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FOREWORD

This report describes models for fuel specific heat and fuel enthalpy. The report will be part of an update to the Materials Properties Handbook which will be published simultaneously with an update of the MATPRO package to include the fuel enthalpy subcode.

The format and numbering scheme used in this report are consistent with its intended use as an update to the MATPRO handbook. Readers who require descriptions of the rest of the material properties package or of the use of this package should consult the code descriptions^{a,b,c} which are published as part of the fuel rod behavior modeling task performed at the Idaho National Engineering Laboratory (INEL).

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- ^a D. L. Hagrman, G. A. Reymann, and R. E. Mason, MATPRO-Version 11 Revision 1: A Handbook of Materials Properties for Use in the Analysis of Light Water Reactor Fuel Rod Behavior, NUREG/CR-0497, TREE-1280, Rev 1 (February 1980).
- ^b G. A. Berna et al, FRAPCON-1: A Code for the Steady-State Analysis of Oxide Fuel Rods, CDAP-TR-78-032-R1, (November 1978).
- ^c L. J. Siefken et al, FRAP-T5: A Computer Code for the Transient Analysis of Oxide Fuel Rods, NUREG/CR-0840, TREE-1281, (June 1979).

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

(C. A. Reymann)

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

1.1 Summary

The specific heat capacity and the enthalpy of nuclear fuel are modeled empirically as functions of four parameters: temperature, composition, molten fraction, and oxygen to metal ratio. Since UO_2 and PuO_2 are the principal LWR fuels, these are the constituents considered. The correlations for fuel specific heat and enthalpy are valid for temperatures from 300 K to more than 4000 K.

The equations for the specific heat and enthalpy of solid UO_2 and PuO_2 are assumed to have the same form, but with different constants. The basic equations are

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

and

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

where

FCP = specific heat capacity (J/kg·K)

FENTHL = fuel enthalpy (J/kg)

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

and the constants are given in Table A-1.I.

TABLE A-1.I
CONSTANTS USED IN THE UO₂ AND PuO₂ HEAT
CAPACITY AND ENTHALPY CORRELATIONS

<u>Constant</u>	<u>UO₂</u>	<u>PuO₂</u>	<u>Units</u>
K ₁	296.7	347.4	J/kg·K
K ₂	2.43 x 10 ⁻²	3.95 x 10 ⁻⁴	J/kg·K ²
K ₃	8.745 x 10 ⁷	3.860 x 10 ⁷	J/kg
e	535.285	571.000	K
E _D	1.577 x 10 ⁵	1.967 x 10 ⁵	J/mol

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

$$FCP = 503 \text{ J/kg}\cdot\text{K.} \quad (\text{A-1.2})$$

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

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

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

1.2 Review of Literature

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

1.2.1 Limitations of the Data Source. The data used by Kerrisk and Clifton cover a wide range of temperatures (483 to 3107 K), but these data are restricted to nearly stoichiometric material (oxygen to metal ratio between about 2.00 and 2.015). The data of Kruger and Savage are limited in that the highest temperature was only 1400 K, which is well below the melting point of about 2600 K for PuO_2 . Their data are also restricted to approximately stoichiometric PuO_2 . The oxygen to metal ratio has been shown to be significant by Gronvold et al^{A-1.4} and by Affortit and Marcon^{A-1.5}.

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

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

1.3 Development of the Model

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

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

$$C_v = \frac{K_1 \theta^2 \exp(\theta/T)}{T^2 [\exp(\theta/T) - 1]^2} \quad (A-1.3)$$

where

C_V = specific heat capacity (J/kg·K)

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

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

$$C_p = C_V + \frac{\alpha^2 V}{\beta} T \quad (\text{A-1.4})$$

where

α = the coefficient of thermal expansion (K^{-1})

β = the coefficient of compressibility (Pa^{-1})

V = the molar volume (m^3).

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

$$C_p = C_V + K_2 T \quad (\text{A-1.5})$$

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

1.3.2 Defect Energy Contribution to the Specific Heat Capacity. Above temperatures of about 1500 K, the specific heat capacity data show a rapid increase not described by Equation (A-1.5). This increase is generally attributed to the energy necessary to form Frenkel defects ^{A-1.7, A-1.8, A-1.9}. Some investigators ^{A-1.4, A-1.8} have suggested that Schottky defects may also contribute to this rapid increase. However, the

assumption made here is that the rapid increase in specific heat capacity above 1500 K is due to formation of Frenkel defects. The functional form of the extra term which should be added to Equation(A-1.5) may be found from the defect energy contribution to the enthalpy given by^{A-1.6}

$$H_D = K_3 \exp (-E_D/RT) \quad (A-1.6)$$

where

$$H_D = \text{defect energy contribution to enthalpy (J)}$$

$$E_D = \text{activation energy for Frenkel defects (J/mol)}$$

$$K_3 = \text{constant to be determined (J)}.$$

R and T were previously defined in Equation (A-1.1). To determine the defect contribution to the specific heat capacity, the derivative of H_D with respect to temperature, C_D , is used. C_D is given by

$$C_D = \frac{K_3 E_D}{RT^2} \exp (-E_D/RT). \quad (A-1.7)$$

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

$$C_p = \frac{K_1 \theta^2 \exp (\theta/T)}{T^2 [\exp (\theta/T) - 1]^2} + K_2 T + \frac{K_3 E_D}{RT^2} \exp (-E_D/RT). \quad (A-1.8)$$

1.3.3 Determination of the Constants in the Model. For UO_2 , the values of the five constants K_1 , K_2 , K_3 , θ , and E_D are taken from Kerrisk and Clifton. For PuO_2 , the constants are determined by fitting the data of Kruger and Savage. In both cases, the fuel was nearly stoichiometric. Data sources for pure PuO_2 are scarce. One potential source is the work of Affortit and Marcon. However, they give only correlations fit to data and not the actual data. Also they do not present an uncertainty analysis.

