.THE UO2 MODULUS WAS REEVALUATED BY C. S. OLSEN IN JULY FEOD0330
C      1975.                                                     FEOD0340
C                                                                FEOD0350
C      EMOD(E,A,B,D,T) = E * (1.00 - A*T) * (1.00 - B * (1.00 - D)) FEOD0360
C      DATA U1,U2,U3/2.262D11,1.131D-4,2.62/                  FEOD0370
C      DATA P1,P2,P3/2.521D11,7.8431D-4,2.03/                 FEOD0380
C      T1 = FTEMP - 273.15                                       FEOD0390
C      D1 = FRADEN                                                FEOD0400
C      IF (COMP .GT. 0.0) GO TO 10                                FEOD0410
C      IF (T1 .GT. 2000.0) GO TO 30                               FEOD0420
C      FELMOD = EMOD(U1,U2,U3,D1,T1)                             FEOD0430
C      GO TO 100                                                  FEOD0440
C 10 IF (T1 .GT. 1271.066) GU TO 30                               FEOD0450
C      FELMOD = EMOD(P1,P2,P3,D1,T1)                             FEOD0460
C      GO TO 100                                                  FEOD0470
C 30 FELMOD=7.0D+8                                                FEOD0480
C      GO TO 100                                                  FEOD0490
C 100 RETURN                                                     FEOD0500
C      END                                                         FEOD0510

```

A-5.4 S. Oldberg, Jr., *BEHAVE-2: Oxide Fuel Performance Code in Two Spatial Dimensions and Time*, GEAP-13788 (February 1972).

A-5.5 A. Padel and C. H. de Novion, "Constantes Elastiques des Carbures, Mitures et Oxydes d'Uranium et de Plutonium", *Journ. Nucl. Mat.*, 33, 40 (1969).

A-5.6 A. W. Nutt, Jr. and A. W. Allen, "Elastic and Anelastic Response of Polycrystalline $\text{UO}_2\text{-PuO}_2$ ", *Journ. Amer. Ceram. Soc.*, 53, 205 (1970).

6. FUEL POISSON'S RATIO (FPOIR)

Poisson's ratio for both UO_2 and $\text{PuO}_2\text{-UO}_2$ fuels is calculated by the routine FPOIR.

Poisson's ratio can be related to Young's modulus and the shear modulus as follows^[A-6.1] :

$$\mu = \frac{E}{2G} - 1 \quad (\text{A-6.1})$$

where

μ = Poisson's ratio (unitless)

E = Young's modulus (N/m^2)

G = shear modulus (N/m^2).

Watchman et al^[A-6.2] reports mean values for the Young's modulus and shear modulus of UO_2 from two experiments as $E = 2.30 \times 10^{12}$ dynes/cm² and $G = 0.874 \times 10^{12}$ dynes/cm². Consequently, the value of Poisson's ratio is 0.316 and the routine FPOIR returns this value for UO_2 . The Watchman et al paper only considers single crystal UO_2 data at 25 C. However, Padel and de Novion^[A-6.3] have reported values of 0.314 and 0.306 for the Poisson's ratio of polycrystalline UO_2 . These values are in reasonable agreement with Watchman's value of 0.316.

Nutt and Allen^[A-6.4] determined Poisson's ratio for $\text{U}_{0.8}\text{Pu}_{0.2}\text{O}_{2-x}$ at room temperature by determining the Young's modulus and the shear modulus and calculating Poisson's ratio using Equation (A-6.1). Nutt and Allen's room temperature Poisson's ratio for $\text{PuO}_2\text{-UO}_2$ fuel of 0.276 ± 0.094 was found to be independent of density and is returned by FPOIR for mixed oxides.

6.1 Poisson's Ratio Subcode FPOIR Listing

The listing for the subcode FPOIR is presented in Table A-6.I.

6.2 References

- A-6.1 I. S. Sokolnifoff, *Mathematical Theory of Elasticity*, Second Edition, New York: McGraw-Hill Book Company, Inc., 1956.
- A-6.2 J. B. Watchman, Jr., M. L. Wheat, H. J. Anderson, J. L. Bates, "Elastic Constants of Single Crystal UO_2 at 25°C", *Journ. Nucl. Mat.*, 16, 1 (1965) p 39.
- A-6.3 A. Padel and C. H. de Novion, "Constantes Elastiques des Carbures, Mitures et Oxydes d'Uranium et de Plutoniuim", *Journ. Nucl. Mat.*, 33, 40 (1969).
- A-6.4 A. W. Nutt and A. W. Allen, "Elastic and Anelastic Response of Polycrystalline $\text{UO}_2\text{-PuO}_2$ ", *Journ. Amer. Ceram. Soc.*, 205 (1970).

TABLE A-6.I

LISTING OF FPOIR SUBCODE

	FUNCTION FPOIR(FTEMP,COMP)	FPIR0010
	IMPLICIT REAL*8(A-H,O-Z)	FPIR0020
C		FPIR0030
C		FPIR0040
C	FPOIR RETURNS POISSON'S RATIO FOR UO ₂ AND MIXED OXIDES.	FPIR0050
C		FPIR0060
C		FPIR0070
C	FTEMP=INPUT FUEL TEMPERATURE(K).	FPIR0080
C	COMP=INPUT PUO ₂ CONTENT, WEIGHT PERCENT.	FPIR0090
C	FPOIR=OUTPUT POISSON'S RATIO FOR UO ₂ .	FPIR0100
C		FPIR0110
C		FPIR0120
C	POISSON'S RATIO FOR UO ₂ USED IN THIS ROUTINE WAS EVALUATED	FPIR0130
C	FROM THE MEAN OF THE DATA PRESENTED BY WATCHMAN ET AL.	FPIR0140
C	REFERENCE:WATCHMAN ET AL.,JOURNAL OF NUCLEAR MATERIALS VOL.16(1)	FPIR0150
C	PP.39-41(1965).	FPIR0160
C		FPIR0170
C		FPIR0180
C	FPOIR WAS CODED BY V. V. BASTON IN MARCH 1974 AND MODIFIED BY	FPIR0190
C	C. S. OLSEN IN FEBRUARY 1975 TO INCLUDE MIXED OXIDE PROPERTIES.	FPIR0200
C		FPIR0210
C		FPIR0220
C	POISSON'S RATIO FOR MIXED OXIDES IS THE VALUE DETERMINED BY NUTT	FPIR0230
C	AND ALLEN. REFERENCE J AMER CERAM SOC VOL 53 205(1970).	FPIR0240
C	T=FTEMP	FPIR0250
	IF (COMP .GT. 0.0) GO TO 10	FPIR0260
	FPOIR=0.316	FPIR0270
	RETURN	FPIR0280
10	FPOIR = 0.276	FPIR0290
	RETURN	FPIR0300
	END	FPIR0310

7. FUEL CREEP (FCREEP)

The fuel creep model FCREEP predicts the steady state creep rate of UO₂ and UO₂-PuO₂ fuel with semiempirical relationships. Because several factors (stress, temperature, grain size, density, and fission rate during irradiation) affect the steady state creep rate, correlations which reflect these parameters are required so that fuel deformation during operation of a fuel rod can be predicted realistically. A theoretically based model is required to provide guidance in the selection of the most appropriate relationships between variables because the data are limited and exhibit much scatter.

Theoretical creep models that have been applied to ceramic materials are discussed in Section 7.1, and experimental UO₂ and mixed oxide creep data are reviewed in Section 7.2. Information regarding out-of-pile and in-pile creep behavior is included in these discussions. In Section 7.3 the FCREEP models for UO₂ and mixed oxide fuels based upon data and theory are presented.

7.1 Theoretical Models for UO₂ Creep

Theoretical creep models for the out-of-pile creep behavior of UO₂ are generally based on the diffusion of vacancies at low stresses and on dislocation climb at high stresses. During irradiation the fissioning process introduces point defects that affect the creep rate. Theoretical models for out-of-pile creep behavior have received more attention than models for in-pile creep behavior.

7.1.1 Models for Out-of-Pile Creep Behavior. Two models have been proposed and applied to out-of-pile UO₂ creep phenomena: a viscous creep model based on diffusion, and a power-law model based on dislocation climb.

The theoretical model [A-7.1, A-7.2] for viscous creep is based on diffusion of vacancies from grain boundaries in tension to grain boundaries in compression. This model results in a creep rate that is (a) proportional to the diffusion coefficient of the rate controlling species, (b) inversely proportional to the square of the grain size, and (c) proportional to stress. Viscous creep using the Arrhenius equation to represent the diffusion coefficient can be written as follows:

$$\dot{\epsilon} = \frac{A_1}{G^2} \sigma e^{-Q_1/RT} \quad (\text{A-7.1})$$

where

- ϵ = steady state creep rate ($\frac{\text{in.}}{\text{in.-hr}}$)
- A_1 = constant
- σ = stress (psi)
- G = grain size (microns)
- R = gas constant (cal/mol-K)
- T = temperature (K)
- Q_1 = activation energy for diffusion (cal/mol).

Equation (A-7.1) is based on the assumption that the diffusion path is through the lattice (volume diffusion). Therefore, this model results in a creep rate that is inversely proportional to the square of the grain size with an activation energy that corresponds to a value for volume diffusion. However, Coble [A-7.3] has shown that if the diffusion path is along grain boundaries, then the creep rate should be inversely proportional to the cube of the grain size with an associated activation energy that corresponds to a value for grain boundary diffusion.

Equation (A-7.1) was derived solely for diffusion of vacancies in UO_2 ; however grain boundary sliding has also been observed to occur during viscous creep deformation of UO_2 [A-7.4, A-7.5]. Both grain boundary sliding and diffusional creep have the characteristics of linear stress dependence and an activation energy nearly that of self-diffusion. Therefore, distinguishing between mechanisms of grain boundary sliding and diffusion is impossible. Regardless of which mechanism predominates, the form of Equation (A-7.1) is still applicable.

At high stresses, the movement of dislocations due to applied shear stresses within the crystal structure results in a macroscopic movement of material. And, at high temperatures, dislocation climb can occur and results in an increase in deformation rate by allowing dislocations to surmount barriers which normally would restrict movement. Weertman [A-7.6] has proposed a power-law model based on dislocation climb which results in a creep rate proportional to stress raised to the 4.5 power. In this case, creep rate is not a function of grain size. This model is represented by Equation (A-7.2):

$$\dot{\epsilon} = A_2 \sigma^{4.5} e^{-Q_2/RT} \quad (\text{A-7.2})$$

where

A_2 = constant

Q_2 = activation energy (cal/mol)

and the other terms are as defined previously.

7.1.2 Models for In-Pile Creep Behavior. A model has been proposed by Speight [A-7.7] for the irradiation enhancement of UO_2 creep. This model considers the effect of local dislocations and voids on the diffusion creep rate when large numbers of atomic displacements and the production of Frenkel defect pairs occur. Under these circumstances, dislocations show a preference for absorbing the irradiation produced interstitials, the excess vacancies being absorbed at voids. To establish equilibrium, the dislocations and voids behave as continuous thermal vacancy sinks and sources, and the resulting interchange of matter is the process that enhances the creep rate.

The principal result from this model is that the diffusion creep rate is enhanced by irradiation although it has the same temperature dependence as unirradiated fuel.

The defect concentration and the creep rate can be considered to depend upon the fission rate [A-7.8]. Creep experiments using Co^{60} gamma-irradiation sources show no creep deformation at temperatures between 100 and 200 C and stresses from 2,880 to 6,305 psi [A-7.9]. These results suggest that the energy from fission events is necessary to move radiation-produced defects at low temperatures.

7.1.3 Conclusions from the Review of Theory. The creep behavior of UO_2 can be represented by the sum of the previously discussed models as indicated by Equation (A-7.3):

$$\dot{\epsilon} = \frac{A_1 \sigma}{G^2} e^{-Q_1/RT} + A_2 \sigma^{4.5} e^{-Q_2/RT} \quad (A-7.3)$$

The constants A_1 , A_2 , Q_1 , and Q_2 must be evaluated for both irradiated and unirradiated fuel.

7.2 Review of Published Creep Data

The general form of the creep equation has been established from the theoretical models previously discussed. The constants in this equation must be evaluated and the grain size dependency must be verified.

Various techniques have been used to determine the creep rate of ceramics. These techniques include either three- or four-point bending tests, tension or compression of helical springs, and compression testing of cylinders. Each of these techniques induces different stresses in the UO_2 specimens, and, consequently, the creep behavior is expected to change with the technique used. Compressive creep of UO_2 cylinders is preferred because this technique is considered to simulate more closely the conditions of stress induced in light water reactor fuel by fission product swelling, fuel thermal expansion, and cladding and fuel restraint. Although the other techniques are not considered representative and may not be appropriate for determining absolute creep rates, they are considered useful for determining the effects of different parameters on the creep rate.

In this section, creep measurements from UO_2 out-of-pile tests, creep measurements from UO_2 in-pile tests, and creep measurements from mixed-oxide tests are discussed and a summary and conclusions are given.

7.2.1 Out-of-Pile UO_2 Creep Data. Scott et al^[A-7.10] used a three-point-bend apparatus to determine the gross differences in the plastic flow properties of 95% dense stoichiometric and nonstoichiometric UO_2 . Stresses up to 7,000 psi and temperatures between 800 and 1,700 C were used. They found that hyperstoichiometric UO_2 can be deformed readily at 800 C, but stoichiometric UO_2 only becomes plastic above 1,600 C. The activation energy for viscous creep, Q_1 , was estimated to be greater than 95,000 cal/mol.

Armstrong et al^[A-7.4] also used a three-point-bending test to determine the plastic behavior of stoichiometric UO_2 for temperatures between 1,250 and 1,400 C and stresses between 700 and 16,000 psi. The influence of grain size (6 to 40 μ) and density (0.933 to 0.980 of theoretical) was also investigated. The creep curves exhibited instantaneous elastic deflection upon application of the load followed by periods of primary and steady state creep. Tertiary creep was observed when samples were subjected to strains greater than 1.5%.

An Arrhenius plot of the Armstrong et al creep data for 10,000 psi resulted in an activation energy of $91,000 \pm 8,000$ cal/mol for the overall flow process. The steady state creep rate was proportional to $\sigma^{1.3}$. For maximum fiber stresses greater than about 10,000 psi, a power-law stress dependence was indicated, but the results were scattered and the fitting of these data into any of the commonly used creep laws was not possible.

Creep rates decreased with an increase in the density of the UO_2 . This effect was noted for specimens that were sintered at 1,650 C, but not for specimens sintered at 1,750 C. Examination of microstructural features disclosed that materials sintered at lower temperatures have irregularly shaped porosity located predominately at grain boundaries, whereas materials sintered at higher temperatures exhibit porosity located primarily within the grains. The enhancement of creep by porosity for specimens sintered at 1,650 C was attributed to grain boundary sliding induced by the pores located in the grain boundaries.

Grain separation was observed in all the samples. Grain separation occurred predominately along grain boundaries lying transverse to the direction of fiber stresses and on the tension side of the neutral axis. Grain separation would not be expected during compressive creep testing.

The effect of density and grain separation in these tests gives the first indication that creep in bending is not representative of the predominately compressive creep behavior during steady state irradiation of UO_2 .

Armstrong and Irvine^[A-7.11] also studied the creep deformation of nonstoichiometric UO_2 by the three-point bend method. Densities of 96 and 97.2% and grain sizes of 6 and 30 μ were used. Desired oxygen-uranium ratios were obtained by equilibrating a UO_2 specimen with U_3O_8 powder. Creep tests were conducted for temperatures between 975 and 1,350 C, stresses up to 7,000 psi, and oxygen-uranium ratios between 2.02 and 2.16.

For the stress range studied, the creep rate was linearly proportional to stress, and the resultant activation energy (for oxygen-uranium ratios up to 2.08) was 55,700 cal/mol, somewhat less than that for stoichiometric UO_2 . This result indicates that the activation energy may be dependent on the oxygen-uranium ratio. The creep rates were reported to be proportional to the oxygen-uranium ratio for ratios up to 2.08.

Grain boundary sliding occurred in nonstoichiometric as well as stoichiometric samples. This result supports the previous suggestions by Armstrong et al^[A-7.4] that grain boundary sliding must accompany the diffusion mechanism.

Poteat and Yust^[A-7.5] related fuel microstructure with the compressive creep deformation of UO_2 . Fine grain polycrystalline specimens were prepared in the form of right-circular cylinders with 97.5% theoretical density and an average grain size of 10 microns. Fine residual porosity was distributed uniformly on grain boundaries. Compressive creep data were obtained for temperatures between 1,430 and 1,666 C and for stresses between 2,000 and 11,000 psi. As shown in Figure A-7.1, their UO_2 samples exhibited two regimes of creep deformation, viscous creep with an approximate linear stress dependence

Fig. A-7.1 Creep rate as a function of stress for creep data from Poteat and Yust [A-7.5].

and a power-law stress dependence. A least squares analysis of the Poteat and Yust data [A-7.5] shows that the stress coefficient, n , varies from 1.10 to 1.76 at low stresses and from 3.0 to 4.0 at high stresses. An estimate of the activation energy at 7,600 psi is 98,700 cal/mol as shown in Figure A-7.2.

The Poteat and Yust results indicate that at least some deformation of the adjoining lattice accompanies grain boundary sliding. In the viscous creep range, intergranular voids resulted from the formation and growth of chains of pores on the grain boundaries. Grain boundary sliding was observed by the displacement of reference marks on the grains. Some dislocation motion in the volume adjacent to the grain boundary is associated with the sliding process.

In a review of creep experiments performed up to 1967, Wolfe and Kaufman [A-7.12] reported additional data obtained from compression testing of UO_2 cylinders. Temperatures varied from 1,600 to 2,000 C and stresses varied from 1,000 to 5,000 psi. Samples with grain sizes of 18 and 55 microns were used with densities of 97.5 and 98.5% TD, respectively.

Fig. A-7.2 Arrhenius plot of Poteat and Yust [A-7.5] data at 7,585 psi.

Figure A-7.3 shows the stress dependence of the Wolfe and Kaufman creep rate data for different temperatures and grain sizes. The stress exponent for the material with an 18- μ grain size is 1.18 at 1,800 C. The stress exponent of the 55- μ material is 4.72 at 1,800 C and 3.58 at 2,000 C. The 1.18 value corresponds to the values expected for viscous creep. The 55- μ grain size material stress exponents are near the 4.5 value expected for dislocation creep. However, because of the large grain size of 55 μ , a different mechanism may be occurring. The activation energy for the 55- μ material at 3,000 psi is 70,500 cal/mol as shown in Figure A-7.4; again, this value is lower than the values between 90,000 and 100,000 determined by other investigators for small grain material. Therefore, the creep models discussed previously may not be applicable for materials with grain sizes larger than about 40 μ .

Bohaby et al [A-7.13] performed compressive creep tests on stoichiometric UO_2 as a function of temperature (1,400 to 1,760 C), stress (1,000 to 15,000 psi), grain size (4 to 35 microns), and theoretical density (92 to 98% theoretical). Bohaby et al like Armstrong, found that at low applied stresses, their measured creep rates were nearly proportional to stress, as shown in Figure A-7.5, and inversely proportional to the square of the grain size, as shown in Figure A-7.6. These results are in line with the viscous creep model proposed by Nabarro [A-7.1] and Herring [A-7.2]. The activation energy was found to be 90,000 cal/mol and consistent with values for self-diffusion of uranium in UO_2 . The creep rate increased with a decrease in theoretical density.

Fig. A-7.3 Creep rate as a function of stress from Wolfe and Kaufman data with different temperatures and grain sizes.

Fig. A-7.4: Arrhenius plot of Wolfe and Kaufman creep data at 3,020 psi.

The creep rates at stress values greater than 8,000 psi were reported by Bohaboy et al. to be proportional to the stress raised to the 4.5 power. The activation energy for the high stress mechanism was reported to be 132,000 cal/mol, considerably higher than values for self-diffusion in UO_2 . No correlation between grain size and deformation rate was found in this regime.

Bohaboy et al. fit the constants in Equation (A-7.3) to their data and obtained the following equation:

$$\dot{\epsilon} = \left(\frac{9.728 \times 10^6}{(-87.7+D)G^2} \right) \sigma \exp(-90,000/RT) + \left(\frac{1.376 \times 10^{-4}}{(-90.5+D)} \right) \sigma^{4.5} \exp(-132,000/RT) \quad (A-7.4)$$

where D is the percent theoretical density and the preceding definitions apply.

Fig. A-7.5 Creep rate versus stress for data normalized to 95% theoretical density and 17-micron grain size (from Bohaboy et al [A-7.13]).

Fig. A-7.6 Creep rate as a function of grain size (from Bohaboy et al [A-7.13]).

7.2.2 Transition Stress. Wolfe and Kaufman [A-7.12] suggested that the stress at which the transition from viscous creep to power-law creep occurs is only mildly dependent upon temperature, but strongly affected by grain size. Seltzer et al [A-7.14, A-7.15], performed an analysis of the transition stress and presented circumstantial evidence for a power-law creep rate with a 4.5 stress coefficient and a viscous creep rate with an inverse dependence on the square of the grain size. At the transition, Equations (A-7.1) and (A-7.2) can be equated:

$$\frac{A_1 \sigma}{G^2} e^{-Q_1/RT} = A_2 \sigma^{4.5} e^{-Q_2/RT} \quad (A-7.5)$$

Equation (A-7.5) can be put in more general terms by letting n replace the exponent on stress and m replace the exponent on grain size. Solving for the stress at the transition:

$$\sigma_t = \left(\frac{A_2}{A_1} \right)^{n-1} G^{-m/n-1} e^{-(Q_2-Q_1)/RT}. \quad (\text{A-7.6})$$

If the activation energies, Q_2 and Q_1 , are about the same magnitude or the temperature interval is small, then the temperature dependence of σ_t would be expected to be small and can be ignored.

Table A-7.I summarizes the values of $-m/n-1$ from various possible values of m and n .

TABLE A-7. I

VALUES OF $-m/n-1$ FROM POSSIBLE VALUES OF m AND n

<u>m</u>	<u>n = 2</u>	<u>n = 3</u>	<u>n = 4</u>	<u>n = 4.5</u>	<u>n = 5</u>
2	-2	-1	-0.667	-0.571	-0.5
3	-3	-1.5	-1.0	-0.857	-0.75

A plot of the logarithm of the transition stress versus the logarithm of the grain size results in a slope equal to $-m/n-1$. Seltzer^[A-7.14] plotted the transition stress for compression testing versus grain size obtained from Poteat and Yust^[A-7.5], Wolf and Kaufman^[A-7.12], and Bohaboy and Asamato^[A-7.16]. As indicated in Figure A-7.7, a slope of -0.61 resulted from a least squares fit of the data. Comparison of this value with those in Table A-7.I shows that an assumption of the grain size to the second power and a value of n between 4 and 4.5 are consistent with this result. However, the results from bend tests (Figure A-7.7) indicate that the transition stress is not a function of grain size. These results are considered anomalous because of the inconsistency with theoretical predictions and with previous experimental results.

Burton and Reynolds^[A-7.17, A-7.18] have studied the creep behavior of UO_2 as a function of grain size and stoichiometry. Compressive creep tests were employed with either cylindrical pellets or with helical springs with square cross sections. The UO_2 samples used for the stoichiometric tests had grain sizes of 7 and 17 microns and were 97% of theoretical density. Hyperstoichiometric control was obtained by equilibrating CO-CO_2 mixtures with the oxide specimens. Specimens tested to determine the effect of grain size on the UO_2 creep were annealed for various times to obtain the desired grain sizes.

Fig. A-7.7 Transition stress as a function of grain size (from Seltzer [A-7:14]).

The stoichiometric samples showed a transition at about 10,000 psi above which the creep was controlled by dislocation motion. Below the transition, the stress dependence of the creep rate diminished as the diffusional creep made an increasing contribution. However, the stress index n ($\partial \log \dot{\epsilon} / \partial \log \sigma$) determined from the Burton and Reynolds data only approached unity at the highest temperatures and over a narrow stress range. Thereafter, n became increasingly large as creep rates fell to very low values. The creep rate was found to be proportional to $(\sigma - \sigma_0)$ where σ_0 is a stress below which diffusional creep does not contribute to strain. Similar results were obtained for the nonstoichiometric samples.

The occurrence of a threshold stress in Burton and Reynold's work seems dubious because they did not distinguish between their different testing techniques. Qualitatively, the threshold stress seems to occur in the region of very low creep rates where the helical spring samples were probably used (with grain sizes larger than those of the cylindrical creep samples).

7.2.3 In-Pile UO₂ Creep Data. Fission-induced creep tests of UO₂ samples at temperatures less than 900 C have been performed by Sykes and Sawbridge^[A-7.19], Clough^[A-7.20], Brucklacher and Dienst^[A-7.21], and Solomon and Gebner^[A-7.22]. In-pile creep measurements were also performed by Perrin^[A-7.23] at higher temperatures between 1,110 and 1,215 C. All these measurements have been summarized by Solomon et al^[A-7.24]. The test conditions are summarized in Table A-7.II.

Solomon et al^[A-7.24] concluded, on the basis of the data, that the in-pile creep of UO₂ is composed of (a) an elevated temperature regime, in which a normal thermal creep mechanism is enhanced, and (b) a low temperature regime, in which the fission process induces significant temperature independent creep.

The results at temperatures less than 900 C indicate that the creep rate is linearly proportional to fission rate and to stress. As shown in Figure A-7.8, all the data appeared to lie within a broad scatter band that is insensitive to temperature at temperatures below about 1400 K. The evidence was insufficient to determine whether the scatter is due primarily to variations of material properties (density, grain size, stoichiometry, and impurity concentration), or test conditions (temperature, stress, and fission rate). In accounting for the experimental uncertainties, Solomon concluded that material variations probably influenced the fission-induced creep.

A linear regression analysis of the data in Figure A-7.8 results in an activation energy of 72,300 cal/mol for Perrin's data and -2,200 cal/mol for the remaining data. The 72,300 cal/mol value is near that for thermal creep in the viscous regime. The -2,200 cal/mol value indicates a relatively temperature-insensitive creep rate, but it cannot be considered very credible because it was determined from data obtained by different testing techniques and from materials with significant grain size and density variations.

Solomon et al^[A-7.24] consolidated the results of Perrin, the results of the low temperature tests, and Bohaboy's equation to arrive at the following expression:

$$\dot{\epsilon} = \frac{(1.38 \times 10^{-4} + 4.6 \times 10^{-17} F)}{(-90.5 + D)} \sigma^{4.5} e^{-132,000/RT} + \frac{(9.73 \times 10^{-6} + 3.24 \times 10^{-6} F)}{(-87.7 + D) G^2} \sigma e^{-90,000/RT} + 7 \times 10^{-23} \sigma F \quad (A-7.7)$$

where F is the fission rate, D is the density in percent TD, and the other symbols are as previously defined. This equation assumes a fivefold increase in creep rate instead of the fourfold increase reported by Perrin at a fission rate of 1.2×10^{13} fissions/cm³-sec. The fivefold increase was also assumed at higher stresses for which dislocation creep occurs and for which no experimental data are available.

Brucklacher et al^[A-7.25] measured the creep rate of stoichiometric UO₂ with a density of 96% TD and a grain size of 10 μ. At a constant fission rate, the fuel temperature was varied from 250 to 500 C. The sample was compressively loaded with stresses from 140

TABLE A-7.II

TEST CONDITIONS OF LOW TEMPERATURE IN-REACTOR UO_2 CREEP EXPERIMENTS

Reference	Test	Grain Size (μ)	Density (% TD)	Stoichiometry	Fission Rate (fission/ $\text{cm}^3\text{-sec}$)	Temperature Range (C)	Stress Range (psi)
Sykes and Sawbridge	Compression of helical springs	8 to 10	>97.5	-	0.08 to 0.17×10^{13}	525 to 880	875 to 1,810
Brucklacher and Dienst	Compression disks	30 to 40	95	-	11.8×10^{13}	400 to 600	1,130 to 2,560
Clough	Three-point bend	8 to 10	96 to 97	2.0005	0.82 to 1.6×10^{13}	595 to 650	3,830 to 4,420
Solomon and Gebner	Tension helical springs	22	96	2.000	0.26×10^{13}	110	5,005

Fig. A-7.8 Arrhenius plot of irradiated UO_2 creep normalized to a fission rate of 1.2×10^{13} fissions/cm³-sec.

to 5,600 psi. The uranium fission rate was 6.9×10^{-9} fissions/U-sec up to 2.5% uranium burnup and 3.5×10^{-9} fissions/U-sec up to a maximum 8.5% burnup.

For burnups up to 2.5%, the radiation-induced creep rate measured by Brucklacher et al depended linearly on the stress and increased slightly with increasing temperature. (The latter result is different than that of Solomon et al^[A-7.24].) An activation energy of 5,200 cal/mol was obtained from the Brucklacher et al irradiation-induced creep data. This very low activation energy suggests a nearly temperature-independent creep rate. However, since the activation energy reported by Brucklacher et al was determined using materials with the same grain size and density, the value of 5,200 cal/mol is probably more credible than the -2,200 cal/mol value discussed previously and indicated in Figure A-7.8.

Brucklacher et al reported the equation for the fission induced creep up to 2.5% burnup as:

$$\dot{\epsilon} = 5.6 e^{-5200/RT} \sigma \dot{F} \quad (\text{A-7.8})$$

where

$\dot{\epsilon}$ = creep rate (in./in.-sec)

σ = stress (kg/mm²)

R = Gas constant (cal/mol-K)

T = temperature (K)

$\dot{F}$ = fission rate (fission/U atom-sec).

For burnups over 3 to 4%, the stress exponent determined from the data of Brucklacher et al was reported to increase from 1 to 1.5. This change was attributed to a possible change in creep mechanism.

7.2.4 Out-of-pile and In-pile Mixed Oxide Creep Data. Vollath^[A-7.26] reported compressive creep measurements on mechanically mixed oxide pellets of two compositions: 19.5 wt% PuO₂ and 19.4 wt% PuO₂; with densities of 94% TD and 95.5% TD, respectively. Grain size was 10 μ for both materials. Test temperatures were between 1,100 and 1,700 C and stresses were between 700 and 7,000 psi. The fuel stoichiometry was 1.94.

The steady state creep-deformation was represented by the following equation:

$$\dot{\epsilon} = A \sigma^{1 \pm 0.15} e^{-(113,000 \pm 6000)/RT} + B \sigma^{4.5 \pm 0.15} e^{-(175,000 \pm 8000)/RT} \quad (\text{A-7.9})$$

Values for A and B were not given.

Slagle^[A-7.27] measured the high temperature creep of coprecipitated UO₂-20 wt% PuO₂ pellets. One series of tests used pellets with a density of $90.5 \pm 1.0\%$ and a grain size of 4 μ . Another series of tests used pellets with a density of $96 \pm 0.5\%$ and a grain size of 17 microns.

The creep measurements were performed under constant load in a four-point bending apparatus with maximum stresses and strain rates computed from elastic theory. For the 90.5% theoretical density material, as shown by Figure A-7.9, the stress exponent was found to be 2.38 at 1,400 and 2.35 at 1,300 C, with an activation energy of 123,000 cal/mol. For a slightly more dense material (91% TD), stress exponents of 1.97 at 1,400 C and 2.21 at 1,300 C were determined as shown in Figure A-7.10. These exponents are slightly higher than the value expected for viscous creep.

Fig. A-7.9 Creep rate versus stress data of Slagle [A-7.27] for 90.5% TD UO_2 -20 wt% PuO_2 material.

Fig. A-7.10. Creep rate versus stress data of Slagle [A-7.27] for 91% TD UO_2 - 20 wt% PuO_2 material.

For the 96% material, the stress exponents varied from 1.14 to 1.53 as shown in Figure A-7.11. These values are in better agreement with the viscous creep model. The analysis of the temperature dependence of the creep of the 96% dense material resulted in an activation energy of 110,000 cal/mol.

Difficulty was encountered by Slagle in obtaining reproducible strain rates on the same sample when the order of loading the sample was varied. The difficulty in getting reproducibility and the high values for the stress exponents place some doubts on the credibility of these experiments.

Fig. A-7.11 Creep rate versus stress data of Slagle [A-7.27] for 96% TD UO_2 -20 wt% PuO_2 material.

Creep experiments on irradiated and unirradiated mixed oxide fuel have been reported by Perrin [A-7.28]. The samples were fabricated from mechanically mixed UO_2 and 22 wt% PuO_2 powder and sintered to yield pellets with 95% theoretical density, a 3-to-5- μ grain size, and an oxygen-to-metal ratio of 1.98. The samples were tested compressively at temperatures from 910 to 1,125 C, stresses of 2,000 psi, and fission rates from 0.7 to 1.2×10^{13} fissions/cm³-sec.

These experiments indicate that the irradiation-enhanced creep rate of mixed oxide fuel is linearly dependent upon fission rate. Perrin compared his in-pile mixed oxide results with in-pile and out-of-pile UO_2 creep data and suggested that at low temperatures the in-pile creep rate of mixed oxides is athermal, or only moderately dependent on temperature, and at high temperatures the in-pile creep rate is strongly dependent on temperature with an activation energy of the order of the out-of-pile creep data. Perrin reported that for the same stress and temperature conditions and a fission rate of 1.0×10^{13} fissions/cm³-sec, the in-pile creep rate is enhanced by a factor of about 30 over that of unirradiated mixed oxides. However, some of the data indicated an enhancement of only a factor of about 9.

