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MASTER

**PROPERTIES FOR
LMFBR SAFETY ANALYSIS**



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ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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PROPERTIES FOR
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March 1976

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PREFACE

This handbook of properties for LMFBR Safety Analysis was prepared to bring together the most current data on thermodynamic, transport, and mechanical properties of reactor materials with primary emphasis on summarizing and selecting data of interest to reactor safety analysts. The working group which performed this task benefited from the efforts of the people who produced the Nuclear Systems Materials Handbook (NSMH) (TID-26666) (J. E. Irvin, Chairman). We have adopted the NSMH property code numbers and have used a similar format for a presentation and discussion of values. Moreover, we intend the data in this handbook, prepared for the convenience of reactor safety analysts, to agree with the data in the NSMH. Where, due to inadvertance, this may not be the case, corrections will be made in future revisions.

The present handbook will be extended, updated, and revised periodically and we welcome comments from users of this material, particularly on how its utility to them could be improved. In many cases, estimates of the uncertainties of the selected values have not been given. We will add such estimates in future revisions. Further, it is hoped, that a compilation of this kind, will reveal those areas in which added experimental and theoretical work is needed.

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INTRODUCTION

Materials and their associated property values have been grouped in this handbook by function, *viz*: fuel, coolant, and structural material. At present, the number of materials included is sufficiently limited that no detailed index has been included and simple tabulation of the materials should suffice.

Fuel

UO₂
(U,Pu)O₂

Coolant

Sodium

Structural Material

Stainless Steel (Type 304)
Stainless Steel (Type 316)

The properties discussed for each material have further been arranged in the numerical order specified by the material property code numbers. There are, however, some exceptions to this ordering. In most cases for which a single number would constitute the entire entry (*e.g.* melting point of a pure substance) several property values have been grouped on a single page at the beginning of relevant material section. We have chosen this scheme for the present edition of the handbook subject to change as needed.

PROPERTY CODE NUMBERS*

- 2000 Mechanical Properties
 - 2100 Static, Short Term Properties
 - 2101 Ultimate Tensile Strength
 - 2102 Yield Strength
 - 2103 Proportional Elastic Limit
 - 2104 Shear Strength
 - 2105 Elongation
 - 2106 Reduction of Area
 - 2107 True Stress-Strain Curves/Equations
 - 2108 Engineering Stress-Strain Curves/Equations
 - 2109 Hardness
 - 2110 Poisson's Ratio
 - 2111 Young's Modulus (modulus of Elasticity)
 - 2112 Shear Modulus (Modulus of Rigidity)
 - 2113 Tangent Modulus
 - 2114 Bulk Modulus
 - 2115 Rupture Modulus
 - 2116 Compressive Strength
 - 2117 Bending Strength
 - 2118 Fracture Strength
 - 2119 Vicat Softening Point (P)
 - 2120 Taber Abrasion (P)
 - 2200 Static, Long Term Properties
 - 2201 Effects of Prior Creep on Residual Tensile Ductility
 - 2202 Stress for Rupture
 - 2203 Burst Pressure (biaxial)
 - 2204 Uniform $\Delta D/D$ (biaxial)
 - 2205 Isochronous Stress-Strain Curve
 - 2206 Creep
 - 2207 Relaxation
 - 2208 Strain at Fracture
 - 2300 Dynamic - Short Term Properties
 - 2301 Strain Rate Effects
 - 2302 Impact Strength

- 2000 Mechanical Properties (Continued)
 - 2303 Brittle to Ductile Transition Temperature
 - 2304 Thermal Shock Resistance
 - 2305 Coefficient of Restitution
 - 2306 Toughness for Tensile Instability
 - 2400 Cyclic Loading Properties
 - 2401 - 2410 Strain-controlled fatigue
 - 2411 - 2420 Stress-controlled fatigue
 - 2421 - 2430 Properties of cyclically hardened material
 - 2421 Equivalent bilinear Yield Strength *vs.* Maximum Strain
 - 2422 Stress-strain for Cyclic Hardened Material - Parameters K_0 and K_1
 - 2423 Stress-strain for Cyclic Hardened Material - Parameters C and C_m
 - 2431 - 2440 Fracture - mechanics parameters
 - 2500 Viscoelastic Properties
 - 2501 Flexural Strength (P)
 - 2502 Flexural Modulus (P)
 - 2503 Breaking Elongation (P)
 - 2504 Deformation Under Load (P)
- 3000 Physical Properties
 - 3100 Thermal Properties
 - 3101 Maximum Service Temperature (P)
 - 3102 Healing Temperature
 - 3103 Melting Point
 - 3104 Heat of Fusion
 - 3105 Boiling Point
 - 3106 Heat of Vaporization
 - 3107 Flammability (P)
 - 3108 Specific Heat
 - 3109 Enthalpy
 - 3110 Thermal Diffusivity
 - 3111 Thermal Emissivity
 - 3112 Thermal Conductivity
 - 3113 Prandtl Number
 - 3114 Thermal Expansion

- 3000 Physical Properties (Continued)
 - 3200 Electrical/Magnetic Properties
 - 3201 Electrical Resistivity
 - 3202 Dielectric Strength
 - 3203 Dielectric Coefficient
 - 3204 Dissipation Factor
 - 3205 Magnetic Permeability
 - 3206 Arc Resistance (P)
 - 3300 Other Physical Properties
 - 3301 Viscosity
 - 3302 Surface Tension
 - 3303 Vapor Pressure
 - 3304 Density
 - 3305 Porosity
 - 3306 Speed of Sound
 - 3307 Isothermal Compressibility
 - 3308 Reflectance (coatings)
 - 3309 Water Vapor Permeability (P)
 - 3310 Water Absorption (P)
 - 3311 Gas Permeability (P)

* From Nuclear Systems Materials Handbook TID-26666

(P) Relates to plastics/elastomers

FUEL

	<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Date: 3/76	Fuel	(U _{.75} Pu _{.25})O ₂	2110 Poisson's Ratio 2112 Shear Modulus 2114 Bulk Modulus

Poisson's Ratio $\gamma = (3K - 2G)/2(3K + G)$

Shear Modulus $G = 76 [1 - (T/2760)^2] (1 - 2P)$ GPa

$G = 11E6 [1 - (T/2760)^2] (1 - 2P)$ psi

Bulk Modulus $K = 140 [1 - .5 (T/2760)^2] (1 - 2P)$ GPa

$K = 20E6 [1 - .5 (T/2760)^2] (1 - 2P)$ psi

T = Temperature, K

P = $1 - \rho$

ρ = Fraction of Theoretical Density

FUNCTION

Fuel

MATERIAL

(U .75 Pu .25)₂O₂

PROPERTY

2110 Poisson's Ratio
2112 Shear Modulus
2114 Bulk Modulus

Date: 3/76

References

HEDL Unpublished Information, 1972.

FUNCTION

MATERIAL

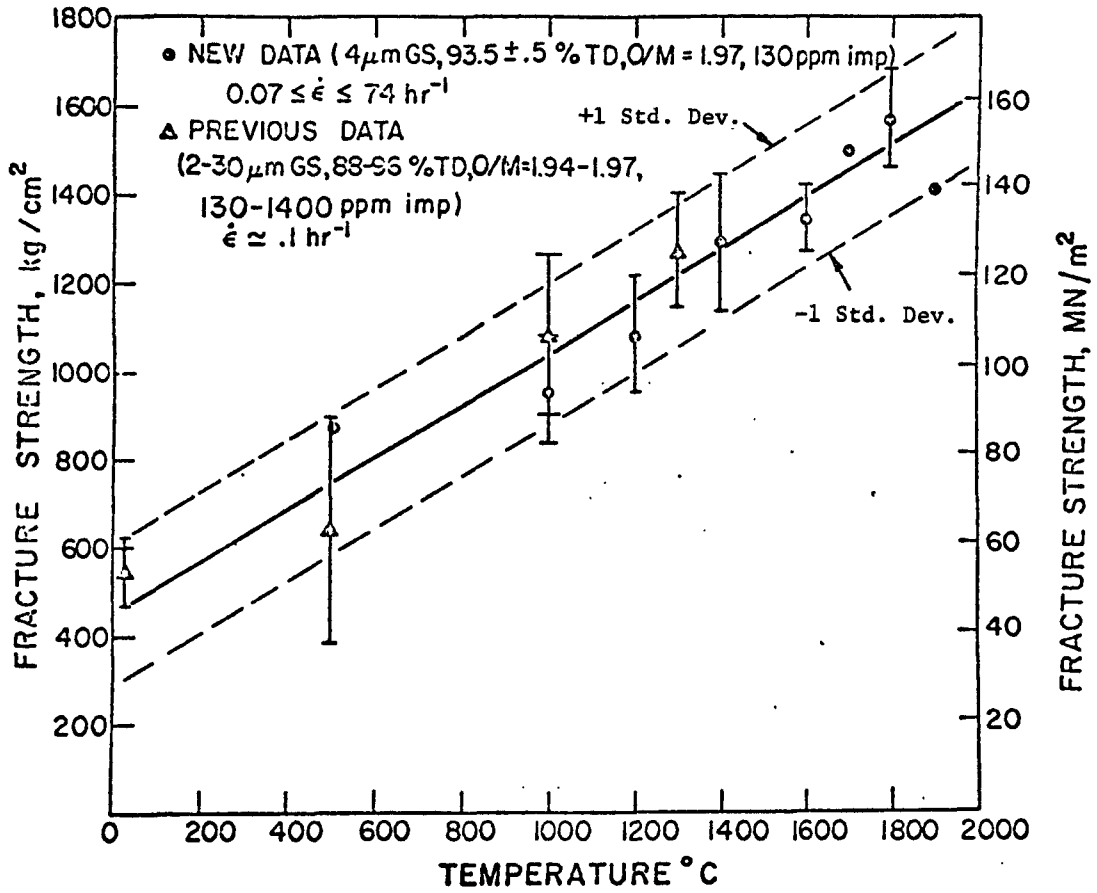
PROPERTY

Fuel

Mixed Oxide

2118 Fracture Strength

Date: 3/76



Temperature dependence of brittle strength of UO₂-20 wt % PuO₂.