Without knowing the number or accuracy of the data on which their correlations are based, it is not possible to estimate what weight to give to their results. Therefore, their correlations were not used to determine the constants of Equation (A-1.8). However, their work was useful for the assessment of the effects of departure from stoichiometry.

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

1.3.4 Effect of Nonstoichiometry. Several investigators have found the oxygen to metal ratio of fuel to influence the specific heat capacity^{A-1.1, A-1.5, A-1.8, A-1.10}. At temperatures above 1300 K, departures from stoichiometry typical of those found in LWR fuel have caused changes in the specific heat capacity greater than the data scatter. The most complete analysis of this effect has been done by Affortit and Marcon. Even though their results are quantitatively different from the sources used to develop this model, they illustrate well the qualitative aspects of this effect. Therefore, Figures A-1.1 and A-1.2, made from their correlations, are presented. Figure A-1.1 is for UO_2 and Figure A-1.2 is for mixed oxide fuels. These figures show that the specific heat capacity increases as the oxygen to metal ratio becomes larger than 2.

Very hyperstoichiometric materials, such as U_4O_9 and U_3O_8 , have specific heat capacities considerably larger than that of UO_2 ^{A-1.4, A-1.11}. In addition, these materials exhibit peaks in specific heat capacity at temperatures which are associated with phase transitions. However, the incidence of these states in light water reactor fuel is infrequent, and their influence is neglected in this model.

In reactor fuel, nonstoichiometry is believed to be due to oxygen interstitials for hyperstoichiometric fuel, and oxygen vacancies for hypostoichiometric fuel^{A-1.8}. Excess oxygen tends to increase and an oxygen deficiency to decrease, the probability of formation of Frenkel and Schottky defects, thereby changing the specific heat capacity. Thus

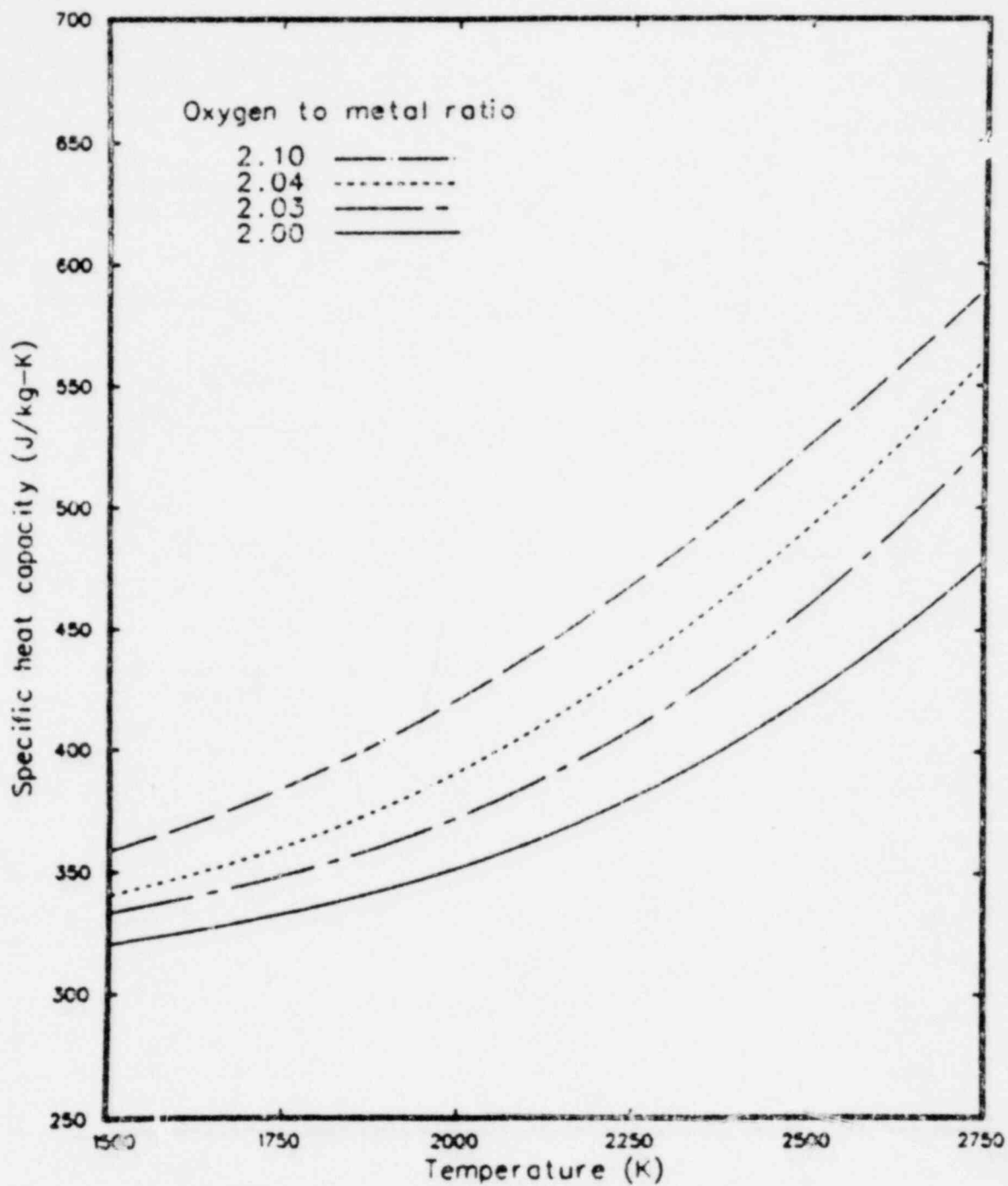


Fig. A-1.1 Specific heat capacity as a function of temperature and oxygen to metal ratio for UO_2 .