Evans et al^[A-7.29] have performed compressive creep tests on coprecipitated mixed oxide fuel containing 10, 20, and 30 wt% PuO₂ and mechanically mixed and sintered pellets containing 20 wt% PuO₂. Table A-7.III lists the characteristics of the samples. The experiments were performed to determine the effects of density, stoichiometry, composition, grain size, and homogeneity on the compressive creep behavior. The data were analyzed in terms of Equation (A-7.3).

The effect of density was found to be much weaker at high stresses than at low stresses. This effect was attributed to grain boundary sliding which would be enhanced by grain boundary porosity.

The effect of stoichiometry on the steady state creep deformation was very pronounced. An eightfold decrease in creep rate occurred when the stoichiometry decreased from 2.00 to 1.95. This decrease was similar in both low and high stress regions and was attributed to a decrease in metal vacancies as anion vacancies increase (when the stoichiometry decreases from 2.00 to 1.95).

On the basis of only three grain sizes, the creep rate was reported to be inversely proportional to the cube of the grain size. This effect is different from the UO₂ results discussed previously for which the creep rate was found to be inversely proportional to the square of the grain size.

The effect of the PuO₂ concentration was to increase the creep rate as the plutonium content increased. The degree of softening appeared to be similar in both the low and high stress regions; however, the plutonium composition did seem to complicate the activation energy. For example, the activation energies for pure PuO₂ were notably smaller than for UO₂-20% PuO₂, being 70 kcal/mol and 100 kcal/mol in the low and high stress regions, respectively, for pure PuO₂.

A comparison of coprecipitated fuel with mechanically mixed fuel could not be made. In addition to containing a potentially unhomogeneous Pu distribution, the mechanically mixed material contained regions of widely different grain sizes. Because of the different grain sizes, the creep behavior could not be correlated.

Evans et al^[A-7.29] described the creep data for mixed oxide fuel with an oxygen-metal ratio of 1.95 to 1.96 by the following equation:

$$\dot{\epsilon} = A\sigma e^{(-100,000/RT)} + B\sigma^{4.5} e^{(-140,000/RT)} \quad (A-7.10)$$

TABLE A-7.III

PROPERTIES OF SINTERED PELLETS^[a]

Composition (wt% Pu)	Density Range (%TD)	Approximate Grain Size (μ)	Sintered Stoichiometry oxygen-metal ratio ± 0.01	Sintered Stoichiometry oxygen-metal ratio ± 0.01
10	93.5 to 94.5	20	1.98	1.98
20	94.5 to 95.5	20	1.98	1.95
	92.5 to 94.0	22	1.98 and 2.00	1.95 and 2.00
	88.0 to 91.0	22	1.98 and 2.00	1.95 and 2.00
	93.8	4	1.98	1.95
30	93.0 to 94.0	18	1.97	1.95
100	93.0	31	1.78	1.78
Physically Mixed	95.0	12	2.00	2.00

[a] Mixed oxide fuel used by Evans et al^[A-7.29] in compressive creep experiments.

where

- $\dot{\epsilon}$ = steady state creep rate (in./in.-hr)
- $A = 3.1 \times 10^7 \exp [33.3(1-D)] \exp (3.56C)/G^3$
- $B = 4.37 \times 10^{-4} \exp [10.3(1-D)] \exp (3.56C)$
- σ = compressive stress (1,000 to 10,000 psi)
- $R = 1.987 \text{ cal/mol} \cdot \text{K}$
- T = temperature (1,473 to 1,898 K)
- D = fractional density (0.86 to 0.95 TD)
- C = grain size (4 to 35 microns)
- $C = \text{Pu}/(\text{Pu} + \text{U}), (0.2 \text{ to } 0.3)$

Routbort et al^[A-7.30] performed compressive creep tests on mechanically mixed oxide fuel containing 25 wt% PuO₂ to determine the effects of grain size, stress, temperature, and oxygen-metal ratio.

Two batches of material were used. One batch contained 93% ²³⁵U with a grain size of 20 μ and a density of 93% $\pm$ 0.5% of theoretical. The other batch contained 65% ²³⁵U with a grain size of 10 μ and density of 95% $\pm$ 0.5% TD. The pellets from both batches had a nonhomogeneous grain size distribution with the average grain size in the peripheral areas of the pellets being smaller by a factor of 2 to 3 than the central grains. Stoichiometry was controlled by equilibrating specimens with different mixtures of hydrogen and water vapor. Tests for oxygen-metal ratios of about 2.00 were performed by equilibrating the samples with CO-CO₂ mixtures.

The creep rate as a function of stress exhibited two regions: a viscous creep region at low stresses ($\dot{\epsilon} \propto \sigma$) and a power-law creep region ($\dot{\epsilon} \propto \sigma^n$) where n was found to be 4.4. An Arrhenius plot indicated that the creep deformation in the viscous region was thermally activated with an activation energy of $92,500 \pm 3,000 \text{ cal/mol}$. Similarly, the Arrhenius plot for the high stress region yielded an activation energy of $136,800 \pm 5,100 \text{ cal/mol}$.

The creep rate was found to be inversely proportional to the square of the grain size. Thus, this effect indicated that lattice diffusion was involved rather than the grain boundary diffusion reported by Evans et al^[A-7.29]. (Six data points were used in this analysis compared to three in Evan's analysis, so that Routbort's analysis appears to be more nearly credible on the basis of sample size.) The analysis performed by Routbort^[A-7.30] based upon the transition stress and the grain size resulted in a ratio $m/n-1$ of 0.51, compared with theoretical value of 0.57 for the stress exponent of 4.5 and $m = 2$. (A theoretical value

of 0.86 results from the stress exponent of 4.5 and $m = 3$.) Therefore, the creep rate as a function of the reciprocal of the square of grain seems to be a more appropriate relationship for mixed oxides.

The effect of the oxygen-metal ratio on the creep rate was very complex. At 1,650 and 1,550 C in the low stress region, the creep rate decreased with a decrease in oxygen-metal ratio to a minimum at an oxygen-metal ratio of 1.94 to 1.96, respectively. The creep rate then increased with further reductions in the oxygen-metal ratio. As the temperature was further reduced to 1,400 C, this trend was not followed. The creep rate increased as the oxygen-metal ratio decreased in the range 2.0 to 1.9. The oxygen-metal ratio did not affect the stress dependency, but the activation energies did vary with the oxygen-metal ratio in a complicated fashion.

Routbort^[A-7.30] proposed the following equation to represent the creep rate of UO_2 -25 wt% PuO_2 fuel pellets with an oxygen-metal ratio of 1.97:

$$\dot{\epsilon} = \frac{2.28 \times 10^7}{G^2} \sigma e^{-92,500/RT} + 1.00 \times 10^{-3} \sigma^{4.4} e^{-136,800/RT}. \quad (\text{A-7.11})$$

7.2.5 Summary of Experimental Data Review. Two different thermal creep mechanisms have been observed. A viscous creep mechanism with some grain boundary sliding operates at low stresses and the creep rate at low stresses is linearly proportional to stress. A mechanism based upon dislocation climb operates at high stresses and the creep rate at high stresses is proportional to the stress raised to about the 4.5 power. The transition stress from viscous creep to dislocation creep is a function of grain size but not temperature.

In the viscous creep regime, creep rate is inversely proportional to the square of grain size and results from lattice diffusion. The reported activation energy for this process varied between 90,000 and 100,000 cal/mol. The only value for the activation energy for the high stress mechanism was reported by Bohaboy to be 132,000 cal/mol.

During irradiation, the fission process enhances the thermal creep mechanisms at high temperatures and induces creep at low temperatures at which out-of-pile thermal creep normally does not occur.

In the viscous regime, the thermal creep rate is enhanced by a factor of four to five and the activation energy is near that of unirradiated fuel. No data are available for the creep enhancement in the dislocation-controlled regime. The same creep enhancement in the viscous regime was assumed by Solomon et al^[A-7.24] in the dislocation-controlled regime but no data exist to substantiate this assumption.

The fission-induced creep rate has been found to be linearly proportional to stress and fission rate. Early experimenters reported the process to be athermal, but suggested that the temperature dependency could be masked by material variations. Later, Brucklacher^[A-7.25] reported a slightly temperature-dependent process with an activation energy of 5,200 cal/mol. Available data are not sufficient to determine the effects of material properties such as grain size and density on the irradiation-induced creep of UO_2 .

The creep rate of mixed oxides exhibits behavior similar to that observed for UO_2 . The creep rate is controlled by viscous creep at low stresses with an activation energy between 90,000 and 125,000 cal/mol and is controlled by dislocation creep at high stresses with an activation energy between 136,000 and 175,000 cal/mol, and a stress exponent of 4.5. The creep rate is inversely proportional to the square of grain size in the viscous regime, and is enhanced by irradiation by a factor of about 9 to 30 in the viscous regime, but data are unavailable to quantify the effect of fission-induced creep at low temperatures or fission enhanced creep in the dislocation-controlled region at high stresses.

7.3 Subcode FCREEP

The subroutine FCREEP incorporates the model proposed by Bohaboy et al [A-7.13] with the modifications suggested by Solomon et al [A-7.24] for fission-enhanced and fission-induced creep. The fission-induced creep constant proposed by Solomon et al has been changed slightly to reflect the slight temperature dependence of fission-induced creep. Also, the model has been changed to remove the temperature dependence in the transition from viscous creep to dislocation-controlled creep. Irradiation-enhanced creep in the dislocation-controlled regime is not assumed in FCREEP because of the lack of data. The following equation is used to calculate UO_2 creep:

$$\dot{\epsilon} = \frac{(A_1 + A_2 F) \sigma e^{-Q_1/RT}}{(A_3 + D) G^2} + \frac{A_4 \sigma^{4.5} e^{-Q_2/RT}}{(A_6 + D)} + A_7 \sigma F e^{-Q_3/RT} \quad (\text{A-7.12})$$

where

$$A_1 = 9.728 \times 10^6$$

$$A_2 = 3.240 \times 10^{-12}$$

$$A_3 = -87.7$$

$$A_4 = 1.376 \times 10^{-4}$$

$$A_6 = -90.5$$

$$A_7 = 9.24 \times 10^{-28}$$

$$Q_1 = 90,000$$

$$Q_2 = 132,000$$

$$Q_3 = 5,200$$

$$F = \text{fission rate } (8.4 \times 10^{17} \text{ to } 1.18 \times 10^{20} \text{ fissions/m}^3\text{-sec})$$

- σ = stress (1,000 to 16,000 psi)
 R = gas constant (cal/mol-K)
 T = temperature (713 to 2,073 K)
 D = density (0.92 to 0.98 TD)
 G = grain size (4 to 35 μ) stoichiometry (2.00 to 2.01).

The transition stress is given by the following expression:

$$\sigma_{\text{trans}} = 24,000G^{-0.5714} \quad (\text{A-7.13})$$

When the stress is less than σ_{trans} , the appropriate stresses are used in the first term of Equation (A-7.12); for stresses greater than σ_{trans} , the transition stress is used in the first term.

The predictions of FCREEP are compared in Figure A-7.12 with experimental data selected from out-of-pile compressive creep experiments for unirradiated stoichiometric UO_2 and from available experiments for irradiated stoichiometric UO_2 . This comparison includes data from Bohaboy et al [A-7.13], Poteat and Yust [A-7.5], Perrin [A-7.23], and Wolf and Kaufman [A-7.12] for unirradiated UO_2 and from Sykes and Sawbridge [A-7.19], Clough [A-7.20], Solomon and Gebner [A-7.22], Brucklacher and Dienst [A-7.21] as reported by Solomon et al [A-7.24] and Perrin [A-7.23] for irradiated fuel. Data from Burton and Reynolds [A-7.17, A-7.18] are not included because of the uncertainty in separating their compressive pellet data from their helical spring data. Good agreement was obtained among all these data except the data from Poteat and Yust [A-7.5] in the high stress region, data for the 55- μ material used by Wolf and Kaufman [A-7.12], and data from Perrin [A-7.23] for unirradiated fuel. Although the discrepancy in the high stress data of Poteat and Yust [A-7.5] and the data for the large grain size material used by Wolf and Kaufman is less than an order of magnitude, the discrepancy in the unirradiated data of Perrin is about two orders of magnitude. No explanation is available for this discrepancy. The solid line shown in Figure A-7.12 represents perfect agreement between experimental and calculated values.

For the creep of mixed oxides, the equation suggested by Evans et al [A-7.29] is adopted with modifications similar to the UO_2 model for the fission-enhanced creep. The constant, B_1 , has been slightly changed to improve the correlation with experimental data. The steady state creep rate for mixed oxides is represented by the following equation:

$$\dot{\epsilon} = \frac{(B_1 + B_2 F)}{G^2} e^{-Q_1/RT} \sigma e^{B_3(1-D)} e^{B_4 C} + (B_5 + B_6 F) \sigma^{4.5} e^{-Q_2/RT} e^{B_7(1-D)} e^{B_4 C} \quad (\text{A-7.14})$$

Fig. A-7.12 Comparison of irradiated and unirradiated UO_2 experimental data with corresponding calculated values from FCREEP.

where

B_1	=	2.5×10^6
B_2	=	1.88×10^{-12}
B_3	=	33.3
B_4	=	3.56
B_5	=	4.37×10^{-4}
B_6	=	0.0
B_7	=	10.3
Q_1	=	110,000
Q_2	=	140,000
$\dot{F}$	=	fission rate (7.0×10^{18} to 1.2×10^{19} fissions/ m^3 -sec)
σ	=	stress (1,000 to 15,000 psi)
R	=	gas constant (cal/mol-K)
T	=	temperature (1,663 to 1,948 K)
G	=	grain size (18 to 25 μ)
C	=	PuO ₂ concentration (0.1 to 0.3)
D	=	density (0.88 to 0.97% TD) stoichiometry (1.95 to 1.96).

In Figure A-7.13 the predictions of FCREEP are compared with mixed oxide creep data selected from compressive experiments with oxygen-metal ratios between 1.95 and 1.98. This comparison includes data from Evans et al^[A-7.29], Routbort et al^[A-7.30], and Perrin^[A-7.28]. Good agreement is obtained for oxygen-metal ratios between 1.95 and 1.96 and grain sizes between 18 and 23 μ . However, measured values for the 4- μ material used by Evans et al^[A-7.29] are one to two orders of magnitude higher than the corresponding values calculated by FCREEP. Also, the high stress data of Routbort^[A-7.30] (in the dislocation-controlled creep regime) compare favorably with FCREEP calculations even though the oxygen-metal ratio is slightly higher than 1.95. The low stress data lie about an order of magnitude higher than that calculated by the FCREEP model indicating the significance of the stoichiometry on the diffusion mechanism in the viscous creep regime. Perrin's^[A-7.28] data were used to determine the constant for fission-enhanced creep in the viscous creep regime (assuming the same amount of creep enhancement for material with a

Fig. A-7.13 Comparison of mixed oxide experimental data with corresponding values from FCREEP.

1.98 oxygen-metal ratio as for material with a 1.95 oxygen-metal ratio). Reasonably good agreement is achieved for the irradiated material but the calculated values for unirradiated material lie about an order of magnitude less than experimental values. The solid line represents the ideal comparison if perfect agreement is achieved between experimental and calculated values.

7.4 Fuel Creep Subcode FCREEP Listing

Table A-7.IV presents a listing of the subcode FCREEP used for calculation of UO₂ and mixed oxide fuel creep.

TABLE A-7.IV

LISTING OF THE FCREEP SUBCODE

	FUNCTION FCREEP(FTEMP,FSTRES,FDENS,FGRN,FIS,COMP)	FCEP0010
C	FCREEP WAS DEVELOPED AND CODED BY C. S. OLSEN IN NOVEMBER 1974.	FCEP0020
	IMPLICIT REAL*8(A-H,O-Z)	FCEP0030
C	THIS FUNCTION CALCULATES THE STEADY-STATE CREEP RATE FOR UO2 OR UO2	FCEP0040
C	-PUO2 FUEL AS A FUNCTION OF STRESS, TEMPERATURE, FISSION RATE,	FCEP0050
C	DENSITY, GRAIN SIZE, AND COMPOSITION.	FCEP0060
C	FCREEP = STRAIN RATE, M/M/SECOND	FCEP0070
C	FTEMP = TEMPERATURE, DEG KELVIN	FCEP0080
C	FSTRES = STRESS, N/M**2	FCEP0090
C	FDENS = DENSITY, KG/CUBIC METER	FCEP0100
C	FGRN = GRAIN SIZE, MICRONS	FCEP0110
C	FIS = FISSION RATE, FISSIONS/CUBIC METER/SECOND	FCEP0120
C	COMP = PUO2 COMPOSITION, WEIGHT PERCENT	FCEP0130
	DIMENSION A(9),Q(5),B(7)	FCEP0140
	DATA A/9.728D06,3.24D-12,-87.7,1.376D-04,4.5,-90.5,9.24D-28,	FCEP0150
	1 24000.0,-.5714/	FCEP0160
	DATA B/2.5D06,1.88D-12,33.3,1.40,4.37D-4,4.5,10.3/	FCEP0170
	DATA Q/-45294.4,-66431.8,-2617.0,-50327.1,-70458.0/	FCEP0180
	EPS1(T,S,D,G,F) = (A(1) + A(2)*F)*S*DEXP(Q(1)/T)/((A(3) + D)*G*G)	FCEP0190
	EPS2(T,S,D) = A(4) * (S**A(5))*DEXP(Q(2)/T)/(A(6) + D)	FCEP0200
	EPS3(T,S,F) = A(7)*F*S*DEXP(Q(3)/T)	FCEP0210
	STRANS(G) = A(8)*G**A(9)	FCEP0220
	EPS4(T,S,D,G,F,C) = (B(1) + B(2)*F)*S*DEXP(Q(4)/T + B(3)*	FCEP0230
	1 (1. - D) + B(4)*C)/(G*G)	FCEP0240
	EPS5(T,S,D,C) = B(5) * (S**B(6))*DEXP(Q(5)/T + B(7)*(1. - D) +	FCEP0250
	1 B(4)*C)	FCEP0260
	DENS(C) = 11.45*C + (1. - C)*10.96	FCEP0270
	T1 = FTEMP	FCEP0280
	S1 = FSTRES/6.894757D03	FCEP0290
	G1 = FGRN	FCEP0300
	F1 = FIS	FCEP0310
	C1 = COMP/100.0	FCEP0320
	IF (C1 .GT. 0.) GO TO 10	FCEP0330
	D1 = FDENS*100.0/(10.96*1.0D03)	FCEP0340
	T = STRANS(G1)	FCEP0350
	IF (S1 .LE. T) QC1 = EPS1(T1,S1,D1,G1,F1)	FCEP0360
	IF (S1 .GT. T) QC1 = EPS1(T1,T,D1,G1,F1)	FCEP0370
	QC = QC1 + EPS2(T1,S1,D1) + EPS3(T1,S1,F1)	FCEP0380
	FCREEP = QC/3600.0	FCEP0390
	GO TO 20	FCEP0400
10	D1 = FDENS/(DENS(C1)*1.0D03)	FCEP0410
	QC = EPS4(T1,S1,D1,G1,F1,C1) + EPS5(T1,S1,D1,C1)	FCEP0420
	FCREEP = QC/3600.0	FCEP0430
20	CONTINUE	FCEP0440
	RETURN	FCEP0450
	END	FCEP0460

7.5 References

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8. FUEL DENSIFICATION (FUDENS)

During the first few thousand hours of reactor operation, some UO_2 fuel has been found to densify, thereby creating axial gaps in the fuel stack^[A-8.1]. The subroutine FUDENS calculates the extent of UO_2 densification as a function of initial fuel density and the fuel pellet sintering temperature during manufacture.

The sintering of cold pressed UO_2 powder compacts may be divided usefully into three regimes: (a) the formation of necks between particles, (b) the decrease of interconnected porosity, and (c) the subsequent densification of isolated pores^[A-8.2]. The last stage begins when about 92 to 93% theoretical density is reached. The porosity in fuels with density below about 92% and which have been sintered at relatively low temperatures is essentially open and located along grain edges. The closed porosity in low density materials sintered at low temperatures is also located along grain boundaries. However, at higher sintering temperatures accelerated grain growth occurs, and the closed porosity may be found inside the grains even in low density compacts^[A-8.3]. The in-reactor densification phenomena involves the third sintering regime in which fine isolated closed porosity, located either at grain boundaries or within the grains, is annihilated.

The applicable literature on the final stage of out-of-pile and in-pile fuel densification is discussed in the following section. As a result of this literature review, the FUDENS model was selected and is described.

8.1 Literature Review

Collins and Hargreaves^[A-8.4] contrasted measurements of out-of-pile sintering rates at temperatures greater than 1,600 K with the sintering rates of fuel irradiated in the Windscale Advance Gas-Cooled Reactor (WAGR). The observed out-of-pile densification was attributed to the sintering of grain boundary porosity and was characterized by an activation energy of 69,200 cal/mol for grain boundary diffusion. Extrapolation of these results to the approximate 1,000 K temperatures of the in-pile material indicated that negligible thermal sintering would be expected after a few hundred hours at this temperature. In addition, no evidence of sintering was observed in out-of-pile anneals at 1,173 K and a pressure of 2.06 MN/m² for several months. However, fuel irradiated to less than 0.3% burnup of heavy atoms at fuel surface temperatures between 1,000 and 1,100 K experienced significant reductions in the pellet diameters. This shrinkage was attributed to irradiation induced sintering of the initial fuel porosity.

From the fuel sintering measurements in the WAGR, Collins and Hargreaves^[A-8.4] arrived at an empirical expression for the volume change of porosity as a function of burnup as follows:

$$V = A V_o e^{-0.002I} + (1-A) V_o \quad (\text{A-8.1})$$

where

V = fuel porosity at burnup I

I = fuel burnup (MWd/MtU)

V_0 = initial porosity of the fuel (%)

A = constant between 0.5 and 0.6.

This expression is reported as appropriate for WAGR fuel in the temperature range between 1,000 and 1,100 K. In this expression, the important densification parameters are burnup and initial density.

Collins and Hargreaves^[A-8.4] suggested that a complete description of the densification rate of uranium dioxide under irradiation demands a knowledge of the initial size distribution of the as-manufactured porosity in addition to the total volume of porosity because of the differing sintering rates of pores of different sizes. However, the morphology of the porosity in the UO_2 fuel they used was not determined.

Pores with diameters less than 3μ were reported by Collins and Hargreaves to be strongly affected by irradiation, causing a change in density, but pores larger than 100μ were reported stable at temperatures below 1,500 K.

Rolstad et al^[A-8.5] measured in the Halden HBWR^[a] the fuel stack shortening of UO_2 with 87 to 95% TD, two different heat ratings, three different degrees of fuel stability as determined by the fuel sintering temperature, and two different gap widths.

The axial length change as a function of burnup for different power levels indicated very little difference in the densification of similar fuel rods operating at quite different power levels. This result suggests that fuel densification is probably independent of fuel temperature. This conclusion is in agreement with the fission-induced sintering rates proposed by Collins and Hargreaves^[A-8.4]. The amount of fuel stack shortening was found to depend mainly on the out-of-pile thermal fuel stability (sintering temperature), initial density, and burnup.

Rolstad et al^[A-8.5] used two equations to correlate their data. The first equation [Equation (A-8.2)] predicts the magnitude of shortening as a function of the percent theoretical density (DENS) and sintering temperature in degrees centigrade (TSINT) at a burnup of 5,000 MWd/Mt UO_2 :

$$\frac{\Delta L}{L} = 22.2 \frac{(100 - \text{DENS})}{(\text{TSINT} - 1,180)} \quad (\text{A-8.2})$$

[a] Test reactor located in Halden, Norway.

The effect of burnup was introduced through the use of a master curve created by shifting all curves vertically to agreement at 5,000 MWd/MtUO₂ and then horizontally to achieve the best agreement at the low burnup portion of the curves. The master curve is described as follows:

$$\frac{\Delta L}{L} = 3.0 - 0.93 e^{-BU} - 2.07 e^{-35BU} \quad (A-8.3)$$

where

BU = the burnup (MWd/kgUO₂).

This equation results in a very fast length change with burnup at low burnup and a much slower length change with burnup at higher burnup levels. After a burnup of 5,000 to 6,000 MWd/MtUO₂ very little additional densification is calculated. Figure A-8.1 shows the comparison of results of this model with Halden data (figure obtained from Reference A-8.5).

Ferrari et al^[A-8.6] measured UO₂ fuel pellet densification using moveable incore flux detectors in commercial reactors and by postirradiation examination of selected Saxton^[a] test rods. Fuel densification was reported to initially occur quite rapidly but to end (become equal to the swelling rate) after about 6,000 to 10,000 MWd/MtU as shown by Figure A-8.2. These results are consistent with the measurements of Rolstad et al^[A-8.5]. For a given density (92%), the extent of densification was reported to vary significantly with microstructure, but no details of the microstructure were reported.

Ferrari et al^[A-8.6] reported that power levels between 1.5 and 17 kW/ft did not significantly affect densification. This result is also in agreement with Collins and Hargreaves^[A-8.4] and Rolstad et al^[A-8.5]. The axial shrinkage was suggested to be controlled by densification in the shoulder of the fuel pellets, a region of the fuel pellets which generally operates at temperatures below 800 C. These temperatures are too low for in-pile densification to be accounted for by thermal mechanisms and Ferrari et al proposed that the kinetics of densification are compatible with irradiation-enhanced diffusion processes.

Metallographic measurements on the Saxton fuel indicated that the irradiation-enhanced densification was associated with the disappearance of fine pores and pore shrinkage significantly decreased with increasing pore size. However, in some fuels not all fine porosity disappears during irradiation because of increased pressure from entrapped gas. Ferrari et al suggested that densification could be reduced through both microstructural control of the fuel pellet and a reduction of the fine porosity content. Both of these factors are influenced by the pellet fabrication process, especially sintering temperature and the use of so called "pore formers". Ferrari reported that experimental fuel of 98% TD has been made and demonstrated in the Saxton reactor to be relatively stable.

[a] A small prototype closed cycle PWR designed by the Westinghouse Electric Corporation and located in Saxton, Pennsylvania.

Fig. A-8.1 Comparison between measured and predicted fuel stack shortening [A-8.5].

Heal et al^[A-8.7] have developed stable-density UO_2 fuel through control of porosity size. They calculated that shrinkage of closed pores would continue until the internal pressure of trapped gas in the pores matched the surface tension forces causing shrinkage. Thus, the criterion for void stability at any temperature is

$$\frac{2\gamma_s}{r} < P < \frac{2\gamma_s}{r} + \sigma_F \quad (\text{A-8.4})$$

where

r = pore radius

γ_s = surface energy of the UO_2

P = gas pressure in the void

σ_F = stress necessary to cause primary creep.

Fig. A-8.2 Fuel stack length changes for 92% TD UO_2 processed by different techniques [A-8.6].

When the void size is $20\ \mu$ or greater, no further shrinkage can occur and even a $10\text{-}\mu$ void is expected to only shrink to 6 to $7\ \mu$ before gas stabilization occurs, according to Heal et al [A-8.7]. A $1.0\text{-}\mu$ void, however, would have to shrink to $0.2\ \mu$ before gas stabilization would occur, thus causing considerable densification [A-8.7].

Fuel pellets with a 91 to 95% TD and porosity sizes greater than $25\ \mu$ manufactured by the controlled porosity method were irradiated by Heal et al [A-8.7] to 1.4×10^{26} fissions/ cm^3 with center temperatures up to $1,600\ \text{C}$. Postirradiation examination of these pellets showed significantly less than 1% volume densification. Other controlled porosity fuel is still being irradiated and results are not available.

Burton and Reynolds [A-8.8] measured the shrinkage of fuel pellets during the final stage of out-of-pile sintering of 96.5% TD UO_2 with isolated porosity located at grain boundaries. The density change as a function of time was measured for three specimens at different temperatures. The densification rate initially occurred very rapidly and then decreased to a much slower rate at longer times. The shapes of these curves are very similar to those for the in-pile densification of UO_2 ; however, in-pile densification apparently occurs at much lower temperatures. This reduction in the sintering rate with time can arise for several reasons: (a) grain boundaries may migrate away from cavities during annealing, thus removing the short-circuiting diffusion path of vacancies away from cavities; (b) when significant entrapped gas is present, cavities may shrink until they become stabilized as the internal gas pressure becomes equal to the surface tension of the cavity as proposed by Heal et al [A-8.7]; or

(c) the number of cavities can become progressively reduced as densification proceeds. The first and second reasons were rejected by Burton and Reynolds because (a) the majority of the cavities in their samples remained on grain boundaries during sintering, and (b) smaller cavities sintered to closure. Therefore, Burton and Reynolds^[A-8.8] suggest that the reduction in the sintering rate with time is due only to the progressive reduction in the number of cavities. In this case, the shape of the sintering curve is expected to be predicted quantitatively from the porosity distribution and a Hull and Rimmer^[A-8.9] relationship:

$$\frac{dV}{dt} = \frac{k w D_{gb}}{T X} \quad (A-8.5)$$

where

- V = volume
- t = time
- w = grain boundary width
- D_{gb} = grain boundary self-diffusivity
- X = mean cavity spacing on the grain boundary
- T = temperature
- k = constant, function of temperature.

Reasonably good agreement was obtained despite the approximations required to evaluate this equation and the errors in determining the porosity distribution of the samples. Both the shape of the predicted curve and the absolute magnitude of the values were reported to be in good agreement, demonstrating that the decrease in sintering rate with time is associated with only the progressive reduction in the number of cavities. However, the calculation was only considered approximate because a constant cavity spacing was assumed for each time step in changing from one volume size to the next one.

The similarity between the out-of-pile densification and in-reactor densification strongly suggests the importance of pore size distribution and volume to in-reactor densification.

Marlowe^[A-8.10] proposed a model for diffusion-controlled densification and modified the model to include fuel swelling contributions to the density changes as well as an irradiation-induced diffusivity which provides atomic mobility for grain growth and densification. His model is expressed by the following equation:

$$\rho = \rho_o \exp(-S F t) + \frac{M}{A} \exp \left[-S \left(\frac{G_o^3}{AD} + F t \right) \right] \left(\frac{1 + AD F t}{G_o^3} \right) \quad (A-8.6)$$

where

S = fractional volumetric fuel swelling per unit exposure

G_0 = initial grain size

M = densification rate constant for the material prior to irradiation $M = (G^3/D) \frac{d\rho}{dt}$

A = grain growth rate constant for the material prior to irradiation $A = 3G^2 \frac{dG^3}{dt}$

F = volumetric fission rate

t = irradiation time

D = diffusion coefficient.

This model is based on densification and grain growth rate parameters, which must be determined experimentally for any particular fuel. The parameters, M and A, strongly affect the predicted in-reactor densification behavior through grain size modification. The model allows for complete pore elimination and, in fact, densities greater than theoretical for the matrix material. Thus, an upper limit to the density must be calculated:

$$\rho_{\max} = \frac{1}{1 + SFt} \quad (\text{A-8.7})$$

The parameters used in this model (grain growth rate, grain size, and diffusion coefficient) strongly imply that material properties affect the extent of densification.

8.2 Conclusions

Fuel densification data are rather scarce. The general mechanics of fuel densification appear to be understood, although a model of the phenomena based on first principles is not available.

Collins and Hargreaves^[A-8.4] suggested that in-reactor densification is radiation induced, whereas Ferrari et al^[A-8.6] proposed irradiation-enhanced thermal densification. However, both authors reported that their in-reactor densification was independent of temperature. Therefore, irradiation-induced densification appears to be the appropriate mechanism. The in-reactor densification rate was observed by Rolstad et al^[A-8.5] and Ferrari et al^[A-8.6] to decrease with burnup and to become zero near 5,000 to 10,000 MWd/MtU. At this burnup, most of the fine porosity has disappeared and the rest of the porosity is beginning to fill with fission gases. Also, fuel swelling may also be compensating for the densification at higher burnups. Empirical exponential equations were proposed by Collins and Hargreaves^[A-8.4], Rolstad et al^[A-8.5], and Marlowe^[A-8.10] to relate densification to burnup.

Collins and Hargreaves^[A-8.4] suggested, and Burton and Reynolds^[A-8.8] showed, for at least thermal sintering, that a complete description of UO₂ fuel densification requires knowledge of the pore size distribution and the associated pore volumes. The work performed by Marlowe^[A-8.10] also suggests that grain size and grain growth parameters may affect the densification rate. However, no material characterizations (porosity distribution, grain size, pore morphology) of the fuel used in any of the irradiated tests were reported. Therefore, no quantitative relationships between densification and material properties can be developed in spite of the allegations by Collins and Hargreaves^[A-8.4], Ferrari et al^[A-8.6], Heal et al^[A-8.7], and Marlowe^[A-8.10] that the material characteristics influence the in-reactor densification rate.

8.3 FUDENS Model

Models for fuel densification were proposed by Collins and Hargreaves^[A-8.4], Rolstad et al^[A-8.5], Burton and Reynolds^[A-8.8], and Marlowe^[A-8.10]. The empirical model proposed by Rolstad et al is the best model considering the state-of-the-art of in-reactor fuel densification. The models of Rolstad et al^[A-8.5] and of Collins and Hargreaves^[A-8.4] are similar except Rolstad's model correlates the fuel characteristics through the fuel sintering temperature. Although Marlowe's model attempts to correlate material properties, this model is still based on diffusion-controlled densification and its application to irradiation-induced densification has not been substantiated. The model of Burton and Reynolds is based on thermal densification and also has not been verified for in-reactor use. The Burton and Reynolds model does predict the same reduction of small pores as observed in-pile, but to relate this reduction to in-reactor densification is difficult.