	<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Date: 3/76	Fuel	Mixed Oxide	2118 Fracture Strength

Discussion

The brittle fracture strength of $(U,Pu)O_2$ may be expressed as a function of temperature T by

$$\sigma_f = 27.4 + 0.059T \text{ (}^\circ\text{K)}$$

where the fracture strength σ_f is in MN/m^2 . This relation is taken from reference (1) which found the fracture strength to be dependent on a largest flaw in the specimen rather than the average porosity,² grain size³ or impurity content.⁴ The brittle fracture strength was also found to be insensitive to loading rate.

FUNCTION

MATERIAL

PROPERTY

Fuel

Mixed Oxide

2118 Fracture Strength

Date: 3/76

References

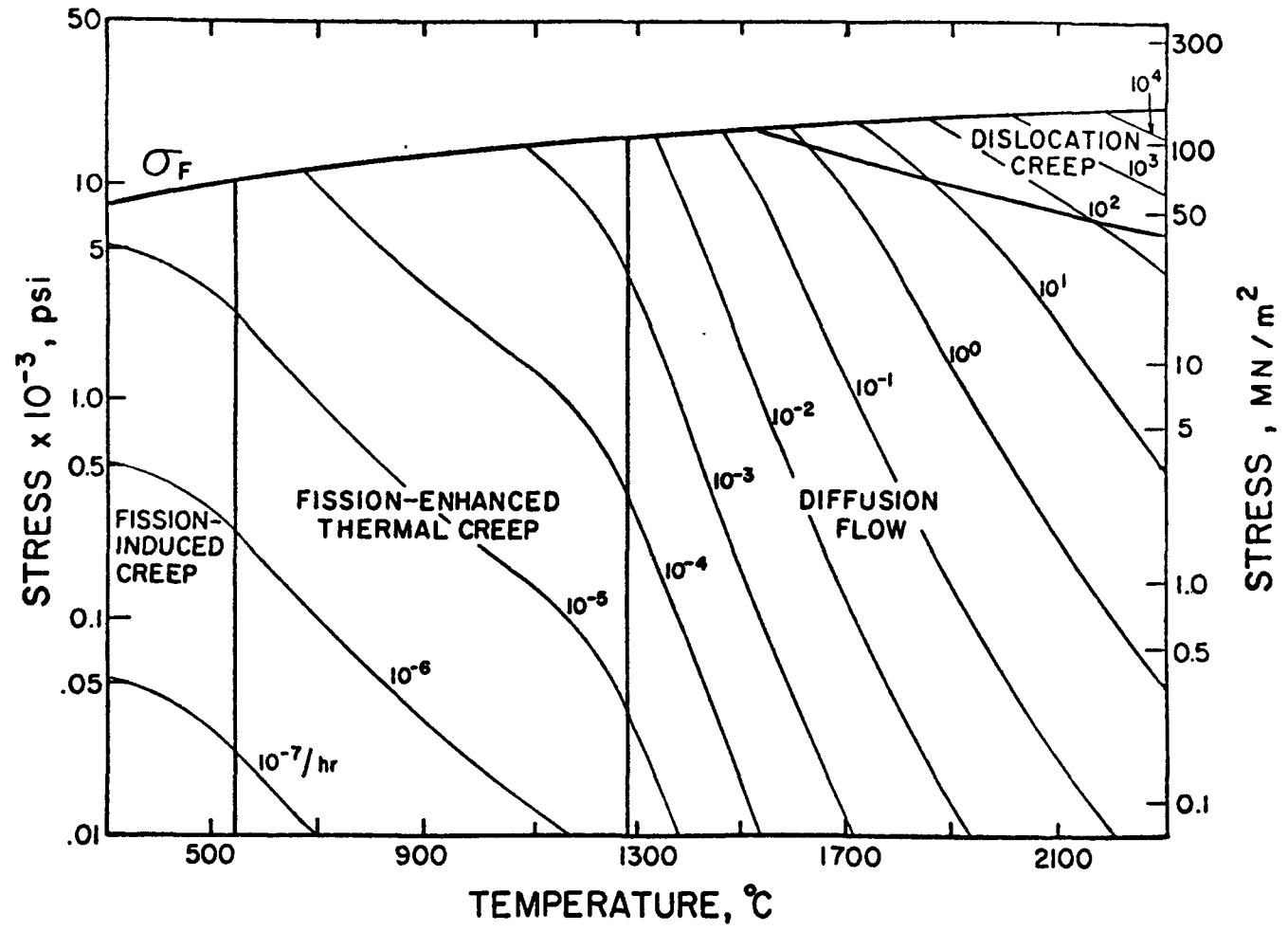
1. J. T. A. Roberts, "Brittle Fracture of Oxide Nuclear Fuel," J. Nucl. Mater., 47(1), 125-128 (May 1973).
2. J. T. A. Roberts and Y. Ueda, "Influence of Porosity on Deformation and Fracture of UO_2 ," J. Am. Ceram. Soc., 55(3), 117-124 (March 1972).
3. J. T. A. Roberts and B. J. Wrona, "Deformation and Fracture of UO_2 -20 wt % PuO_2 ," ANL-7945 (June 1972).
4. A. A. Solomon, "Influence of Impurity Particles on the Fracture of UO_2 ," J. Am. Ceram. Soc., 55(12), 622-627 (December 1972).

Date: 3/76

FUNCTION
Fuel

MATERIAL
Mixed Oxide

PROPERTY
2206 Creep



Deformation Map of 4- μm 96% TD UO_2 -25 wt % PuO_2 Subjected to Fission Rate of 5×10^{13} fissions/ cm^3 -sec.

Properties for LMFBR Safety Analysis

FUNCTIONMATERIALPROPERTY

Fuel

Mixed Oxide

2206 Creep

Date: 3/76

Discussion

The steady-state creep rate of mixed-oxide fuel may be expressed as the sum of several linearly additive terms

$$\dot{\epsilon}_{\text{total}} = \dot{\epsilon}_{\text{TL}} = \dot{\epsilon}_{\text{TH}} + \dot{\epsilon}_{\text{FT}} + \dot{\epsilon}_{\text{FA}} \quad (1)$$

The values of parameters used in these terms are given for a specific fuel composition, impurity concentration, pore morphology and O/M ratio. The effect of plutonium concentration has been reported,¹ but is not included in the present report because the creep rate in the diffusion flow region varies only ~15% in the concentration range of 20-30 wt % PuO₂. Primary creep has not been considered in the above relation although contributions from this mechanism may be significant.

Viscous creep ($\dot{\epsilon}_{\text{TL}}$) may be described by the relation

$$\dot{\epsilon}_{\text{TL}} = \frac{A}{d^2} [1 + 2.11 (97 - \zeta)] \sigma \exp (-Q_1/RT) \quad (2)$$

where

$\dot{\epsilon}_{\text{TL}}$ = steady-state creep due to diffusional flow (hr⁻¹)

A = 3.23 x 10⁹ (for UO₂-25 wt % PuO₂)

d = grain size (10-47 μm)

ζ = density (88-95% TD)

σ = stress (6.9-110 MN/m²)

Q₁ = 92500 cal/mole (O/M = 1.97)

R = gas constant (1.987 calories per °K per mole)

T = temperature (1573 - 1973°K)

Properties for LMFBR Safety Analysis

FUNCTIONMATERIALPROPERTY

Fuel

Mixed Oxide

2206 Creep

Date: 3/76

Discussion (Contd.)

The effect of density is based on work reported in Ref. 1. These data are extrapolated to 97% TD and normalized to the same figure. The other experimental parameters were obtained from Ref. 2.

Power-law creep ($\dot{\epsilon}_{TH}$) may be described by the relation

$$\dot{\epsilon}_{TH} = B[1 + 0.22(97 - \zeta)] \sigma^{4.4} \exp(-Q_2/RT) \quad (3)$$

where

$\dot{\epsilon}_{TH}$ = steady-state creep due to dislocation motion (hr^{-1})

B = 3.24×10^6 (for UO_2 -25 wt % PuO_2)

Q_2 = 136,800 cal/mole

Other variables are the same as Eq. (2).

The density dependence is also based on Ref. 1 data which have been extrapolated and normalized to 97% TD. The remaining experimental parameters were taken from Ref. 3.

Radiation-enhanced thermal creep ($\dot{\epsilon}_{FT}$) can be expressed as

$$\dot{\epsilon}_{FT} = C \sigma \dot{F} \exp(-Q_3/RT) \quad (4)$$

where

$\dot{\epsilon}_{FT}$ = fission enhanced thermal creep (hr^{-1}) for 95% TD, 4 μm grain size
 UO_2 -22 wt % PuO_2

C = 2.84×10^{-17}

\dot{F} = fission-rate (fissions/ cm^3 -sec)

FUNCTIONMATERIALPROPERTY

Fuel

Mixed Oxide

2206 Creep

Date: 3/76

Discussion (Contd.)

This relation describes Ref. 4 data within a factor of two.