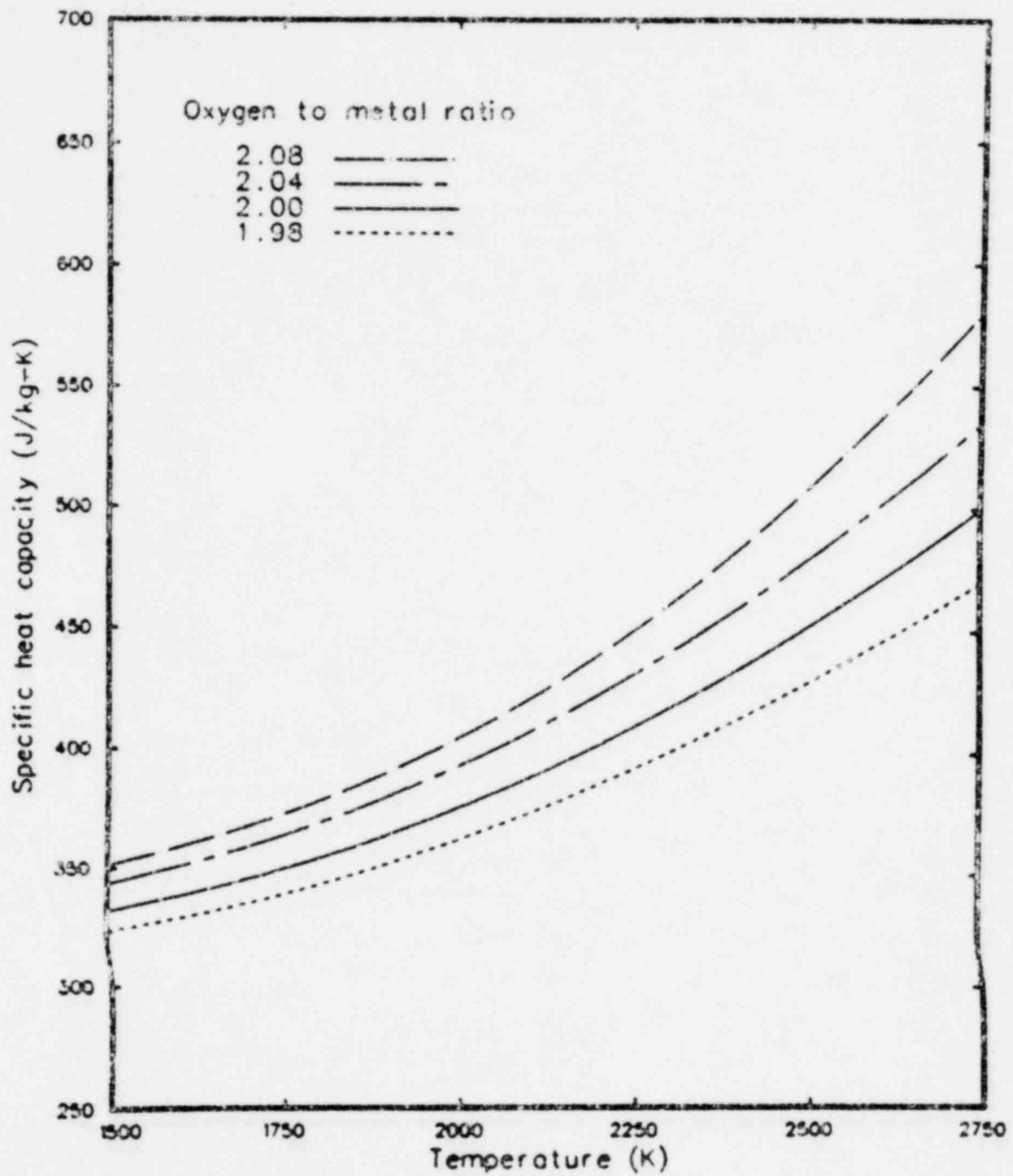


Fig. A-1.2 Specific heat capacity as a function of temperature and oxygen to metal ratio for $(U_{0.8}Pu_{0.2})O_{2+x}$.

the logical adjustment to Equation (A-1.8) to account for the oxygen to metal ratio effect is in its last term, which includes the effect of defect formation. By multiplying the term by the oxygen to metal ratio divided by 2.0, the following desirable features are produced:

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

Therefore, this correction has been made to Equation (A-1.8) giving Equation (A-1.1a). This is the model used for the specific heat capacity of solid UO_2 and PuO_2 .

If the fuel consists of a mixed oxide (MO_2) with a weight fraction of PuO_2 equal to $FCOMP$, then the specific heat capacity of the mixed oxide fuel is calculated by the expression

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

If the fuel temperature is greater than the fuel melting temperature, $FTMELT$, plus the liquid-solid coexistence temperature, then the fuel specific heat capacity is not calculated using Equation (A-1.1a) but set equal to the specific heat of liquid fuel, 503 J/kg·K for both UO_2 and PuO_2 fuel. If the fuel temperature is equal to the fuel melting temperature, $TMELT$, then the specific heat capacity is calculated by the expression

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

where

R = fraction of fuel which is molten

F_{CPMOL} = specific heat capacity of liquid fuel

= 503 J/kg·K.