The Rolstad et al model^[A-8.5], as originally proposed, is solved graphically as indicated in Figure A-8.3. The curves in Figure A-8.3a are defined by Equation (A-8.8) for various sintering temperatures and the curve in Figure A-8.3b is defined by Equation (A-8.9):

$$(\Delta L/L) = 22.2 \times \frac{(100 - \text{DENS})}{(\text{TSINT} - 1,180.0)} \quad (\text{A-8.8})$$

$$\left(\frac{\Delta L}{L}\right) = -3.0 + 0.93 e^{-\text{BU}} + 2.07 e^{-35\text{BU}} \quad (\text{A-8.9})$$

where

$\Delta L/L$ = length change (%)

TSINT = fuel sintered temperature (C)

DENS = initial density (%TD)

BU = burnup (MWd/kg UO₂).

Fig. A-8.3 Graphical solution of Rolstad's model [A-8.5], where TD is percent of theoretical density, TS is sintering temperature (C), and BU is burnup.

The use of these equations to find the length change as a function of burnup (for fuel having an initial density, DENS, after sintering at temperature, TSINT) is shown in Figure A-8.3. For an initial density of 91% TD and sintering temperature of 1,500 C, the left scale of Figure A-8.3 shows that the eventual length change will be about 0.6%. To determine the change as a function of burnup, new axes are drawn in Figure A-8.3b as shown by the dashed lines. With the (x,y) origin of these new axes interpreted to be zero burnup and zero length change, the solid curve in Figure A-8.3b then gives $\Delta L/L$ as a function of burnup. The 0.6% fractional length change is then seen to require about 5,000 MWd/MtU burnup.

The numerical equivalent to this graphical solution is incorporated into the subroutine FUDENS. Newton's method^[A-8.11] was selected for the iterative determination of the new origin because of its rapid convergence. Between four and ten iterations are typically required to determine the position of the new axes with a 0.0002% convergence criterion defined by

$$\text{ERR} = 100 (X - X_1)/X \quad (\text{A-8.10})$$

where

X = current value of BU in Equation (A-8.9)

X_1 = preceding value of BU in Equation (A-8.9).

Predicted values from FUDENS are compared with experimental data in Figure A-8.4. Although the data and model are based upon axial length measurements, the fuel can be considered isotropic and, therefore, the model can be applied to the fuel radius.

8.4 Fuel Densification Subcode FUDENS Listing

The listing of the subcode FUDENS used to calculate fuel densification is shown in Table A-8.I. In the event that a sintering temperature is not provided, the routine assumes a temperature of 1,600 C.

8.5 References

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Fig. A-8.4 Comparison of experimental [A-8.5] and FUDENS calculated values of length change.

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TABLE A-8.I

LISTING OF THE FUDENS SUBCODE

```

C      FUNCTION FUDENS(TSINT,FDENS,BU,TTIME)                                FUDS0010
C                                                                              FUDS0020
C      FUDENS IS A SUBROUTINE THAT CALCULATES THE EXTENT OF FUEL          FUDS0030
C      DENSIFICATION AS A FUNCTION OF BURNUP, SINTERING TEMPERATURE,      FUDS0040
C      AND INITIAL DENSITY.                                                FUDS0050
C      N = NUMBER OF ITERATIONS AND                                       FUDS0060
C      M = NUMBER OF INTERVALS FOR NEWTON'S SOLUTION METHOD WHERE          FUDS0070
C      EPS = CONVERGENCE CRITERIA                                         FUDS0080
C      FUDENS WAS DEVELOPED AND PROGRAMMED BY C. S. OLSEN IN JANUARY 1975 FUDS0090
C      UPDATED AND CORRECTED BY B. W. BURNHAM. OCTOBER 1975              FUDS0100
C      FUDENS = DIMENSIONAL CHANGE, PERCENT                              FUDS0110
C      TSINT = FUEL SINTERING TEMPERATURE, DEG K.                        FUDS0120
C      FDENS = FUEL DENSITY, KG/CUBIC METER                               FUDS0130
C      BU = BURNUP. MEGAWATT-SECONDS/KG URANIUM                           FUDS0140
C      TTIME = TIME, SECONDS                                              FUDS0150
C      IMPLICIT REAL*8 (A-H,O-Z)                                          FUDS0160
C      DIMENSION A(3),B(5)                                                FUDS0170
C      DATA A/22.2,100.,1180./                                           FUDS0180
C      DATA B/3.0,0.93,1.0,2.07,35.0/                                    FUDS0190
C      DLEN1(TSIN,DENS) = A(1)*(A(2) - DENS)/(TSIN - A(3))                FUDS0200
C      DLEN2(ALEN,BU,ABU) = -B(1) + ALEN + B(2)*DEXP(-B(3)*(BU + ABU))    FUDS0210
C      1 + B(4)*DEXP(-B(5)*(BU + ABU))                                     FUDS0220
C      DLEN3(BU) = -B(2)*B(3)*DEXP(-B(3)*BU) - B(4)*B(5)*DEXP(-B(5)*BU) FUDS0230
C      FUDENS IS BASED UPON A MODEL PROPOSED BY ROISTAD ET AL IN PAPER    FUDS0240
C      PRESENTED AT THE ENLARGED HPG MEETING ON COMPUTER CONTROL AND FUEL FUDS0250
C      RESEARCH, JUNE 4-7,1974                                             FUDS0260
C      FBU = BU * 1.0202D-05                                              FUDS0270
C      IF (TTIME .GT. 0.) GO TO 40                                         FUDS0280
C      TS = TSINT - 2.7315D02                                             FUDS0290
C      IF TSINT IS NOT DEFINED BY USER. THE DEFAULT VALUE IS 1600 DEG    FUDS0300
C      CENTIGRADE                                                         FUDS0310
C      IF (TSINT .LE. 0.0) TS = 1600.0                                     FUDS0320
C      DE = FDENS/1.096D03                                                 FUDS0330
C      N = 50                                                              FUDS0340
C      EPS = 0.0002                                                        FUDS0350
C      H = 1.00                                                            FUDS0360
C      M = 6                                                                FUDS0370
C      X3 = 0.0                                                            FUDS0380
C      X4 = H                                                              FUDS0390
C      AL1 = DLEN1(TS,DE)                                                  FUDS0400
C      AL3 = 3.0 - AL1                                                     FUDS0410
C      AL4 = 0.0                                                           FUDS0420
C      IF (AL1 .LE. 4.27D-03) GO TO 30                                     FUDS0430
C
10  CONTINUE                                                              FUDS0440
    DO 15 I = 1,M                                                         FUDS0450
      Y2 = DLEN2(AL3,X4,AL4)                                               FUDS0460
      Y1 = DLEN2(AL3,X3,AL4)                                               FUDS0470
      IF (Y1*Y2 .LE. 0.) GO TO 20                                          FUDS0480
      X3 = X4                                                             FUDS0490
      X4 = X4 + H                                                         FUDS0500
      IF (I .EQ. M) GO TO 45                                              FUDS0510
15  CONTINUE                                                              FUDS0520
20  CONTINUE                                                              FUDS0530
    X1 = X3                                                                FUDS0540
    DO 25 J = 1,N                                                         FUDS0550
      X = X1 - DLEN2(AL3,X1,AL4)/DLEN3(X1)                                FUDS0560
      Y = DLEN2(AL3,X,AL4)                                                FUDS0570
      ERR = DABS((X - X1)*100.0/X1)                                       FUDS0580
      IF (ERR .LE. EPS) GO TO 35                                          FUDS0590
      X1 = X                                                              FUDS0600
25  CONTINUE                                                              FUDS0610

```

TABLE A-8.I (contd.)

LISTING OF THE FUDENS SUBCODE

C		FUDS0620
30	AL3 = 2.996	FUDS0630
	AL2 = 5.384	FUDS0640
	GO TO 40	FUDS0650
35	AL2 = X	FUDS0660
40	IF (FBU .LT. AL2) FUDENS = 0.0	FUDS0670
	IF (FBU .GE. AL2) FUDENS = DLEN2(AL3,FBU,AL2)	FUDS0680
	GO TO 50	FUDS0690
45	PRINT 100	FUDS0700
100	FORMAT (1X,/' NO ROOTS HAVE BEEN FOUND BETWEEN 0. AND 6000. MWD/MT	FUDS0710
	1 UO2')	FUDS0720
	FUDENS = 0.0	FUDS0730
50	CONTINUE	FUDS0740
	AL5 = FUDENS	FUDS0750
	RETURN	FUDS0760
	END	FUDS0770

- A-8.7 T. J. Heal, J. E. Littlechild, R. H. Watson, "Development of Stable Density UO_2 Fuel", *Paper No. 52, presented at BNES Nuclear Fuel Performance Conference, London, October 15-19, 1973.*
- A-8.8 B. Burton and G. L. Reynolds, "The Sintering of Grain Boundary Cavities in Uranium Dioxide", *Journ. Nucl. Mat.*, 45 (1972/73) pp 10-14.
- A-8.9 D. Hull and D. E. Rimmer, "The Growth of Grain-Boundary Voids Under Stress", *Phil Mag.*, 4 (1959) p 673.
- A-8.10 M. O. Marlowe, "Predicting In-Reactor Densification Behavior of UO_2 ", *Trans. Amer. Nucl. Soc.*, 17 (November 1973) pp 166-169.
- A-8.11 R. W. Hamming, *Introduction to Applied Numerical Analysis*, New York: McGraw-Hill Book Company, Inc., 1971.

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APPENDIX B
CLADDING MATERIAL PROPERTIES

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APPENDIX B

CLADDING MATERIAL PROPERTIES

Fourteen material properties of light water reactor cladding (zircaloy-2 or -4) have been modeled for inclusion in MATPRO. The approaches taken range from: (a) a choice of experimental data and linear interpolation of those data; to (b) a semiempirical correlation employing an analytical expression suggested by theory, with constants determined by comparison with data.

All fourteen properties are modeled as a function of temperature, with only creep rate and zirconium oxide emissivity having additional dependent arguments. Some of the subcodes are interconnected, employing in part identical or very similar correlations (for example, strain versus stress, stress versus strain, and cladding ultimate strength). Some subcodes call upon others described in this appendix (for example, strain versus stress and shear modulus).

1. CLADDING SPECIFIC HEAT CAPACITY (CCP)

The specific heat of zircaloy cladding is required to determine fuel rod temperatures during nonsteady state conditions. Zircaloy heat capacity data have been reported by Brooks and Stansbury^[B-1.1] up to temperatures of 700 C and by Deem and Eldridge^[B-1.2] up to 1,050 C. The Deem and Eldridge data are of particular interest because the effects of the α - β transformation region are included, whereas the Brooks and Stansbury data do not include this region. At temperatures up to 700 C, the Brooks and Stansbury data agree with the Deem and Eldridge data within 3%. Above the α - β transus (about 975 C) and up to about 1,050 C, a constant value of 355.7 J/kg-K was reported by Deem and Eldridge. This value agrees well with a value of 365.3 reported by Coughlin and King^[B-1.3] for pure zirconium, for the overlapping temperature range of 862 to 1,127 C.

The MATPRO cladding heat capacity subcode CCP employs the Deem and Eldridge^[B-1.2] data in tabular form. Linear interpolation is performed by the routine POLATE (Appendix D) to return the heat capacity at the required temperature. Above 1,248 K, a constant value of 355.7 J/kg-K is returned by CCP. The heat capacity of zircaloy as calculated by CCP is shown in Figure B-1.1.

The lack of symmetry in the data precluded the use of a polynomial equation to describe heat capacity over the temperature range of interest in accident analyses.

1.1 Cladding Specific Heat Capacity Subcode CCP Listing

The subcode CCP is listed in Table B-1.1.

Fig. B-1.1 Heat capacity of zircaloy as calculated by CCP.

TABLE B-1.I

LISTING OF THE CCP SUBCODE

```

FUNCTION CCP(CTEMP)                                CCP 0010
IMPLICIT REAL*8 (A-H,O-Z)                          CCP 0020
C                                                    CCP 0030
C  CCP CALCULATES THE CONSTANT PRESSURE HEAT CAPACITY (SPECIFIC HEAT)    CCP 0040
C  OF ZIRCALOY AS A FUNCTION OF TEMPERATURE                             CCP 0050
C                                                    CCP 0060
C  CTEMP = INPUT CLADDING MESH POINT TEMPERATURE, K                    CCP 0070
C  CCP   = OUTPUT SPECIFIC HEAT OF ZIRCALOY, JOULES/KG-K                CCP 0080
C                                                    CCP 0090
C  DATA FOR THIS CORRELATION WERE TAKEN FROM                           CCP 0100
C  H.W. DEEM AND E.A. ELDRIDGE, "SPECIFIC HEAT MEASUREMENTS"           CCP 0110
C  R.W. DAYTON AND R.F. DICKERSON, EDITORS "PROGRESS RELATING TO       CCP 0120
C  CIVILIAN APPLICATIONS DURING AUGUST 1963"                            CCP 0130
C  USAEC REPORT BMI-1644 (SEPT 1963) PP V-1 TO V-2                     CCP 0140
C                                                    CCP 0150
C  CCP CODED BY R.L. MILLER 'OCT '74                                    CCP 0160
C                                                    CCP 0170
C  DIMENSION CPDATA(38)                                                CCP 0180
C  DATA CPDATA/ 288.70, 273.15, 297.1, 373.15, 305.5, 473.15,        CCP 0190
C  * 313.8, 573.15, 326.38, 673.15, 330.6, 773.15, 338.9, 843.15,    CCP 0200
C  * 338.9, 843.15, 359.90, 873.15, 359.9, 1083.15, 502.1, 1093.15,    CCP 0210
C  * 590.0, 1113.15, 615.10, 1133.15, 719.7, 1153.15, 816.0, 1173.15, CCP 0220
C  * 769.9, 1193.15, 619.30, 1213.15, 468.7, 1233.15, 355.7, 1248.15/ CCP 0230
C  DATA NPCP, IU / 19,1 /                                              CCP 0240
C  IF(CTEMP.GE.1248.0) GO TO 2                                          CCP 0250
C  CCP = POLATE(CPDATA,CTEMP,NPCP,IU)                                   CCP 0260
C  RETURN                                                                CCP 0270
2  CCP = 355.7                                                           CCP 0280
C  RETURN                                                                CCP 0290
END                                                                      CCP 0300

```

1.2 References

- B-1.1 C. R. Brooks and E. E. Stansbury, "The Specific Heat of Zircaloy-2 from 50 to 700°C", *Journal Nuclear Material*, 18 (1966) p 223.
- B-1.2 H. W. Deem and E. A. Eldridge, "Specific Heat Measurements", *Progress Relating to Civilian Applications during August 1963*, R. W. Dayton and R. F. Dickerson, eds., USAEC Report BMI-1644 (September 1963) pp V-1 to V-2.
- B-1.3 J. P. Coughlin and E. G. King, "High-Temperature Heat Contents of Some Zirconium-Containing Substances", *Journal American Chemical Society*, 72 (1950) p 2262.

2. CLADDING THERMAL CONDUCTIVITY (CTHCON)

Calculation of the temperature distribution in the fuel and cladding requires a model for the thermal conductivity of the zircaloy cladding. The model developed for MATPRO describes zircaloy thermal conductivity from room temperature to the melting point and is based on the data of Chirigos et al^[B-2.1], Feith^[B-2.2], and Scott^[B-2.3].

Chirigos et al^[B-2.1] reported the thermal conductivity of zircaloy-4 at temperatures from 100 to 850 C. These data, shown in Table B-2.I, compare favorably with other thermal conductivity data for zircaloy.

Feith^[B-2.2] measured the thermal conductivity of zircaloy-4 at selected temperatures from 300 to 1,500 C. His results are shown in Figure B-2.1 along with the relatively low temperature results of Scott^[B-2.3]. The average values of these data are reported to be within $\pm 5\%$ of the smoothed curve^[B-2.4]. A marked increase in Feith's conductivity was observed to occur above about 1,000 C^[B-2.4]. The reason for this increase is not apparent but may be due to differences in the thermal conductivity of the α and β zircaloy-4 phases.

Scott^[B-2.3] reported the thermal conductivity of zircaloy-4 at selected temperatures from 80 to 790 C and performed a linear least squares fit of his data. His correlation is

$$k = 7.97 + 0.00316 T \quad (B-2.1)$$

where

k = thermal conductivity (Btu/hr-F)

T = temperature (F).

TABLE B-2.1

THERMAL CONDUCTIVITY OF ZIRCALOY-2 AND -4
AS A FUNCTION OF TEMPERATURE^[B-2.1]

Temperature (C)	Thermal Conductivity ($\frac{W}{cm-C}$)	
	Zircaloy-4	Zircaloy-2
100	0-136	0-134
200	0-143	0-145
300	0-152	0-156
400	0-164	0-170
500	0-180	0-184
600	0-201	0-199
700	0-225	0-215
800	0-252	0-231
850	0-266	0-231

Fig. B-2.1 Thermal conductivity of zircaloy-4 as a function of temperature^[B-2.2].

This correlation and its supporting data base are shown in Figure B-2.2. The data are reported to be within $\pm 5\%$ of the correlation.

Fig. B-2.2 Thermal conductivity of zircaloy-4 as a function of temperature[B-2.3].

The correlation developed for the CTHCON subcode combines all of the preceding data. A least squares fit of the data to a third-order polynomial resulted in the correlation of Equation (B-2.2):

$$k = 7.848 + 2.200 \times 10^{-2} T - 1.676 \times 10^{-5} T^2 + 8.712 \times 10^{-9} T^3 \quad (\text{B-2.2})$$

where

k = cladding thermal conductivity (W/m-K)

T = temperature (K).

This correlation and its supporting data base are shown in Figure B-2.3. These data are considered reliable up to about 850 C. Between this temperature and 1,500 C, the correlation is less accurate because fewer data are available. Above 1,500 C, data are not available, and the correlation is an extrapolation of the lower temperature data.

Fig. B-2.3 Thermal conductivity of zircaloy-4 as calculated by CELMOD with its supporting data base [B-2.1,-2.2,-2.3] and 95% confidence limits.

TABLE B-2.II

LISTING OF THE CTHCON SUBCODE

	FUNCTION CTHCON(CTEMP, TIME, FLUX, COLDW)	CTON0010
	IMPLICIT REAL*8(A-H, O-Z)	CTON0020
C		CTON0030
C	CTHCON CALCULATES CLADDING THERMAL CONDUCTIVITY AS A FUNCTION OF	CTON0040
C	TEMPERATURE. TIME, FLUX AND COLD WORK ARE PRESENTLY DUMMY	CTON0050
C	VARIABLES	CTON0055
C		CTON0060
C	CTEMP = INPUT CLADDING MESHPOINT TEMPERATURE (DEG K)	CTON0070
C	FLUX = INPUT FAST NEUTRON FLUX, N/M**2-SEC.	CTON0080
C	TIME = INPUT TIME AT TEMPERATURE AND FLUX, SECONDS.	CTON0090
C	CTHCON = OUTPUT THERMAL CONDUCTIVITY OF ZIRCALLOY-4. WATTS/M-K	CTON0100
C		CTON0110
C	THE DATA USED TO GENERATE THIS THIRD DEGREE CORRELATION OF	CTON0120
C	THERMAL CONDUCTIVITY AS A FUNCTION OF TEMPERATURE WERE TAKEN FROM	CTON0130
C	(1) J.N. CHIRIGOS, ET AL. DEVELOPMENT OF ZIRCALLOY-4, FUEL ELEMENT	CTON0140
C	FABRICATION-1. INTERNATIONAL ATOMIC ENERGY AGENCY. 1961. P 45.	CTON0150
C	(2) A.D. FEITH, HIGH TEMPERATURE MATERIALS PROGRAM PROGRESS	CTON0160
C	REPORT NO 61, GE-NMPO, USAEC REPORT GEMP-61, SEPT 30, 1966, P 153	CTON0170
C		CTON0180
C	THIS VERSION OF CTHCON DEVELOPED BY R.L. MILLER, MARCH, MAY '74	CTON0190
C	CORRECTED BY R.L. MILLER FEB '75	CTON0200
C	UPDATED AND CORRECTED BY B.W. BURNHAM, OCTOBER 1975	CTON0205
C		CTON0210
C		CTON0220
	CTHCON = 7.8476185D0 + CTEMP * (2.2004485D-2 + CTEMP	CTON0230
	Z * (-1.6760128D-5 + CTEMP * 8.7117277D-9))	CTON0240
	RETURN	CTON0250
	END	CTON0260

If the calculated thermal conductivity of the zircaloy-4 is inaccurate by as much as 20% at steady state operating conditions, the estimated surface temperature at the outer surface of the cladding will not be in error by more than about 5 C, however.

2.1 Cladding Thermal Conductivity Subcode CTHCON Listing

The subcode CTHCON is listed in Table B-2.II.

2.2 References

- B-2.1 J. N. Chirigos, S. Kass, W. W. Kirk, G. J. Salvaggio, "Development of Zircaloy-4", *Fuel Element Fabrication*, New York: Academic Press, 1961, pp 19-55.
- B-2.2 A. D. Feith, "Thermal Conductivity and Electrical Resistivity of Zircaloy-4", *High-Temperature Materials Program Progress Report No. 61*, USAEC Report GEMP-61 (September 1966) pp 153-155.
- B-2.3 D. B. Scott, *Physical and Mechanical Properties of Zircaloy-2 and -4*, USAEC Report WCAP-3269-61 (May 1965) pp 5-8.
- B-2.4 H. C. Brassfield, J. F. White, L. Sjodahl, J. T. Bittel, *Recommended Property and Reaction Kinetics Data for Use in Evaluating a Light Water-Cooled Reactor Loss-of-Coolant Incident Involving Zircaloy-4 or 304-SS Clad UO₂*, USAEC Report GEMO-482 (April 1968) p 23.

3. ZIRCONIUM OXIDE EMISSIVITY (ZOEMIS)

The transfer of heat from a fuel rod during an off-normal transient may be dependent upon convection and radiation. The rate of radiation heat transfer is directly proportional to the emissivity of the rod surface. An oxide layer forms on zircaloy tubing when the tubing is exposed to oxygen in the atmosphere or in a reactor coolant. This layer thickens with time and determines the emissivity of the rod surface. Two forms of zirconium oxide form during normal reactor operation. A black oxide which is substoichiometric forms during the early life of the rod. This oxide has markedly different emissivity properties from the stoichiometric white oxide that forms after extended irradiation or under severe, off-normal operating conditions.

The emissivity of initially black substoichiometric oxide was reported by Juenke and Sjodahl^[B-3.1] as a function of time at temperature and forms the basis for the MATPRO model. Their data are presented in Figure B-3.1. These data were gathered on zircaloy during steam oxidation. The test conditions suggest that these data may be particularly applicable to loss-of-coolant accident (LOCA) analyses. At temperatures greater than about 1,200 C, the emissivity decreases rapidly with time suggesting that white oxide may be forming or the surface oxygen is diffusing into the substrate zircaloy. Data were read from Figure B-3.1 and analyzed using least squares techniques. The correlations derived from these data are the basis of the MATPRO subcode ZOEMIS for estimation of the emissivity of zirconium oxide.

Fig. B-3.1 Total hemispherical emittance of zircaloy-4 versus time at temperature in steam[B-3.1].

The present data are limited to the temperature range of 850 to 1,300 C. Although some trends exist in the data, they are not well enough defined to establish reliable correlations below 850 C or above 1,300 C. The model in ZOEMIS sets temperatures less than 850 C equal to 850 C, and calculates emissivity on the basis of data for this temperature. For temperatures above 1,300 C, a cladding emissivity is calculated using the 1,300 C data. The data for 850 C extend to 100 minutes, whereas the data at 1,300 C are limited to 5 minutes. Typical LOCA analyses are limited to even shorter times. Thus, the extrapolation of the 1,300 C data to long time periods is not necessary. However, the second-degree equation for the 1,300 C data appears reasonable up to times of about 20 minutes, and this extrapolation is allowed in the subcode for calculational continuity. For temperatures above 1,200 C and times longer than 20 minutes, a cladding emissivity is calculated using the equation at 20 minutes. For temperatures below 1,200 C and times longer than 100 minutes, a cladding emissivity is calculated using the 100-minute data.

The technique used in ZOEMIS for calculation of emissivity at temperatures between those listed on Figure B-3.1 is to select the temperature range which includes the input surface cladding temperature. The two bounding values of emissivity for this range are then calculated using an appropriate input time. The correct emissivity of the zirconium oxide is then estimated by linear interpolation between the bounding values of emissivity.

The calculated values of emissivity are compared in Table B-3.I with the values indicated in Figure B-3.1.

3.1 Zirconium Oxide Emissivity Subcode ZOEMIS Listing

The listing of the subcode ZOEMIS is presented in Table B-3.II.

3.2 Reference

- B-3.1. E. F. Juenke and L. H. Sjodahl, "Physical and Mechanical Properties: Emittance Measurements", *AEC Fuels and Materials Development Program*, USAEC Report GEMP-1008 (1968) pp 239-242.

TABLE B-3.I

COMPARISON OF EMISSIVITY OF ZrO_2 AS CALCULATED BY ZOEMIS WITH EXPERIMENTAL
VALUES REPORTED BY JUENKE AND SJODAHL

Time (min)	850 C		1,000 C		1,100 C		1,200 C		1,300 C	
	Measured	ZOEMIS	Measured	ZOEMIS	Measured	ZOEMIS	Measured	ZOEMIS	Measured	ZOEMIS
0	0.740	0.740	0.715	0.712	0.751	0.765	0.65	0.776	0.672	0.672
3.5	-	-	-	-	-	-	-	-	0.620	0.620
5	-	0.743	-	0.736	-	0.777	0.795	0.792	0.600	0.600
10	-	0.746	0.750	0.756	0.808	0.788	0.780	0.789	-	0.544
15	-	0.750	-	0.772	0.815	0.796	0.775	0.766	-	0.502
20	0.755	0.755	0.773	0.784	0.780	0.802	0.722	0.725	-	0.476
30	-	0.765	0.795	0.798	-	0.803				
40	0.775	0.775	-	0.802	-	0.805				
50	-	0.784	-	0.797	0.798	0.793				
60	-	0.792	0.790	0.786	0.775	0.773				
70	-	0.797	0.775	0.772						
80	-	0.798	0.738	0.758						
90	-	0.794	0.755	0.746						
100	0.785	0.785	0.740	0.739						

TABLE B-3.II

LISTING OF THE ZOEMIS SUBCODE

	FUNCTION ZOEMIS(CTEMP,TIME)	ZOES0010
	IMPLICIT REAL*8(A-H, O-Z)	ZOES0020
C		ZOES0030
C	ZOEMIS CALCULATES THE EMISSIVITY OF ZIRCONIUM OXIDE AS A	ZOES0040
C	FUNCTION OF TEMPERATURE AND TIME	ZOES0050
C		ZOES0060
C	CTEMP = INPUT MESH POINT TEMPERATURE (K)	ZOES0070
C	TIME = INPUT TIME (SECONDS)	ZOES0080
C	ZOEMIS = OUTPUT ZIRCONIUM OXIDE EMISSIVITY (UNITLESS)	ZOES0090
C		ZOES0100
C	DATA FOR THIS CORRELATION WERE TAKEN FROM	ZOES0110
C	GEMP-1008	ZOES0120
C		ZOES0130
C	ZOEMIS CODED BY R.L. MILLER SEPT '74	ZOES0140
C		ZOES0150
	TT = TIME/6.0D1	ZOES0160
	T = CTEMP - 273.15	ZOES0170
	IF(T - 850.0) 850,850,200	ZOES0180
200	IF(T - 1000.0) 1000,1000,300	ZOES0190
300	IF(T - 1100.0) 1100,1100,400	ZOES0200
400	IF(T - 1200) 1200,1200,500	ZOES0210
500	IF(T - 1300) 1300,1300,600	ZOES0220
850	IF (TT.GE.100.0) TT = 100.0	ZOES0230
	ZOEMIS = 7.4D-1+TT*(4.916667D-4+ TT *(1.625D-5-TT* 1.6666D-7))	ZOES0240
	RETURN	ZOES0250
1000	IF (TT.GE.100.0) TT = 100.0	ZOES0260
	E850 = 7.4D-1+TT*(4.916667D-4+ TT *(1.625D-5-TT* 1.6666D-7))	ZOES0270
	E1000 = 7.107608D-1+TT*(5.411616D-3+TT*(-9.65268D-5+	ZOES0280
Z	TT*4.526029D-7))	ZOES0290
	ZOEMIS = (T-8.5D2)/1.5D2*(E1000-E850) + E850	ZOES0300
	RETURN	ZOES0310
1100	IF (TT.GE.100.0) TT = 100.0	ZOES0320
	E1000 = 7.107608D-1+TT*(5.411616D-3+TT*(-9.65268D-5+	ZOES0330
Z	TT*4.526029D-7))	ZOES0340
	E1100 = 7.65D-1+TT*(2.7106D-3+TT*(-4.2885D-5))	ZOES0350
	ZOEMIS = (T - 1.0D3)/1.0D2 * (E1100 - E1000) + E1000	ZOES0360
	RETURN	ZOES0370
1200	IF (TT.GE.100.0) TT = 100.0	ZOES0380
	E1100 = 7.65D-1+TT*(2.7106D-3+TT*(-4.2885D-5))	ZOES0390
	E1200 = 7.663143D-1+TT*(6.794286D-3-TT*4.457143D-4)	ZOES0400
	ZOEMIS = (T - 1.1D3)/1.0D2 * (E1200 - E1100) + E1100	ZOES0410
	RETURN	ZOES0420
1300	IF(TT.GE.20.0) TT = 20.0	ZOES0430
	E1200 = 7.663143D-1+TT*(6.794286D-3-TT*4.457143D-4)	ZOES0440
	E1300 = 6.72D-1 + TT * (-1.5924D-2 + TT * 3.0476D-4)	ZOES0450
	ZOEMIS = (T - 1.2D3)/1.0D2 * (E1300 - E1200) + E1200	ZOES0460
	RETURN	ZOES0470
600	IF(TT.GE.20.0) TT = 20.0	ZOES0480
	ZOEMIS = 6.72D-1 + TT * (-1.5924D-2 + TT * 3.0476D-4)	ZOES0490
	RETURN	ZOES0500
	END	ZOES0510

4. ZIRCONIUM OXIDE THERMAL CONDUCTIVITY (ZOTCON)

The transfer of heat from fuel pellet to coolant is dependent in part on the thermal resistance of the oxide layer that forms on the rod surface. Accurate predictions of fuel rod temperature profiles require knowledge of the oxide thermal conductivity.

Kingery et al. [B-4.1] reported the thermal conductivity of zirconium oxide stabilized with calcium oxide over the temperature range 100 to 1,400 C. A least squares analysis of his data resulted in the correlation

$$k = 1.96 - 2.41 \times 10^{-4} T + 6.43 \times 10^{-7} T^2 - 1.95 \times 10^{-10} T^3 \quad (B-4.1)$$

where

k = zirconium oxide thermal conductivity (W/in-K)

T = temperature (K).

This correlation and its supporting data are shown in Figure B-4.1. Equation (B-4.1) is used in the ZOTCON subroutine of MATPRO for calculating zirconium oxide thermal conductivity.

Maki [B-4.2] and Lapshov and Bashkatov [B-4.3] have also reported the thermal conductivity of zirconium oxide films. Maki's data presented in Table B-4.I, cover a much smaller temperature range, show a strong temperature dependence, and generally exhibit larger values of thermal conductivity than the data of Kingery et al. Lapshov and Bashkatov experimented with films formed by plasma sputtering of zirconium oxide on tungsten substrates. Although their data, shown in Figure B-4.2, cover the range of 300 to 1,500 C, the data exhibit much greater scatter and are substantially smaller in value than those of both References B-4.1 and B-4.2. The reason for the discrepancy between the data of Lapshov and Bashkatov and that of Kingery et al and Maki may be due to the fact that the sputtered or sprayed coatings are quite porous, poorly consolidated, and not very adherent to the tungsten substrate.

4.1 Zirconium Oxide Thermal Conductivity Subcode ZOTCON Listing

A listing of the ZOTCON subcode is given in Table B-4.III.

Fig. B-4.1 Thermal conductivity of zirconium oxide as a function of temperature as calculated by the ZOTCON subcode. Data are from Kingery et al^[B-4.1].

TABLE B-4.I

THERMAL CONDUCTIVITY OF ZIRCONIUM OXIDE FROM MAKI^[B-4.2]

Specimen	Linear Heat Rate (W/cm)	Coolant Temperature (C)	Temperature Inside Tube (C)	Apparent Thermal Conductivity (W/cm-C)
2	80.8	110.3	142.8	0.0076
	167.8	140.2	173.7	0.0514
	292.5	200.4	229.5	0.0673
	293.6	249.0	272.4	0.162
	361.9	298.6	324.4	0.941
3	86.8	110.8	152.5	0.0088
	168.7	151.7	186.0	0.0181
	306.7	199.9	239.7	0.0326
	280.9	249.0	279.1	0.0396
	392.9	300.1	335.1	0.0633

TABLE B-4.I (contd.)