Radiation-induced creep ($\dot{\epsilon}_{FA}$) may be described as

$$\dot{\epsilon}_{FA} = D \dot{F} \sigma \quad (5)$$

where

$\dot{\epsilon}_{FA}$ = fission-induced creep

$D = 5.40 \times 10^{-21}$ based on UO_2 for $T < 600^\circ K^5$

The following notes of caution should be observed in using these relations: (1) In general, the effect of fuel parameters such as composition, impurity concentration, pore morphology and O/M ratio have not been included; (2) Primary creep has not been considered; (3) No experimental data exists for $\sigma < 1000$ psi or $T > 2000^\circ K$.

FUNCTION

Fuel

MATERIAL

Mixed Oxide

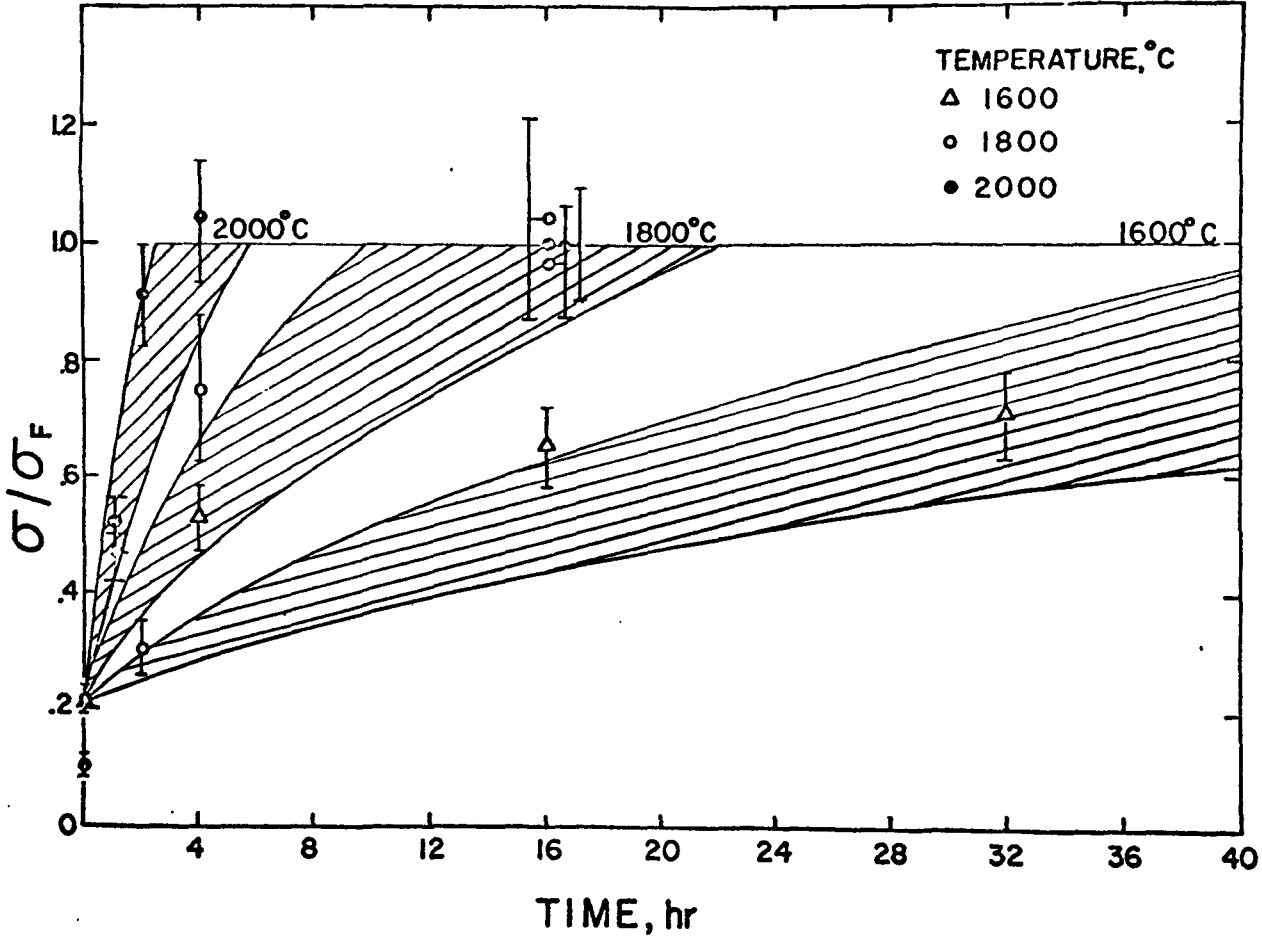
PROPERTY

2206 Creep

Date: 3/76

References

1. S. K. Evans, P. E. Bohaboy, and R. A. Laskiewicz, "Compressive Creep of Urania-Plutonia Fuels," GEAP-13732 (1971).
2. J. L. Routbort, N. A. Javed, and J. C. Voglewede, "Compressive Creep of Mixed-oxide Fuel Pellets," J. Nucl. Mater. 44(3), 247-259 (Sept 1972).
3. J. L. Routbort and J. C. Voglewede, "Creep of Mixed-oxide Fuel Pellets at High Stress," J. Am. Ceram. Soc. 56(6), 330-333 (June 1973).
4. J. S. Perrin, "Effect of Irradiation on the Creep of UO_2 - PuO_2 ," J. Nucl. Mater. 42, 101-104 (1972).
5. A. A. Solomon, "Radiation-Induced Creep of UO_2 ," J. Am. Ceram. Soc. 56(3), 164-171 (Mar 1973).



Recovery of Strength in UO_2 as a Function of Annealing Time and Temperature

Date: 3/76

FUNCTION
Fuel

MATERIAL
 UO_2

PROPERTY
3102 Crack Healing

	<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Date: 3/76	Fuel	UO ₂	3102 Crack Healing

Discussion

The recovery in strength of thermally shocked UO₂ specimens has been studied as a function of time and isothermal annealing temperature.¹ The strength recovery is expressed as a fraction of the unshocked strength of the material.

$$\left[\frac{\sigma(t)}{\sigma_f} \right]^2 - \left[\frac{\sigma_o}{\sigma_f} \right]^2 + \left[\frac{At}{\sigma_f^2} \right] \exp(-Q/RT)$$

where

$\sigma(t)$ = the time dependent fracture strength of thermally shocked UO₂,
kg/cm²

σ_f = fracture strength of unshocked UO₂, kg/cm²

σ_o = fracture strength of thermally shocked UO₂ (at t=0) equals
 $\approx 0.2 \sigma_f$

A = $6.5 \pm 2.7 \times 10^{10}$ kg² cm⁻⁴ hr⁻¹

t = time (hrs)

Q = 55000 cal/mole

R = gas constant (1.987 calories per °K per mole)

T = temperature °K

FUNCTIONMATERIALPROPERTY

Fuel

UO₂

3102 Crack Healing

Date: 3/76

References

1. J. T. A. Roberts and B. J. Wrona, "Crack Healing in UO₂," J. Am. Cer. Soc., 56 (6), 297-299 (June 1973).

FUNCTION

Fuel

MATERIAL

UO₂

PROPERTY

Vapor Pressure

(3303)

Date: 1/76

Vapor Pressure over UO₂

T(K)	ρ (atm)
2000	9.29×10^{-8}
2500	1.25×10^{-4}
3000	1.52×10^{-2}
3500	0.344
4000	2.45
4500	10.7
5000	33.1
5500	77.6
6000	151