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

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

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

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

$$FENTHL_{MO_2} = FENTHL_{UO_2} (1 - F_{COMP}) + FENTHL_{PuO_2} * F_{COMP} \quad (A-1.12)$$

If the fuel temperature is equal to the fuel melting temperature, FT_{MELT}, then the fuel enthalpy is calculated by the expression

$$FENTHL = FENTHL(T = FT_{MELT}) + FHEFUS * FACMOT \quad (A-1.13)$$

where

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

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

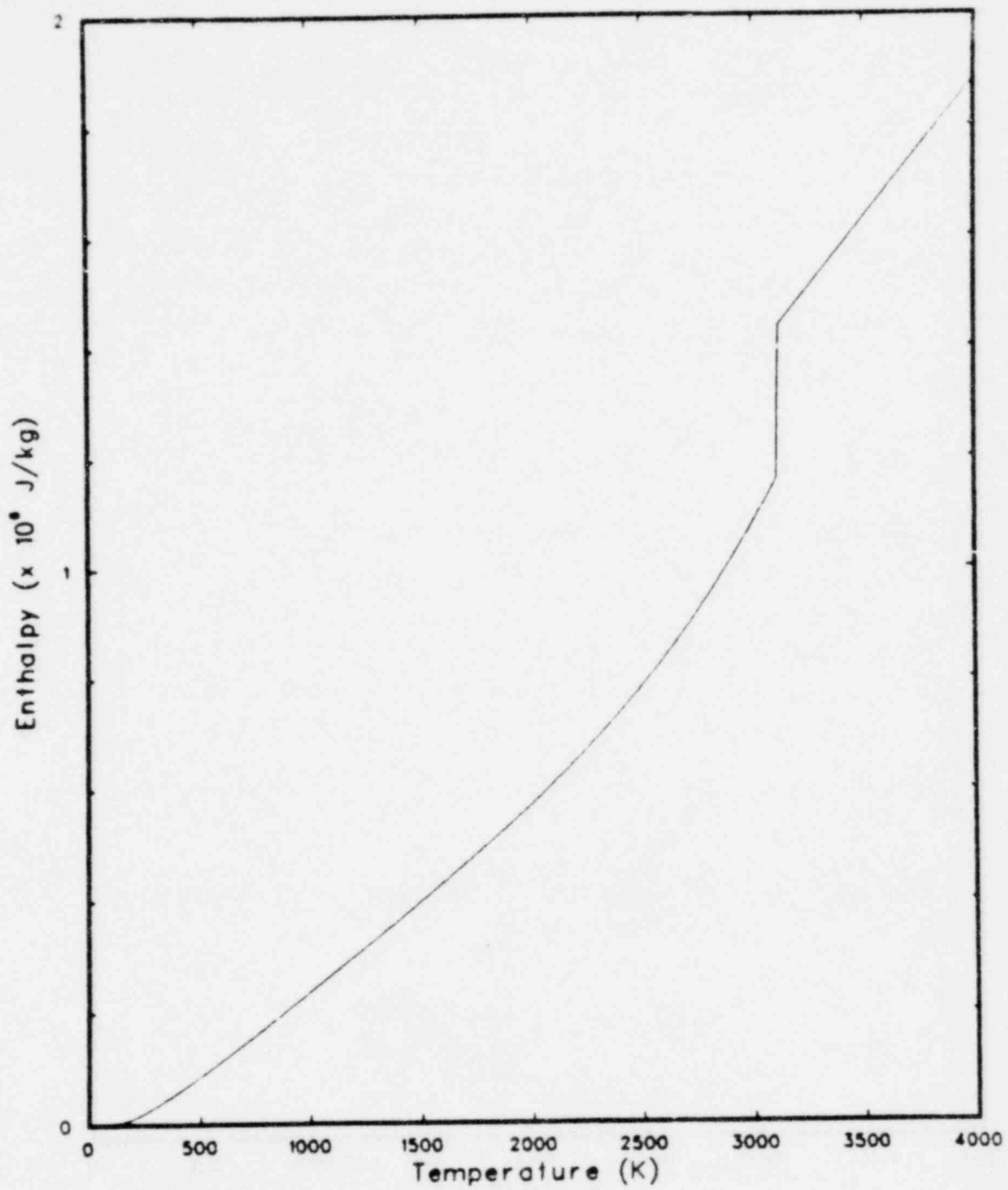


Fig. A-1.3 Enthalpy of UO_2 as a function of temperature to 4000 K.

If the fuel temperature, F_{TEMP} , is greater than the fuel melting temperature, then the fuel enthalpy is calculated by the expression

$$\begin{aligned} F_{ENTHL} = & F_{ENTHL} (T = F_{TMELT}) + F_{HEFUS} \\ & + (F_{TEMP} - F_{TMELT}) * F_{CPMOL} \end{aligned} \quad (A-1.14)$$

where

$$F_{CPMOL} = \text{specific heat capacity of molten fuel (J/kg}\cdot\text{K)}.$$

1.4 Comparisons of the Model with Data

Figure A-1.4 shows the specific heat capacity correlation, F_{CP} , for UO_2 compared with data from three sources^{A-1.4, A-1.12, A-1.13}. These data were taken from stoichiometric UO_2 . At the high end of the temperature interval, a few hundred kelvin below the melting temperature, the data fall below the model calculations. This is probably the result of partial melting due to a nonuniform temperature distribution within the sample. In such a case, the measured specific heat capacity would be smaller because in a liquid the specific heat capacity is considerably lower than in a solid. A similar comparison is shown in Figure A-1.5 for PuO_2 . In this instance, the correlation is compared with its own data base. This was necessary due to the lack of a broad data base for PuO_2 fuel. A better test of the accuracy of the model is found by comparing its predictions with mixed oxide data^{A-1.5, A-1.10, A-1.14}, as is done in Figure A-1.6. None of the data shown in this figure were used in the development of the model. The agreement is relatively good except for the low values reported by Affortit and Marcon. Other experimenters^{A-1.3, A-1.10} have pointed out that the results of Affortit and Marcon are generally low when compared with their data and have excluded the Affortit and Marcon measurements from their data base. No one has proposed an adequate explanation for the discrepancy. On the other hand, at least one investigator^{A-1.9} has given considerable weight to the work done by Affortit and Marcon. Herein, the Affortit and Marcon results are used only in the analysis of the effect of departure from stoichiometry on the specific heat capacity.