THERMAL CONDUCTIVITY OF ZIRCONIUM OXIDE FROM MAKI^[B-4.2]

Specimen	Linear Heat Rate (W/cm)	Coolant Temperature (C)	Temperature Inside Tube (C)	Apparent Thermal Conductivity (W/cm-C)
4	86.5	110.3	145.6	0.0070
	168.3	151.3	176.0	0.0478
	287.2	200.1	228.8	0.0635
	288.1	250.0	274.6	0.0541
	383.3	299.6	329.7	0.0545
5	76.2	109.9	144.5	0.0107
	159.4	151.2	177.3	0.0450
	292.9	200.7	233.9	0.0576
	277.5	249.0	275.7	0.0611
	355.5	299.9	331.6	0.0627
6	81.0	110.1	143.1	0.0120
	171.7	151.1	178.0	0.0395
	277.2	200.6	231.5	0.0410
	295.9	249.1	278.9	0.0312
	414.3	299.7	336.6	0.0400

4.2 References

- B-4.1. W. D. Kingery, J. Francl, R. L. Coble, T. Vasilos, "Thermal Conductivity: X, Data for Several Pure Oxide Materials Corrected to Zero Porosity", *Journal American Ceramic Society*, 37 (1954) pp 107-110.
- B-4.2. H. Maki, "Heat Transfer Characteristics of Zircaloy-2 Oxide Film". *Journal Nuclear Science and Technology*, 10 (1973) pp 107-175.
- B-4.3. V. N. Lapshov and A. V. Bashkatov, "Thermal Conductivity of Coatings of Zirconium Dioxide Applied by the Plasma Sputtering Method", *Heat Transfer, Soviet Research*, 5 (1973) pp 19-22.

Fig. B-4.2 Temperature dependence of the thermal conductivity of zirconium oxide according to Lapshov and Bashkatov[B-4.3], showing the trend line.

TABLE B-4.II

LISTING OF THE ZOTCON SUBCODE

	FUNCTION ZOTCON(CTEMP)	Z00N0010
	IMPLICIT REAL*8(A-H, O-Z)	Z00N0020
C		Z00N0030
C		Z00N0040
C	ZOTCON CALCULATES ZIRCONIUM OXIDE THERMAL CONDUCTIVITY AS A	Z00N0050
C	FUNCTION OF TEMPERATURE.	Z00N0060
C		Z00N0070
C		Z00N0080
C	CTEMP = INPUT CLADDING MESHPOINT TEMPERATURE (DEG K)	Z00N0090
C	ZOTCON= OUTPUT THERMAL CONDUCTIVITY OF ZIRCONIUM OXIDE. WATTS/M-K	Z00N0100
C		Z00N0110
C	THE DATA USED TO GENERATE THIS THIRD DEGREE CORRELATION OF	Z00N0120
C	THERMAL CONDUCTIVITY AS A FUNCTION OF TEMPERATURE WERE TAKEN FROM	Z00N0130
C	W.D. KINGERY, J. FRANCL, R.L. COBLE AND T. VASILOS	Z00N0140
C	J. OF THE AMERICAN CERAMIC SOCIETY, VOL 37 NO. 1. FEB(1954) P 107-1	Z00N0150
C		Z00N0160
C	ZOTCON WAS CODED BY R.L.MILLER IN MARCH 1974.	Z00N0170
C	MODIFIED BY R.L.MILLER. APRIL '74. MAY '74	Z00N0180
C		Z00N0190
C	USE CAUTION ABOVE 1400 C	Z00N0200
C		Z00N0210
C	ZOTCON = 1.9599 -CTEMP*(2.41D-4 -CTEMP*(6.43D-7-CTEMP*1.946D-10))	Z00N0220
	RETURN	Z00N0230
	END	Z00N0240

5. CLADDING AXIAL THERMAL EXPANSION (CATHEX)

Thermal expansion correlations are required to estimate geometry changes in the cladding as a function of temperature. For calculational continuity in accident analyses, the correlations must span the range from room temperature to the melting temperature of the cladding. Due to the strong texture (preferred crystallographic orientation) of cold-worked zircaloy, the thermal expansion is different in the axial and radial directions. Figure B-5.1 shows the directions which may exhibit differences in texture for rolled plate and drawn tubing. The textures and, therefore, the thermal expansions in the axial direction of tubing

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Fig. B-5.1 Nomenclature for directions in rolled plate and drawn tubing.

and the longitudinal direction of rolled plate are similar. The textures and thermal expansions in the long transverse direction in rolled plate and the circumferential direction of tubing are similar. And, the texture and thermal expansion in the radial direction of tubing and the short transverse direction of plate are similar. However, it should not be assumed that the textures in the analogous directions of zircaloy plates and tubes are exactly the same.

Mehan and Cutler^[B-5.1] reported data for the axial thermal expansion of zircaloy-2 plate. These data are recapitulated by Mehan and Wiesinger^[B-5.2] and Scott^[B-5.3] and form the basis of the MATPRO subcode CATHEX. The thermal expansion of zircaloy tubing has not been measured and reported. Figure B-5.2 presents the Mehan and Cutler data. Values were taken from this figure and used to generate the following second-degree polynomial least squares fit of the data from room temperature to about 1,073 K:

$$\Delta L/L = 1.708 \times 10^{-3} + T [5.224 \times 10^{-6} + T (1.204 \times 10^{-9})] \quad (B-5.1)$$

where

$\Delta L/L$ = cladding axial thermal expansion (m/m)

T = cladding meshpoint temperature (K).

The assumption is made that this equation will adequately describe both zircaloy-2 and zircaloy-4 tubing since these materials are quite similar.

Additional data were taken from the figure to generate a table of data describing the thermal expansion over the temperature range where alpha zircaloy is transforming to beta zircaloy. (Interpolation in this data set is accomplished through use of the subroutine POLATE described in Appendix D.) Above about 1,290 K, the assumption was made that zircaloy had completely transformed to the beta phase and that the thermal expansion of zirconium would adequately describe the thermal expansion of zircaloy. A constant value of the coefficient of thermal expansion of zirconium of $9.7 \times 10^{-6} \text{K}^{-1}$, as recommended by Lustman and Kerze^[B-5.4], was used to generate the following linear equation describing the thermal expansion of zircaloy from about 1,290 K to the melting point of 2,125 K:

$$\Delta L/L = -8.208 \times 10^{-3} + (9.683 \times 10^{-6}) T. \quad (B-5.2)$$

The large contraction during the α - β transition prevents the use of a single analytical function to describe the thermal expansion of zircaloy over the entire temperature range of interest.

Fig. B-5.2 Axial thermal expansion of zircaloy-2 plate from Reference B-5.1.

Figure B-5.3 summarizes the results of CATHEX calculations of axial thermal expansion for zircaloy from room temperature to the melting point of the alloy. These results are compared with those for cladding diametral thermal expansion in Figure B-6.3.

5.1 Axial Thermal Expansion Subcode CATHEX Listing

The listing for the subcode CATHEX is presented in Table B-5.I.

Fig. B-5.3 Axial thermal expansion of zircaloy tubing as calculated by CATHEX.

TABLE B-5.1

LISTING OF THE CATHEX SUBCODE

```

C      FUNCTION CATHEX (CTEMP)
C      IMPLICIT REAL*8 (A-H,O-Z)
C      CATHEX CALCULATES THE AXIAL THERMAL EXPANSION OF ZIRCALOY AS A
C      FUNCTION OF TEMPERATURE
C
C      CTEMP = INPUT CLADDING MESH POINT TEMPERATURE (K)
C      CATHEX = OUTPUT THERMAL EXPANSION OF ZIRCALOY. (METERS/METER)
C
C      DATA FOR THE CORRELATION FROM ROOM TEMPERATURE TO 1000 C ARE
C      TAKEN FROM R.L. MEHAN AND G.L. CUTLER, "THERMAL EXPANSION OF
C      ZIRCALOY-2 BETWEEN ROOM TEMPERATURE AND 1000 DEG C"
C      USAEC REPORT KAPL-M-RLM-15, 1958
C      ABOVE 1000 C THE THERMAL EXPANSION USED IS THE CONSTANT
C      VALUE 9.7D-6 (M/M/DEG C) RECOMMENDED BY
C      B. LUSTMAN AND F. KERZE, "THE METALLURGY OF ZIRCONIUM"
C      MCGRAW-HILL BOOK CO., NEW YORK, 1955 PP 355
C
C      CATHEX USES A LINEAR INTERPOLATION BETWEEN VALUES OF THERMAL
C      EXPANSION AS A FUNCTION OF TEMPERATURE. THE VALUE RETURNED IS
C      A UNITLESS MULTIPLIER OF LENGTH
C
C      CATHEX CODED BY R.L. MILLER OCT '74
C
C      DIMENSION CATXD (30)
C      DATA CATXD/
C      * 0.53200D-02, 1073.1, 0.55700D-02, 1098.1,
C      * 0.55600D-02, 1133.1, 0.55500D-02, 1143.1,
C      * 0.54700D-02, 1153.1, 0.53800D-02, 1173.1,
C      * 0.50500D-02, 1193.1, 0.45000D-02, 1213.1,
C      * 0.41800D-02, 1223.1, 0.40800D-02, 1233.1,
C      * 0.40700D-02, 1243.1, 0.40700D-02, 1253.1,
C      * 0.40800D-02, 1263.1, 0.41200D-02, 1273.1 /
C      DATA NPCATX, III / 15.1 /
C      IF(CTEMP.LE.1073.15)GO TO 1
C      IF(CTEMP.GE.1273.15) GO TO 2
C      CATHEX = POLATE(CATXD,CTEMP,NPCATX.IU)
C      RETURN
C 1  CATHEX = -1.708257D-3 + CTEMP*(5.223606D-6 + CTEMP*1.204285D-9)
C      RETURN
C 2  CATHEX = -8.208037D-3 + CTEMP*9.683099D-6
C      RETURN
C      END

```

5.2 References

- B-5.1. R. L. Mehan and G. L. Cutler, *Thermal Expansion of Zircaloy-2 between Room Temperature and 1000°C*, USAEC Report KAPL-M-RLM-15 (1958).
- B-5.2. R. L. Mehan and F. W. Wiesinger, *Mechanical Properties of Zircaloy-2*, USAEC Report KAPL-2110 (February 1961).
- B-5.3. D. B. Scott, *Physical and Mechanical Properties of Zircaloy-2 and -4*, USAEC Report WCAP-3269-41 (May 1965) pp 8-12.
- B-5.4. B. Lustman and F. Kerze, Jr., *The Metallurgy of Zirconium*, New York: McGraw-Hill Book Company, Inc., 1955, p 355.

6. CLADDING DIAMETRAL THERMAL EXPANSION (CDTHEX)

Due to the strong texture (preferred crystallographic orientation) of cold-worked zircaloy tubing, the thermal expansion is different in the axial and diametral directions. Figure B-6.1 shows the directions which may show differences in texture for rolled plate and drawn tubing. As discussed in Section B.5, the texture and, therefore, the thermal expansion in the axial direction of tubing and the longitudinal direction of rolled plate are similar. The texture and thermal expansion in the long transverse direction in rolled plate and in the circumferential direction of tubing are similar. And, the texture and thermal expansion in the radial direction of tubing and in the short transverse direction of plate material are similar. Diametral thermal expansion in tubing is a combination of circumferential and radial thermal expansion.

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Fig. B-6.1 Nomenclature used to describe directions in rolled plate and drawn tubing.

Mehan and Wiesinger^[B-6.1] measured the radial thermal expansion of zircaloy-2 plate from room temperature to 1,100 F. These data are recapitulated by Scott^[B-6.2], and form the basis of the MATPRO subcode CDTEX for temperatures below 1,100 K. (Again, no zircaloy tube data are available.) These data are summarized in Figure B-6.2. Data were taken from Figure B-6.2 and used to generate the following third-degree polynomial least squares fit of the Mehan and Wiesinger data up to a temperature of 1,050 K:

$$\Delta D/D = 8.208 \times 10^{-4} + T \left\{ (-7.856 \times 10^{-6} + T [1.924 \times 10^{-8} - T (6.141 \times 10^{-12})]) \right\} \quad (\text{B-6.1})$$

Fig. B-6.2 Experimental thermal expansion of zircaloy-2 tubing in the radial direction according to Mehan and Wiesinger^[B-6.1].

where

$\Delta D/D$ = the thermal expansion in the diametral direction

T = cladding meshpoint temperature (K).

The assumption is made that the diametral thermal expansion is parallel to the axial thermal expansion curve shown in Figure B-5.3 from about 1,050 K to a temperature at which the beta phase is well formed, about 1,290 K. This assumption was used to generate a data table to describe the thermal expansion of zircaloy from 1,050 to 1,290 K. CDTHEX then employs the subroutine POLATE (described in Appendix D) to linearly interpolate between points in the data set.

From 1,290 K to the melting temperature, the assumption is made that the coefficient of thermal expansion of zircaloy is the same as for zirconium. A constant value of the coefficient of thermal expansion, $9.7 \times 10^{-6} \text{K}^{-1}$ as recommended by Lustman and Kerze^[B-6.3], was used to generate the following linear equation for the thermal expansion of zircaloy from 1,290 to 2,125 K:

$$\Delta D/D = -6.514 \times 10^{-3} + (9.701 \times 10^{-6})T. \quad (\text{B-6.2})$$

The large contraction during the α - β transition prevents the use of a single analytical function to describe the thermal expansion of zircaloy over the entire temperature range of interest.

Figure B-6.3 summarizes the results of CDTHEX calculations of zircaloy diametral thermal expansion from room temperature to the melting point of the alloy and also shows the axial thermal expansion model (Appendix B-5) for the purpose of comparison.

6.1 Diametral Thermal Expansion Subcode CDTHEX Listing

The listing of CDTHEX is given in Table B-6.I.

6.2 References

- B-6.1. R. L. Mehan and F. W. Wiesinger, *Mechanical Properties of Zircaloy-2*, USAEC Report KAPL-2110 (February 1961).
- B-6.2. D. B. Scott, *Physical and Mechanical Properties of Zircaloy-2 and -4*, USAEC Report WCAP-3269-41 (May 1965) pp 8-12.
- B-6.3. B. Lustman and F. Kerze, Jr., *The Metallurgy of Zirconium*, New York: McGraw-Hill Book Company, Inc., p 355.

Fig. B-6.3 Comparison of diametral thermal expansion of zircaloy tubing from 300 to 2,125 K as calculated by CDTHX with axial thermal expansion of zircaloy tubing over the same temperature range as calculated by CATHEX.

TABLE B-6.I

LISTING OF THE CDTEX SUBCODE

	FUNCTION CDTEX(CTEMP)	CDTX0010
	IMPLICIT REAL*8 (A-H,O-Z)	CDTX0020
C	CDTEX CALCULATES THE DIAMETRAL THERMAL EXPANSION OF ZIRCALOY	CDTX0030
C	AS A FUNCTION OF TEMPERATURE	CDTX0040
C		CDTX0050
C	CTEMP = INPUT CLADDING MESH POINT TEMPERATURE (K)	CDTX0060
C	CDTEX = OUTPUT THERMAL EXPANSION OF ZIRCALOY (METERS/METER)	CDTX0070
C		CDTX0080
C	DATA FOR THE CORRELATION FROM ROOM TEMPERATURE TO 1100 K ARE	CDTX0090
C	OF ZIRCALOY-2, USAEC REPORT KAPL-2110 (FEB 1961)	CDTX0100
C	TAKEN FROM R.L. MEHAN AND F.W. WEISINGER, MECHANICAL PROPERTIES	CDTX0110
C	ABOVE 1290 K THE THERMAL EXPANSION USED IS THE CONSTANT	CDTX0120
C	VALUE 9.7D-6 (M/M/DEG C) RECOMMENDED BY	CDTX0130
C	B. LUSTMAN AND F. KERZE, "THE METALLURGY OF ZIRCONIUM"	CDTX0140
C	MCGRAW-HILL BOOK CO., NEW YORK, 1955 PP 355	CDTX0150
C		CDTX0160
C	CDTEX USES A LINEAR INTERPOLATION BETWEEN VALUES OF THERMAL	CDTX0170
C	EXPANSION AS A FUNCTION OF TEMPERATURE. THE VALUE RETURNED	CDTX0180
C	IS A UNITLESS MULTIPLIER OF LENGTH, DELTA L/L.	CDTX0190
C		CDTX0200
C	CDTEX CODED BY R.L. MILLER NOV '74	CDTX0210
C	UPDATED AND CORRECTED BY B.W. BURNHAM, OCTOBER 1975	CDTX0215
C		CDTX0220
	DIMENSION RTHEXP (42)	CDTX0230
	DATA RTHEXP/	CDTX0240
	* 7.28D-3,1100., 7.30D-3,1110., 7.30D-3,1120., 6.67D-3,1050.,	CDTX0250
	* 7.26D-3,1140., 7.23D-3,1150., 7.18D-3,1160., 7.10D-3,1170.,	CDTX0260
	* 7.00D-3,1180., 6.80D-3,1170., 6.56D-3,1200., 6.27D-3,1210.,	CDTX0270
	* 6.03D-3,1220., 5.87D-3,1230., 5.78D-3,1240., 5.77D-3,1250.,	CDTX0280
	* 5.80D-3,1260., 5.84D-3,1270., 5.93D-3,1280., 6.00D-3,1290./	CDTX0290
	DATA NPREXP, IU / 21,1 /	CDTX0300
	IF(CTEMP.LT.1050.0) GO TO 1	CDTX0310
	IF(CTEMP.GT.1290.0) GO TO 2	CDTX0320
	CDTEX = POLATE(RTHEXP, CTEMP, NPREXP, IU)	CDTX0330
	RETURN	CDTX0340
1	CDTEX = 8.2076D-4 + CTEMP * (-7.856D-6 + CTEMP * (1.9236D-8	CDTX0350
2	- CTEMP * 6.1409D-12))	CDTX0360
	RETURN	CDTX0370
2	CDTEX = -6.513772D-3 + CTEMP * 9.700599D-6	CDTX0380
	RETURN	CDTX0390
	END	CDTX0400

7. CLADDING ELASTIC MODULUS (CELMOD)

The modulus of elasticity is required to calculate mechanical properties of zircaloy cladding at stresses less than the yield stress. The elastic modulus is defined by Hooke's law as the ratio of stress to strain-for stresses below the yield point. The data available are for unirradiated material and span the range from room temperature to about 800 C, although they are less reliable above 400 C.

Busby[B-7.1] reported values of the elastic modulus for zircaloy-4 between 24 and 371 C for five combinations of cold work and heat treatment. Too few data were reported to allow separation of the contribution of cold work and heat treatment from the effects of temperature, however. A linear least squares fit of Busby's data resulted in the correlation

$$E = 1.472 \times 10^7 - 5.152 \times 10^3 T \quad (\text{B-7.1})$$

where

E = Young's modulus (psi)

T = temperature (F).

Busby's data and the least squares fit are shown in Figure B-7.1.

Spasic et al[B-7.2] studied the elastic modulus of zircaloy-2 in the unirradiated condition from room temperature to 400 C. They reported the correlation

$$E = 8.25 E_0 T^{-0.369} \quad (\text{B-7.2})$$

Fig. B-7.1 Temperature dependence of the elastic modulus of zircaloy-4 according to Busby[B-7.1] with a linear least squares fit of the data.

where

E = Young's modulus (kgf/cm^2)

T = temperature (K)

E_0 = experimental value of Young's modulus (kgf/cm^2) at room temperature
(27 C) = $1.01 \times 10^6 \frac{\text{kgf}}{\text{cm}^2}$.

The Spasic et al data are reported to fall within $\pm 3\%$ of their calculated curve [B-7.2]. Their correlation (Equation B-7.2) and supporting data are shown in Figure B-7.2. The elastic modulus calculated by this correlation decreases slowly after about 900 K and is probably not valid much beyond the limits of its data base. The material used by Spasic et al was not characterized as to amount of cold work, and the assumption is made that unirradiated material in the annealed condition was used in the tests.

Fig. B-7.2 Elastic modulus of zircaloy-2 as a function of temperature showing the data and correlation of Spasic et al [B-7.2].

Mehan^[B-7.3] and Mehan and Wiesinger^[B-7.4] reported elastic modulus data in the range of room temperature to 1,500 F. These data were gathered on unirradiated, vacuum-annealed zircaloy-2. Brassfield et al^[F-7.5] reported the following correlation of Mehan and Wiesinger's^[F-7.4] data:

$$E = 9.841 \times 10^5 - 578 T \quad (B-7.3)$$

where

E = Young's modulus (kgf/cm²)

T = temperature (C).

This correlation is shown in Figure B-7.3.

In the temperature range over which the data base of the preceding correlations overlap, the agreement is within about 10%. The CELMOD correlation is a linear relation of the elastic modulus as a function of temperature and represents a combination of the available correlations. The relation is

$$E = 1.148 \times 10^{11} - 5.99 \times 10^7 T \quad (B-7.4)$$

where

E = Young's modulus (N/m²)

T = temperature (K).

This function is used to represent the elastic modulus of zircaloy-4 in the α -phase region (that is, in the region up to 862 C) and thus involves an extrapolation over a considerable temperature range. This relation is plotted in Figure B-7.3 along with the correlations from which it was derived.

Another extrapolation was made from the value at the α - β transus temperature to about zero at the melting point. This extrapolation is used to represent elastic modulus in the β -phase region and is given by

$$E = 1.005 \times 10^{11} - 4.725 \times 10^7 T \quad (B-7.5)$$

where E is given in N/m² and T is in degrees kelvin.

This relation is shown in Figure B-7.4 along with the correlation for the α -phase region.

Fig. B-7.3 Zircaloy elastic modulus as a function of temperature showing the correlation of Busby, Spasic et al, Mehan and Weisinger, and CELMOD for the α -phase of zircaloy.

Fig. B-7.4 Elastic modulus of zircaloy as a function of temperature as calculated by the CELMOD subcode.

The change in the elastic modulus at the α - β transus temperature is unknown. The extrapolation of the elastic modulus from the α - β transus temperature to the melting point is for calculational convenience, and large uncertainties exist in values calculated using the code in the β -phase region.

7.1 Cladding Elastic Modulus Subcode CELMOD Listing

A listing of the MATPRO subcode CELMOD, Equations (B-7.4) and (B-7.5), is presented in Table B-7.I.

7.2 References

- B-7.1. C. C. Busby, in *Properties of Zircaloy-4 Tubing*, C. R. Woods (ed.), USAEC Report WAPD-TM-585 (December 1966) p 65ff.
- B-7.2. Z. Spasic, M. Pavlovic, G. Simis, *Conference on the Use of Zirconium Alloys in Nuclear Reactors*, Pizen, Check., cataloged as a USAEC Report CONF-681086 (1968) pp 277-84.
- B-7.3. R. L. Mehan, *Modulus of Elasticity of Zircaloy-2 Between Room Temperature and 1,000°F*, USAEC Report KAPL-M-RLM-16 (July 1958).

TABLE B-7.I

LISTING OF THE CELMOD SUBCODE

	FUNCTION CELMOD(CTEMP, TIME, FLUX, COLDW)	CEOD0010
	IMPLICIT REAL*8(A-H, O-Z)	CEOD0020
C		CEOD0030
C		CEOD0040
C	CELMOD CALCULATES CLADDING ELASTIC MODULUS AS A FUNCTION OF	CEOD0050
C	TEMPERATURE. TIME, FLUX AND COLD WORK ARE PRESENTLY DUMMY	CEOD0060
C	VARIABLES	CEOD0070
C		CEOD0080
C	CTEMP = INPUT CLADDING MESHPOINT TEMPERATURE (DEG K)	CEOD0090
C	FLUX = INPUT FAST NEUTRON FLUX, N/M**2-SEC.	CEOD0100
C	TIME = INPUT TIME AT TEMPERATURE AND FLUX, SECONDS.	CEOD0110
C	CELMOD = OUTPUT MODULUS OF ELASTICITY FOR ZIRCALOY-4 (N/M**2)	CEOD0120
C		CEOD0130
C	THE MODULUS OF ELASTICITY USED IN THIS SUBROUTINE IS TAKEN FROM	CEOD0140
C	THE DATA AND CORRELATIONS FROM THE FOLLOWING REFERENCES	CEOD0150
C	(1) C.C. BUSBY, IN WAPD-TM-585, PROPERTIES OF ZIRCALOY-4 TUBING,	CEOD0160
C	C.R. WOODS, ED. PAGES 65FF.	CEOD0170
C	(2) Z. SPASIC, M. PAVLOVIC, G. SIMIC, CONFERENCE ON THE USE OF	CEOD0180
C	ZIRCONIUM ALLOYS IN NUCLEAR REACTORS, PIZEN, CZECH, 1968, PP 277-84	CEOD0190
C	CATALOGUED AS USAEC REPORT CONF-681086	CEOD0200
C	(3) R.L. MEHAN AND F.W. WIESINGER, MECHANICAL PROPERTIES OF	CEOD0210
C	ZIRCALOY-2, USAEC REPORT KAPL-2110.	CEOD0220
C		CEOD0230
C	CELMOD WAS CODED BY R.L. MILLER IN MARCH 1974.	CEOD0240
C	MODIFIED BY R.L. MILLER, APRIL 1974	CEOD0250
C	UPDATED AND CORRECTED BY B.W. BURNHAM, OCTOBER 1975	CEOD0255
C		CEOD0260
C	CAUTION SHOULD BE EXERCISED IN USING THIS CORRELATION BEYOND	CEOD0270
C	700 DEG K (800 DEG F).	CEOD0280
C		CEOD0290
C	CALL PHYPRO(FTMELT, FHEFUS, CTMELT, CHEFUS, CTRANB, CTRANE, CTRANZ,	CEOD0300
C	Z FDELTA, BU, COMP)	CEOD0302
C	IF(CTEMP.GT.CTRANZ) GO TO 20	CEOD0340
C	CELMOD = 1.148D11 - CTEMP * 5.99D7	CEOD0350
C	RETURN	CEOD0360
C	20 CELMOD = 1.0050D11 - CTEMP * 4.7245178D7	CEOD0370
C	RETURN	CEOD0380
C	END	CEOD0390

B-7.4. R. L. Mehan and F. W. Wiesinger, *Mechanical Properties of Zircaloy-2*, USAEC Report KAPL-2110 (February 1961) pp 11-12.

B-7.5. H. C. Brassfield, J. F. White, L. Sjodahl, J. T. Bittel, *Recommended Property and Reaction Kinetics Data for Use in Evaluating a Light Water-Cooled Reactor Loss-of-Coolant Accident Involving Zircaloy-4 or 304-SS-Clad UO₂*, USAEC Report GEMP-482 (April 1968).

8. CLADDING STRAIN VERSUS STRESS (CSTRAN)

In the subroutine, CSTRAN strain is calculated as a function of stress by two different equations, one for the elastic region and another for the plastic region. In the elastic region, Hooke's law is used:

$$\epsilon = \sigma/E \quad (\text{B-8.1})$$

where

ϵ = true strain

σ = true stress

E = the modulus of elasticity.

In the plastic region, the strain is calculated by a power law:

$$\epsilon = \left(\frac{\sigma}{K} \right)^{1/n} \quad (\text{B-8.2})$$

where

K = the strength coefficient.

n = the strain hardening coefficient.

The transition from the elastic to the plastic region is found by comparing the values of true strain calculated by Equations (B-8.1) and (B-8.2). The plastic region begins when the true strain calculated by Equation (B-8.2) is greater than that calculated by Equation (B-8.1). The true strain can then be calculated as a function of true stress over the temperature range for which relations for E , K , and n exist.

Values for the modulus of elasticity as a function of temperature are obtained from the subcode CELMOD (Appendix B-7). As discussed in the description of CELMOD, the correlation for elastic modulus has an uncertainty of about 10% below 900 K, and larger uncertainties above that temperature.

Values for n up to 755 K are obtained from Busby^[B-8.1]. The value of n at higher temperatures is assumed to be constant and equal to the value at 755 K, namely 0.057. Although in principle, n would be expected to decrease to zero for temperatures near the melting point, no data are available in the elevated temperature region. In addition, the calculation of strain by the power law in Equation (B-8.2) becomes unstable as n becomes small. The data points and the correlation curve for n are presented in Figure B-8.1.

Fig. B-8.1 Correlation of work hardening coefficient with temperature for zircaloy stress relieved at 783 K [B-8.1].

K is calculated in CSTRAN using Equation (B-8.3) where K is in N/m^2 and T is in degrees kelvin.

For temperatures less than 755 K:

$$K = 1.398 \times 10^9 - 1.220 \times 10^6 T - 96.62 T^2 \quad (\text{B-8.3a})$$

For temperatures between 755 and 866 K:

$$K = 2.538 \times 10^9 - 2.794 \times 10^6 T. \quad (\text{B-8.3b})$$

For temperatures above 866 K:

$$K = 1.180 \exp (25.12 - 9.216 \times 10^{-3} T + 1.678 \times 10^{-6} T^2) \quad (\text{B-8.3c})$$

The data for K up to 755 K were obtained by Busby^[B-8.1] from tensile tests on tubes cold worked to about 75% and stress relieved at 783 K. Equation (B-8.3) is a simple least squares fit to the data of Busby^[B-8.1]. From 866 K to the melting point, the value of K was calculated from the ultimate tensile strength data from Brassfield et al^[B-8.2] which are based primarily on experiments using annealed sheet material. K was calculated from the ultimate tensile strength data by assuming in Equation (B-8.2) that when $E = n = 0.057$, $\sigma = \sigma_{uts}$, where σ_{uts} is the ultimate tensile strength. Then:

$$K = \frac{\sigma_{uts}}{(0.057)^{0.057}} = 1.18 \sigma_{uts} \quad (B-8.4)$$

Equation (B-8.3b) represents a linear interpolation between the values at 755 and 866 K given by the low and high temperature correlations.

Figure B-8.2 indicates that the ultimate tensile strength of cold-worked and stress-relieved zircaloy is equivalent to that of annealed material above 866 K. This fact provides some justification for the use of annealed data from Brassfield et al^[B-8.2] for the high temperature correlation. The results for K [Equation (B-8.3)] programmed in CSTRAN are shown graphically in Figure B-8.3.

A second set of data for n and K from Busby^[B-8.1] for tubes recrystallized at 922 K has been correlated with temperature in Equations (B-8.5) and (B-8.6), again employing the Brassfield^[B-8.2] ultimate tensile strength data.

For temperatures less than 775 K:

$$n = 0.3380 - 0.1726 \times 10^{-2} T + 0.4097 \times 10^{-5} T^2 - 0.3020 \times 10^{-8} T^3 \quad (B-8.5a)$$

For temperatures greater than 775 K:

$$n = 0.056 \quad (B-8.5b)$$

For temperatures up to 2,000 K:

$$k = e^{[7.090 + 0.4216 \times 10^{-3} T - 0.5000 \times 10^{-5} T^2 + 0.1475 \times 10^{-8} T^3]} \quad (B-8.6)$$

where

T = temperature (K).

Fig. B-8.2 Ultimate tensile strength as a function of temperature showing annealing of cold work at temperatures above 866 K.

Fig. B-8.3 Strength coefficient as a function of temperature for zircaloy as used in CSTRAN.

These correlations for annealed zircaloy, shown as functions of temperature in Figures B-8.4 and B-8.5, can be substituted for those of the stress-relieved material in CSTRAN, if desired.

Fig. B-8.4 Work hardening coefficient as a function of temperature for zircaloy recrystallized at 922 K^[B-8.1].

Fig. B-8.5 Strength coefficient as a function of temperature for zircaloy recrystallized at 922 K^[B-8.1, B-8.2].

Failure is defined in terms of the total circumferential elongation (TCE) at rupture in a biaxial burst test. TCE data from isothermal^[B-8.3] and temperature transient^[B-8.4, B-8.5] burst tests in which one end of the tube was closed and free of restraint were correlated with temperature to define the failure point on the stress-strain diagram. The TCE correlations are shown in Figure B-8.6 along with the isothermal data of Busby and Marsh^[B-8.3], the 28 C/sec heating rate data of Hobson and Rittenhouse^[B-8.5], and the 25 C/sec heating rate data of Hardy^[B-8.4]. Values of the TCE are transformed to true strain by the relation:

Fig. B-8.6 Total circumferential elongation (TCE) to failure as a function of temperature as modeled in CSTRAN.

$$\epsilon = \ln (1+e) \quad (\text{B-8.7})$$

where

ϵ = the true strain

e = the engineering strain.

The output of CSTRAN is presented in Figure B-8.7 as a series of true stress - true strain curves at various temperatures. Both true and engineering strain are calculated for each input value of true stress.

Fig. B-8.7 True stress - true strain curves as calculated by CSTRAN for various temperatures.

8.1 Cladding Strain Subcode CSTRAN Listing

A listing of the subcode CSTRAN used for calculating strain as a function of stress is given in Table B-8.I.