FUNCTION

Fuel

MATERIAL

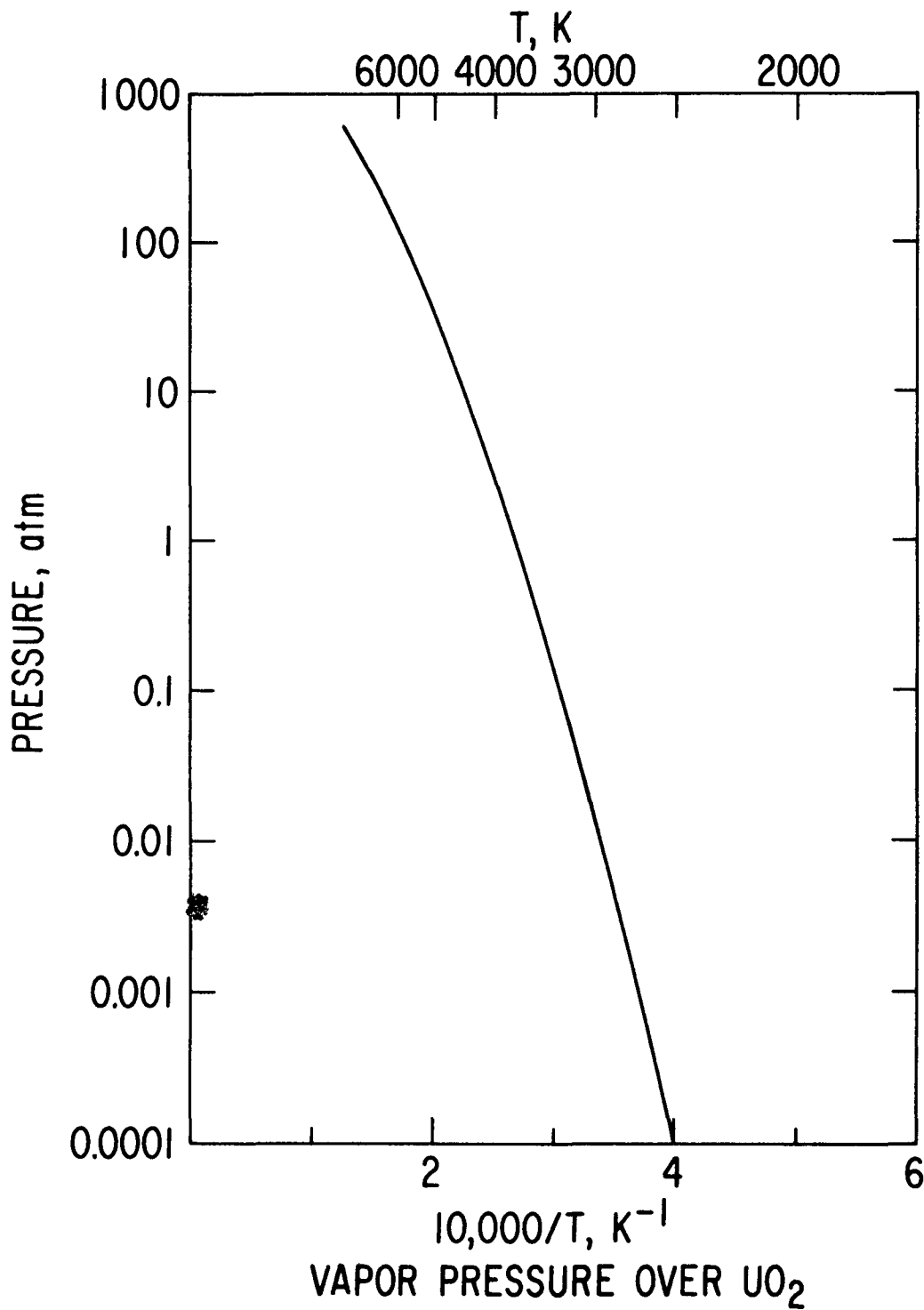
UO₂

PROPERTY

Vapor Pressure

(3303)

Date: 1/76



FUNCTION

Fuel

MATERIALUO₂PROPERTY

Vapor Pressure (3303)

Date: 1/76

Data Source

The values of vapor pressure below the melting point of UO₂ (3123K) come from the experimental work of Tetenbaum and Hunt;¹ $\log P(\text{atm}) = (-31284/T) + 8.61$; T is in K. The value at 3500K is based on the experimental work of Reedy and Chasanov;² $\log p(\text{atm}) = (-27426/T) + 7.373$. The values at 4000K and above are based on the liquid UO₂ equation of state developed by Gillian.³

Discussion

There have been a large number of experimental determinations of the vapor pressure over UO₂, notably the work of Ackermann *et al.*,⁴ Ohse,⁵ Tetenbaum and Hunt,¹ Pattoret *et al.*,⁶ and Reedy and Chasanov.² The last set of experiments extended in the liquid UO₂ temperature range. The experimental methods employed were Knudsen effusion, mass spectrometry, and transpiration. More recently several experiments above 4000K have employed laser pulse heating techniques; these include the work of Ohse *et al.*⁷ and that of Bober *et al.*⁸ A quite different approach using matrix isolation spectroscopic data to calculate pressures over UO₂ has been employed by Gabelnick.⁹ Breitung¹⁰ has used an oxygen potential theory method. There have been a number of purely calculational approaches based on employing corresponding states theory to extrapolate low temperature pressure data to the reactor accident temperature regime; notable among these efforts are the calculations of Booth¹¹ and Menzies¹². A recent paper by Gillian³ employs Significant Structures theory to calculate the equation of state of liquid UO₂.

To represent the pressures over solid UO₂, we have chosen the values of Tetenbaum and Hunt.¹ These data are in reasonable agreement with the work of other experimenters in this temperature range and they agree well with the high temperature liquid UO₂ experiments of Reedy and Chasanov.³ For 4000K and above, there are many sets of calculated values to choose from; some of these are displayed in the following table.

T(K)	Calculated $p(\text{atm})$					
	Gabelnick ⁹	Ohse ⁷	Booth ¹¹	Menzies ¹²	Breitung ¹⁰	Gillian ^{3*}
4000	2.24	5.31	6.01	2.63	6.08	2.45
5000	29.1	132	98.9	46.5	150	33.1
6000	171	1120	554	272	-	151

*Using Tetenbaum and Hunt data as basis for calculation.

FUNCTION

Fuel

MATERIALUO₂PROPERTY

Vapor Pressure (3303)

Date: 1/76

Discussion (cont'd.)

The relatively good agreement between Gabelnick's and Gillian's results (which were arrived at by very different calculational methods) resulted in the use of Gillian's values in the recommended vapor pressure table. It must be kept clearly in mind, however, that all these values are based on some kind of calculational scheme, and until reliable experimental data are obtained at these upper temperatures, the recommended values are probably uncertain by a factor of two or three.

References

1. M. Tetenbaum and P. D. Hunt, J. Nucl. Mater. 34, 86 (1970).
2. G. T. Reedy and M. G. Chasanov, J. Nucl. Mater. 42, 341 (1972).
3. M. J. Gillian, "Thermodynamics of Nuclear Materials 1974," Vol. I, p. 269, International Atomic Energy Agency, Vienna, 1975.
4. R. J. Ackermann, P. W. Gilles, and R. J. Thorne, J. Chem. Phys. 25, 1089 (1956).
5. R. W. Ohse, J. Chem. Phys. 44, 1375 (1966).
6. A. Pattoret, I. Drowart, and S. Smoes, "Thermodynamics of Nuclear Materials 1967," p. 613, International Atomic Energy Agency, Vienna, 1967.
7. R. W. Ohse, P. G. Berrie, H. G. Bogensberger, and E. A. Fischer, "Thermodynamics of Nuclear Materials 1974," Vol. I, p. 307, International Atomic Energy Agency, Vienna, 1975.
8. M. Bober, H. V. Karow, and K. Schretzmann, Nuclear Technol. 26, 237 (1975).
9. M. G. Chasanov, D. F. Fischer, D. R. Fredrickson, S. D. Gabelnick, R. Kumar, L. Leibowitz, G. T. Reedy, F. A. Cafasso, and L. Burris, "Chemical Engineering Division Reactor Safety and Physical Properties Studies Annual Report, July 1973 - June 1974," ANL-8120, p. 60.
10. W. Breitung, "Calculation of Vapor Pressures of Oxide Fuels up to 5000K for Equilibrium and Nonequilibrium Evaporation," KFK2091, 1975.
11. D. L. Booth, "The Thermodynamic Properties of UO₂ and Sodium," TRG Report 1871 (R/X), 1969.
12. D. C. Menzies, "The Equation of State of Uranium Dioxide at High Temperatures and Pressures," TRG Report 1119 (D).

FUNCTIONMATERIALPROPERTY

Fuel

 $(U_{0.8}Pu_{0.2})O_{1.96}$

Vapor Pressure

(3303)

Date: 1/76

Vapor Pressure over $(U_{0.8}Pu_{0.2})O_{1.96}$

T(K)	ρ (atm)
2000	1.2×10^{-7}
2500	2.1×10^{-4}
3000	3.6×10^{-2}
3500	0.91
4000	9.1
4500	49
5000	170
5500	500*
6000	1000*

*Extrapolated from values at lower temperatures

FUNCTION

Fuel

MATERIAL

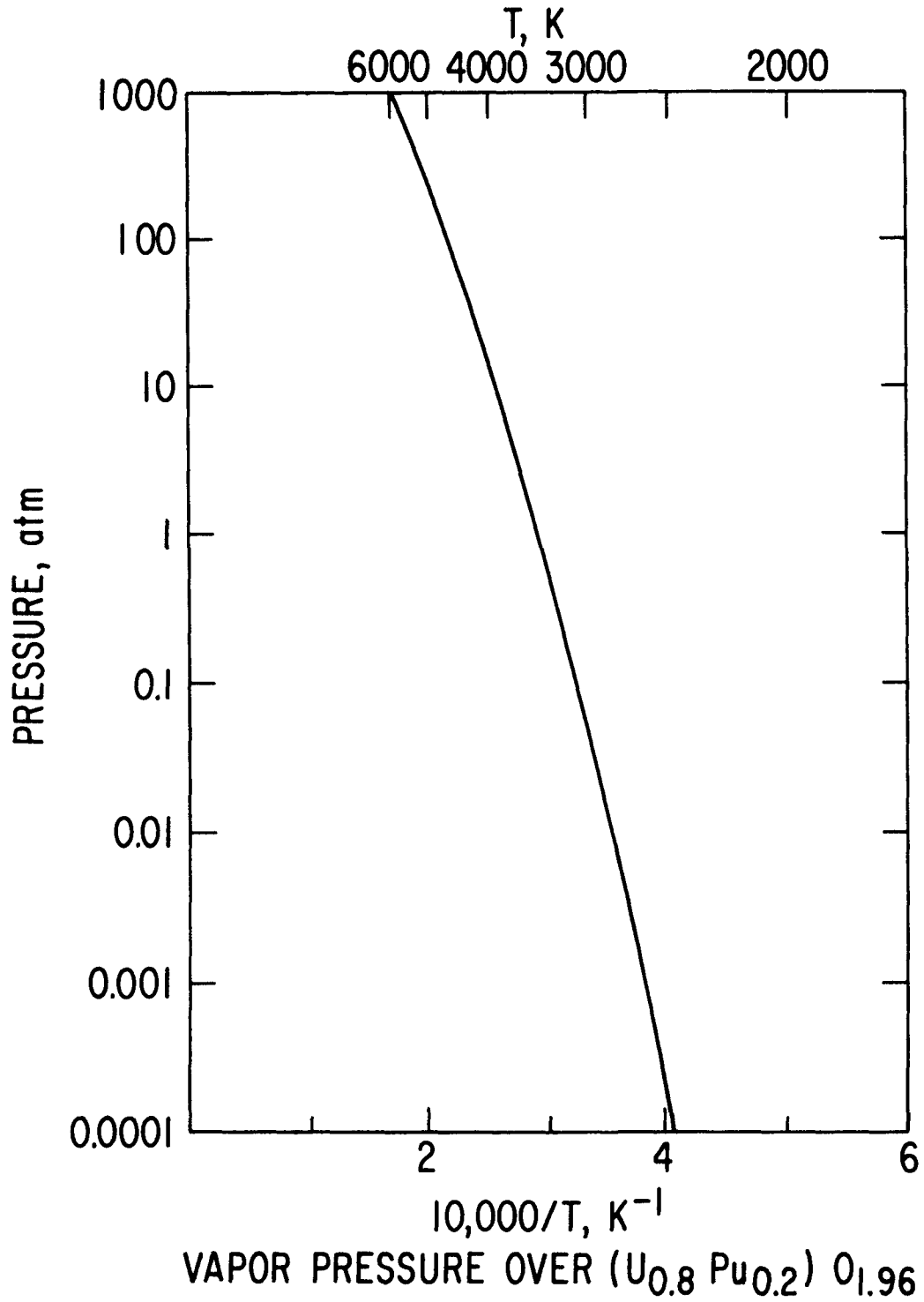
$(U_{0.8}Pu_{0.2})O_{1.96}$

PROPERTY

Vapor Pressure

(3303)