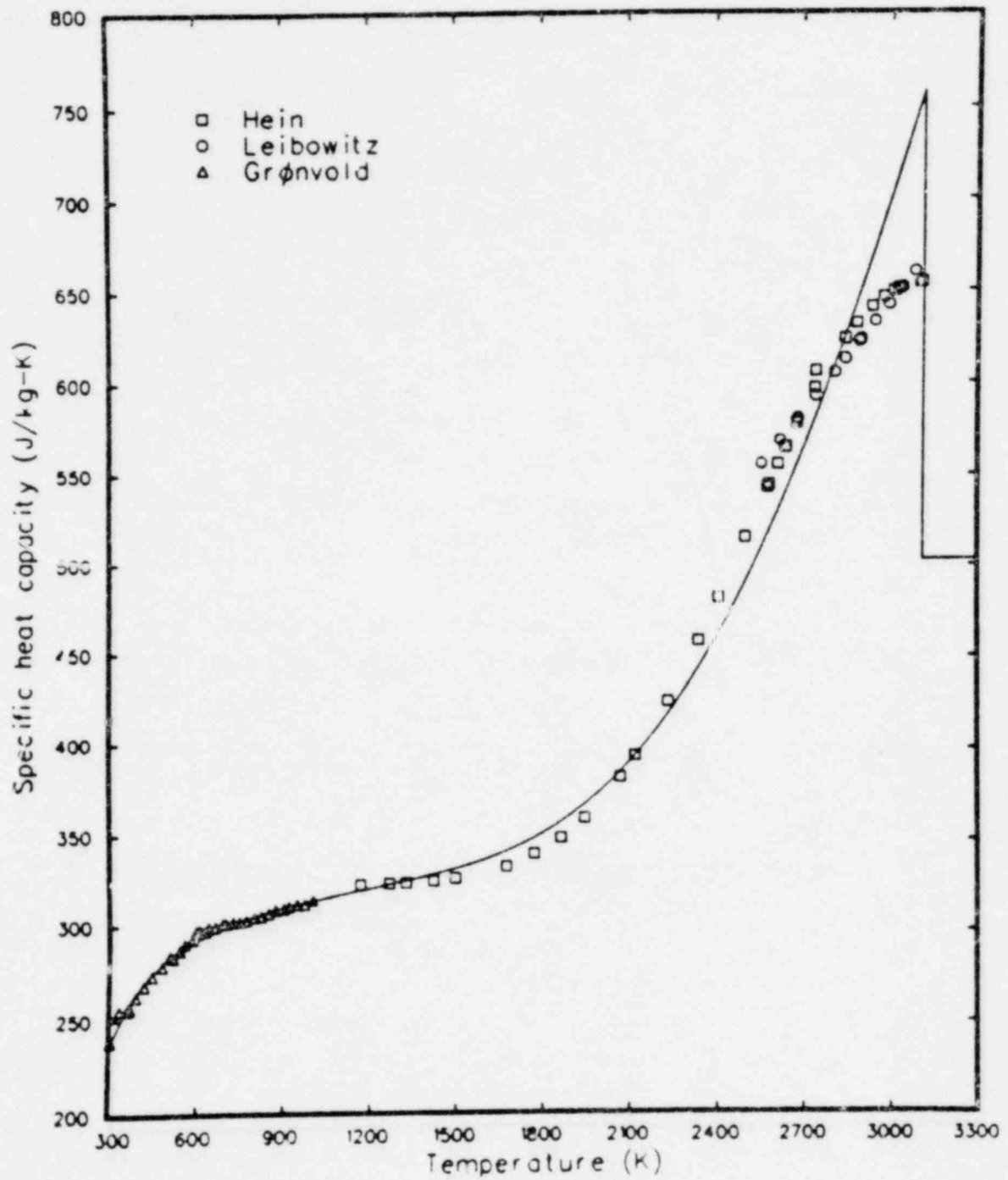


Fig. A-1.4 Specific heat capacity of UO_2 from three experimenters with the FCP correlation (solid line) for UO_2 .