TABLE B-8.I

LISTING OF THE CSTRAN SUBCODE

SUBROUTINE CSTRAN(CTEMP,CSTRES,STRANE,STRANT,STRNUE,STRNUT)	CSAN0010
IMPLICIT REAL*8(A-H, O-Z)	CSAN0020
C	CSAN0030
C CSTRAN CALCULATES CLAD STRAIN AS A FUNCTION OF CLAD STRESS AND	CSAN0040
C TEMPERATURE.	CSAN0050
C	CSAN0060
C CTEMP = INPUT CLADDING MESHPOINT TEMPERATURE (DEG K)	CSAN0070
C CSTRES = INPUT CLADDING MESHPOINT STRESS (N/M**2)	CSAN0080
C CELMOD = INPUT MODULUS OF ELASTICITY FOR ZIRCALOY-4 (N/M**2)	CSAN0090
C STRANE = OUTPUT ENGINEERING STRAIN, UNITLESS RATIO OF LENGTHS	CSAN0100
C STRANT = OUTPUT TRUE STRAIN, UNITLESS RATIO OF LENGTHS	CSAN0110
C STRNUE = OUTPUT ENGINEERING STRAIN AT RUPTURE, UNITLESS RATIO OF	CSAN0120
C LENGTHS	CSAN0130
C STRNUT = OUTPUT TRUE STRAIN AT RUPTURE, UNITLESS RATIO OF LENGTHS	CSAN0140
C CONVERSION TO PSI = (N/M**2)*1.4505E-4(PSI/(N/M**2))	CSAN0150
C	CSAN0160
C IN THIS SUBROUTINE STRAIN IS CALCULATED BY TWO DIFFERENT EQUATIONS,	CSAN0170
C ONE FOR THE ELASTIC REGION AND ANOTHER FOR THE PLASTIC REGION.	CSAN0180
C IN THE ELASTIC REGION HOOKES LAW IS USED: STRANT = CSTRES/CELMOD.	CSAN0190
C WHERE CELMOD IS THE ELASTIC MODULUS OF THE CLADDING.	CSAN0200
C IN THE PLASTIC REGION A POWER LAW IS EMPLOYED:	CSAN0210
C CSTRAN = (CSTRES/AK)**RAN, WHERE AK IS THE STRENGTH COEFFICIENT.	CSAN0220
C AND RAN IS THE RECIPROCAL OF THE WORK HARDENING COEFFICIENT, AN.	CSAN0230
C	CSAN0240
C THE VALUES OF AN AND AK ARE FROM C.C. BUSBY, IN WAPD-TM-585,	CSAN0250
C PROPERTIES OF ZIRCALOY-4 TUBING, C.R. WOODS, ED., PAGES 65FF.	CSAN0260
C ADDITIONAL USEFUL INFORMATION ON THE ANALYSIS OF THE PLASTIC	CSAN0270
C DEFORMATION OF ZIRCALOY CAN BE FOUND IN A.L. BEMENT, JR., EFFECTS	CSAN0280
C OF COLD WORK AND NEUTRON IRRADIATION ON THE TENSILE PROPERTIES OF	CSAN0290
C ZIRCALOY-2, USAEC REPORT HW-74955.	CSAN0300
C VALUES OF AK ABOVE 866 DEG K ARE CALCULATED FROM THE ULTIMATE	CSAN0310
C STRENGTH DATA OF H.C. BRASSFIELD, ET AL. USAEC REPORT GEMP-482(1968)	CSAN0320
C STRAIN AT RUPTURE DATA ARE FROM C.C. BUSBY AND K.B. MARSH,	CSAN0330
C "HIGH TEMPERATURE DEFORMATION AND BURST CHARACTERISTICS OF	CSAN0340
C RECRYSTALLIZED ZIRCALOY -4 TUBING". WAPD-TM-900, JANUARY 1970	CSAN0350
C D.G. HARDY, "HIGH TEMPERATURE EXPANSION AND RUPTURE BEHAVIOR OF	CSAN0360
C ZIRCALOY TUBING" IN TOPICAL MEETING ON WATER REACTOR SAFETY,	CSAN0370
C SALT LAKE CITY, AMERICAN NUCLEAR SOCIETY, MARCH 26-28, 1973. CONF-7303	CSAN0380
C D.O. HOBSON AND P.L. RITTENHOUSE, "DEFORMATION AND RUPTURE BEHAVIOR	CSAN0390
C OF LIGHT-WATER REACTOR FUEL CLADDING", ORNL-4727, OCTOBER 1971.	CSAN0400
C	CSAN0410
C CSTRAN WAS CODED BY R.L. MILLER AND R.R. HOBBS IN MARCH 1974.	CSAN0420
C MODIFIED BY R.L. MILLER, APRIL 1974, R.R. HOBBS JUNE 1974.	CSAN0430
C MODIFIED BY R.R. HOBBS, MARCH 1975	CSAN0440
C CODING REVISED BY R.C. YOUNG MAY 75	CSAN0450
C	CSAN0460
C CAUTION SHOULD BE EXERCISED IN USING THIS CORRELATION BEYOND	CSAN0470
C 800 DEG K.	CSAN0480
C	CSAN0490
C DATA TIME, FLUX, COLDW / 3*0. /	CSAN0500
C ELMOD = CELMOD(CTEMP, TIME, FLUX, COLDW)	CSAN0510
C T = CTEMP	CSAN0520
C STRESS = CSTRES	CSAN0530
C AN = 0.05657400	CSAN0540
C IF (T.GT.866.) GO TO 20	CSAN0550
C IF (T.GT.755.) GO TO 10	CSAN0560
C AK = 1.398304D09 - T*(1.219965D06 + T*96.6206)	CSAN0570
C AN = -1.3498D-2 + T*(5.1521D-4 - 5.5947D-7*T)	CSAN0580
C GO TO 30	CSAN0590

TABLE B-8.1 (contd.)

LISTING OF THE CSTRAN SUBCODE

10	AK = 2.53829D9 - T * 2.79378D6	CSAN0600
	GO TO 30	CSAN0610
20	AK = 1.1800 * DEXP(25.1225D0 + T*(-9.21627D-3 + T*1.61799D-6))	CSAN0620
30	IF (STRESS.GT.AK) STRESS = AK	CSAN0630
	RAN = 1.0/AN	CSAN0640
	STRANT = STRESS / ELMOD	CSAN0650
	STRAN2 = (STRESS / AK) ** RAN	CSAN0660
	IF (STRAN2.GT.STRANT) STRANT = STRAN2	CSAN0670
	STRANE = STRANT	CSAN0680
	IF (STRANT.GT.2.E-4) STRANE = DEXP(STRANT) - 1.0	CSAN0690
C	CALCULATE ULTIMATE STRAIN	CSAN0700
	IF (T.GT. 1126.) GO TO 40	CSAN0710
	STRNUE = 38.6164D-2+T*(-0.154553D-03+T*0.596470D-06)	CSAN0720
	GO TO 50	CSAN0730
40	IF (T.GT. 1180.) GO TO 42	CSAN0740
	STRNUE = -9646.080D-2+T*(18.1175D-2-T*0.840563D-4)	CSAN0750
	GO TO 50	CSAN0760
42	IF (T.GT. 1330.) GO TO 44	CSAN0770
	STRNUE = -554.943D-2 + T*0.493585D-2	CSAN0780
	GO TO 50	CSAN0790
44	IF (T.GT. 1672.) GO TO 46	CSAN0800
	STRNUE = 586.489D-2+T*(-0.616648D-2+T*0.190107D-05)	CSAN0810
	GO TO 50	CSAN0820
46	STRNUE = 86.9D-2	CSAN0830
50	CONTINUE	CSAN0840
	STRNUT = DLOG(1.0+STRNUE)	CSAN0850
	IF (STRANT.LT. STRNUT) GO TO 60	CSAN0860
	STRANT = STRNUT	CSAN0870
	STRANE = STRNUE	CSAN0880
60	RETURN	CSAN0890
	END	CSAN0900

8.2 References

- B-8.1. C. C. Busby, "Longitudinal Uniaxial Tensile and Compressive Properties", *Properties of Zircaloy-4 Tubing*, C. R. Woods (ed.), WAPD-TM-585 (December 1966).
- B-8.2. H. C. Brassfield, J. F. White, L. Sjodahl, J. T. Bittel, *Recommended Property and Reaction Kinetics Data for Use in Evaluating a Light Water Cooled Reactor Loss-of-Coolant Incident Involving Zircaloy-4 or 304-SS-Clad UO₂*, IISAFEC Report GEMP-482 (April 1968).
- B-8.3. C. C. Busby and K. B. Marsh, *High Temperature Deformation and Burst Characteristics of Recrystallized Zircaloy-4 Tubing*, WAPD-TM-900 (January 1970).
- B-8.4. D. G. Hardy, "High Temperature Expansion and Rupture Behavior of Zircaloy Tubing" *Topical Meeting on Water Reactor Safety, Salt Lake City, American Nuclear Society*, March 26-28, 1973, CONF-730304.
- B-8.5. D. O. Hobson and P. L. Rittenhouse, *Deformation and Rupture Behavior of Light-Water Reactor Fuel Cladding*, ORNL-4727 (October 1971).

9. CLADDING STRESS VERSUS STRAIN (CSTRES)

The subroutine CSTRES calculates true stress as a function of true strain based on the idealized stress-strain relation shown in Figure B-9.1. The diagram is divided into three regions: I, elastic; II, uniform plastic; and III, unstable plastic. In the elastic region, stress is calculated using Hooke's law:

$$\sigma = \epsilon E \quad (\text{B-9.1})$$

where

σ = true stress

ϵ = true strain

and E = Young's modulus.

Fig. B-9.1 Schematic of true stress - true strain curve modeled by CSTRES, indicating an elastic region (I), a uniform plastic region (II), and an unstable plastic region (III).

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In the uniform plastic and unstable plastic regions, the stress is calculated using a power law:

$$\sigma = K\epsilon^n \quad (B-9.2)$$

where

K – strength coefficient

n = strain hardening coefficient.

The transition to the uniform plastic region occurs at Point A in Figure B-9.1 when the stress calculated by Equation (B-9.2) is less than that calculated by Equation (B-9.1). The transition to the unstable plastic region occurs at Point B when the stress [calculated by Equation (B-9.2)] reaches the magnitude of the strength coefficient.

The stress versus strain relations calculated by CSTRES may differ slightly from those calculated by CSTRAN (Appendix B-8). In CSTRAN, Equation (B-9.2) is employed until a strain at failure criterion is met, and the resulting stress versus strain curves (Figure B-8.7) have a negative curvature until failure. In CSTRES the maximum (ultimate) stress is limited to a value equal to the strength coefficient K.

In the CSTRES code, values of Young's modulus are obtained from CELMOD (Appendix B-7) and the correlations for K and n described in CSTRAN (Appendix B-8) are used. Figure B-9.2 shows typical true stress – true strain diagrams calculated by CSTRES. In these cases the failure criterion as described in Appendix B-8 is met prior to Point B of Figure B-9.1 being attained.

9.1 Cladding Stress Subcode CSTRES Listing

A listing of the subcode CSTRES for calculating true stress as a function of true strain is given in Table B-9.I.

Fig. B-9.2 True stress - true strain diagrams as calculated by CSTRES for various temperatures.

TABLE B-9.1

LISTING OF CSTRES SUBCODE

	FUNCTION CSTRES (CTEMP, STRANT)	CSTS0010
	IMPLICIT REAL*8(A-H, O-Z)	CSTS0020
C		CSTS0030
C	CSTRES CALCULATES TRUE CLAD STRESS AS A FUNCTION OF TRUE CLAD	CSTS0040
C	STRAIN AND TEMPERATURE.	CSTS0050
C		CSTS0060
C	CTEMP = INPUT CLADDING MESHPOINT TEMPERATURE (DEG K)	CSTS0070
C	STRANT = INPUT TRUE STRAIN, UNITLESS RATIO OF LENGTHS	CSTS0080

TABLE B-9.I (contd.)

LISTING OF CSTRES SUBCODE

C	CSTRES = OUTPUT CLADDING TRUE MESHPOINT STRESS (N/M**2)	CSTS0090
C	CELMO = INPUT MODULUS OF ELASTICITY FOR ZIRCALOY-4 (N/M**2)	CSTS0100
C		CSTS0110
C	IN THIS SUBROUTINE STRESS IS CALCULATED BY TWO DIFFERENT EQUATIONS,	CSTS0120
C	ONE FOR THE ELASTIC REGION AND ANOTHER FOR THE PLASTIC REGION.	CSTS0130
C	IN THE ELASTIC REGION HOOKES LAW IS USED: CSTRES = STRANT*CELMO ,	CSTS0140
C	WHERE CELMO IS THE ELASTIC MODULUS OF THE CLADDING.	CSTS0150
C	IN THE PLASTIC REGION A POWER LAW IS EMPLOYED:	CSTS0160
C	CSTRES = AK*(STRANT)**AN , WHERE AK IS THE STRENGTH COEFFICIENT,	CSTS0170
C	AND AN IS THE WORK HARDENING COEFFICIENT.	CSTS0180
C		CSTS0190
C	THE VALUES OF AN AND AK ARE FROM C.C. BUSBY, IN WAPD-TM-585,	CSTS0200
C	PROPERTIES OF ZIRCALOY-4 TUBING, C.R. WOODS, ED., PAGES 65FF.	CSTS0210
C		CSTS0220
C	CSTRES WAS ADAPTED FROM CSTRAN (A SUBROUTINE BY R.L. MILLER AND	CSTS0230
C	R.R. HOBBS) BY G.A. BERNA IN APRIL 1975	CSTS0240
C		CSTS0250
C	CAUTION SHOULD BE EXERCISED IN USING THIS CORRELATION BEYOND	CSTS0260
C	800 DEG K.	CSTS0270
C		CSTS0280
C	DATA TIME, FLUX, COLDW / 3*0. /	CSTS0290
C	ELMOD = CFIMODICTEMP, TIME, FLUX, COLDW)	CSTS0300
C	T = CTEMP	CSTS0310
C	AN = 0.05657400	CSTS0320
C	IF (T.GT.866.) GO TO 20	CSTS0330
C	IF (T.GT.755.) GO TO 10	CSTS0340
C	AK = 1.398304009 - T*(1.219965006 + T*96.620A1)	CSTS0350
C	AN = -1.34980-2 + T*(5.15210-4 -5.59470-7 *T)	CSTS0360
C	GO TO 30	CSTS0370
C	10 AK = 2.5382909 - T*2.7937806	CSTS0380
C	GO TO 30	CSTS0390
C	20 AK = 1.1800 * DEXP(25.122500 + T*(-9.216270-3 + T*1.677990-6))	CSTS0400
C	30 CONTINUE	CSTS0410
C	CSTRS1 = ELMOD * STRANT	CSTS0420
C	CSTRES = AK * STRANT**AN	CSTS0430
C	CSTRES = DMIN1(CSTRS1,CSTRES)	CSTS0440
C	IF(CSTRES .GT. AK) CSTRES = AK	CSTS0450
C	RETURN	CSTS0460
C	END	CSTS0470

10. CLADDING ULTIMATE STRENGTH (CULTST)

As discussed in the two preceding sections, the plastic stress-strain relationship used in MATPRO for calculating the deformation of zircaloy cladding is based on the power law

$$\sigma = K\epsilon^n \quad (B-10.1)$$

where

σ = stress (N/m²)

ϵ = strain (m/m)

K = strength coefficient (N/m²)

n = work hardening exponent (unitless).

Plastic instability is assumed to set in when the work hardening exponent is equal to the strain. The stress causing this strain is the ultimate stress. The ultimate stress may then be calculated using the relation

$$\sigma_{ult} = K \epsilon^n \quad (B-10.2)$$

where

σ_{ult} = ultimate strength of cladding.

Equation (B-10.2) is the equation used in the CULTST subcode.

Values for n up to 755 K are obtained from Busby [B-10.1]. The value of n above 755 K is assumed to be constant and equal to the value at 755 K, namely 0.057. Although in principle n would be expected to decrease to zero near the melting point, no data are available in the high temperature region to permit accurate modeling. However, the value of n^n approaches unity as n approaches zero and is 0.85 when n is 0.057. The uncertainty due to lack of knowledge concerning n is limited to the order of 10%.

Data for K up to 755 K are also obtained from Busby [B-10.1]. These data were obtained from tensile tests on tubes that were cold worked to about 75% and relieved at 783 K. From 866 K to the melting point, the value of K is calculated from the ultimate tensile strength data reported by Brassfield et al [B-10.2] which are based primarily on annealed sheet material. K is calculated from that ultimate strength data by assuming in Equation (B-10.2) that when $\epsilon=n=0.057$, $\sigma=\sigma_{uts}$. The value of K over the range 755 to 866 K is linearly interpolated between the values at the two extremes. The correlations for K and n are discussed in greater detail in Appendix B-8 (CSTRAN).

10.1 Cladding Ultimate Strength Subcode CULTST Listing

A listing of the subcode CULTST for calculating the deformation of zircaloy cladding is presented in Table B-10.I.

10.2 References

- B-10.1. C. C. Busby, "Longitudinal Uniaxial Tensile and Compressive Properties", *Properties of Zircaloy-4 Tubing*, C. R. Woods (ed.), WAPD-TM-585 (December 1966) p 65.
- B-10.2. H. C. Brassfield, J. F. White, L. Sjodahl, J. T. Bittel, *Recommended Property and Reaction Kinetics Data for Use in Evaluating a Light Water Cooled Reactor Loss-of-Coolant Incident Involving Zircaloy-4 or 304-SS-Clad UO₂*, USAEC Report GEMP-482 (April 1968).

TABLE B-10.I

LISTING OF THE CULTST SUBCODE

	FUNCTION CULTST(CTEMP)	CUST0010
	IMPLICIT REAL*8(A-H, O-Z)	CUST0020
C		CUST0030
C	CULTST CALCULATES ULTIMATE STRENGTH OF ZIRCALOY AS A FUNCTION OF	CUST0040
C	TEMPERATURE.	CUST0050
C		CUST0060
C	CTEMP = INPUT CLADDING MESH POINT TEMPERATURE (DEG K)	CUST0070
C	CULTST = OUTPUT ZIRCALOY ULTIMATE STRENGTH SI UNITS N/M**2	CUST0080
C		CUST0090
C	THE MODEL FOR CALCULATING ZIRCALOY ULTIMATE STRENGTH IS THE	CUST0100
C	POWER LAW USED FOR PLASTIC STRAIN IN THE CSTRAN SUBCODE	CUST0110
C		CUST0120
C	STRESS = STRENGTH COEFFICIENT * STRAIN**STRAIN HARDENING COEFFICIENT	CUST0130
C	AK = STRENGTH COEFFICIENT	CUST0140
C	AN = STRAIN HARDENING COEFFICIENT	CUST0150
C		CUST0160
C	THE POINT OF PLASTIC INSTABILITY AND ULTIMATE STRENGTH IS	CUST0170
C	IS ASSUMED TO OCCUR WHEN STRAIN EQUALS THE STRESS HARDENING	CUST0180
C	COEFFICIENT	CUST0185
C	THE REFERENCES TO THE CULTST MODEL ARE IN THE CSTRAN SUBCODE	CUST0190
C		CUST0200
C	CULTST CODED BY R.L.MILLER JUNE'74	CUST0210
C	UPDATED AND CORRECTED BY B.W.BURNHAM, OCTOBER 1975	CUST0215
C		CUST0220
	T = CTEMP	CUST0230
	IF(CTEMP - 755.0) 100,100,200	CUST0240
200	IF(CTEMP - 866.0) 250,250,300	CUST0250
100	AK = 1.398304D09 - T*(1.219965D06 + T*96.6206)	CUST0260
	AN = -1.3498D-02+T*(5.1521D-04-T*5.5947D-07)	CUST0270
	CULTST = AK * AN**AN	CUST0280
	RETURN	CUST0290
250	CULTST =(2.53829D9 - T*2.79378D6)*0.84934643200	CUST0300
	RETURN	CUST0310
300	CULTST=1.180*DEXP(25.1225-T*(9.21627D-3-T*1.67799D-6))*0.84934643	CUST0320
	RETURN	CUST0330
	END	CUST0340

11. CLADDING CREEP RATE (CCRPR)

The subroutine CCRPR calculates the in-reactor transverse creep rate of biaxially stressed cold-worked zircaloy tubes as a function of flux, stress, temperature, and time.

The most reliable experiments in which the time dependence of the in-reactor creep strain rate were determined were performed by Ibrahim in 1973^[B-11.1]. The zircaloy tube used by Ibrahim was 20% cold drawn. The basal poles were oriented in the transverse-radial plane of the tube. This texture is similar to that found in most commercial fuel cladding. Contrary to the conclusions of previous workers that the in-reactor creep rate became constant after about 1,000 hours, Ibrahim found that the creep rate continuously decreased with time.

The CCRPR relation for transverse creep strain rate of 20% cold drawn zircaloy-2 tube, based on the Ibrahim time dependence, is given in Equation (B-11-1):

$$\dot{\epsilon} = K \phi (\sigma + B e^{C\sigma}) \exp (-10,000/RT) t^{-1/2} \quad (B-11.1)$$

where

ϵ = transverse creep strain rate ($\frac{m}{m-sec}$)

K = 5.129×10^{-29}

B = 7.252×10^2

C = 4.967×10^{-8}

R = $1.987 \left(\frac{cal}{mol-K} \right)$

T = temperature (K)

t = time (sec)

ϕ = fast neutron flux $\left(\frac{n}{m^2-sec} \right) E > 1.0 \text{ MeV}$

σ = transverse stress (N/m^2).

11.1 Discussion

In the absence of data to the contrary, the assumption was made that each of the variables (time, stress, temperature, and flux) independently affects the creep rate. The effect of each variable on the creep rate is discussed in the following subsections.

11.1.1 Time Dependence. Ibrahim's creep curves can be represented by equations of the form

$$\dot{\epsilon} = \beta t^m \quad (B-11.2)$$

where

t = time

β = constant for the particular creep curve

m = power function equal to the slope of a log-log creep plot.

Ibrahim found a good fit of log strain versus log time plots with a weighted mean m value of 0.47. Further support for the decreasing creep rate with time has been provided by Wood^[B-11.2]. Analysis of the SGHWR zircaloy-2 pressure tubes, for times greater than two years, showed an m value of 0.6. The CCRPR model uses an m -value of 0.5.

11.1.2 Stress Dependence. Ibrahim's tubular creep data were obtained at stresses from 111 to 261 MN/m^2 (16.1 to 36.8 ksi). The data at all stresses can be fitted well by Equation (B-11.1). However, the 95% confidence band is about three times as large at the highest stress level (261 MN/m^2) as at lower stress levels. A plot of creep rate at 5,000 hours versus stress was found to be linear for cold drawn zircaloy for stresses up to 170 MN/m^2 (24.7 ksi) as shown in Figure B-11.1.

Fig. B-11.1 Effect of stress on 20% cold drawn zircaloy-2 creep rates at 5,000 hours in a fast neutron flux of 2.9×10^{17} $n/(\text{m}^2\text{-sec})$ ($E > 1$ MeV) and at 263 C (536 K)^[B-11.1].

Thus, in this stress range:

$$\dot{\epsilon} = A\sigma^n \quad (\text{B-11.3})$$

where

σ = transverse stress

A = a constant for the specific test condition

n = stress exponent (approximately unity).

In order to account for the nonlinear stress dependence of the creep rate above 170 MN/m², the stress function in the CCRPR model was determined by fitting the 5,000-hour tubular creep data in Figure B-11.1 by an equation of the form

$$\dot{\epsilon} = A(\sigma + B e^{C\sigma}) \quad (\text{B-11.4})$$

where

A, B, and C = constants

σ = transverse stress.

The pressure tube equation for in-reactor creep of zircaloy, developed by Ross-Ross and Hunt^[B-11.3], shows the same stress dependence up to the maximum stress of 121 MN/m² available in their data.

Their pressure tube equation is

$$\dot{\epsilon} = 4 \times 10^{-25} \sigma (T-433) \phi \quad (\text{B-11.5})$$

where

$\dot{\epsilon}$ = transverse creep rate (%/hr)

ϕ = fast neutron flux at energies greater than 1 MeV [from 0.5 to 3.5 x 10¹³ n/(cm²-sec)]

σ = transverse stress (to 20,000 psi)

T = temperature (from 523 to 573 K).

11.1.3 Temperature Dependence. Ross-Ross and Hunt consider the flux and stress dependence to be reasonably well defined within the previously mentioned limits, but the effect of temperature is not. The use by Ross-Ross and Hunt of a linear temperature dependence (T-433 K) is equivalent to the commonly used form $\exp(-Q/RT)$ where Q, the "apparent activation energy", is 6,500 cal/mol at 573 K. The value of Q in the literature varies widely with temperature, based on uniaxial creep data. Fidleris^[B-11.4] reports Q values from 5,000 to 10,000 cal/mol in the temperature range 373 to 573 K, and from 40,000 to 60,000 cal/mol between 620 and 690 K. At temperatures near 620 K, the pressure tube equation [Equation (B-11.5)] was found to underpredict the creep strain of the Saxton Plutonium Program zircaloy-4 fuel cladding by about 40% at 10,000 hours. The use of the CCRPR equation with Q = 10,000 cal/mol makes the agreement excellent, however, and this value has been chosen for use in the model:

11.1.4 Flux Dependence. The CCRPR flux dependence is probably not accurate at fluxes below 0.5×10^{13} n/cm²-sec^[B-11.3]. It is probably too high for temperatures above 620 K because of the strong temperature dependence of the thermal creep component and the fact that relatively little irradiation acceleration of zircaloy creep occurs at high temperatures. However, the temperature factor used in CCRPR may be too low for temperatures above 620 K^[B-11.4], and the two uncertainties tend to compensate.

For applications requiring creep rates at higher temperatures, such as in engineering tests, an out-of-reactor model would be preferred. An unpublished out-of-reactor uniaxial creep model due to Ibrahim for use above 673 K (400 C) has the form

$$\epsilon_u = At^m \exp(B) \quad (B-11.6)$$

where

ϵ_u = uniaxial creep strain (%)

A = $5.84 \times 10^{-3} - 1.1177 \times 10^{-5}T$

T = temperature (C)

m = $(3.35 \times 10^{-3}T - 0.811)$

t = time (hr)

B = $(3.12 \times 10^{-6}T - 1.15 \times 10^{-3}) \sigma_u$

σ_u = uniaxial stress (psi).

The range of test data on which the Ibrahim equation is based is as follows:

623 K (350 C)	104-207 MPa(15 to 30 ksi)
673 K (400 C)	34-104 MPa(5 to 15 ksi)
723 K (450 C)	17-69 MPa(2.5 to 10 ksi)

The use of Equation (B-11.6) outside of these limits is not recommended. The Ibrahim out-of-reactor model, Equation (B-11.6), is based on longitudinal tests of cold-worked zircaloy-2 pressure tube material.

11.1.5 Uniaxial Creep. In 1968, Ross-Ross and Hunt^[B-11.3] presented a pessimistic picture of correlating uniaxially and biaxially stressed creep results. Others expressed the same pessimism and, as a result, creep tests which provide critical design data have been performed using only biaxially stressed internally pressurized tubes (one end closed).

In later work, Ibrahim^[B-11.5] correlated uniaxial creep data with biaxial tube data using a mechanistic approach and Fidleris, Ross-Ross, and Fraser^[B-11.6] used a continuum mechanics approach. The two approaches agree within the accuracy of the data available. Fidleris et al recommend the use of a factor of 0.4 to convert uniaxial creep rates in cold-worked zircaloy to the transverse creep rates in biaxially stressed tubes. This factor is applicable to tubes with textures (basal poles are oriented radially) typical of those used in commercial power reactors. Thus, approximate uniaxial strain rates can be obtained by multiplying $\dot{\epsilon}$ in CCRPR by a factor of 2.5.

11.1.6 Evaluation of Model. The data used in formulation of the model are based primarily on expansion creep data developed for the evaluation of the behavior of pressure tubes such as those used in CANDU reactors. Service conditions for these reactors involve temperatures near 573 K, transverse stresses near 138 MPa(20 ksi), and fluxes slightly less than 1×10^{14} n/cm²-sec. The model is considered to be very good at these conditions. In the range of 573 to 623 K, the temperature dependence may be less accurate; however, the CCRPC model predicts very well the Saxton Plutonium Program zircaloy-4 creep strain data at 10,000 hours and 620 K. At stresses above 250 MPa(36 ksi), the model may also be less accurate.

11.1.7 Graphical Representation of CCRPR. In order to visualize the creep strains and strain rates predicted by CCRPR, Figures B-11.2 and B-11.3 are presented. Figure B-11.2 compares the creep strain predicted by CCRPR and the pressure-tube equation presented in Reference B-11.3 at the same flux (2.4×10^{17} n/m²-sec), temperature (573 K), and stress (138 MPa, 20 ksi). A log creep rate versus log time plot for the CCRPR model is shown in Figure B-11.3.

Fig. B-11.2 Biaxial creep strain as a function of time at 573 K, at a stress of 138 MN/m² (20 ksi), and at a fast neutron flux of 2.4×10^{17} n/m²-sec, comparing the CCRPR calculation with the pressure tube equation of Reference B-11.3.

11.2 Cladding Creep Rate Subcode CCRPR Listing

A listing of the subcode CCRPR is given in Table B-11.I.

11.3 References

- B-11.1. E. F. Ibrahim, "In Reactor Tubular Creep of Zircaloy-2 at 260 to 300 C", *Journal Nuclear Material*, 46 (1973) pp 169-182.
- B-11.2. D. S. Wood (M.K.A.E.A. REML, RISLEY) "Discussion on Session 1", *Proceedings of the Conference on Nuclear Fuels, British Nuclear Energy Society, November 9-10, 1972*.
- B-11.3. P. A. Ross-Ross and C. E. L. Hunt, "The In-Reactor Creep of Cold-Worked Zircaloy-2 and Zirconium-2.5 wt.% Niobium Pressure Tubes", *Journal Nuclear Material*, 26, (1968) pp 2-17.
- B-11.4. V. Fidleris, *Summary of Experimental Results on In-Reactor Creep and Irradiation Growth of Zirconium Alloys*, Report AECL-4766 (1974).

Fig. B-11.3 CCRPR biaxial creep-strain rate as a function of time at 573-K for various stresses and fluxes.

B-11.5. E. F. Ibrahim, *In-Reactor Creep of Zirconium-Alloy Tubes and its Correlation with Uniaxial Data*, ASTM-STP-458 (1969) pp 18-36.

B-11.6. P. A. Ross-Ross, V. Fidleris, D. E. Fraser, *Canadian Metallurgical Quarterly*, 11 (1972) pp 101-111.

TABLE B-11.I

LISTING OF THE CCRPR SUBCODE

	FUNCTION CCRPR(CTEMP,CTSRSS,CFLUX,TIME)	CCRPO010
	IMPLICIT REAL*8 (A-H,O-Z)	CCRPO020
C		CCRPO030
C	CCRPR CALCULATES TRANSVERSE CLADDING CREEP STRAIN AS A FUNCTION	CCRPO040
C	OF TRANSVERSE CLADDING STRESS (CTSRSS), TEMPERATURE (CTEMP),	CCRPO050
C	FAST NEUTRON FLUX (CFLUX) AND TIME	CCRPO060
C	CTEMP = INPUT CLADDING MESHPOINT TEMPERATURE (K)	CCRPO070
C	CTSRSS = INPUT CLADDING STRESS (NEWTONS/M**2. (PASCALS))	CCRPO080
C	CFLUX = FAST NEUTRON FLUX (NEUTRONS/M**2/SEC)	CCRPO090
C	TIME = INPUT TIME AT TEMPERATURE (SECONDS)	CCRPO100
C		CCRPO110
C	THE CREEP RATE EQUATION USED IN THIS SUBROUTINE WAS BASED ON :	CCRPO120
C	THE TIME AND STRESS DEPENDENCE TAKEN FROM "INREACTOR TUBULAR	CCRPO130
C	CREEP OF ZIRCALOY-2 AT 260 TO 3000". E.F. IBRAHIM, J. NUCL. MATER	CCRPO140
C	VOL 46 (1973) PP 169-182	CCRPO150
C	THE FLUX DEPENDENCE WAS BASED ON ROSS-ROSS AND HUNT, J. NUCL.	CCRPO160
C	MATER. VOL 26 (1968) PP 2 - 17	CCRPO170
C	THE TEMPERATURE DEPENDENCE, $\text{DEPX}(-Q/RT)$, WAS BASED ON A VALUE	CCRPO180
C	OF $Q = 10000 \text{ CAL/MOLE}$ NEAR 573K FROM FIOLERIS, AECL-4766	CCRPO190
C		CCRPO200
C	CCRPR CODED BY C.E.DIXON, JUNE'75, AND MODIFIED BY B.BURNHAM,6-75	CCRPO210
C		CCRPO220
	CCRPR = $5.129D-29 * \text{CFLUX} * (\text{CTSRSS} + 7.252D2 * \text{DEXP}(4.967D-8 * \text{CTSRSS}))$	CCRPO230
Z	* $\text{DEXP}(-5.03271D3/CTEMP) / \text{DSQRT}(TIME)$	CCRPO240
	RETURN	CCRPO250
	END	CCRPO260

12. CLADDING POISSON'S RATIO (CPOIR)

Poisson's ratio is defined as the ratio of transverse to axial strain and is dimensionless. The theoretical value of Poisson's ratio for isotropic or ideal materials has been reported as 0.5 by van Vlack^[B-12.1], 0.25 by Dieter^[B-12.2], and 0.33 by Shanley^[B-12.3]. Dieter notes that most metals have a Poisson's ratio of about 0.33.

Scott^[B-12.4], Shober et al^[B-12.5], and Johnson^[B-12.6] have reported experimental data for the Poisson's ratio of zircaloy. Scott^[B-12.4] reported data and a correlation for the Poisson's ratio of zircaloy-4 from 70 to 750 F using annealed, unirradiated material. These data show a decrease in Poisson's ratio with increasing temperature. Shober^[B-12.5] reported values for Poisson's ratio of 0.368 to 0.380 at 27 C and 0.425 to 0.460 at 150 C using annealed, unirradiated zircaloy-2; that is, an increase in Poisson's ratio was reported for increasing temperature. Johnson^[B-12.6] reported values of Poisson's ratio of 0.325 ± 0.015 at room temperature for annealed, unirradiated zircaloy-2. Since Johnson's data were derived from shear modulus test data, they may be less applicable than the data of Scott and Shober et al. The data of Scott, Shober et al, and Johnson and the correlation of Scott are shown in Figure B-12.1. The cause of the differences between the reported data is not apparent, and a value judgment would be difficult to make or justify until more data or correlations become available.