Date: 1/76



<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>	
Fuel	$(U_{0.8}Pu_{0.2})O_{1.96}$	Vapor Pressure	(3303)

Date: 1/76

Data Source

The values of vapor pressure over $(U_{0.8}Pu_{0.2})O_{1.96}$ were taken from the calculated tables of values given by Breitung.¹ The values above 5000K were obtained by graphical extrapolation of his lower temperature results.

Discussion

While there are experimental data^{2,3} available for pressures over mixed oxide at temperatures up to ~2400K, above the melting point of fuel only the recent values of Ohse et al.⁴ are available. While the latter experiments extended to 7000K, there remain many questions relating to the interpretation of the results of these laser-evaporation experiments. The vapor pressure equation of Ohse et al.⁴ thus was not used for calculation of the above recommended values; however, this equation is presented here for those who may wish to consider its use:

$$\log p(\text{atm}) = 7.966 - \frac{28137}{T},$$

where T is in Kelvins.

Gabelnick⁵ calculated vapor pressures over mixed oxides using the same methods he employed for UO_2 (see UO_2 vapor pressures). However, the application of this method becomes more tenuous in the case of mixed oxides since Gabelnick had to estimate thermodynamic parameters for the plutonium-bearing vapor species as well as for the oxygen potentials. Because of these imponderable uncertainties, Gabelnick's estimated vapor pressures were also not used in this compilation. Breitung¹ has made thermodynamic calculations of mixed oxide vapor pressures using oxygen potential theory. His calculated values fall in between those of Gabelnick⁵ and Ohse et al.⁴ at the highest temperatures and Breitung's calculations have been chosen as the recommended values. A comparison of these different calculated vapor pressures is given below:

Calculated ρ (atm)			
T(K)	Ohse <u>et al.</u> ⁴	Breitung ¹	Gabelnick ⁵
4000	8.5	9.1	3.9
5000	220	170	44
6000	1900	1000	260

Until more experimental work is completed on the vapor pressures of mixed oxides at high temperatures, especially greater clarification of the oxygen potentials over the non-stoichiometric fuels, these recommended mixed oxide vapor pressure values remain more uncertain than those for UO_2 (cf.).

FUNCTION

Fuel

MATERIAL $(U_{0.8}Pu_{0.2})O_{1.96}$ PROPERTY

Vapor Pressure (3303)

Date: 1/76

References

1. W. Breitung, "Calculation of Vapor Pressure of Oxide Fuels up to 5000K for Equilibrium and Nonequilibrium Evaporation," KFK 2091, 1975.
2. J. E. Battles, W. A. Shinn, P. E. Blackburn, and R. K. Edwards in "Plutonium 1970" Nuclear Metallurgy, Vol. 17, Pt. II, p. 733 (1971).
3. R. W. Ohse and W. M. Olsen, ibid., p. 743.
4. R. W. Ohse, P. G. Berrie, H. G. Bogensberger, and E. A. Fischer, "Thermodynamics of Nuclear Materials 1974," Vol. I, p. 307, International Atomic Energy Agency, Vienna, 1975.
5. M. G. Chasanov, D. F. Fischer, D. R. Fredrickson, S. D. Gabelnick, R. Kumar, L. Leibowitz, G. T. Reedy, F. A. Cafasso, and L. Burris, "Chemical Engineering Division, Reactor Safety and Physical Property Studies Annual Report, July 1973 - June 1974," ANL-8120.

FUNCTION

MATERIAL

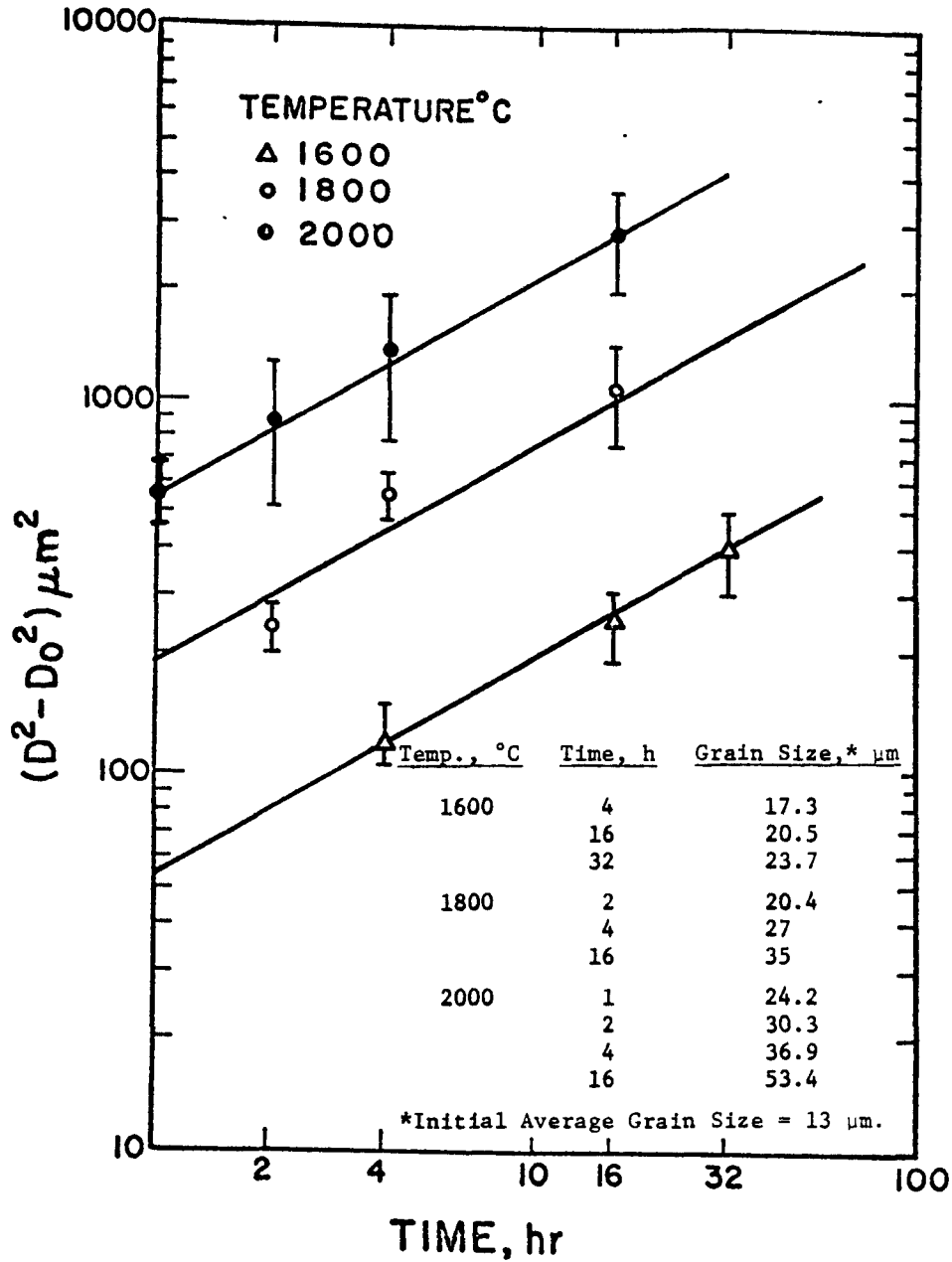
PROPERTY

Fuel

UO₂

4201 Grain Growth

Date: 3/76



Grain Growth in UO₂ Plotted as $\ln(D^2 - D_0^2)$ vs $\ln t$.