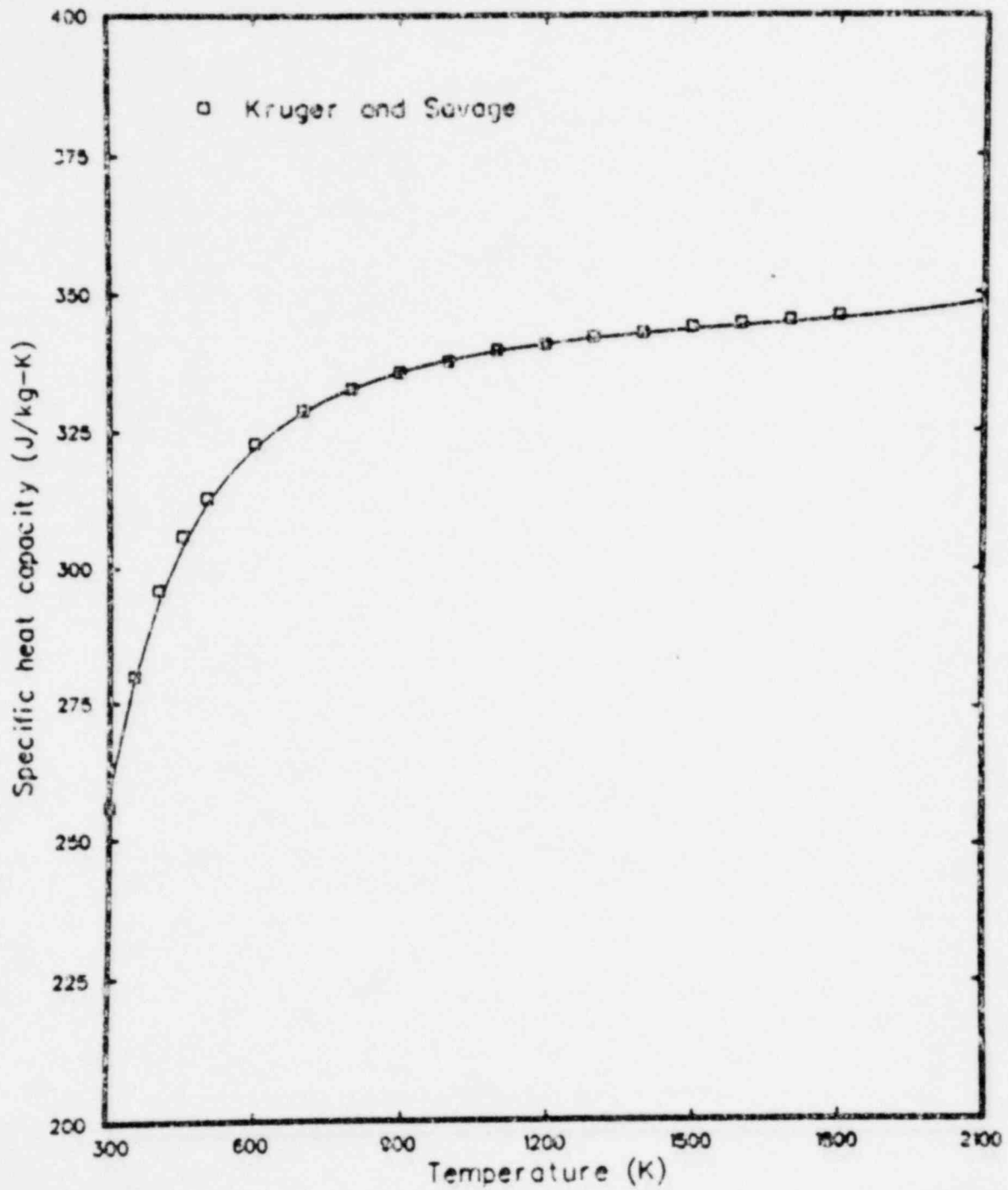


Fig. A-1.5 Specific heat capacity of PuO_2 from Kruger and Savage compared to FCP correlation (solid line) for PuO_2 .

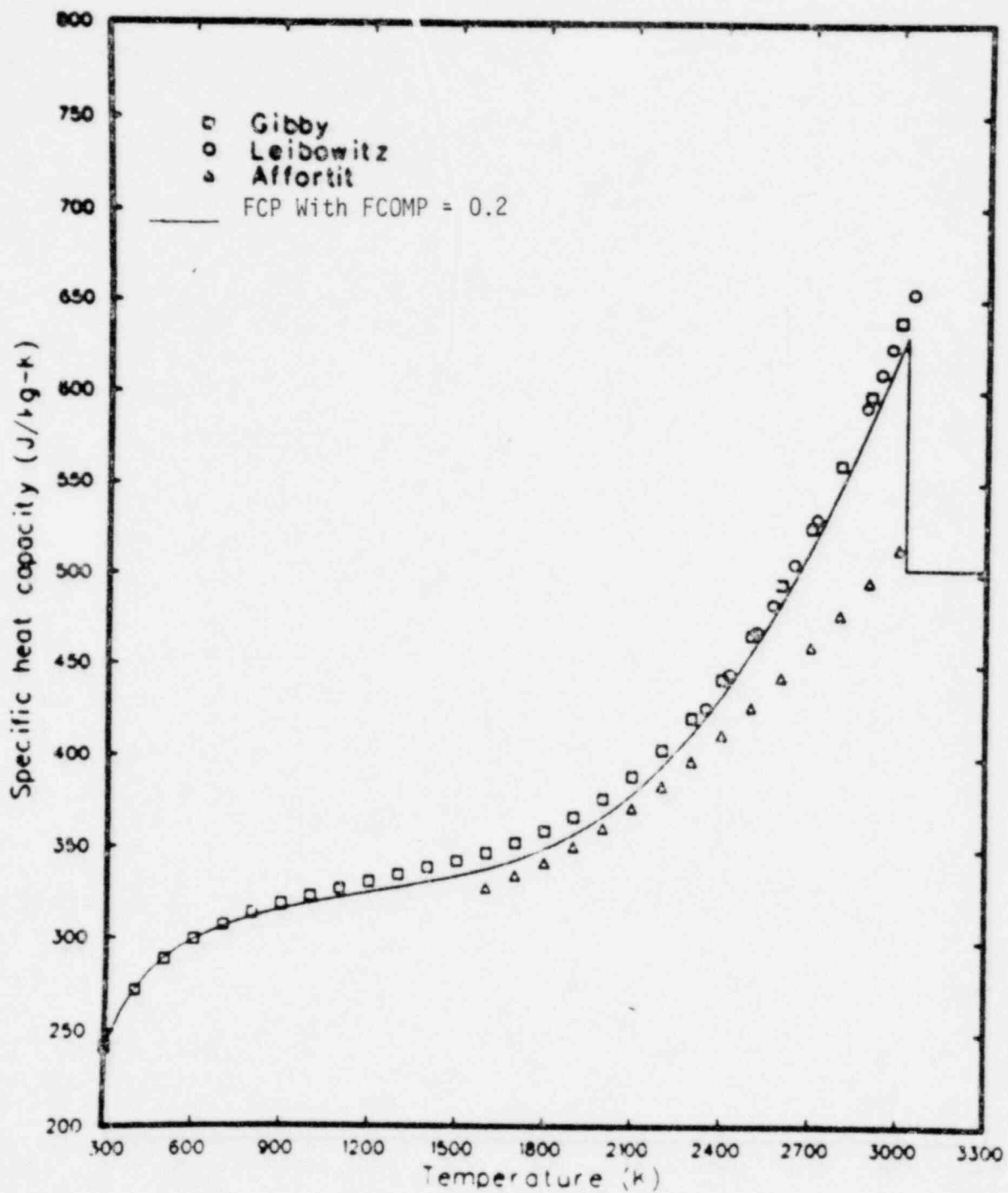


Fig. A-1.6 Specific heat capacity of $(U_{0.8}Pu_{0.2})O_2$ from three experimenters compared with the FCP correlation (solid line) for mixed oxides.