Fig. B-12.1 Temperature dependence of Poisson's ratio for zircaloy as used in the CPOIR subcode.

Because Scott's [B-12.4] data are more extensive, his correlation was used in the CPOIR subcode to estimate Poisson's ratio as a function of temperature; that is:

$$\text{Poisson's ratio} = 0.301 - 7.03 \times 10^{-5} T \quad (\text{B-12.1a})$$

where

$$T = \text{temperature (F)}$$

or

$$\text{Poisson's ratio} = 0.333 - 1.26 \times 10^{-4} T \quad (\text{B-12.1b})$$

where

$$T = \text{temperature (K)}$$

12.1 Cladding Poisson's Ratio Subcode CPOIR Listing

The subcode CPOIR is listed in Table B-12.I. Due to the relatively large data scatter and to the lack of data at higher temperatures, Poisson's ratio at temperatures above 750 F (670 K) is assumed to be 0.248, the value given by Equation (B-12.1) at $T = 750$ F.

TABLE B-12.1

LISTING OF THE CPOIR SUBCODE

	FUNCTION CPOIR(CTEMP)	CPIR0010
	INPLICIT REAL*8(A-H, O-Z)	CPIR0020
C		CPIR0030
C		CPIR0040
C	CPOIR CALCULATES CLADDING POISSON RATIO AS A FUNCTION OF	CPIR0050
C	TEMPERATURE.	CPIR0060
C		CPIR0070
C		CPIR0080
C	CTEMP = INPUT CLADDING MESH POINT TEMPERATURE (DEG K)	CPIR0090
C	CPOIR = OUTPUT VALUE OF POISSON'S RATIO, UNITLESS	CPIR0100
C	NEGATIVE RATIO OF LATERAL STRAIN TO AXIAL STRAIN	CPIR0110
C	THIS CORRELATION FOR POISSON'S RATIO IS REPORTED BY D.B. SCOTT IN	CPIR0120
C	IN PHYSICAL AND MECHANICAL PROPERTIES OF ZIRCALOY-2 AND 4,	CPIR0130
C	USAEC REPORT WCAP-3269-41, MAY, 1965	CPIR0140
C		CPIR0150
C	CPOIR WAS CODED BY R.L.MILLER IN MARCH 1974.	CPIR0160
C	MODIFIED BY R.L.MILLER, APRIL '74, MAY '74	CPIR0170
C		CPIR0180
C		CPIR0190
	T = (CTEMP * 1.8) - 459.67	CPIR0200
	IF(T.GT.750.0) GO TO 20	CPIR0210
	CPOIR = 0.301 - T * 7.030-05	CPIR0220
	RETURN	CPIR0230
20	CPOIR = 0.248	CPIR0240
	RETURN	CPIR0250
	END	

12.2 References

- B-12.1. L. H. van Vlack, *Materials Science for Engineers*, Reading: Addison-Wesley Publishing Company, 1971, pp 190-191.
- B-12.2. G. E. Dieter, Jr., *Mechanical Metallurgy*, New York: McGraw-Hill Book Company, Inc., 1961, p 36.
- B-12.3. F. R. Shanley, *Strength of Materials*, New York: McGraw-Hill Book Company, Inc., 1957, pp 138-139.
- B-12.4. D. B. Scott, *Physical and Mechanical Properties of Zircaloy-2 and -4*, USAEC Report WCAP-3269-41 (May 1965).
- B-12.5. F. R. Schober, J. A. Van Echo, L. L. Marsh Jr., J. R. Keeler, *The Mechanical Properties of Zirconium and Zircaloy-2*, USAEC Report BMI-1168 (February 1957).
- B-12.6. R. E. Johnson, *The Torsional Properties of Zircaloy-2 and Zircaloy-4*, USAEC Report WAPD-BT-10 (October 1958) pp 49-56.

13. CLADDING SHEAR MODULUS (CSHEAR)

Johnson^[B-13.1] reported values of the shear modulus of zircaloy-2 and -4 from tests conducted on both tube and solid specimens. His values of the shear modulus varied from 3.599 to 3.647×10^{10} N/m² for the zircaloy-2 tubing and from 4.089 to 4.309×10^{10} N/m² for the solid specimens. The average shear modulus was $3.61 \pm 0.3 \times 10^{10}$ N/m² for zircaloy-2.

CSHEAR employs the following relationships^[B-13.2]:

$$G = \frac{E}{2(1+\nu)} \quad (B-13.1)$$

where

- G = shear modulus (N/m²)
- E = elastic modulus (N/m²)
- ν = Poisson's ratio (unitless).

The elastic modulus and Poisson's ratio are given as functions of temperature by the CELMOD and CPOIR subcodes (Appendixes B-7 and B-12). Although Equation (B-13.1) strictly applies to isotropic materials, only its value for G at room temperature, 3.74×10^{10} N/m², agrees well with Johnson's results^[B-13.1].

Figure B-13.1 shows the temperature dependence of the shear modulus as calculated by CSHEAR.

13.1 Cladding Shear Modulus CSHEAR Listing

A listing of the subcode CSHEAR is given in Table B-13.I.

13.2 References

B-13.1. R. E. Johnson, *The Torsional Properties of Zircaloy-2 and Zircaloy-4*, USAEC Report WAPD-BT-10 (October 1958) pp 49-56.

B-13.2. T. Baumeister, (ed.), *Mechanical Engineers' Handbook*, New York: McGraw-Hill Book Company, Inc., 1958, pp 5-25.

Fig. B-13.1 The CSHEAR correlation for the shear modulus of zircaloy.

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TABLE B-13.I

LISTING OF THE CSHEAR SUBCODE

FUNCTION CSHEAR (CELMOD, CPOIR, CTEMP)	CSAR0010
IMPLICIT REAL*8(A-H, O-Z)	CSAR0020
C	CSAR0030
C CSHEAR CALCULATES THE SHEAR MODULUS OF ZIRCALOY-4 AS	CSAR0040
C A FUNCTION OF TEMPERATURE	CSAR0050
C THE UNITS OF SHEAR MODULUS ARE N/M**2, PASCALS	CSAR0060
C	CSAR0070
C CELMOD=INPUT VALUE OF CLADDING ELASTIC MODULUS AS CALCULATED	CSAR0080
C BY THE CELMOD SUBPROGRAM, CELMOD HAS UNITS OF N/M**2	CSAR0090
C CPOIR=INPUT VALUE OF CLADDING POISSON'S RATIO AS CALCULATED	CSAR0100
C BY THE CPOIR SUBPROGRAM, CPOIR HAS NO UNITS	CSAR0110
C SCHEAR = OUTPUT SHEAR MODULUS OF ZIRCALOY, N/M**2	CSAR0120
C	CSAR0130
C FOR PURPOSES OF INITIAL CODE DEVELOPMENT ZIRCALOY IS ASSUMED	CSAR0140
C TO BE AN ISOTROPIC ALLOY. FOR AN ISOTROPIC MATERIAL	CSAR0150
C	CSAR0160
C ELASTIC MODULUS	CSAR0170
C SHEAR MODULUS = $\frac{\text{ELASTIC MODULUS}}{2 (1 + \text{POISSON'S RATIO})}$	CSAR0180
C	CSAR0190
C	CSAR0200
C	CSAR0210
C SCHEAR WAS CODED BY R.L.MILLER, JUNE '74	CSAR0220
C	CSAR0230
C ELMOD = CELMOD(CTEMP, TIME, FLUX, COLDW, CTRANZ)	CSAR0240
C POIR = CPOIR(CTEMP)	CSAR0250
C CSHEAR = (ELMOD/2.0)/(1 + POIR)	CSAR0260
C RETURN	CSAR0270
C END	CSAR0280

14. CLADDING MEYER HARDNESS (CMHARD)

One of the parameters required for calculating a fuel-sheath contact conductance is hardness. As the contact pressure between the two surfaces increases, the points of contact become enlarged due to localized plastic deformation, and the solid-to-solid thermal conductance is improved. The Meyer hardness is used by Ross and Stoute^[B-14.1] in their heat transfer correlation as an indication of the hardness or resistance to deformation of the softer (zircaloy) material.

The Meyer hardness number is a measure of indentation hardness and is defined by the equation $L = ad^n$ where L is the load, d is the diameter of impression at the surface of a specimen in a static ball test, n is the Meyer work hardening coefficient, and a is the Meyer constant or Meyer hardness number. Other defined hardness numbers are available; for example, Brinell, Rockwell, . . . , and conversion from one to another is possible. However, the routine CMHARD was created to provide information required by the Ross and Stoute gap conductance model.

The hardness of zircaloy was assumed to be proportional to the yield strength of zircaloy:

$$MH = MH_{RT} \left(\frac{YS_T}{YS_{RT}} \right) \quad (B-14.1)$$

where

MH = Meyer hardness number at temperature of interest (N/m^2)

MH_{RT} = Meyer hardness number at room temperature (N/m^2)

YS_{RT} = zircaloy yield strength at room temperature (N/m^2)

YS_T = zircaloy yield strength at temperature of interest (N/m^2).

Meyer hardness numbers for temperatures from 298 to 1,000 K were determined by using the room temperature Meyer hardness value presented by Ross and Stoute and the yield strength data (YS_{RT} and YS_T) of Zima^[B-14.2]. A regression analysis of the Meyer hardness values versus temperature was performed to obtain the analytical expression that is used in CMHARD for the temperature range of 298 to 1,000 K. The Meyer hardness number is assumed to take on constant values outside this temperature range. The correlation used in CMHARD is given by Equations (B-14.2) through (B-14.4).

For $T < 298$ K:

$$MH = 1.96 \times 10^9 \text{ N/m}^2 \quad (B-14.2)$$

For $298 < T < 1,000$ K:

$$\begin{aligned} MH = & 6.51 \times 10^9 - 2.36 \times 10^7 T + 3.29 \times 10^4 T^2 \\ & - 15.68 T^3 \text{ N/m}^2. \end{aligned} \quad (\text{B-14.3})$$

For $T > 1,000$ K:

$$MH = 1.0 \times 10^8 \text{ N/m}^2. \quad (\text{B-14.4})$$

Figure B-14.1 illustrates these relations.

Fig. B-14.1 The CMHARD correlation for the Meyer hardness of zircaloy.

14.1 Cladding Meyer Hardness Subcode CMHARD Listing

Table B-14.I provides a listing of the subcode CMHARD.

TABLE B-14.1

LISTING OF THE CMHARD SUBCODE

FUNCTION CMHARD(CTEMP)	CMRD0010
IMPLICIT REAL*8(A-H,O-Z)	CMRD0020
	CMRD0030
	CMRD0040
THE ROUTINE CMHARD CALCULATES MEYER HARDNESS AS A FUNCTION OF	CMRD0050
CLADDING TEMPERATURE.	CMRD0060
	CMRD0070
	CMRD0080
CTEMP=INPUT CLADDING TEMPERATURE (K).	CMRD0090
CMHARD=OUTPUT MEYER HARDNESS OF ZIRCALOY CLADDING (N/MM**2).	CMRD0100
	CMRD0110
THE CORRELATION OF MEYER HARDNESS AS A FUNCTION OF TEMPERATURE	CMRD0120
USED IN THIS ROUTINE IS BASED ON THE APPROXIMATION THAT HARDNESS	CMRD0130
IS PROPORTIONAL TO YIELD STRENGTH SUGGESTED BY ROSS&STOUTE(AECL-	CMRD0140
1552). THE YIELD STRENGTH DATA WAS TAKEN FROM ZIMA(HW-60908). THE	CMRD0150
CORRELATION USED IS A THIRD ORDER POLYNOMIAL FIT TO THE CALCULAT	CMRD0160
ED VALUES FOR MEYER HARDNESS(MH) FROM THE ASSUMPTION THAT MH AT	CMRD0170
ROOM TEMPERATURE MULTIPLIED BY THE RATIO OF YIELD STRENGTH AT	CMRD0180
TEMPERATURE OF INTEREST TO YIELD STRENGTH AT ROOM TEMPERATURE	CMRD0190
EQUALS MH AT TEMPERATURE OF INTEREST. THE YIELD STRENGTH DATA OF	CMRD0200
ZIMA ONLY COVERS THE TEMPERATURE RANGE OF 298K TO 773K. CONSEQUENT	CMRD0210
LY EXTRAPOLATION OF THE CORRELATION BEYOND THIS RANGE IS NOT	CMRD0220
RECOMMENDED. FURTHERMORE MH IS SET EQUAL TO 1.E8 FOR ALL TEMPERAT	CMRD0230
URES ABOVE 1000K. REFERENCES:A.M.ROSS&R.L.STOUTE.HEAT TRANSFER	CMRD0240
COEFFICIENT BETWEEN UO2 AND ZIRCALOY-2(AECL-1552)1962. G.E.ZIMA,	CMRD0250
A REVIEW OF THE PROPERTIES OF ZIRCALOY-2(HW-60908)1959.	CMRD0260
	CMRD0270
	CMRD0280
CMHARD WAS CODED BY V.F.BASTON IN MAY 1974.	CMRD0290
	CMRD0300
	CMRD0310
T=CTEMP	CMRD0320
IF(T.LT.298) GO TO 10	CMRD0330
IF(T.GT.1000) GO TO 20	CMRD0340
CMHARD=6.513D9-2.365D7*T+3.2931D4*T**2-15.6832*T**3	CMRD0350
GO TO 30	CMRD0360
10 CMHARD=1.9613D9	CMRD0370
GO TO 30	CMRD0380
20 CMHARD=1.008	CMRD0390
30 RETURN	CMRD0410
END	CMRD0420

14.2 References

B-14.1. A. M. Ross and R. L. Stoute, *Heat Transfer Coefficient Between UO₂ and Zircaloy-2*, AECL-1552 (June 1962).

B-14.2. G. E. Zima, *A Review of the Properties of Zircaloy-2*, HW-60908 (October 1959) p 61.

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APPENDIX C

GAS AND FUEL ROD PROPERTIES

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APPENDIX C

GAS AND FUEL ROD PROPERTIES

Three properties of the internal gas or fuel-to-cladding gap of light water reactor fuel pins have been included in MATPRO. The thermal conductivity of seven gases (and their mixture in any combination) is modeled, as is gas viscosity and gap conductance.

The gap conductance model employs the MATPRO gas thermal conductivity predictions and reflects pellet cracking phenomena. The amount of pellet-to-cladding contact is given as a function of burnup, with some contact assured at beginning of life due to early pellet cracking. Gas viscosity and thermal conductivity have been modeled as functions of both temperature and gas composition.

In addition to these three models, a physical property subroutine (PHYPRO) is reported in this appendix. This subroutine provides the melting temperatures and heats of fusion for light water reactor fuels and cladding, and also includes phase transformation temperatures for zircaloy cladding. A number of MATPRO models call upon this subroutine for needed data, some of which are given in PHYPRO as a function of burnup and material composition.

1. GAS THERMAL CONDUCTIVITY (GTHCON)

The cladding-fuel gap conductance is, in part, dependent on the thermal conductivity of the gap gas mixture. Thermal conductivity relations for seven gases have been taken from the literature as has a scheme for calculating the conductivity of mixtures of those gases. The thermal conductivities of the light gases, hydrogen and helium, have been adjusted to allow for imperfect energy transfer between solids and gas in the Knudsen regime.

1.1 Conductivity of Gases and Gas Mixtures

The MATPRO relationship for calculating the thermal conductivity of a monatomic gas mixture is based on the work of Brokaw^[C-1.1] :

$$k_{mix} = \sum_{i=1}^n \left(\frac{k_i}{1 + \sum_{\substack{j=1 \\ j \neq i}}^n \psi_{ij} \frac{x_j}{x_i}} \right) \quad (C-1.1)$$

where

$$\psi_{ij} = \phi_{ij} \left[1 + 2.41 \frac{(M_i - M_j)(M_i - 0.142 M_j)}{(M_i + M_j)^2} \right] \quad (C-1.2)$$

and

$$\psi_{ij} = \frac{\left[1 + \left(\frac{k_i}{k_j} \right)^{1/2} \left(\frac{M_i}{M_j} \right)^{1/4} \right]^2}{2^{3/2} \left(1 + \frac{M_i}{M_j} \right)^{1/2}} \quad (C-1.3)$$

and

n = number of components in mixture

M = molecular weight

x = mole fraction

k = thermal conductivity.

The thermal conductivity equations of the individual rare gases are based on the correlative work of Gandhi and Saxena^[C-1.2]. The resulting expressions are^[C-1.3]:

$$k_{\text{helium}} = 3.366 \times 10^{-3} T^{0.668} \quad (C-1.4)$$

$$k_{\text{argon}} = 3.421 \times 10^{-4} T^{0.701} \quad (C-1.5)$$

$$k_{\text{xenon}} = 4.0288 \times 10^{-5} T^{0.872} \quad (C-1.6)$$

$$k_{\text{krypton}} = 4.726 \times 10^{-5} T^{0.923} \quad (C-1.7)$$

where

k = thermal conductivity (W/m-K)

T = gas temperature (K).

In addition, the following conductivity equations for air, nitrogen, hydrogen, and steam [C-1.3, C-1.4] are used:

$$k_{\text{air}} = 2.091 \times 10^{-4} T^{0.846} \quad (\text{C-1.8})$$

$$k_{\text{N}_2} = 2.091 \times 10^{-4} T^{0.846} \quad (\text{C-1.9})$$

$$k_{\text{H}_2} = 1.6355 \times 10^{-3} T^{0.8213} \quad (\text{C-1.10})$$

$$\begin{aligned} k_{\text{water}} = & (-2.8516 \times 10^{-8} + 9.424 \times 10^{-10} T \\ & - 6.004 \times 10^{-14} T^2) \frac{P}{T} + \frac{1.009 P^2}{T^2 (T-273)^{4.2}} \\ & - 8.4083 \times 10^{-3} - 1.19998 \times 10^{-5} T \\ & - 6.706 \times 10^{-8} T^2 - 4.51 \times 10^{-11} T^3 \end{aligned} \quad (\text{C-1.11})$$

where

P = gas pressure (N/m²).

The thermal conductivity of monatomic gases has been measured by a large number of workers. Gandhi and Saxena, through the facilities of the Thermophysical Properties Research Center of Purdue University, developed a consistent, correlated set of thermal conductivity data for each rare gas through careful evaluation of experimental techniques, review of viscosity data and kinetic theory, and intercomparison of various data. The data on which the Gandhi and Saxena analysis was based are: helium (References C-1.5 through -1.22), argon (References C-1.5, -1.9 through -1.12, -1.17 through -1.21, -1.23 through -1.35), krypton (References C-1.9, -1.14, -1.17 through -1.19, -1.25, -1.26, -1.28, -1.29, -1.31, and -1.36), and xenon (References C-1.9, -1.10, -1.13, -1.14, -1.17 through -1.19, -1.28, -1.36, and -1.37).

The equations based on the correlative work of Gandhi and Saxena have also been compared with the results of the review of experimental and theoretical rare gas conductivities published by Anders and Calvert [C-1.38]. Little difference was noted.

Figure C-1.1 compares the conductivities of the xenon-helium mixture at 520 C (as a function of mole fraction) calculated by GTHCON with those measured and calculated by other investigators (References C-1.1, -1.39 through -1.44 as summarized in Reference C-1.38). The GTHCON values compare well with other published theoretical and experimental values.

1.2 Conductivities in the Knudsen Domain

The thermal conductivity of the gas mixture plays an important role in determining so-called "contact" gap conductance as well as "open" gap conductance in a fuel rod. When the ratio of the mean free path of the gas molecules to the characteristic dimension (gap) of the body exceeds about 0.01, normal heat flow formulas become inaccurate. Heat transfer from a solid to a gas in this Knudsen domain is then dependent on an accommodation coefficient which is defined as the ratio of the actual energy interchange to the maximum possible energy interchange between a surface and a gas. Generally, the accommodation coefficient of a heavy gas such as argon or xenon is near unity and this effect can be neglected. But the effect cannot be neglected when the gap is filled with a light gas such as helium. Dean^[C-1.44] has presented the following factor by which the bulk thermal conductivity of the light gases, helium and hydrogen, should be divided when temperature drops are calculated in the Knudsen domain:

$$f = 1 + \frac{\alpha_1 + \alpha_2 - \alpha_1 \alpha_2}{\alpha_1 \alpha_2} \frac{4}{c_p + c_v} \frac{k \lambda}{\mu \zeta} \quad (\text{C-1.12})$$

where

- α_1 = accommodation coefficient of the fuel
- α_2 = accommodation coefficient of the cladding
- c_p = constant pressure heat capacity
- c_v = constant volume heat capacity
- k = gas thermal conductivity
- μ = gas viscosity
- λ = mean path
- ζ = characteristic dimension (gap).

Fig. C-1.1 Thermal conductivity of xenon-helium mixtures at 520 C.

The mean path (λ) can be written as

$$\lambda = \frac{3\mu}{\rho} \sqrt{\frac{\pi M}{8KT g_c}} \quad (C-1.13)$$

where

- μ = gas viscosity
- T = gas temperature
- M = mass of the molecule
- K = Boltzman constant
- ρ = density of gas
- g_c = gravitational constant.

If λ and ρ are substituted in Equation (C-1.12) and c_p and c_v are assumed to be temperature independent, then Equation (C-1.12) can be rewritten as

$$f = 1 + C \frac{k\sqrt{T}}{P\zeta} \quad (C-1.14)$$

where

- k = thermal conductivity (W/m-K)
- T = temperature (K)
- P = pressure (n/m²)
- ζ = characteristic dimension (m)
- C = empirical constant.

The characteristic dimension, ζ , is essentially equal to the gap dimension and during pellet-to-cladding contact should be equal to the root mean square of the surface roughness, approximately 4.389×10^{-6} meters in most commercial fuel rods. A value for C of approximately $0.2103 \text{ N-K}^{1/2}/\text{W}$ ($8.5 \times 10^{-4} \text{ psi-ft}^2\text{-hr-}^\circ\text{F}^{1/2}/\text{Btu}$) was determined in conjunction with the development of the cracked pellet gap conductance model discussed in Section C-3. C was determined by comparing fuel centerline temperature predictions with thermocouple measurements of centerline temperatures in helium-filled test rods with

strong pellet-cladding mechanical interaction and high contract pressure. These comparisons are presented in Section C-3.2.

Values for the thermal accommodation coefficients of the uranium oxide fuel and zircaloy cladding, α_1 and α_2 , of approximately 0.3 and 0.07, respectively, are obtained by equating Equations (C-1.12) and (C-1.14). Eckert and Drake^[C-1.45] have published thermal accommodation coefficients for glass (a ceramic) and helium of approximately 0.3, as well as coefficients ranging from 0.011 to approximately 0.2 for tungsten or nickel and helium. Thus the accommodation coefficient values determined by comparison of measured and predicted in-pile temperatures compare favorably with the limited thermal accommodation coefficient data published for similar materials.

The effect of heat transfer in the Knudsen domain on fuel temperatures is indicated in Figure C-1.2. Campbell and DesHaies^[C-1.46] performed an experiment in which the fuel rod internal gas pressure was reduced from about 150 atmospheres during irradiation thereby allowing the cladding to collapse onto the fuel. Fuel temperatures near the pellet surface and cladding circumferential strain were continuously monitored. As the internal pressure was decreased, the gap width became smaller (as indicated in Figure C-1.2), the gap conductance increased, and the fuel surface temperature decreased. Further pressure reduction from about ten atmospheres results in increasingly imperfect energy exchange between the fill gas and the fuel and cladding, however. This effect more than compensates for the decreased gap width and the fuel temperature, and then the fuel radius is seen to increase. Continued reduction in fill gas pressure increased fuel temperatures until heat transfer through mating asperity points became dominant. At pressures below approximately 0.01 atmosphere, the heat transfer was primarily through contact conductance and the temperatures stabilized.

1.3 Gas Thermal Conductivity Subcode GTHCON Listing

A listing of the MATPRO subcode GTHCON is presented in Table C-1.1.

1.4 References

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- C-1.2 J. M. Gandhi and S. C. Saxena, "Correlated Thermal Conductivity Data of Rare Gases and Their Binary Mixtures at Ordinary Pressures", *Journ. of Chem. and Eng. Data*, 13, 3 (1968).
- C-1.3 Wisconsin Electric Power Company, "Fuel Densification", Point Beach Nuclear Plant, Unit 2, Docket No. 50301-78 (December 1972).
- C-1.4 *Thermodynamic and Transport Properties of Steam*, New York: American Society of Mechanical Engineers, 1968.

Fig. C-1.2 Effect of measured internal gas pressure on fuel temperatures near the pellet surface [C-1.46]

TABLE C-1.1

LISTING OF THE GTHCON SUBCODE

FUNCTION GTHCON(GMIX, GTEMP, GPRES, GPTHK)	GTON0010
IMPLICIT REAL*8(A-H,O-Z)	GTON0020
	GTON0030
	GTON0040
GTHCON CALCULATES GAS THERMAL CONDUCTIVITY AS A FUNCTION OF	GTON0050
TEMPERATURE AND GAS FRACTION FOR SEVEN GASES:	GTON0060
	GTON0070
GTHCON=OUTPUT GAS THERMAL CONDUCTIVITY (W/M-K).	GTON0080
	GTON0090
GMIX(I) =INPUT MOLE FRACTIONS OF THE GAS MIXTURE	GTON0100
THE SEVEN ELEMENTS OF GMIX MUST SUM TO 1.0	GTON0110
CONSTITUENT GAS NUMBER KEY	GTON0120
1 HELIUM	GTON0130
2 ARGON	GTON0140
3 KRYPTON	GTON0150
4 XENON	GTON0160
5 HYDROGEN	GTON0170
6 AIR	GTON0180
7 WATER VAPOR	GTON0190

TABLE C-1.I (contd.)

LISTING OF THE GTHCON SUBCODE

C		GTON0200
C	GTEMP=INPUT GAS TEMPERATURE (K)	GTON0210
C	GPRES=INPUT GAS PRESSURE (N/M**2)	GTON0220
C	USED FOR KNUDSEN DOMAIN CORRECTION AND FOR STEAM	GTON0230
C	NOT USED IF 0.	GTON0240
C	GPTHK=INPUT EFFECTIVE GAP THICKNESS FOR KNUDSEN DOMAIN (M)	GTON0250
C	= MAX(GAP DIMENSION, SURFACE ROUGHNESS)	GTON0260
C	NOT USED IF 0.	GTON0270
C		GTON0280
C		GTON0290
C	FORMULA FOR GAS MIXTURES IS FROM R.S.BROKAW, REPORT NASA TR R-81	GTON0300
C	(1961). CONDUCTIVITY OF RARE GASES IS BASED ON J.M.GANDHI AND	GTON0310
C	S.C.SAXENA, JOUR. CHEM. & ENG. DATA, VOL.13, NO.3 (1968)	GTON0320
C	ALSO: WISCONSIN ELECTRIC POWER CO., DOCKET NO. 50-301 (JAN 1973)	GTON0330
C	THE ACCOMMODATION FACTOR IS FROM R.A.DEAN, CVNA-127 (1962)	GTON0340
C	STEAM EQUATION IS FROM MAYER, ET.AL., "THERMODYNAMIC AND	GTON0350
C	TRANSPORT PROPERTIES OF STEAM", THE AMERICAN SOCIETY OF	GTON0360
C	MECHANICAL ENGINEERS (1967)	GTON0370
C		GTON0380
C		GTON0390
C	GTHCON CODED BY R.C.YOUNG (INEL) MAR 1975	GTON0400
C	ADAPTED FROM ROUTINE CMIX BY P.E.MACDONALD	GTON0410
C		GTON0420
C	DIMENSION GMIX(7), A(7), C(7), R(7), AA(6), BB(6)	GTON0430
C	DATA A / 4.003D0, 39.944D0, 83.80D0, 131.30D0, 2.016D0, 28.8D0,	GTON0440
C	& 18.016D0 /	GTON0450
C	R = SQRT(A)	GTON0460
C	DATA R / 2.00075D0, 6.3201D0, 9.1542D0, 11.4586D0, 1.41986D0,	GTON0470
C	1 5.3666D0, 4.2445D0 /	GTON0480
C		GTON0490
C	DATA AA/1.314D-3, 1.31D-4, 1.588D-5, 1.395D-5, 5.834D-4, 7.35D-5 /	GTON0500
C	DATA BB / .668D0, .701D0, .92331D0, .872D0, .8213D0, .846D0 /	GTON0510
C	DATA EPS / 1.0-9 /	GTON0520
C		GTON0530
C	CONVERT TEMP TO RANKINE	GTON0540
C	TR = GTEMP * 1.8D0	GTON0550
C	IF (TR.GT.10000.) GO TO 90	GTON0560
C	IF (TR.GT.0.) GO TO 5	GTON0570
C	90 WRITE (6,95) GTEMP, GMIX	GTON0580
C	95 FORMAT(25HIGTHCON INPUT BAD. GTEMP=,1PE12.4,2H K, /	GTON0590
C	& 10HOFRACIONS, (10E12.4))	GTON0600
C	CALL FABEND	GTON0610
C	5 L = 0	GTON0620
C	CALCULATE SMALL GAP CORRECTION	GTON0630
C	FACC = GPRES * GPTHK	GTON0640
C	IF (FACC.GT.EPS) FACC = DSQRT(TR) * 1.7863D0 / FACC	GTON0650
C	DO 10 I = 1,6	GTON0660
C	IF (GMIX(I) .LE. EPS) GO TO 10	GTON0670
C	L = I	GTON0680
C	C(I) = AA(I) * TR**BB(I)	GTON0690
C	IF (FACC .LE. 0.) GO TO 10	GTON0700
C	IF (I.EQ.1 .OR. I.EQ.5)	GTON0710
C	1 C(I) = C(I) / (1.0 + C(I) * FACC)	GTON0720
C	10 CONTINUE	GTON0730
C	IF (GMIX(7) .LE. EPS) GO TO 15	GTON0740
C	L = 7	GTON0750
C		GTON0760
C		GTON0770
C	TC = GTEMP - 273.15D0	GTON0780
C	C(7) = 17.6D-3 + TC*(5.87D-5 + TC*(1.04D-7 - 4.51D-11*TC))	GTON0790
C	IF (GPRES.LE.1.E5) GO TO 8	GTON0800
C	USE IDEAL GAS LAW FOR DENSITY - OK FOR CORRECTION AT HI TEMP.	GTON0810
C	DEN = 2.1668D-6 * GPRES / GTEMP	GTON0820
C	C(7) = C(7) + DEN*(103.51D-3 + TC*(0.4198D-3 - 2.771D-8*TC)	GTON0830
C	1 + 2.1482D11 * DEN / TC**4.20D0)	GTON0840
C	8 C(7) = C(7) / 1.73073467D0	GTON0850
C	15 IF (L.LE.0) GO TO 90	GTON0860
C		

TABLE C-1.I (contd.)

LISTING THE GTHCON SUBCODE

	GTHCON = 0.	GT0N0870
	DO 30 I = 1,L	GT0N0880
	IF (GMIX(I) .LE. EPS) GO TO 30	GT0N0890
	SUM = 0.	GT0N0900
	DO 25 J=1,L	GT0N0910
	IF (J .EQ. I) GO TO 25	GT0N0920
	IF (GMIX(J) .LE. EPS) GO TO 25	GT0N0930
	RC = C(I) / C(J)	GT0N0940
	RA = A(I) / A(J)	GT0N0950
	FIJ = 1. + 2.41D0*(RA-1.)*(RA-.142D0) / (1.+RA)**2	GT0N0960
	GIJ = (1. + DSQRT(RC*R(I)/R(J)))**2 / DSQRT(8.*(1.+RA))	GT0N0970
	SUM = SUM + FIJ * GIJ * GMIX(J)	GT0N0980
25	CONTINUE	GT0N0990
	GTHCON = GTHCON + C(I) * GMIX(I) / (GMIX(I) + SUM)	GT0N1000
30	CONTINUE	GT0N1010
C	CONVERT FROM BTU/HR.FT. ² TO W/M. ² K	GT0N1020
	GTHCON = GTHCON * 1.73073467D0	GT0N1030
	RETURN	GT0N1040
	END	GT0N1050
C-1.5	H. Cheung, L. A. Bromley, C. R. Wilke, "Thermal Conductivity of Gas Mixtures", <i>AIChE Journ.</i> , 8 (1962) pp 221-228.	
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2. GAS VISCOSITY (GVISCO)

Viscosity is an important parameter in describing the dynamic behavior of fluids. According to kinetic theory for a gas having a net mass motion, molecules tend to lose forward momentum due to proximity of stationary surfaces. This loss is described in terms of a viscosity, and it is pertinent to the flow of gas in a fuel-cladding gap as well as through a cladding rupture. In particular, the rate at which gas flows into the ballooning section of a fuel rod is inversely proportional to the fill gas viscosity for narrow gaps, becoming less dependent on the gas viscosity as the gap widens and flow becomes turbulent.