FUNCTION

Fuel

MATERIALUO₂PROPERTY

4201 Grain Growth

Date: 3/76

Discussion

Unpublished data of J. T. A. Roberts and B. J. Wrona of A.N.L. has been used to develop an expression for grain growth in UO₂. In the undisturbed and equiaxed regions

$$D^2 = D_o^2 + K t^n \exp(-Q/RT) \quad (1)$$

where

D = time and temperature dependent grain size, μm

D_o = initial grain size, μm

K = 3×10^7

t = time (hrs)

n = 0.61

Q = 49400 kcal/mole

R = gas constant (1.987 calories per °K per mole)

T = temperature °K

For the columnar region,

$$\bar{D} = \sqrt{D_b \times R_c}$$

this relation assumes that the columnar grain length equals the zone radius R_c and the grain width equals the equiaxed grain size D_b and is based on a formulation used by Ashby and Raj for asymmetric grains in diffusion creep theory.¹

FUNCTION

MATERIAL

PROPERTY

Fuel

UO₂

4201 Grain Growth

Date: 3/76

References

1. M. F. Ashby and R. Raj, Tech. Rept. 2, Div. of Eng. and Appl. Phys. Harvard U, Cambridge, Mass. (June 1970).

COOLANT

FUNCTION

Coolant

MATERIAL

Sodium

PROPERTY

Miscellaneous Properties

Date: 1/76

<u>Property</u>	<u>Value</u>	<u>Reference</u>	<u>Property Code</u>
Melting Point	370.98 K	1	3103
Heat of Fusion	621.8 cal/mol	1	3104
Boiling Point	1154.6 K	1	3105
Heat of Vaporization	21.280 Kcal/mol	1	3106
Critical Temperature	2733K	2	
Critical Pressure	408.2 atm	2	
Critical Density	0.1818 g/cm ³	2	

FUNCTION

Coolant

MATERIAL

Sodium

PROPERTY

Miscellaneous Properties

Date: 1/76

References

1. O. J. Foust, Editor, "Sodium-NaK Engineering Handbook Volume 1," Gordon and Breach, New York, 1972.
2. D. Miller, A. B. Cohen, and C. E. Dickerman, "Estimation of Vapor and Liquid Density and Heat of Vaporization of the Alkali Metals to the Critical Point," International Conference on the Safety of Fast Breeder Reactors, Aix-en-Provence, France, September 19-22, 1967.

	<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Date: 1/76	Coolant	Sodium	Heat Capacity (3108)
	T(K)	C_p (cal/mol K)	C_v (cal/mol K)
	400	7.53	6.73
	500	7.30	6.31
	600	7.12	5.95
	700	6.99	5.64
	800	6.92	5.39
	900	6.89	5.19
	1000	6.92	5.05
	1100	6.99	4.96
	1200	7.11	4.93
	1300	7.29	4.94
	1400	7.51	5.00
	1500	7.78	5.11
	1600	8.11	5.26
	1700	8.38	5.28
	1800	8.60	5.14
	1900	8.88	4.99
	2000	9.24	4.83
	2100	9.72	4.67
	2200	10.4	4.50
	2300	11.4	4.35
	2400	13.1	4.24
	2500	16.3	4.23
	2600	25.1	4.61
	2700	135	8.55

FUNCTION

MATERIAL

PROPERTY

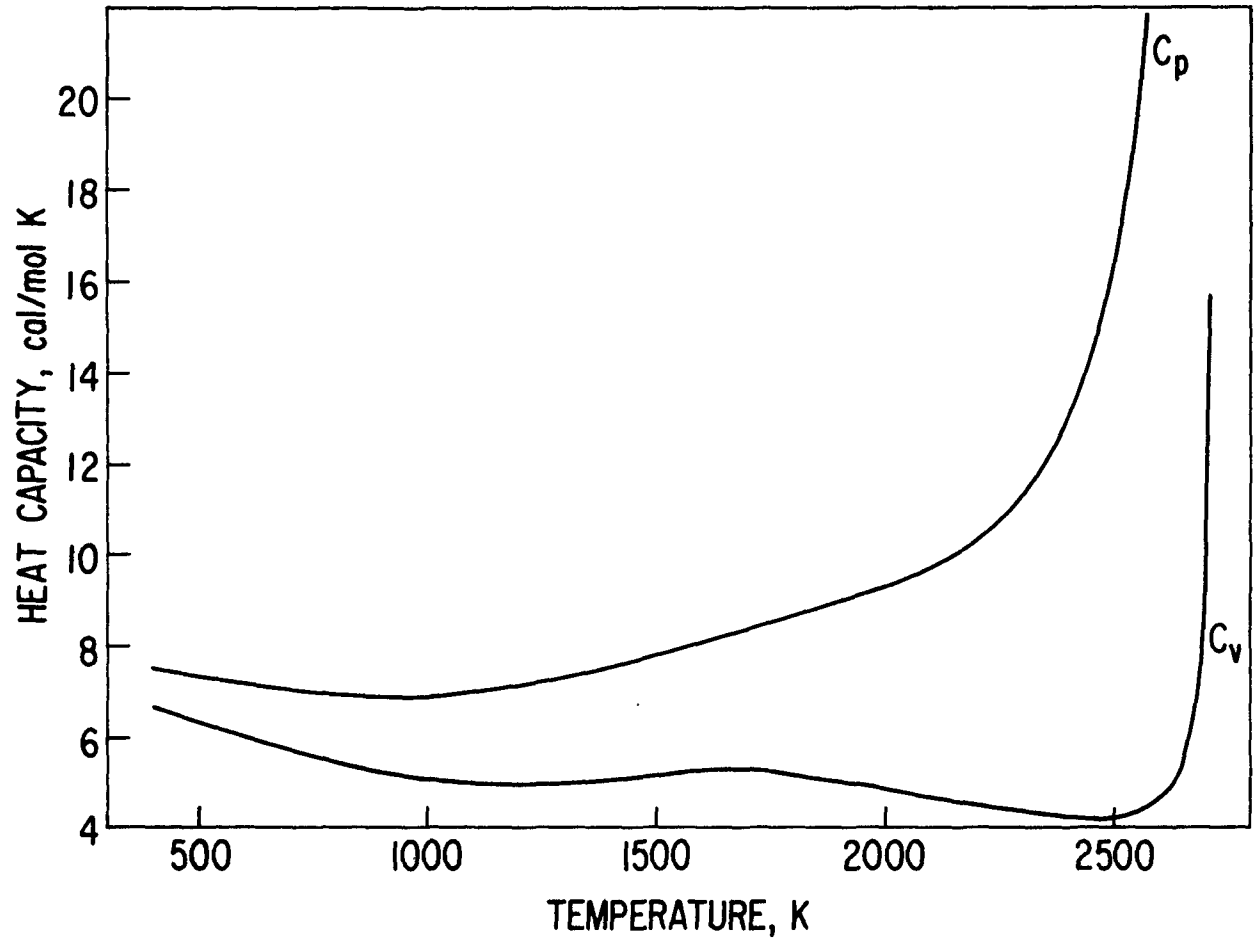
Coolant

Sodium

Heat Capacity

(3108)

Date: 1/76



HEAT CAPACITY FOR SATURATED SODIUM LIQUID

FUNCTION

Coolant

MATERIAL

Sodium

PROPERTY

Heat Capacity

(3108)

Date: 1/76

Data Source

The values for C_p and C_v came from Reference 1.

Discussion

C_p and C_v came from Reference 1 and are based on values recommended by Golden and Tokar,² who in turn used Ginnings et al.'s³ experimental data (up to 900°C) as extended by Stone et al.⁴ Padilla (Ref. 1) extrapolated the values of Ref. 2 to obtain the results shown. The range of experimental specific heat data has since been extended to 1232°C by Fredrickson and Chasanov.⁵ These newer data should be included in revisions of Padilla's calculations. It must be kept in mind, however, that the extrapolation of the experimental data beyond the range of measurement involves a significant dependence on estimated critical parameters of sodium. This is clearly demonstrated by the work of Gabelnick,⁶ which shows the variations in C_p and C_v with choice of critical parameters. The curves shown in Reference 1 are based on Miller's estimates⁷ ($T_c = 2733K$, $P_c = 408.2$ atm, $\rho_c = 0.1818$ g/cm³). Above 1700°C, these specific heat values should be used with caution since current experiments at Columbia under Bonilla⁸ may result in markedly different critical parameters and in resultantly higher specific heats in the region between 1700°C and the critical temperature.

References

1. A. Padilla, "High Temperature Thermodynamic Properties of Sodium," ANL-8095, 1974.
2. G. H. Golden and J. V. Tokar, "Thermophysical Properties of Sodium," ANL-7323, 1967.
3. D. C. Ginnings, T. B. Douglas, and A. F. Ball, J. Res. N.B.S.R.P. 2110 45, 23 (1950).
4. J. P. Stone, C. T. Ewing, J. R. Spann, E. W. Steinkuller, D. D. Williams, and R. R. Miller, "High Temperature Properties of Sodium," NRL Report 6241, September 24, 1965.
5. D. R. Fredrickson and M. G. Chasanov, J. Chem. Thermodynamics 6, 629 (1974).
6. M. G. Chasanov, D. F. Fischer, D. R. Fredrickson, S. D. Gabelnick, R. Kumar, L. Leibowitz, G. T. Reedy, F. A. Cafasso, and L. Burris, "Chemical Engineering Division, Reactor Safety and Physical Property Studies Annual Report, July 1973 - June 1974," ANL-8120.

FUNCTION

MATERIAL

PROPERTY

Coolant

Sodium

Heat Capacity (3108)

Date: 1/76

References

7. D. Miller, A. B. Cohen, and C. E. Dickerman, "Estimation of Vapor and Liquid Density and Heat of Vaporization of the Alkali Metals to the Critical Point," International Conference on the Safety of Fast Breeder Reactors, Aix-en-Provence, France, September 19-22, 1967.
8. C. F. Bonilla, private communication.