1.5 Uncertainty of the Model

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

1.5.1 Uncertainty in UO_2 Model. Kerrisk and Clifton report an accuracy of $\pm 3\%$ for their correlation over the temperature range 300 to 3000 K, with an approximately uniform distribution relative to temperature. When the calculations of the correlation are compared with the data of Groenveld et al for stoichiometric oxide, the agreement is even better, having a standard error of only 2.0 J/kg·K. This is a good test of the model since these data were not used to develop the correlation. The paper by Affortit and Marcon gives correlations fit to their data. Arbitrarily taking 200 K intervals over their temperature range from 600 to 3000 K and using their correlations, the standard error is 46 J/kg·K. Affortit and Marcon's predictions are smaller at all temperatures and the residuals increase with temperature.

1.5.2 Uncertainty in the Mixed Oxide Model. Because of the limited number of data for PuO_2 , the accuracy of the correlation for mixed oxide fuel was used as a test for this correlation. Data were taken from Leibowitz et al^{A-1.14}, Gibby et al^{A-1.10}, and Affortit and Marcon. The model presented in this paper, using a weighted sum of the UO_2 and PuO_2 results, calculates specific heat capacities that are slightly larger than all but two of the 55 data reported by Gibby and Leibowitz. At the highest and lowest applicable temperatures (3000 K and 300 K) the differences are negligible, less than 1.0 J/kg·K. At intermediate temperatures around 1600 K the residuals are about 10.0 J/kg·K, falling off smoothly from this temperature. The standard error of the model relative to these three data sets is 5.6 J/kg·K. This is equivalent to a maximum percentage error of less than 2.5%. Since these residuals are smaller than the scatter in the data, the model represents these data sets adequately. When the model is compared with that of Affortit

and Marcon, again taking 200 K steps from 1600 K to melting, the standard error is 46 J/kg·K. Affortit and Marcon always have the smaller value and the residuals increase with increasing temperature, as with the UO₂ results. Because of the lack of actual data, the results of Affortit and Marcon are not included in the standard error estimate.

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

A listing of the FCP subcode is given in Table A-1.II and the FENTHL subcode in Table A-1.III. The function EMFCP is the evaluation model fuel specific heat (which is not part of the best estimate materials properties package) and the subroutine DIALOT is part of the uncertainty analysis package.

POOR ORIGINAL

TABLE A-1.II

LISTING OF THE FCP SUBCODE

FUNCTION FCP (FTEMP, FACMOT, FOTMTL, FRADEN)

THE FUNCTION FCP IS USED TO CALCULATE THE SPECIFIC HEAT CAPACITY OF UO₂, PUO₂, AND (U,PU)O₂ FUELS AS A FUNCTION OF TEMPERATURE, FRACTION OF FUEL WHICH IS MOLTEN, PUO₂ CONTENT, AND OXYGEN-TO-METAL RATIO.

FCP = OUTPUT FUEL SPECIFIC HEAT CAPACITY (J/(KG*K))

FTEMP = INPUT FUEL MELTING POINT TEMPERATURE (K)

FACMOT = INPUT FUEL FRACTION MOLTEN (UNITLESS)

FACMOT = 1.0 - FUEL IS ALL MOLTEN

FACMOT = 0.0 - FUEL IS ALL SOLID

FOTMTL = INPUT OXYGEN TO METAL RATIO (UNITLESS)

FOTMTL = (ATOMS OXYGEN)/(ATOMS METAL) IF NOT KNOWN,

ENTER 2.0

FRADEN = INPUT FUEL DENSITY (RATIO OF ACTUAL DENSITY TO THEORETICAL DENSITY)

UFCP = ESTIMATED STANDARD ERROR FOR UO₂ (J/(KG*K)) (NOT CURRENTLY RETURNED)

PUFCP = ESTIMATED STANDARD ERROR FOR PUO₂ (J/(KG*K)) (NOT CURRENTLY RETURNED)

THE EQUATIONS USED IN THIS FUNCTION ARE BASED ON DATA FROM:
(1) J. KEPPIK AND J. CLIFTON, NUCLEAR TECHNOLOGY, 16 (1972).
(2) D. KRUGER AND H. SAVAGE, JOURNAL OF CHEMICAL PHYSICS, 45 (1968).

THE EFFECT OF OXYGEN-TO-METAL RATIO WAS ESTIMATED FROM EQUATIONS PUBLISHED BY:

(3) C. AFFORTIT AND J. MARCON, REVUE INTERNATIONALE DES HAUTES TEMPERATURES ET DES REFRACTAIRES, 7 (1970).

THE SPECIFIC HEAT CAPACITY OF MOLTEN UO₂ WAS TAKEN FROM

(4) L. LEIBOWITZ ET AL, JOURNAL OF NUCLEAR MATERIALS, 39 (1970)

FCP WAS ORIGINALLY CODED BY V.F. BASTON IN MARCH 1974.
LAST MODIFIED BY G.A. REYMANN IN MAY 1978.

COMMON / PHYPRO / FTMELT, FHEFUS, CTMELT, CHEFUS, CTRANB, CTRANE, CTRANZ, FDELTA, BU, COMP, DELOXY

THE PHYPRO COMMON BLOCK IS SET BY CALL TO THE SUBROUTINE PHYPRO WHICH IS PART OF THE MATERIALS PROPERTIES PACKAGE USED AT THE INEL.

QUANTITIES CONTAINED IN IT USED IN THIS SUBCODE ARE:

FTMELT = FUEL MELTING TEMPERATURE (K)

FDELTA = LIQUID-SOLID COEXISTENCE TEMPERATURE (K)

COMP = PUO₂ CONTENT (WT. %)

WHEN THE FUNCTION FCP IS USED ALONE, NOT AS PART OF THE INEL CODE, VALUES FOR FTMELT, FDELTA, AND COMP MUST BE INPUT.