Bretznajder^[C-2.1], Bird et al^[C-2.2], and Hirschfelder et al^[C-2.3] have discussed in detail the functional relationships of viscosity, which in summary show dependence on temperature, pressure, and gas composition. The formulation used in the routine GVISCO was taken from Bird et al^[C-2.2] and is as follows:

$$\mu_{mix} = 0.1 \sum_{i=1}^n \frac{X_i \mu_i}{\sum_{j=1}^n X_j \Phi_{ij}} \quad (C-2.1)$$

where

- μ_{mix} = viscosity of gas mixture (kg/m-sec)
- n = number of chemical species in the mixture
- X_i, X_j = the mole fractions of species i and j
- μ_i, μ_j = the viscosities of species i and j (g/cm-sec)

and Φ_{ij} is a dimensionless parameter defined as

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2 \quad (C-2.2)$$

where

$M_i, M_j =$ the molecular weights of species i and j (g/mol).

The viscosity of a pure monatomic species may be expressed as

$$\mu_i = 2.6693 \times 10^{-5} \frac{\sqrt{MT}}{\sigma^2 k T/\epsilon} \quad (C-2.3)$$

where

M = molecular weight of species (g/mol)

σ = the collision diameter (Å)

T = absolute temperature (K)

ϵ = the maximum energy of attraction between a pair of molecules (ergs/molecule)

k = Boltzmann's constant = 1.38×10^{-16} (ergs/molecule-K).

Bird et al^[C-2.2] states that Equations (C-2.1) through (C-2.3) are useful for computing viscosities of nonpolar gases and gas mixtures at low density from their tabulated values of the intermolecular force parameters σ and ϵ . Figure C-2.1 shows the viscosities for three different cases calculated from Equation (C-2.1): (a) helium only, (b) an equal molar mixture of helium and xenon, and (c) an equal molar mixture of helium, argon, krypton, and xenon. The routine GVISCO currently allows seven gases to be considered: helium, argon, krypton, xenon, hydrogen, air, and steam. Additional nonpolar gases may be readily added to GVISCO if desired.

The viscosity of steam, μ_s , is taken from Meyer et al^[C-2.4]:

$$\mu_s = 80.4 + 0.407 T \quad (C-2.4)$$

where

T = temperature (C).

A density correction could be applied, but examination of tabular data indicates the correction is small at typical fuel rod temperatures.

Fig. C-2.1 Gas viscosity as a function of temperature for pure helium; a binary mixture of helium and xenon; and an equal molar mixture of helium, argon, krypton, and xenon.

2.1 Gas Viscosity Subcode GVISCO Listing

The listing for the subcode GVISCO used for calculating gas viscosity is presented in Table C-2.I.

TABLE C-2.I

LISTING OF THE GVISCO SUBCODE

C	FUNCTION GVISCO(GMIX, GTEMP)	GVIS0010
C		GVIS0020
C	FUNCTION GVISCO CALCULATES GAS VISCOSITY AS A FUNCTION OF	GVIS0030
C	TEMPERATURE AND GAS MOLE FRACTIONS.	GVIS0040
C		GVIS0050
C	GVISCO=OUTPUT GAS VISCOSITY (KG/M-SEC).	GVIS0060
C		GVIS0070
C	GMIX(I) = INPUT ARRAY OF GAS MOLAR FRACTIONS	GVIS0080
C	THE SEVEN ELEMENTS OF GMIX MUST SUM TO 1.0	GVIS0090
C	I = 1 HELIUM	GVIS0100
C	I = 2 ARGON	GVIS0110
C	I = 3 KRYPTON	GVIS0120
C	I = 4 XENON	GVIS0130
C	I = 5 HYDROGEN	GVIS0140
C	I = 6 AIR	GVIS0150
C	I = 7 STEAM - FROM 1967 ASME AT 1 BAR PRESSURE	GVIS0160
C	GTEMP=INPUT GAS TEMPERATURE (K).	GVIS0170
C		GVIS0180
C	IMPLICIT REAL*8(A-H,O-Z)	GVIS0190
C		GVIS0200
C	THE GAS VISCOSITY RELATIONSHIPS USED IN THIS FUNCTION ROUTINE	GVIS0210
C	ARE THOSE STATED BY BIRD, STEWART, AND LIGHTFOOT.	GVIS0220
C	"TRANSPORT PHENOMENA", P.26 AND P.258 (1960).	GVIS0230
C	BIRD, HIRSCHFELDER, CURTISS, TRANS. ASME 76(1954)1011-1038,	GVIS0240
C	OR HANDBOOK OF PHYSICS, CHAPTER 5.5 (MCGRAW-HILL) 1954.	GVIS0250
C		GVIS0260
C	STEAM EQUATION IS FROM MAYER, ET.AL., "THERMODYNAMIC AND	GVIS0270
C	TRANSPORT PROPERTIES OF STEAM". THE AMERICAN SOCIETY OF	GVIS0280
C	MECHANICAL ENGINEERS (1967)	GVIS0290
C		GVIS0300
C	CODED BY R.C.YOUNG AT INEL IN MAR 1975.	GVIS0310
C		GVIS0320
C	DIMENSION SIGMA2(6), EOK(6), IM(6)	GVIS0330
C	DIMENSION A(7), R(7), VIS(7), GMIX(7)	GVIS0340
C	DIMENSION TABLE(164)	GVIS0350
C	DATA EPS, NT, IM / 1.E-8, 82, 6*1 /	GVIS0360
C		GVIS0370
C	DATA SIGMA / 2.576, 3.418, 3.498, 4.055, 2.915, 3.617/	GVIS0380
C	DATA SIGMA2 / 6.635776, 11.682724, 12.236004, 16.443025,	GVIS0390
C	1 8.497225, 13.082689/	GVIS0400
C	DATA EOK / 10.2, 124., 225., 229., 38.0, 97.0/	GVIS0410
C	DATA A / 4.003, 39.944, 83.80, 131.3, 2.016, 28.97, 18.016/	GVIS0420
C	R = SQRT(A)	GVIS0430
C	DATA R / 2.00075D0, 6.32010D0, 9.1542D0, 11.4586D0, 1.41986D0,	GVIS0440
C	1 5.3666D0, 4.2445D0/	GVIS0450
C		GVIS0460
C	DATA TABLE / 2.785,.30, 2.628,.35, 2.492,.40, 2.368,.45, 2.257,.5,	GVIS0470
C	A2.156,.55, 2.065,.60, 1.982,.65, 1.908,.70, 1.841,.75, 1.780,.80,	GVIS0480
C	B1.725,.85, 1.675,.90, 1.629,.95, 1.587,1.0, 1.549,1.05,1.514,1.1,	GVIS0490
C	C1.482,1.15,1.452,1.2, 1.424,1.25,1.399,1.3, 1.375,1.35,1.353,1.4,	GVIS0500
C	D1.333,1.45,1.314,1.5, 1.296,1.55,1.279,1.6, 1.264,1.65,1.248,1.7,	GVIS0510
C	E1.234,1.75,1.221,1.8, 1.209,1.85,1.197,1.9, 1.186,1.95,1.175,2.0,	GVIS0520
C	F1.156,2.1, 1.138,2.2, 1.122,2.3, 1.107,2.4, 1.093,2.5, 1.081,2.6,	GVIS0530

TABLE C-2.I (contd.)

LISTING OF THE GVISCO SUBCODE

	G1.069,2.7, 1.058,2.8, 1.048,2.9, 1.039,3.0, 1.030,3.1, 1.022,3.2,	GVIS0540
	H1.014,3.3, 1.007,3.4, .9999,3.5, .9932,3.6, .9870,3.7, .9811,3.8,	GVIS0550
	I.9755,3.9, .9700,4.0, .9649,4.1, .9600,4.2, .9553,4.3, .9507,4.4,	GVIS0560
	J.9464,4.5, .9422,4.6, .9382,4.7, .9343,4.8, .9305,4.9, .9269,5.0,	GVIS0570
	K.8963,6.0, .8727,7.0, .8538,8.0, .8379,9.0, .8242,10., .7432,20.,	GVIS0580
	L.7005,30., .6718,40., .6504,50., .6335,60., .6194,70., .6076,80.,	GVIS0590
	M.5973,90., .5882,100., .5320,200., .5016,300., .4811,400./	GVIS0600
C		GVIS0610
	L = 0	GVIS0620
	DO 10 I = 1,6	GVIS0630
	IF (GMIX(I) .LE. EPS) GO TO 10	GVIS0640
	L = I	GVIS0650
	TKOE = GTEMP / EOK(I)	GVIS0660
	IF (TKOE.GT.400.) TKOE=400.	GVIS0670
	OMEGA = POLATE(TABLE, TKOE, NT, IM(I))	GVIS0680
	VIS(I) = 2.6693D-6 * DSQRT(A(I)*GTEMP) / (SIGMA2(I)*OMEGA)	GVIS0690
10	CONTINUE	GVIS0700
	IF (GMIX(7) .LE. EPS) GO TO 15	GVIS0710
	L = 7	GVIS0720
C	VIS(7) = 1.E-7 * (0.407*(GTEMP-273.15) + 80.4)	GVIS0730
	VIS(7) = 0.407D-7 * GTEMP - 30.77 D-7	GVIS0740
15	IF (L.LE.0) CALL FABEND	GVIS0750
	GVISCO=0.0	GVIS0752
C		GVIS0760
	DO 30 I = 1,L	GVIS0770
	IF (GMIX(I) .LE. EPS) GO TO 30	GVIS0780
	SUM = 0.	GVIS0790
	DO 20 J = 1,L	GVIS0800
	IF (J .EQ. I) GO TO 20	GVIS0810
	IF (GMIX(J) .LE. EPS) GO TO 20	GVIS0820
	RV = VIS(I) / VIS(J)	GVIS0830
	PHI = (1. + DSQRT(RV*R(J)/R(I)))*2 / DSQRT(8.*(1.+A(I)/A(J)))	GVIS0840
	SUM = SUM + GMIX(J) * PHI	GVIS0850
20	CONTINUE	GVIS0860
	GVISCO = GVISCO + GMIX(I) * VIS(I) / (GMIX(I) + SUM)	GVIS0870
30	CONTINUE	GVIS0880
	RETURN	GVIS0890
	END	GVIS0900

2.2 References

- C-2.1 S. Bretsznajder, *Prediction of Transport and Other Physical Properties of Fluids*, New York: Pergamon Press, 1971.
- C-2.2 R. B. Bird, W. E. Stewart, E. N. Lightfoot, *Transport Phenomena*, New York: John Wiley & Sons, Inc. 1954.
- C-2.3 J. O. Hirschfelder, C. F. Curtiss, R. B. Bird, *Molecular Theory of Gases and Liquids*, New York: John Wiley & Sons, Inc., 1954.
- C-2.4 C. A. Meyer, R. B. McClintock, G. J. Silvestri, R. C. Spencer, Jr., *Thermodynamic and Transport Properties of Steam*, New York: The American Society of Mechanical Engineers, 1967.

3. GAP HEAT TRANSFER (GAPHTR)

GAPHTR calculates the fuel-to-cladding thermal gap conductance as a function of burnup. The model encompasses geometries ranging from an open gap with partial fuel-to-cladding contact to a closed gap with hard contact. Pellet cracking is implicitly considered in the model.

Fuel pellets crack extensively upon irradiation both because of the thermal stresses induced by power changes and, at high burnup, the accumulation of gaseous fission products at grain boundaries. Therefore, the distance between the fuel and cladding will be circumferentially nonuniform, varying between that calculated for an annular gap in an intact fuel rod and essentially zero (fuel segments lying against the cladding wall). Since uranium dioxide pellets tend to crack in the radial direction, the pellet thermal conductivity will be only slightly influenced by this phenomenon. However, the fuel-to-cladding gap thermal conductance will be strongly increased and will generally correspond to a value reflecting both contact and open gas gap conductance.

Efforts to calculate fuel temperatures for rods with large hot gaps based on conductance across an annular gap between the cladding and the fuel using the Ross and Stoute or similar models [C-3.1, C-3.2] have given poor agreement with available inpile high burnup temperature measurements. Calculated fuel temperatures are much higher than observed, and the calculated effect of fill-gas conductivity is greater than that measured. This disagreement between predictions and measurements is not surprising, because pellet cracking in effect moves the gap thermal resistance towards the center of the pellet and replaces, to a certain extent, gap gas conduction with contact conduction. Calculated fuel temperatures using the cracked pellet gap conductance model compare well with data throughout burnup.

3.1 Analytical Model

If a nominal open hot gap is calculated, a fraction of the fuel pellet is assumed to be in contact with the cladding at zero contact pressure and an effective fuel-to-cladding gap conductance is calculated as follows:

$$h_{\text{gap}} = (1-F)h_o + F h_c \quad (\text{C-3.1})$$

where

h_{gap} = net gap conductance ($\text{W}/\text{m}^2\text{-K}$)

h_o = nominal open gap conductance ($\text{W}/\text{m}^2\text{-K}$)

h_c = contact gap conductance (zero contact pressure) (W/m²-K)

F = fraction of pellet circumference in contact with the cladding.

The nominal open gap conductance is determined from

$$h_o = \frac{k_{mix}}{\Delta r + \delta} \quad (C-3.2)$$

where

k_{mix} = thermal conductivity of gas mixture as determined by the GTHCON subroutine described in Section C-1. (W/m-K)

Δr = nominal hot radial gap width (m)

δ = root mean square of the fuel and the cladding surfaces roughness. (A value of 4.4×10^{-6} m was used in this study).

The nominal hot radial gap width, Δr , is a gap width calculated assuming radial fuel cracking and fuel-cladding symmetry but no movement of the fuel segments. The zero pressure contact gap conductance, h_c , is determined from the equation for contact gap conductance discussed subsequently. Radiation heat transfer is assumed negligible.

The fraction of pellet circumference in light contact [P equals zero in Equation (C-3.6)] with the cladding, F , is assumed to be an inverse power law function of the ratio of the nominal hot radial gap and the hot pellet radius as follows:

$$F = \frac{1}{a_1 \left(\frac{\Delta r}{R_F} \right)^{a_2 + 1.429}} + 0.3 \quad (C-3.3)$$

where

R_F = hot radius of the fuel pellet (m)

a_1 and a_2 = empirical constants determined from data.

The relationships for a_1 and a_2 as a function of burnup when the burnup is greater than 600 MWd/MtU are described by Equations (C-3.4) and (C-3.5), respectively:

$$a_1 = 100 - 98 F' \quad (C-3.4)$$

$$a_2 = 4 - 0.5 F' \quad (C-3.5)$$

where

$$F' = 1 - \frac{1}{\left(\frac{x - 600}{1,000}\right)^4 + 1}$$

x = burnup in MWd/MtU

when the burnup is less than or equal to 600 MWd/MtU, then

$$a_1 = 100 \text{ and } a_2 = 4.$$

The fraction of pellet-cladding contact, Equation (C-3.3) is plotted in Figure C-3.1 for both beginning and end of life. The burnup relationship, F' , is plotted in Figure C-3.2. Equations (C-3.4) and (C-3.5) combined with Equation (C-3.3) yield a family of curves between the two curves shown in Figure C-3.1. Thus the fraction of the pellet circumference in contact with the cladding is calculated to increase with both decreasing nominal hot radial gas gap and burnup. The asymptotic value of pellet-cladding contact for large gaps, $F = 0.3$, and the empirical constants a_1 and a_2 , were determined empirically by comparison of predictions with the fuel centerline temperature data discussed in Section C-3.2.

When the fuel and cladding are in contact, the Mikic theory [C-3.3, C-3.4] of thermal conductance with modifications as proposed by Jacobs and Todreas [C-3.5] for ceramic fuel elements is used. The governing equation for contact conductance is thus

$$h_c = C_1 p^n + \frac{k_{\text{mix}}}{\delta} \quad (\text{C-3.6})$$

where

C_1 = 2.7 for stainless steel cladding and 3.4 for zircaloy-2 and zircaloy-4 cladding

P = pellet-cladding contact pressure and is zero when F is less than one (psi)

n = 1 for $0 \leq P \leq 1,000$ psi and $1/2$ for $P > 1,000$ psi.

The value of the exponent, n, is governed by the behavior of the fuel and cladding at the interface of the contact points. An exponent of 1.0 is valid only if the surface peaks of one of the materials are flowing plastically. This type of behavior is consistent with the Ross and Stoute [C-3.1] theory of contact conductance. If the contact points of both materials are behaving elastically, the correct value for the exponent, n, is approximately $1/2$. The

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Fig. C-3.1 Fraction of pellet circumference in contact with the cladding as a function of the ratio of the nominal hot radial gap to the hot pellet radius.

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Fig. C-3.2 Effect of burnup on fraction of pellet circumference in contact with cladding.

experimental results of Fenech and Rohsenow^[C-3.4] support this value and also indicate that for metal-ceramic pairs, the transition pressure from plastic to elastic flow is about 1,000 psi. The parameter k_{mix}/δ in Equation (C-3.6) accounts for heat conduction through the gas in the gaps between contact points.

3.2 Comparison of Predictions with Experimental Data

Measured fuel centerline temperatures are compared with calculations obtained through use of both the cracked pellet and the Ross and Stoute^[C 3.1,C 3.2] gap conductance models. Only well characterized rods with known power levels and measured system coolant conditions or cladding temperatures were considered. The following fuel rod conditions are reflected in the data: pellet density (92-96% TD), cold diametral gap (2-13 mils), and initial internal gas composition (helium and fission gas). The burnup ranged from 0 to about 15,300 MWd/MtU.

The data comparisons are grouped according to initial fill gas and burnup: (a) fission gas-filled test rods with little burnup; (b) helium-filled rods at beginning of life; and (c) helium-filled rods at various burnups. The initial fuel rod conditions for each comparison are summarized on the figure showing that comparison.

Figures C-3.3 through C-3.7 present temperature data from Reference C-3.6 for six capsules. Although the data were taken at relatively low power levels, typical commercial fuel rod dimensions and coolant conditions (except for initial gas composition) are represented. The calculated values obtained using the cracked pellet model are in much better agreement with data from those Reference C-3.6 test rods initially filled with fission gas than are the values calculated using the Ross and Stoute model. Predictions with both models are in reasonable agreement with the data for the helium-filled rod (Figure C-3.7). These results lend support to the concept that pellet cracking and relocation effectively increase the gap conductance and that a significant proportion of the heat is transferred through mating asperity points rather than by gas gap conduction, even in rods with relatively large initial pellet-to-cladding gaps.

The comparisons of model predictions with data presented in Figures C-3.8 through C-3.11 show centerline temperature data from helium-filled rods that were irradiated in the Halden HBWR to about 4,200 MWd/MtU^[C-3.7]. These rods experienced periodic ramps to moderate power levels (about 13 kW/ft at the location of temperature measurement) throughout the irradiation period. Figures C-3.8 through C-3.11 show reasonable agreement between the prediction and the measurement for both gap conductance models. In Figures C-3.8 and C-3.9 hard fuel-cladding contact is predicted for a major portion of the power ramps (above 4 to 5 kW/ft). The cracked pellet gap conductance model calculated slightly increased centerline temperatures and changes in temperature with power as compared with the Ross and Stoute model. This result is obtained because of the assumption in the Mikic model of elastic behavior of the mating asperity points at contact pressures above 1,000 psi.

Fig. C-3.3 Measured and predicted fuel centerline temperature versus power for Rod 22-14 [C-3.6]

Figures C-3.12 and C-3.13 compared predictions obtained using both models with measured fuel centerline data reported in Reference C-3.8. Both models show excellent agreement with the data from these large gap helium-filled rods.

Data from the Halden test assembly IFA-226 [C-3.9] were used to evaluate both models at burnups up to 15,300 MWd/MtU. Figure C-3.14 presents the IFA-226 fuel centerline temperature data versus power during the first power ramp (zero to full power in 12 hours). Except for a very few points, the response is continuous and almost linear. The data extrapolate to the system temperature at zero power. Compared with one another, Rod AO and AA temperatures show similar relationships with power [a]. Temperatures for the high density fuel Rod AK are somewhat lower, and the temperatures for the large

[a] Both are rods of standard PWR design: 8-mil gap, 92.8% dense fuel.

Fig. C-3.4 Measured and predicted fuel centerline temperature versus power for Rod 22-15^[C-3.6].

pellet-to-cladding gap Rod AE are somewhat higher than the temperatures of Rods AO and AA as expected. Figure C-3.15 presents the IFA-226 pellet centerline temperature versus power data for these same rods during the following 25-hour period (nearly full power for 9 hours, decreasing power for 16 hours). This figure suggests considerable pellet cracking and relocation. Centerline temperatures for the large pellet-to-cladding gap Rod AE are now similar to those of the standard Rods AO and AA. Figure C-3.16 presents Rod AK centerline fuel temperature measurements taken during both increasing and decreasing power during the first four power ramps. The hysteresis effect at 10 to 14 kW/ft apparently is due to cracked pellet healing at high temperatures, followed by reformation of the pellet-to-cladding gap upon power reduction, followed in turn by the reinitiation of pellet cracking during temperature changes at lower power levels or during the subsequent power ramp.

Fig. C-3.5 Measured and predicted fuel centerline temperature versus power for Rods 22-2 and 22-9 [C-3.6].

The fuel centerline temperature data from the first four days of irradiation, (four power ramps) of Rods AA, AO, AE, and AK and model predictions are shown in Figures C-3.17 through C-3.20, respectively. The centerline temperature at a given power increased slightly (compared with the preceding power ramp) during the first three power ramps and then stabilized in all four rods. This small increase in the fuel temperatures during the first three power ramps may have been due to slight changes in the fuel thermal conductivity caused by pellet cracking. In any case, the predictions, obtained using both gap conductance models, are in good agreement with these data after the temperatures stabilize (Ramps 3 and 4).

Comparisons of model predictions with IFA-226 fuel centerline temperature data at various burnups to 15,300 MWd/MtU are shown in Figures C-3.21 through C-3.27. These data indicate that burnup effects on pellet cracking and relocation (and possibly UO_2 thermal conductivity which is not considered) reduce the temperature at a given power in a nonlinear fashion. The effects of burnup do not become noticeable in the experimental data until about 1,000 MWd/MtU of burnup and become constant after 10,000 MWd/MtU. Figures C-3.21 through C-3.27 also suggest that, as burnup increases, the Ross and Stoute gap conductance model becomes progressively more conservative. At a burnup of about 15,300 MWd/MtU, the Ross and Stoute gap conductance model overpredicts measured fuel centerline temperatures by at least 1,000 F. The calculated release of fission product gases

Fig. C-3.6 Measured and predicted fuel centerline temperature versus power for Rod 22-7^[C-3.6].

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Fig. C-3.7 Measured and predicted fuel centerline temperatures versus power for Rod 22-4 [C-3.6].

degrades the fill gas conductivity at high burnup and, therefore, substantially decreases the Ross and Stoute calculated gap conductance values. Predictions obtained using the cracked pellet gap conductance model compare well with the IFA-226 temperature data throughout burnup suggesting that increased pellet cracking and relocation with burnup compensates for the degradation in gap gas thermal conductivity.

3.3 Gap Heat Transfer Subcode GAPHTR Listing

A listing of the subcode GAPHTR is presented in Table C-3.I.

3.4 References

- C-3.1 A. M. Ross and R. L. Stoute, *Heat Transfer Coefficient Between UO_2 and Zircaloy-2*, AECL-1552, Chalk River, Ontario, Canada (June 1962).
- C-3.2 C. R. Hann, C. E. Beyer, L. J. Parchen, *GAPCON-THERMAL-1: A Computer Program for Calculating the Gap Conductance in Oxide Fuel Pins*, BNWL-1778 (September 1973).

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Fig. C-3.8 Measured and predicted fuel centerline temperature versus power for Rod HBB [C-3.7].

- C-3.3 B. B. Mikic and W. M. Rohsenow, *Thermal Contact Resistance*, DSR 74542-41, Mechanical Engineering Dept., Massachusetts Institute of Technology (1966).
- C-3.4 H. Fenech and W. M. Rohsenow, "Prediction of Thermal Conductance of Metallic Surface in Contact", Paper 62-HT-32, *Trans. ASME, Journ. of Heat Transfer* (March 1963).
- C-3.5 G. Jacobs and N. Todreas, "Thermal Contact Conductance in Reactor Fuel Elements", *Nuclear Science and Engineering*, 50 (1973).

Fig. C-3.9 Measured and predicted fuel centerline temperature versus power for Rod HCD^[C-3.7].

Fig. C-3.10 Measured and predicted fuel centerline temperature versus power for Rod HBC^[C-3.7].

Fig. C-3.11 Measured and predicted fuel centerline temperature versus power for Rod HCC^[C-3.7].

- C-3.6 I. Cohen, B. Lustman, J. O. Eichenberg, *Measurement of the Thermal Conductivity of Metal-Clad Uranium Oxide Rods During Irradiation*, WAPD-228 (1960).
- C-3.7 G. Kjaerheim and E. Rolstad, *In-File Determination of UO_2 Thermal Conductivity, Density Effects and Gap Conductance*, HPR-80 (December 1967).
- C-3.8 I. Devold, *A Study of the Temperature Distribution in UO_2 Reactor Fuel Elements*, Report AE-318, Akticbolaget Atomenergi, Stockholm, Sweden (1968).
- C-3.9 E. T. Laats, P. E. MacDonald, W. J. Quapp, *USNRC-OECD Halden Project Fuel Behavior Test Program – Experiment Data Report for Test Assemblies IFA-226 and IFA-239*, ANCR-1270 (December 1975).

Fig. C-3.12 Measured and predicted fuel centerline temperature versus power for the IFA-3 rod^[C-3.8].

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Fig. C-3.13 Measured and predicted fuel centerline temperature versus power for the IFA-4 rod^[C-3.8]

Fig. C-3.14 IFA-226 fuel centerline temperature data versus power during the initial startup power cycle [C-3.9].

Fig. C-3.15 IFA-226 fuel centerline temperature data versus power during the 25-hour period following the initial startup power ramp [C-3.9].

Fig. C-3.16 Measured fuel centerline temperature versus power for Rod AK during the first four power ramps^[C-3.9].

Fig. C-3.17 Measured and predicted fuel centerline temperature versus power for Rod AA at 0 to 100 MWd/MtU [C-3.9].

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Fig. C-3.18 Measured and predicted fuel centerline temperature versus power for Rod A0 at 0 to 100 MWd/MtU [C-3.9]

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Fig. C-3.19 Measured and predicted fuel centerline temperature versus power for Rod AE at 0 to 70 MWd/MtU^[C-3.9].

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Fig. C-3.20 Measured and predicted fuel centerline temperature versus power for Rod AK at 0 to 100 MWd/MtU^[C-3.9]

Fig. C-3.21 Measured and predicted fuel centerline temperature versus power for Rod AA at 1,100 MWd/MtU [C-3.9].

Fig. C-3.22 Measured and predicted fuel centerline temperature versus power for Rod A0 at 1,700 MWd/MtU [C-3.9].

Fig. C-3.23 Measured and predicted fuel centerline temperature versus power for Rod A0 at 2,900 MWd/MtU^[C-3.9].

Fig. C-3.24 Measured and predicted fuel centerline temperature versus power for Rod AA at 6700 MWd/MtU [C-3.9]

Fig. C-3.25 Measured and predicted fuel centerline temperature versus power for Rod AA at 10,900 MWd/MtU^[C-3.9]

Fig. C-3.26 Measured and predicted fuel centerline temperature versus power for Rod AA at 12,500 MWd/MtU [C-3.9]

Fig. C-3.27 Measured and predicted fuel centerline temperature versus power for Rod AA at 15,300 MWd/MtU [C-3.9].

TABLE C-3.1

LISTING OF THE GAPHTR SUBCODE

```

SUBROUTINE GAPHTR (BU      ,PRES      ,GASES      ,DELH      ,DPH      ,GAPC0020
1      ,GPTH      ,HGAP      ,ICM      ,PINNM      ,TP      ,TX      ,GAPC0040
2      ,TAGK      ,DELBU      )      ,GAPC0060
C      ,GAPC0080
C      IMPLICIT REAL*8 (A-H,O-Z)      ,GAPC0100
C      ,GAPC0101
C      GAPHTR CALCULATES THE FUEL/CLADDING GAP HEAT CONTUCTANCE AS A      ,GAPC0102
C      FUNCTION OF BURN-UP, HOT DIAMETRAL GAP AND FILL GAS CONDUCTIVITY.      ,GAPC0103
C      ,GAPC0104
C      ,GAPC0120
C      *****      ,GAPC0140
C      INPUT VARIABLES      ,GAPC0160
C      *****      ,GAPC0180
C      ,GAPC0200
C      BU      - BURN-UP (MWD/MTU)      ,GAPC0220
C      DELBU      - ROD AVERAGE BURNUP DURING TIME STEP (MWD/MTU)      ,GAPC0240
C      DELH      - TIME STEP SIZE (SEC)      ,GAPC0260
C      DPH      - HOT AXIAL NODE DIAMETER (M)      ,GAPC0280
C      GASES      - MOLE FRACTIONS OF THE GAP GASES      ,GAPC0300
C      (1) - HELIUM      ,GAPC0320
C      (2) - ARGON      ,GAPC0340
C      (3) - KRYPTON      ,GAPC0360
C      (4) - XENON      ,GAPC0380
C      (5) - HYDROGEN      ,GAPC0400
C      (6) - AIR      ,GAPC0420
C      (7) - WATER VAPOR      ,GAPC0440
C      GPTH      - GAP THICKNESS (DIAMETRAL) (M)      ,GAPC0460
C      ICM      - CLAD MATERIAL INDEX      ,GAPC0480
C      ICM=1 - STAINLESS STEEL      ,GAPC0500
C      ICM=2 - ZIRCALOY-2      ,GAPC0520
C      ICM=4 - ZIRCALOY-4      ,GAPC0540
C      PINNM      - INTERFACIAL PRESSURE (N/M**2)      ,GAPC0560
C      PRES      - ROD INTERNAL GAS PRESSURE (N/M**2)      ,GAPC0580
C      TAGK      - AVERAGE GAP GAS TEMPERATURE (K)      ,GAPC0600
C      TP      - TIME TO BEGINNING OF TIME STEP (SEC)      ,GAPC0620
C      TX      - TIME TO POINT OF CREEP CALCULATION (SEC)      ,GAPC0640
C      ,GAPC0660
C      *****      ,GAPC0680
C      OUTPUT VARIABLES      ,GAPC0700
C      *****      ,GAPC0720
C      ,GAPC0740
C      HGAP      - GAP CONDUCTANCE (W/M**2-K)      ,GAPC0760
C      ,GAPC0780
C      *****      ,GAPC0781
C      ,GAPC0782
C      THE CRACKED PELLET GAP CONDUCTANCE MODEL USED IN THIS SUBROUTINE      ,GAPC0783
C      WAS DEVELOPED BY BROUGHTON AND MACDONALD, REFERENCE - A CRACKED      ,GAPC0784
C      PELLET GAP CONDUCTANCE MODEL - COMPARISON OF FRAP-S CALCULATIONS      ,GAPC0785
C      WITH MEASURED FUEL CENTERLIN TEMPERATURES, BY MACDONALD,P.E.,      ,GAPC0786
C      BROUGHTON, J.M., ENLARGED HALDEN PROGAAMME GROUP MEETING, GEILO,      ,GAPC0787
C      NORWAY, MARCH 16+H-21ST,1975.      ,GAPC0788
C      ,GAPC0789
C      ,GAPC0790
C      GAPHTR WAS CODED BY G.A. BERNA.,      ,GAPC0791
C      ,GAPC0792
C      DIMENSION A(6)      ,GAPC0800
C      ,GAPC0820
C      DATA      A(1)/100.00/ ,A(2)/4.00/ ,A(3)/2.00/ ,A(4)/3.500/ ,GAPC0840
C      ,GAPC0860
C      CGASCL = GTHCON( GASES , TAGK , PRES , 4.389D-6)      ,GAPC0920

```

TABLE C-3.I (contd.)