	<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Date: 1/76	Coolant	Sodium (relative to the standard state at 0K)	Enthalpy (3109)
T(K)		H _{liquid} (Kcal/mol)	H _{vapor} (Kcal/mol)
400		2.898	27.58
500		3.639	28.03
600		4.359	28.40
700		5.065	28.68
800		5.760	28.90
900		6.450	29.08
1000		7.139	29.24
1100		7.834	29.41
1200		8.539	29.59
1300		9.260	29.78
1400		10.000	29.96
1500		10.766	30.12
1600		11.563	30.24
1700		12.392	30.35
1800		13.243	30.44
1900		14.119	30.51
2000		15.024	30.54
2100		15.964	30.54
2200		16.949	30.50
2300		17.994	30.39
2400		19.120	30.21
2500		20.373	29.89
2600		21.855	29.35
2700		24.004	28.14
2733 (critical temperature)		26.229	26.229

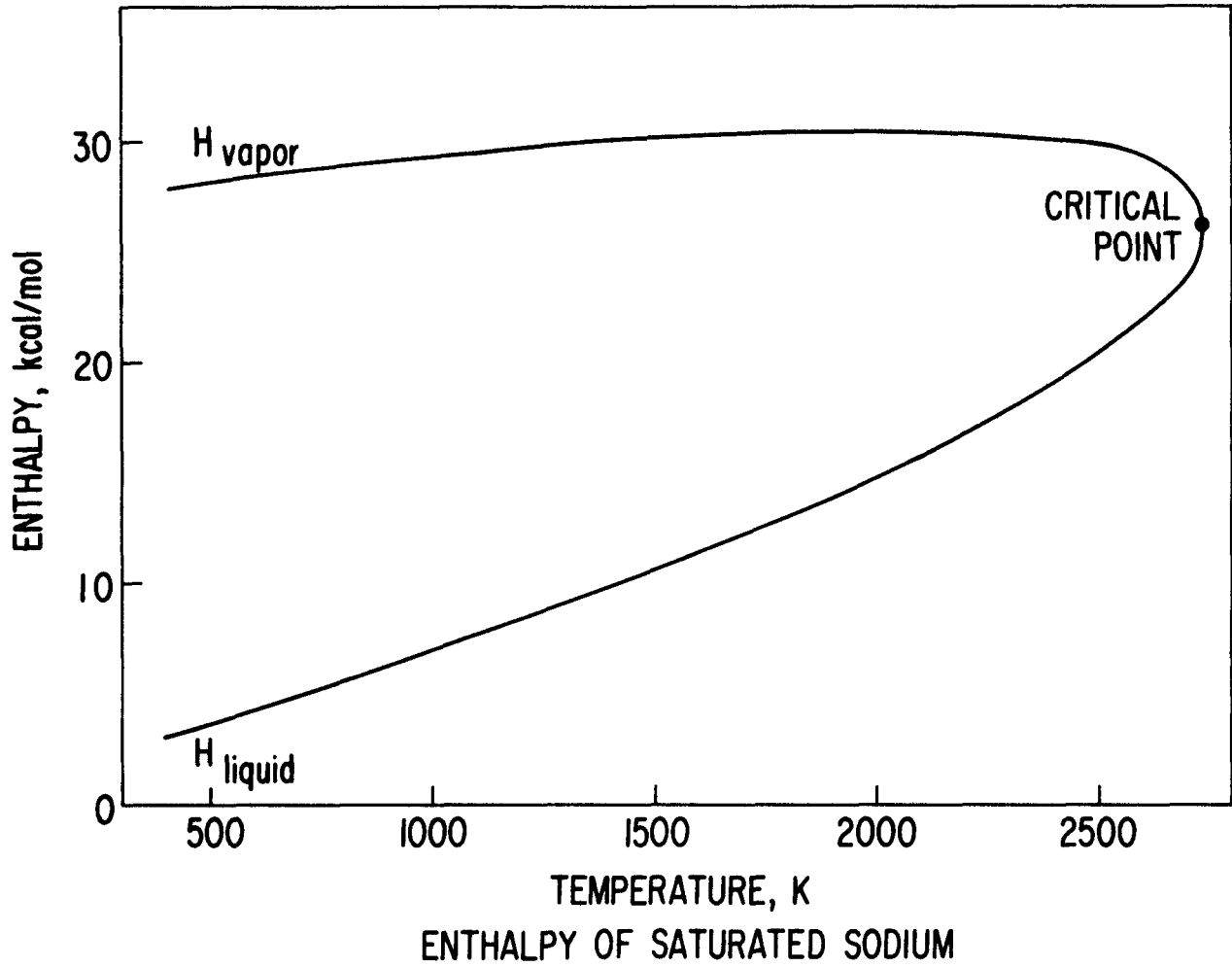
FUNCTION
Coolant

MATERIAL
Sodium

PROPERTY
Enthalpy

(3109)

Date: 1/76



<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>	
Coolant	Sodium	Enthalpy	(3109)

Date: 1/76

Data Source

The values for the enthalpy of saturated sodium came from Reference 1.

Discussion

Padilla in Reference 1 combined liquid enthalpies recommended by Golden and Tokar² with computed vapor enthalpies from the same source to obtain average enthalpy values. The average enthalpy was then extrapolated to the critical temperature assumed by Miller et al.³ (2733K) and extrapolated liquid and vapor enthalpies were obtained by the addition or subtraction of half the heat of vaporization. The heat of vaporization used for this calculation was based on that recommended by Miller et al.³ Padilla's values (Ref. 1) are represented by the equations:

$$H_{liq}(J/g) = H_{avg} - \Delta H_{vap}/2$$

$$H_{vap}(J/g) = H_{avg} + \Delta H_{vap}/2$$

where: $H_{avg}(J/g) = 3841.9 + 0.85563[T(k) - 1644.31]$

$$\Delta H_{vap} = 5.050 RT_c (1 - T/T_c)^{0.4262}$$

T_c = critical temperature

= 2733K (estimate of Miller et al.³)

The above enthalpies are relative to the standard state at 0°K. However, it is clear that the results of Reference 1 are quite dependent on the choice of the critical parameters; Gabelnick⁴ has shown the marked effect of variation of critical temperature on the enthalpy of the system above ~1700°C (see property code 3108 for a discussion of current experimental work in this area). Thus the user of these enthalpy values should be aware of these uncertainties; a quantitative estimate of them can be obtained by consulting Gabelnick's study.⁴

References

1. A. Padilla, "High Temperature Thermodynamic Properties of Sodium," ANL-8095, 1974.
2. G. H. Golden and J. V. Tokar, "Thermophysical Properties of Sodium," ANL-7323, 1967.

FUNCTION
Coolant

MATERIAL
Sodium

PROPERTY
Enthalpy

(3109)

Date: 1/76

References

3. D. Miller, A. B. Cohen, and C. E. Dickerman, "Estimation of Vapor and Liquid Density and Heat of Vaporization of the Alkali Metals to the Critical Point," International Conference on the Safety of Fast Breeder Reactors, Aix-en-Provence, France, September 19-22, 1967.
4. M. G. Chasanov, D. F. Fischer, D. R. Fredrickson, S. D. Gabelnick, R. Kumar, L. Leibowitz, G. T. Reedy, F. A. Cafasso, and L. Burris, "Chemical Engineering Division Reactor Safety and Physical Property Studies Annual Report, July 1973 - June 1974," ANL-8120.

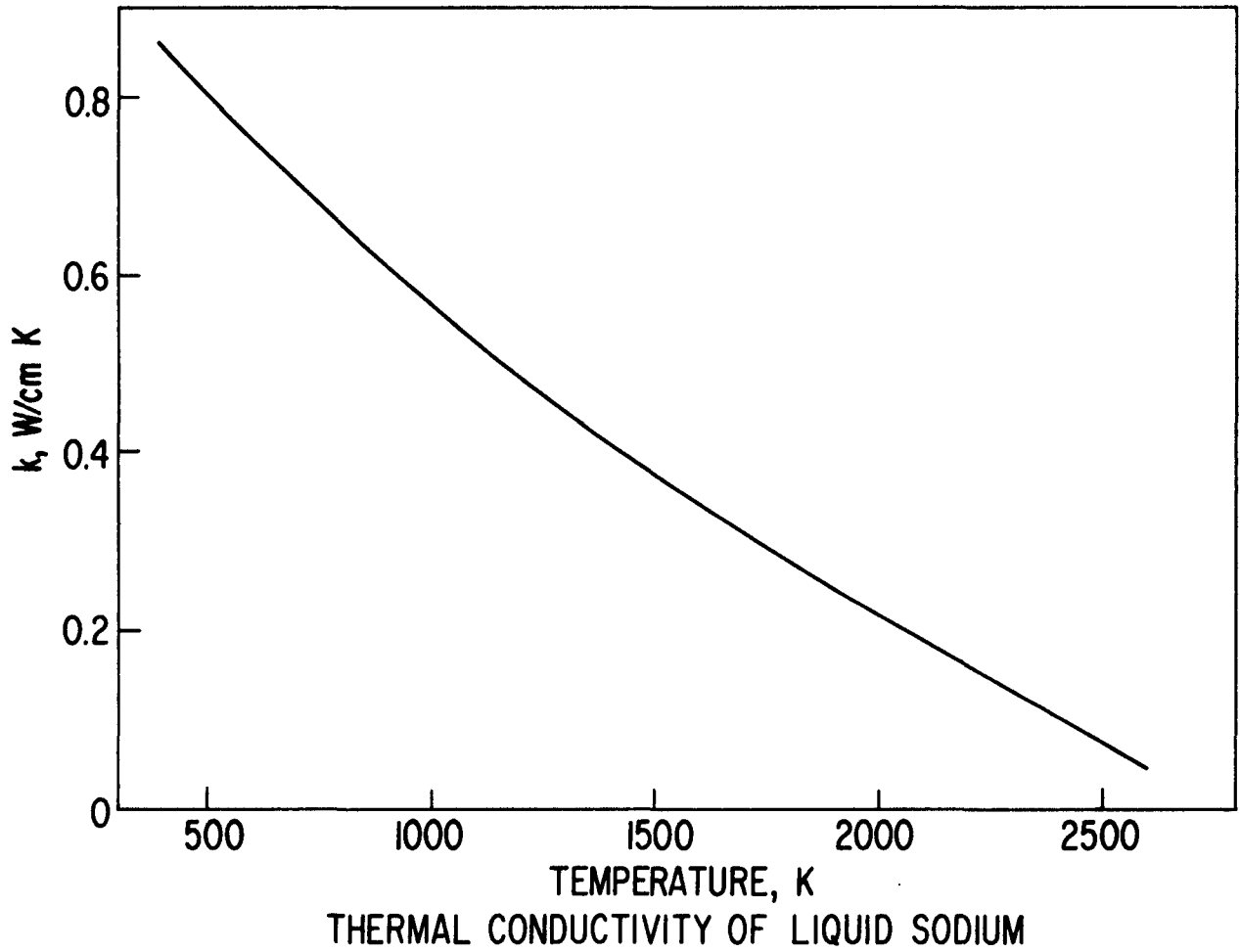
<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>	(3113)
Coolant	Sodium	Liquid Thermal Conductivity	
Date: 1/76			
T(K)		k(w/cm K)	
400		0.858	
500		0.804	
600		0.753	
700		0.703	
800		0.656	
900		0.612	
1000		0.570	
1100		0.530	
1200		0.492	
1300		0.457	
1400		0.41	
1500		0.38	
1600		0.34	
1700		0.31	
1800		0.29	
1900		0.26	
2000		0.22	
2100		0.20	
2200		0.17	
2300		0.14	
2400		0.11	
2500		0.078	
2600		0.042	
2700		0.013	