POOR ORIGINAL

TABLE A-1.II (Contd.)

```

C LICENSING ASSISTANCE COMMON BLOCK.
C ADD TO MAINLINE
-----
C COMMON /LACMOL/ MAXIDX, EMFLAG(21)
-----
C DATA ON / 24ON /,
# OFF / 3HOFF /,
-----
C # LOCIDX / 3 /
-----
C DATA C1U ,C2U ,C3U ,THU ,EDU / 296.7 , 2.43E-02, 8.745E07,
# 535.285, 1.577E05 /
-----
C DATA C1PU,C2PU,C3PU,THPU,EDPU/ 347.4 , 3.95E-04, 3.860E07,
# 571.0 , 1.967E05 /
-----
C CP(C1,C2,C3,TH,ED,T,FOOTMTL) =
# C1*(TH**2)*EXP(TH/T)/((T**2)*((EXP(TH/T)-1.)**2)) + C2*T
# + (FOOTMTL/2.)*(C3*ED/(8.314*(T**2)))*EXP(-ED/(8.314*T))
-----
C IF (EMFLAG(LOCIDX) .EQ. ON)
# FCP = EMFCP(FTEMP,FACMOT,FTMELT,FRADEN)
-----
C IF (EMFLAG(LOCIDX) .EQ. ON) GO TO 100
-----
C T = FTEMP
R = FACMOT
TM = FTMELT
FCOMP = COMP/100.0
FCPMOL = 503.0
-----
C FCPMOL = SPECIFIC HEAT CAPACITY OF MOLTEN FUEL (J/(KG*K))
-----
C IF (T .GT. (TM+FDelta)) GO TO 50
-----
C FCP = CP(C1U ,C2U ,C3U ,THU ,EDU ,T,FOOTMTL)*(1.0 - FCOMP) +
# CP(C1PU,C2PU,C3PU,THPU,EDPU,T,FOOTMTL)*FCOMP
-----
C IF (T .LT. (TM-0.1)) GO TO 100
FCP = (1.0 - R)*FCP + R*FCPMOL
GO TO 100
-----
C 50 FCP = FCPMOL
UFCP = 2.0
PUFCP = 5.6
-----
C 100 CALL DIALOT(FTEMP,1,FDIALA,FDIALM)
FCP=(FCP+FDIALA)*FDIALM
RETURN
END

```


POOR ORIGINAL

TABLE A-1.III

LISTING OF THE FENTHL SUBCODE

```
FUNCTION FENTHL (TEMP, FCOMP, FOTMTL, FTMELT, FACMOT)
1
IMPLICIT REAL * 8 (A-H, O-Z)
*****
THIS FUNCTION IS CALLED BY SUBROUTINE ENERGY AND COMPUTES THE
ENTHALPY OF FUEL AT A POINT RELATIVE TO ZERO DEGREES ABSOLUTE
TEMPERATURE
*****
INPUT ARGUMENTS
*****
FACMOT - FRACTION OF MOLTEN FUEL
FCOMP - PUO2 FRACTION OF THE FUEL
FHEFUS - HEAT OF FUSION OF THE FUEL (J/KG)
FOTMTL - FUEL OXYGEN TO METAL RATIO
FTMELT - FUEL MELTING TEMPERATURE (K)
TEMP - LOCAL TEMPERATURE (K)
*****
OUTPUT
*****
FENTHL - LOCAL FUEL ENTHALPY RELATIVE TO ZERO DEGREES-K (J/KG)
*****
FENTHL WAS ORIGINALLY CODED BY G.A. BERNA IN NOVEMBER 1979
IT WAS UPDATED BY L.J. SIEFKEN IN DECEMBER 1979
FURTHER UPDATED BY G.A. REYMANN IN FEBRUARY 1980
FCPMOL = SPECIFIC HEAT CAPACITY OF MOLTEN FUEL ( J/(KG*K) )
DATA FCPMOL / 503.00 /
THE FOLLOWING DATA STATEMENTS CONTAIN CONSTANTS FROM MATPRO-11 FCP
DATA C1U, C2U, C3U, THU, EDU / 296.7, 2.43E-02, 8.745E07,
535.285, 1.577E05 /
DATA C1PU, C2PU, C3PU, THPU, EDPU / 347.4, 3.95E-04, 3.860E07,
571.0, 1.967E05 /
THE FOLLOWING EQUATION IS THE INTEGRAL OF THE FUEL SPECIFIC HEAT
WITH RESPECT TO TEMPERATURE
CPDT(C1, TH, C2, OTM, ED, T, C3) =
# C1*TH * ( 1. / (EXP(TH/T)-1.))
# + C2 * T * T / 2.00
# + C3 * OTM * EXP(-ED / (T * 8.314E0)) / 2.00
C
```

POOR ORIGINAL

TABLE A-1.III (Contd.)

```
TX=TEMP
IF(TX.GT.FTMELT)TX=FTMELT
C
# FENTHL = CPDT(C1U      ,THU      ,C2U      ,FOTMTL      ,EDU
  ,TX      ,C3U      ) * ( 1.E0 - FCOMP )
C
# IF( FCOMP .GT. 0.E0 ) FENTHL = FENTHL + CPDT(C1PU      ,THPU
  ,C2PU      ,FOTMTL      ,EDPU      ,TX      ,C3PU ) * FCOMP
C
IF( TEMP .LE. FTMELT - 2.E0 ) GO TO 10J
C
FENTHL = FENTHL + FHEFUS * FACMOT
IF(TEMP.LE.(FTMELT+2.))GO TO 100
C
100 FENTHL=FENTHL+(TEMP-FTMELT)*FCPMCL
CONTINUE
C
RETURN
END
```

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1.8 Bibliography

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