LISTING OF THE GAPHTR SUBCODE

C	IF(PINNM .EQ. 0.0) GO TO 10	GAPC0940
C		GAPC0960
C	CONVERT FROM W/M-K TO BTU/HR-FT-F	GAPC0980
C	CGASCL = CGASCL/1.7296	GAPC1000
C	CONVERT FROM N/M**2 TO PSI	GAPC1020
C	PIN = PINNM/6894.76	GAPC1040
C		GAPC1060
C	IF(ICM .EQ. 1.AND. PIN .LE. 1000.) HGAP = 0.475 * PIN +	GAPC1080
1	CGASCL/14.4D-6	GAPC1100
C		GAPC1120
C	IF(ICM .EQ. 1.AND. PIN .GT. 1000.) HGAP = 475. + .475 *	GAPC1140
1	DSQRT(PIN - 1000.) + CGASCL/14.4D-6	GAPC1160
C		GAPC1180
C	IF(ICM .EQ. 1.AND. PIN .GT. 5.64D+6) HGAP = 2375. +	GAPC1200
1	CGASCL/14.4D-6	GAPC1220
C		GAPC1240
C	IF(ICM .GE. 2.AND. PIN .LE. 1000.) HGAP = 0.6 * PIN +	GAPC1260
1	CGASCL/14.4D-6	GAPC1280
C		GAPC1300
C	IF(ICM .GE. 2.AND. PIN .GT. 1000.) HGAP = 600. + 0.6 *	GAPC1320
1	DSQRT(PIN - 1000.) + CGASCL/14.4D-6	GAPC1340
C		GAPC1360
C	IF(ICM .GE. 2.AND. PIN .GT. 9.D6) HGAP = 3000. +	GAPC1380
1	CGASCL/14.4D-6	GAPC1400
C		GAPC1420
C	CONVERT FROM BTU/HR-FT**2-F TO W/M**2-K	GAPC1440
C	HGAP = HGAP*5.6745	GAPC1460
C	RETURN	GAPC1480
C		GAPC1500
C		GAPC1520
C		GAPC1540
C	10 CONTINUE	GAPC1560
	GPTHM = DMAX1(GPTH/2.D0 , 4.389D-6)	GAPC1580
	CGASOP = GTHCON(GASES , TAGK , PRES , GPTHM)	GAPC1600
	BU1 = (TX - TP)*DELBU/DELH + BU - DELBU	GAPC1640
	IF(BU1 .GT. 600.) GO TO 20	GAPC1660
	FRCBU = 0.00	GAPC1680
	GO TO 30	GAPC1700
	20 FRCBU = 1.00-1.00/((((BU1- 600.)/1000.))**4) + 1.00)	GAPC1720
	30 CONTINUE	GAPC1740
C		GAPC1760
C	DO 40 I=1,2	GAPC1780
40	A(I+4) = (A(I+2) - A(I))*FRCBU + A(I)	GAPC1800
C		GAPC1820
C	CA = 1./(A(5) * (GPTH * 100./DPH)**A(6) + 1.42857D0) + 0.3	GAPC1840
C		GAPC1860
C		GAPC1880
C	HGAP1 = CGASOP/((GPTH/2.) + 4.389D-6)	GAPC1900
	HGAP2 = CGASCL/4.389D-6	GAPC1920
C		GAPC1940
C	HGAP = HGAP1 * (1. - CA) + HGAP2 * CA	GAPC1960
	RETURN	GAPC1980
	END	GAPC2000

4. PHYSICAL PROPERTIES (PHYPRO)

The routine PHYPRO returns melting temperatures and heats of fusion for UO_2 , $\text{UO}_2\text{-PuO}_2$, and zircaloy and returns α to β transformation temperatures for zirconium and zircaloy. The fuel melting temperatures are modeled as a function of burnup and for mixed oxides as a function of plutonium content.

4.1 UO_2 and $\text{UO}_2\text{-PuO}_2$ Melting Point

The melting point of unirradiated UO_2 has been measured by several investigators with varying results. Brassfield et al^[C-4.1] and Lyons et al^[C-4.2] have published compilations and discussions of several recent experimental results and have listed "best" value UO_2 melting points of 2,840 and $2,860 \pm 15$ C, respectively, for burnups less than 10,000 MWd/MtU. The routine PHYPRO uses Brassfield et al's recommendation of 3,113 K for the melting temperature of unirradiated UO_2 .

Lyon and Bailly^[C-4.3] determined the phase diagram for stoichiometric $\text{UO}_2\text{-PuO}_2$ mixed oxides. The temperature data for the solidus and for the liquidus boundaries were fit by least squares techniques to a parabolic equation and these results are given for the solidus and liquidus boundaries by Equations (C-4.1) and (C-4.2), respectively.

$$T (\text{solidus}) = 2,840.0 - 5.414 C + 7.468 \times 10^{-3} T^2 \quad (\text{C-4.1})$$

$$T (\text{liquidus}) = 2,840.0 - 3.219 C - 1.449 \times 10^{-2} T^2 \quad (\text{C-4.2})$$

where

C = the mole percent of PuO_2

T = temperature (C).

The solidus curve is used for the melting point of mixed oxides and the difference between the liquidus and solidus boundaries defines the temperature range in which solid and liquid coexist. Figure C-4.1 shows the solidus and liquidus boundaries.

Christensen^[C-4.4, C-4.5] established that the melting point of his UO_2 samples decreased with fuel burnup. The largest decrease measured by Christensen was about 32 C per 10,000 MWd/MtU. Krankota and Craig^[C-4.6] have also reported a 50 to 100 C decrease in the melting point of irradiated mixed oxide test samples for burnups between 55,000 and 85,000 MWd/MtM. However, these results are not in accord with those of Reavis and Green^[C-4.7] who reported no significant reduction in the melting point of UO_2 due to irradiation. Since a fission event results in the accumulation of cationic fission products together with some liberation of oxygen, a lowering of the melting point of UO_2 during irradiation is expected. Therefore, the melting point of UO_2 and mixed oxides is decreased 32 C per 10,000 MWd/MtM in PHYPRO.

Fig. C-4.1 Phase diagram for stoichiometric mixed uranium plutonium oxides.

4.2 UO₂ and UO₂-PuO₂ Heat of Fusion

The two calorimetrically determined values for the heat of fusion of unirradiated UO₂ are in good agreement. Specifically, Hein and Flagella [C-4.8] measured a UO₂ heat of fusion of 18.2 ± 0.5 kcal/mol and Leibowitz et al [C-4.9] reported a value of 17.7 kcal/mol. These results suggest that the heat of fusion of unirradiated UO₂ is adequately known from present analyses. The routine PHYPRO uses Leibowitz et al's calorimetry data of 2.74×10^5 J/kg for the heat of fusion of UO₂.

Leibowitz et al [C-4.10] determined a heat of fusion for mixed oxides of 16 kcal/mol from three tests (as compared with 17.7 kcal/mol for UO₂). The 10% agreement

between the UO_2 and mixed oxide values for the heat of fusion is quite reasonable and suggests that until more data become available, the UO_2 value can be used for the heat of fusion of mixed oxides. Similar values for the mixed oxide and UO_2 heats of fusion are theoretically expected because of the similarity in crystal structure and atomic bonding.

4.3 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^[C-4.11], and small amounts of iron, nickel, or chromium decrease the solidus temperatures of a binary mixture about 70 C for each 0.1% addition of solute^[C-4.12]. These results are for the binary mixtures of zirconium and one solute: tin, iron, chromium, or nickel. In the zircaloy five component 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 1,825 C, and this value is returned by PHYPRO.

Pure zirconium isothermally transforms from the α phase to the β phase at 862 C^[C-4.13]. The routine PHYPRO returns 1,135.15 K for the zirconium transformation temperature when the variable CTRANZ is called. Zircaloy, however, undergoes the same transformation over a range of temperatures. PHYPRO returns the beginning of the α - β transformation (1,083.15 K) using the variable CTRANB and the end of the α - β transformation (1,243.15 K) using the variable CTRANE^[C-4.14].

4.4 Zircaloy Heat of Fusion

The heat of fusion of zircaloy will depend to some extent on its composition and the extent of oxidization. Brassfield et al^[C-4.1] 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 4.9 kcal/mol. However, Quill^[C-4.15] lists the heat of fusion of zirconium as 5.5 kcal/mol with uncertainty. The routine PHYPRO returns Brassfield et al's^[C-4.1] listed heat of fusion for zirconium of 2.25×10^5 J/kg when called.

4.5 Physical Properties Subcode PHYPRO Listing

The subcode PHYPRO is listed in Table C-4.I.

4.6 References

- C-4.1 H. C. Brassfield, J. F. White, L. Sjodahl, J. T. Bittle, *Recommended Property and Reactor Kinetics Data for Use in Evaluating a Light-Water-Cooled Reactor Loss-of-Coolant Incident Involving Zircaloy-4 of 304-SS-Clad UO_2* , GEMP-482 (April 1968).
- C-4.2 M. F. Lyons, R. F. Boyle, J. H. Davies, V. E. Hazel, T. C. Rowland, "UO₂ Properties Affecting Performance", *Nuc. Eng. and Design*, 21 (1972) p 167.

TABLE C-4.I

LISTING OF THE PHYPRO SUBCODE

```

SUBROUTINE PHYPRO(FTMELT,FHEFUS,CTMELT,CHEFUS,CTRANB,CTRANE,
C CTRANZ,FDELTA,BU,COMP)
C IMPLICIT REAL*8(A-H,O-Z)
C
C PHYPRO RETURNS UO2, MIXED OXIDE FUEL, AND ZR CLAD MELTING POINTS
C AND HEATS OF FUSION, AND ZIRCONIUM AND ZIRCALOY ALPHA TO BETA
C TRANSITION TEMPERATURES.
C
C FTMELT=OUTPUT UO2 OR MIXED OXIDE FUEL MELTING POINTS (K)
C FHEFUS=OUTPUT UO2 OR MIXED OXIDE FUEL HEAT OF FUSION(J/KG)
C CTMELT=OUTPUT ZR CLAD MELTING POINT (K).
C CHEFUS=OUTPUT ZR CLAD HEAT OF FUSION (J/KG).
C CTRANB=OUTPUT BEGIN OF ZR-4 ALPHA-BETA TRANSUS TEMPERATURE (K)
C CTRANF=OUTPUT END OF ZR-4 ALPHA-BETA TRANSUS TEMPERATURE (K)
C CTRANZ=OUTPUT ZR ISOTHERMAL ALPHA-BETA TRANSUS TEMPERATURE (K)
C FDELTA=OUTPUT LIQUID-SOLID COEXISTANCE TEMPERATURE RANGE (K)
C BU=BURNUP, MEGAWATT-SECONDS/KG URANIUM
C COMP=PUO2 CONTENT, WEIGHT PERCENT
C
C THE UO2 FUEL AND ZR CLAD MELTING POINTS AND HEATS OF FUSION ARE
C TAKEN FROM THE FOLLOWING REFERENCES. UO2 FUEL MELTING POINT OF
C 2840C FROM H.C.BRASSFIELD ETAL.-GEMP-482. UO2 FUEL HEAT OF FUSION
C OF 17.7KCAL/MOLE FROM L.LEIBOWITZ ETAL.-J.NUC.MAT. VOL39 P.115
C (1971). ZR CLAD MELTING POINT OF 1825C FROM M.L. PICKLESIMER
C PRIVATE COMMUNICATION. ZR CLAD HEAT OF FUSION OF 4.9 KCAL/MOLE
C FROM BRASSFIELD ET AL. -GEMP-482.
C BEGINNING OF ZIRCALOY ALPHA-BETA TRANSUS TEMPERATURE IS 1490 F
C DATA TAKEN FROM M.L. PICKLESIMER, U. S. PATENT 2,894,866
C END OF ZIRCALOY ALPHA-BETA TRANSUS TEMPERATURE IS 1780 F
C DATA TAKEN FROM M.L. PICKLESIMER, U. S. PATENT 2,894,866
C ISOTHERMAL ZIRCONIUM ALPHA-BETA TRANSUS TEMPERATURE IS 862C
C DATA TAKEN FROM B.LUSTMAN&F.KERZE "THE METALLURGY OF ZIRCONIUM"
C MCGRAW-HILL BOOK CO., NEW YORK, 1955
C
C PHYPRO WAS CODED BY V.F. BASTON IN MAY 1974 AND MODIFIED BY R.L.
C MILLER IN JUNE 1974.
C
C PHYPRO WAS FURTHER MODIFIED BY C. S. OLSEN IN FEBRUARY 1975 TO
C INCLUDE MIXED OXIDE MELTING POINTS AND THE EFFECT OF IRRADIATION
C UPON UO2 AND UO2-PUO2 MELTING POINTS AND MODIFICATIONS TO THE
C ZIRCALOY MELTING POINT AND PHASE TRANSITION TEMPERATURES.
C
C MIXED OXIDE MELTING POINTS WAS OBTAINED FROM LYON ET AL, REFERENCE
C IS J NUCL MAT VOL 22 (1967) PG. 332.
C
C MOLE(C) = (C/269.96/(C/269.96 + (100. - C)/270.04))*100.
C SLOUS(C) = 2840.0 - 5.41395*C + 7.468390-3*C*C
C LIQDUS(C) = 2840.0 - 3.2186*C - 1.4485180-2*C*C
C FBU = BU/86.4
C IF (COMP.GT. 0.0) GO TO 10
C FTMELT=3113.15 - 32.0*FBU/10000.0
C FDELTA = 1.00-10
C GO TO 20
10 C1 = MOLE(COMP)
C FTMELT = SLOUS(C1) + 273.15 - 32.0*FBU/10000.0
C FDELTA = LIQDUS(C1) - SLOUS(C1) - 32.0*FBU/10000.0
20 FHEFUS=27.40+4
C CTMELT=2098.15
C CHEFUS=22.50+4
C CTRANB = 1083.15
C CTRANF = 1243.15
C CTRANZ = 1135.15
C RETURN
C END

```

- C-4.3 W. L. Lyon and W. E. Baily, "The Solid-Liquid Phase Diagram for the $\text{UO}_2\text{-PuO}_2$ System", *Journ. Nucl. Mat.*, 22, 332 (1967).
- C-4.4 J. A. Christensen, *Radiation Effects on UO_2 Melting*, HW-69234, Hanford Atomic Products Operation (March 1962).
- C-4.5 J. A. Christensen, R. J. Allio, A. Biancheria, *Melting Point of Irradiated Uranium Dioxide*, WCAP-6065 (1965).
- C-4.6 J. L. Krankota and C. N. Craig, "Melting Point of High Burnup $\text{PuO}_2\text{-UO}_2$ ", *Trans. Amer. Nucl. Soc.*, 11 132 (1968).
- C-4.7 J. G. Reavis and J. L. Green, "Transformation Temperatures of Irradiated $\text{UO}_2\text{-PuO}_2$ Fast Reactor Fuels", *Trans. Amer. Nucl. Soc.*, 14 593 (1971).
- C-4.8 R. A. Hein and P. N. Flagella, *Enthalpy Measurements of UO_2 and Tungsten to 3,260°K*, GE-NMPO-578 (February 1968).
- C-4.9 L. Leibowitz, M. G. Chasanov, L. W. Mishler, D. F. Fischer, "Enthalpy of Liquid Uranium Dioxide to 3,500°K", *Journ. Nucl. Mat.*, 39 (1971) p 115.
- C-4.10 L. Leibowitz, D. F. Fischer, M. G. Chasanov, *Enthalpy of Molten Uranium-Plutonium Oxide*, ANL-8082, Argonne National Laboratory (February 1975).
- C-4.11 D. J. McPherson and M. Hansen, "The System Zirconium-Tin", *Trans. ASM*, 45, 915 (1953).
- C-4.12 E. T. Hayes, A. H. Roberson, O. G. Paasche, "The Zirconium-Nickel Phase Diagram", *Trans. ASM*, 45, 893 (1953).
- C-4.13 B. Lustman and F. Kerze, *The Metallurgy of Zirconium*, New York: McGraw-Hill Book Company, Inc., 1955.
- C-4.14 M. L. Picklesimer, "Method of Annealing and Rolling Zirconium-Base Alloys", U.S. Patent 2,894,866 (July 14, 1959).
- C-4.15 L. L. Quill, *Chemistry and Metallurgy of Miscellaneous Materials, Thermodynamic, National Nuclear Energy Series, Div. IV, Vol. 19B*, New York: McGraw-Hill Book Company, Inc., 1950.

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APPENDIX D
SUPPORTING MATERIAL FOR MATPRO

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APPENDIX D

SUPPORTING MATERIAL FOR MATPRO

This Appendix contains a list of input and output arguments for each of the MATPRO subcodes, the base and derived SI units used in MATPRO, and the linear interpolation routine (FOLATE).

1. INPUT-OUTPUT ARGUMENTS OF MATPRO SUBCODES

Input and output arguments for each of the MATPRO subcodes are given in the following table. This description provides a summary of the FORTRAN subcodes that are described in detail in Appendixes A, B, and C.

TABLE D-1.I

INPUT-OUTPUT ARGUMENTS OF MAIPRO SUBCODES

Subcode	Arguments	I/O ^[a]	Description
<u>Fuel Subcodes</u>			
Fuel Specific Heat Capacity (FCP)	FTEMP	I	Fuel temperature (K)
	FACMOT	I	Fuel fraction that is molten: FACMOT = 1 for all molten fuel, FACMOT = 0 for all solid fuel
	BU ^[b]	I	Burnup of uranium (MW-s/kg)
	COMP	I	Plutonium oxide content in the fuel (wt%)
Fuel Thermal Conductivity (FTHCON)	FCP	O	Specific heat capacity (J/kg-K)
	FTEMP	I	Fuel temperature (K)
	CONINP	I	Conductivity integral (W/m)
	FRADEN	I	Fractional fuel density -- ratio of actual density to theoretical density
	COMP	I	Plutonium oxide content in the fuel (wt%)
	BU ^[b]	I	Burnup of uranium (MW-s/kg)
	CON	O	Fuel thermal conductivity (W)

[a] I/O distinguishes between input and output arguments.

[b] Used to call the fuel melting temperature from PHYPRO.

TABLE D-1.I (contd.)

INPUT-OUTPUT ARGUMENTS OF MATPRO SUBCODES

Subcode	Arguments	I/O ^[a]	Description
<u>Fuel Subcodes (contd.)</u>			
Fuel Thermal Conductivity (FTHCON) (contd.)	CONINT	O	Integral of thermal conductivity with respect to temperature (W/M)
	CONINU	O	Temperature as a function of the integral of the thermal conductivity (K)
Fuel Emissivity (FEMISS)	FTEMP	I	Fuel temperature (K)
	FEMISS	O	Fuel emissivity (unitless)
Fuel Thermal Expansion (FTHEXP)	FTEMP	I	Fuel temperature (K)
	FACMOT	I	Fraction of fuel molten. FACMOT = 1 for all fuel molten, FACMOT = 0 for all fuel solid
	BU ^[b]	I	Burnup of uranium (MW-s/kg)
	COMP	I	Plutonium oxide content in the fuel (wt%)
	FTHEXP	O	Fuel thermal expansion (unitless)
Fuel Elastic Modulus (FELMOD)	FTEMP	I	Fuel temperature (K)
	FRADEN	I	Fractional fuel density - ratio of actual density to theoretical density

[a] I/O distinguishes between input and output arguments.

[b] Used to call the fuel melting temperature from PHYPRO.

TABLE D-1.I (contd.)

INPUT-OUTPUT ARGUMENTS OF MATPEO SUBCODES

Subcode	Arguments	I/O ^[a]	Description
<u>Fuel Subcodes (contd.)</u>			
Fuel Elastic Modulus (FELMOD) (contd.)	COMP	I	Plutonium oxide content in the fuel (wt%)
	FELMOD	O	Fuel elastic modulus (N/m^2)
Fuel Poisson's Ratio (FPOIR)	FTEMP	I	Fuel temperature (K)
	COMP	I	Plutonium oxide content in the fuel (wt%)
	FPOIR	O	Fuel Poisson's ratio (unitless)
Fuel Creep (FCREEP)	FTEMP	I	Fuel temperature (K)
	FSTRESS	I	Fuel stress, (N/m^2)
	FDENS	I	Fuel density, (kg/m^3)
	FGRN	I	Fuel grain size (μ)
	FIS	I	Fission rate (fissions/ $\text{m}^3\text{-s}$)
	COMP	I	Plutonium oxide composition (wt%)
	FCREEP	O	Fuel creep strain rate (m/m-s)
Fuel Densification (FUDENS)	TSINT	I	Fuel sintering temperature (K)

[a] I/O distinguishes between input and output arguments.

TABLE D-1, I (contd.)

INPUT-OUTPUT ARGUMENTS OF MATPRO SUBCODES

Subcode	Arguments	I/O [a]	Description
<u>Fuel Subcodes (contd.)</u>			
Fuel Densification (FUDENS) (contd.)	FDENS	I	Fuel density (kg/m^3)
	BU	I	Burnup of uranium (MW-s/kg)
	TTIME	I	Time (s)
	FUDENS	O	Fuel density (kg/m^3)
<u>Cladding Subcodes</u>			
Cladding Specific Heat Capacity (CCP)	CTEMP	I	Cladding temperature (K)
	CCP	O	Cladding specific heat capacity (J/kg-K)
Cladding Thermal Conductivity (CTHCON)	CTEMP	I	Cladding temperature (K)
	TIME		Time (s) - not presently operational but must be supplied as a dummy variable in the argument linkage
	FLUX		Fast neutron flux ($\text{N/m}^2\text{-s}$) - not presently operational but must be supplied as a dummy variable in the argument linkage
	COLDW		Cold work (unitless) - not presently operational but must be supplied as a dummy variable in the argument linkage
	CTHCON	O	Cladding thermal conductivity (W/m-K)

[a] I/O distinguishes between input and output arguments.

TABLE D-1.I (contd.)

INPUT-OUTPUT ARGUMENTS OF MATPRO SUBCODES

Subcode	Arguments	I/O ^[a]	Description
<u>Cladding Subcodes (contd.)</u>			
Zirconium Oxide	CTEMP	I	Cladding temperature (K)
Emissivity (ZOEMIS)	TIME	I	Time (s)
	ZOEMIS	O	Zirconium oxide emissivity (unitless)
Zirconium Oxide Thermal Conductivity (ZOTCON)	CTEMP	I	Cladding temperature (K)
	ZOTCON	O	Zirconium oxide thermal conductivity (W/m-K)
Cladding Axial Thermal Expansion (CATHEX)	CTEMP	I	Cladding temperature (K)
	CATHEX	O	Zircaloy axial thermal expansion (m/m)
Cladding Diametral Thermal Expansion (CDTHEX)	CTEMP	I	Cladding temperature (K)
	CDTHEX	O	Zircaloy diametral thermal expansion (m/m)
Cladding Elastic Modulus (CELMOD)	CTEMP	I	Cladding temperature (K)
	TIME		Time (s) - not presently operational but al must be supplied as dummy variable in the e argument linkage
	FLUX		Fast neutron flux (N/m^2-s) - not presently operational but must be supplied as dummy variable in the argument linkage
	COLDW		Cold work (unitless) - not presently opera- tional but must be supplied as dummy variable in the argument linkage

[a] I/O distinguished between input and output arguments.

TABLE D-1.I (contd.)

INPUT-OUTPUT ARGUMENTS OF MATPRO SUBCODES

Subcode	Arguments	I/O ^[a]	Description
<u>Cladding Subcodes (contd.)</u>			
Cladding Elastic Modulus (CELMOD)	CELMOD	O	Zircaloy elastic modulus (N/m^2)
Cladding Strain versus Stress (CSTRAN)	CTEMP	I	Cladding temperature (K)
	CSTRES	I	Cladding meshpoint stress (N/m^2)
	STRANE	O	Engineering strain (unitless ratio of lengths)
	STRANT	O	True strain (unitless ratio of lengths)
	STRNUE	O	Engineering strain at rupture (unitless ratio of lengths)
Cladding Stress versus Strain (CSTRES)	STRNUT	O	True strain at rupture (unitless ratio of lengths)
	CTEMP	I	Cladding temperature (K)
	STRANT	I	True strain (unitless ratio of lengths)
Cladding Ultimate Strength (CULTST)	CSTRES	O	Cladding true stress (N/m^2)
	CTEMP	I	Cladding temperature (K)
	CULTST	O	Cladding ultimate strength (N/m^2)

[a] I/O distinguishes between input and output arguments.

TABLE D-1.I (contd.)

INPUT-OUTPUT ARGUMENTS OF MATPRO SUBCODES

Subcode	Arguments	I/O ^[a]	Description
<u>Cladding Subcodes (contd.)</u>			
Cladding Creep Rate (CCRPR)	CTEMP	I	Cladding temperature (K)
	STSRSS	I	Cladding transverse stress (N/m ²)
	CFLUX	I	Fast neutron flux (N/m ² -s)
	TIME	I	Time (s)
	CCRPR	O	Cladding creep strain rate (m/m-s)
Cladding Poisson's Ratio (CPOIR)	CTEMP	I	Cladding temperature (K)
	CPOIR	O	Cladding Poisson's ratio (unitless)
Cladding Shear Modulus (CSHEAR)	CTEMP	I	Cladding temperature (K)
	CSHEAR	O	Cladding shear modulus (N/m ²)
Cladding Meyer Hardness (CMHARD)	CTEMP	I	Cladding temperature (K)
	CMHARD	O	Cladding Meyer hardness (N/m ²)
<u>Gas and Fuel Rod Property Subcodes</u>			
Gas Thermal Conductivity (GTHCON)	GMIX	I	Mole fraction of the following gases: helium, argon, krypton, xenon, hydrogen, air, and water vapor

[a] I/O distinguishes between input and output arguments.

TABLE D-1.I (contd.)

INPUT-OUTPUT ARGUMENTS OF MATPRO SUBCODES

Subcode	Argument	I/O ^[a]	Description
<u>Gas and Fuel Rod Property Subcodes</u>			
	GTEMP	I	Gas temperature (K)
	GPRES	I	Gas pressure (N/m^2)
	GPTHK	I	Effective gas gap thickness for Knudsen domain (m)
	GTHCON	O	Gas thermal conductivity (W/m-K)
Gas Viscosity (GVISCO)	GMIX	I	Mole fraction of the following gases: helium, argon, krypton, xenon, hydrogen, air, and steam
	GTEMP	I	Gas temperature (K)
	GVISCO	O	Gas viscosity (kg/m-s)
Gap Heat Transfer (GADHTR)	BU	I	Burnup of uranium (MW-s/kg)
	DELBU	I	Rod average burnup during time step (MW-s/kg)
	DELH	I	Time step size (s)
	DPH	I	Hot pellet diameter (m)

[a] I/O distinguishes between input and output arguments.

TABLE D-1.I (contd.)

INPUT-OUTPUT ARGUMENTS OF MATPRO SUBCODES

Subcode	Arguments	I/O ^[a]	Description
<u>Gas and Fuel Rod Property</u> <u>Subcodes (contd.)</u>			
Gap Heat Transfer (GADHTR) (contd.)	GASES	I	Mole fractions of the gap gases (1) - helium (2) - argon (3) - krypton (4) - xenon (5) - hydrogen (6) - air (7) - water vapor
	GPTH	I	Gap thickness (diametral) (m)
	ICM	I	Cladding material index ICM=1 - stainless steel ICM=2 - zircaloy-2 ICM=4 - zircaloy-4
	PINNM	I	Fuel-cladding interfacial pressure (N/m^2)
	PRES	I	Rod internal gas pressure (N/m^2)
	TAGK	I	Average gap gas temperature (K)
	TP	I	Time to beginning of time step (s)
	TX	I	Time to point of creep calculation (s)
	HGAP	O	Gap conductance ($\text{W/m}^2\text{-K}$)

[a] I/O distinguishes between input and output arguments.

TABLES D-1.I (contd.)

INPUT-OUTPUT ARGUMENTS OF MATPRO SUBCODES

<u>Subcode</u>	<u>Arguments</u>	<u>I/O^[a]</u>	<u>Description</u>
<u>Gas and Fuel Rod Property</u> <u>Subcodes (contd.)</u>			
Physical Properties (PHYPRO)	FTMELT	0	UO ₂ or mixed oxide fuel melting points (K)
	FHEFUS	0	UO ₂ or mixed oxide fuel heat of fusion (27.4 x 10 ⁴ J/kg)
	CTMELT	0	Zircaloy cladding melting point (2,098 K)
	CHEFUS	0	Zircaloy cladding heat of fusion (22.5 x 10 ⁴ J/kg)
	CTRANB	0	Temperature of the beginning of the zircaloy-4 α ₁ -β transus (1,083 K)
	CTRANE	0	Temperature of the end of the zircaloy-4 α-β transus (1,243.15 K)
	CTRANZ	0	Zirconium isothermal α-β transus temperature (1,135.15 K)
	FDELTA	0	Liquid-solid coexistence temperature range (K)
	BU	I	Burnup of uranium (MW-s/kg)
	COMP	I	Plutonium oxide content in the fuel (wt%)

[a] I/O distinguishes between input and output arguments.

2. BASE AND DERIVED SI UNITS USED IN MATPRO

The intent of materials properties work for MATPRO has been to code correlations in the Standard International System (SI) of Units. However, in some cases relationships are reported in other units as taken directly from the literature. This latter practice has been frequently followed in the case of graphical presentations. Table D-2.I indicates the SI units employed in MATPRO subcodes; Table D-2.II indicates some conversion factors that may be useful in interpreting other units.

TABLE D-2.I

SI UNITS FOR USE IN MATPRO

Quantity	Unit	SI Symbol	Formula
<u>Base Units</u>			
length	meter	m	
time	second	s	
mass	kilogram	kg	
thermodynamic temperature	kelvin	K	
amount of substance	mole	mol	
<u>Derived Units</u>			
area	square meter		m^2
density	kilogram per cubic meter		kg/m^3
energy	joule	J	N-m
force	newton	N	$kg-m/s^2$
power	watt	W	J/s
pressure	pascal	Pa	N/m^2
specific heat	joule per kilogram-kelvin		J/kg-K
stress	pascal	Pa	N/m^2
thermal conductivity	watt per meter-kelvin		W/m-K
velocity	meter per second		m/s
viscosity (dynamic)	pascal-second		Pa-s
volume	cubic meter		m^3

TABLE D-2.II
CONVERSION FACTORS

<u>To Convert From</u>	<u>To</u>	<u>Multiply By</u>
foot ²	meter ² (m ²)	9.29030E-02
pound-mass/foot ³	kilogram/meter ³ (kg/m ³)	1.60185E+01
pound-force-foot	joule (J)	1.35582E+00
pound-force	newton (N)	4.44822E+00
pound-force-foot/sec	watt (W)	1.35582E+00
pound-force/foot ²	pascal (Pa)	4.78803E+01
pound-force/inch ²	pascal (Pa)	6.89476E+03
British thermal unit pound mass-Fahrenheit	joule/kilogram-kelvin (J/kg-K)	4.18400E+03
calorie/gram-Centigrade	joule/kilogram-kelvin (J/kg-K)	4.18400E+03
British thermal unit- inch/hour-foot ² - Fahrenheit	watt/meter-kelvin (W/m-K)	1.44131E-01
foot/second	meter/second (m/s)	3.04800E-01
pound-mass-foot/second	pascal-second (Pa-s)	1.48816E+00
foot ³	meter ³ (m ³)	2.83168E-02

3. LINEAR INTERPOLATION ROUTINE (POLATE)

A number of the MATPRO subcodes contain tables of data for a property rather than analytical expressions. Examples are cladding axial and radial thermal expansion in the region of 800 to 1,000 C and cladding specific heat capacity. In these cases discontinuities exist in the temperature range of the α and β phase transformation. Theory-based analytical expressions are not available, and interpolation of reported data is simpler than use of an empirical equation.

A listing of the subcode POLATE which performs this function is given in Table D-3.I.

TABLE D-3.I

LISTING OF POLATE SUBCODE

	FUNCTION POLATE (XY,XX,NN,KK)	POLA0010
	IMPLICIT REAL*8 (A-H,O-Z)	POLA0020
C		POLA0030
	DIMENSION XY(2)	POLA0040
C		POLA0050
C	XY IS A TABLE OF Y(1), X(1), Y(2), X(2), ... Y(NN), X(NN)	POLA0060
C	XX IS THE GIVEN VALUE FOR X	POLA0070
C	NN IS THE NUMBER OF PAIRS OF ENTRIES IN XY	POLA0080
C	KK IS BOTH THE POSITION GUESS AND THE FINAL VALUE	POLA0090
C		POLA0100
	DATA ZERO , DM10 / 0. , 1.0-10 /	POLA0104
C		POLA0105
	1 X = XX	POLA0110
	2 N = NN	POLA0120
	3 M = IABS(N)	POLA0125
	4 K = KK	POLA0130
C	IF (K .LE. 0) K = 1	
C	IF (K .GT. N) K = N	
C		POLA0140
C	IS CONSTANT WANTED	POLA0141
	IF (M-1) 5,6,10	POLA0142
	5 POLATE = ZERO	POLA0143
	RETURN	POLA0144
	6 POLATE = XY(1)	POLA0145
	RETURN	POLA0146
C		POLA0147
C	LOOP TO DECREASE INDEX	POLA0150
	10 IF (XY(2*K)-X) 20,20,11	POLA0160
	11 K = K - 1	POLA0170
	12 IF (K) 30,30,10	POLA0180
C		POLA0190
C	LOOP TO INCREASE INDEX	POLA0195
	20 IF (X-XY(2*K+2)-DM10)100,100,21	POLA0200
	21 K = K + 1	POLA0210
	22 IF (K-M)20,20,40	POLA0220
C		POLA0230
C	TEST FOR EXTRAPOLATION	POLA0231
	30 IF (N) 31,5,180	POLA0232
	31 K = 1	POLA0233
	GO TO 100	POLA0234
	40 IF (N) 41,5,190	POLA0235
	41 K = M - 1	POLA0236
C		POLA0240

TABLE D-3.1 (contd.)

LISTING OF POLATE SUBCODE

C	EVERYTHING OK, GET ANSWER	POLA0250
100	KK = K	POLA0260
101	POLATE = XY(2*K-1) + (X-XY(2*K)) * (XY(2*K+1)-XY(2*K-1))	POLA0270
1	/ (XY(2*K+2)-XY(2*K))	POLA0280
102	RETURN	POLA0290
C		POLA0300
C	POLATE FAILURE, SEARCH OUT OF BOUNDS	POLA0310
180	POLATE = XY(1)	POLA0311
	GO TO 200	POLA0312
190	POLATE = XY(2*M-1)	POLA0313
200	CONTINUE	
C	200 WRITE (6,210) KK, K, N, X, (XY(2*I),I=1,N)	POLA0320
C	201 CALL FAIL	POLA0330
202	RETURN	POLA0340
210	FORMAT(16H ERROR IN POLATE / 16HINITIAL INDEX =, I6, 10X,	POLA0350
	113HFINAL INDEX =, I6, 10X, 14HARRAY LENGTH =, I6, 10X,	POLA0360
	210HARGUMENT =, E14.6 / 20HOTABLE OF X VALUES = / (8E15.6))	POLA0370
C		POLA0380
	END	POLA0390

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