FUNCTION
Coolant

MATERIAL
Sodium

PROPERTY
Liquid Thermal
Conductivity (3113)

Date: 1/76



FUNCTIONMATERIALPROPERTY

Coolant

Sodium

Liquid Thermal
Conductivity

(3113)

Date: 1/76

Data Source

The values of thermal conductivity given for liquid sodium are based on the work of Golden and Tokar¹ and Grosse.³

Discussion

Golden and Tokar¹ developed an equation for the thermal conductivity of liquid sodium based on their analysis of the experimental data. Their equation was proposed for the liquid range up to 1643K:

$$k(\text{w/cm K}) = 0.930 - 0.581 \times 10^{-3} (T - 273) + 1.173 \times 10^{-7} (T - 273)^2 .$$

Above the boiling point, Foust² recommends a semi-empirical method developed by Grosse³ for estimation of thermal conductivities. The values presented in the preceding table were obtained from the Golden and Tokar¹ equation up to 1300K; the values from 1400K were obtained by graphical interpolation of Grosse's³ calculated results. It should be borne in mind that Grosse's method depends strongly on the choice of critical temperature; he used a value of 2800K, slightly greater than the value recommended by Miller.⁴ In addition, Grosse's method is based on the Wiedemann-Franz-Lorenz law. In the absence of experimental data at the higher temperatures, Grosse's approach seems preferable to some of the other extrapolative methods (see Foust²).

References

1. G. H. Golden and J. V. Tokar, "Thermophysical Properties of Sodium," ANL-7323 (1967).
2. O. J. Foust, Editor, "Sodium-NaK Engineering Handbook, Vol. 1," Gordon and Breach, New York, 1972.
3. A. V. Grosse, Rev. Hautes Temp. et Refract. 3, 115 (1966).
4. D. Miller, A. B. Cohen, and C. E. Dickerman, "Estimation of Vapor and Liquid Density and Heat of Vaporization of the Alkali Metals to the Critical Point," International Conference on the Safety of Fast Breeder Reactors, Aix-en-Provence, France, September 19-22, 1967.

FUNCTIONMATERIALPROPERTY

Coolant

Sodium

Thermal Expansivity (3114)

Date: 1/76

T(K)	$\alpha_p(K^{-1}) \times 10^4$
400	2.533
500	2.616
600	2.719
700	2.814
800	2.912
900	3.012
1000	3.114
1100	3.220
1200	3.329
1300	3.444
1400	3.565
1500	3.694
1600	3.833
1700	4.090
1800	4.492
1900	4.993
2000	5.634
2100	6.486
2200	7.670
2300	9.430
2400	12.33
2500	18.00
2600	33.97
2700	250.6

FUNCTION

MATERIAL

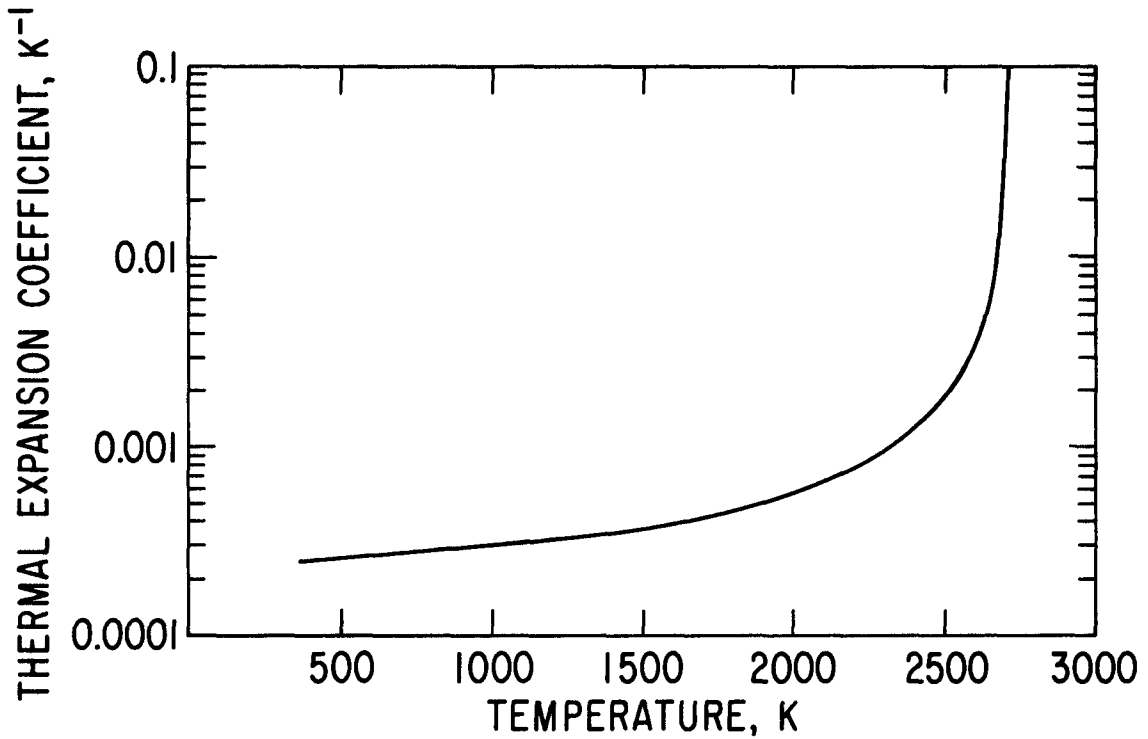
PROPERTY

Coolant

Sodium

Thermal Expansivity (3114)

Date: 1/76



VOLUMETRIC THERMAL EXPANSION COEFFICIENT
FOR SATURATED SODIUM LIQUID

FUNCTION

Coolant

MATERIAL

Sodium

PROPERTY

Thermal Expansivity (3114)

Date: 1/76

Data Source

The values for the volumetric coefficient of thermal expansion came from Reference 1.

Discussion

The volumetric thermal expansion coefficient along the saturation curve can be obtained directly from density data (see Property Code 3304 for density discussion). However, the thermodynamic volumetric coefficient of expansion differs from that along the saturation curve by the product of the isothermal compressibility and the thermal pressure coefficient along the saturation curve (see Ref. 2); this difference becomes significant at high temperatures. Thus, since Padilla in Ref. 1 required critical temperature and pressure data for extrapolation of vapor pressure, speed of sound, and density data to the high temperature regions near the critical point, there are compounded uncertainties in using the values he generated.

Gabelnick³ has shown the effect of different critical parameter choice on the expansion coefficient; Padilla's values are based on the Miller et al.⁴ critical parameters ($T_c = 2733K$, etc.). Fortunately, except at a few hundred degrees near the critical temperature, the thermal expansion coefficient remains relatively unchanged on a wide range of temperatures.

References

1. A. Padilla, "High Temperature Thermodynamic Properties of Sodium," ANL-8095, 1974.
2. J. S. Rowlinson, "Liquids and Liquid Mixtures, 2nd Ed.," Plenum Press, New York, 1969.
3. M. G. Chasanov, D. F. Fischer, D. R. Fredrickson, S. D. Gabelnick, R. Kumar, L. Leibowitz, G. T. Reedy, F. A. Cafasso, and L. Burris, "Chemical Engineering Division, Reactor Safety and Physical Property Studies Annual Report, July 1973 - June 1974," ANL-8120.
4. D. Miller, A. B. Cohen, and C. E. Dickerman, "Estimation of Vapor and Liquid Density and Heat of Vaporization of the Alkali Metals to the Critical Point," International Conference on the Safety of Fast Breeder Reactors, Aix-en-Provence, France, September 19-22, 1967.

<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>	
Coolant	Sodium	Saturated Vapor Pressure	(3303)
Date: 1/76			
T(K)		p(atm)	
800		0.01	
900		0.05	
1000		0.19	
1100		0.59	
1200		1.48	
1300		3.20	
1400		6.17	
1500		10.9	
1600		17.8	
1700		27.4	
1800		40.4	
1900		57.2	
2000		78.4	
2100		105	
2200		136	
2300		173	
2400		217	
2500		266	
2600		323	
2700		386	
2733 (critical temperature)		408	

FUNCTION

MATERIAL

PROPERTY

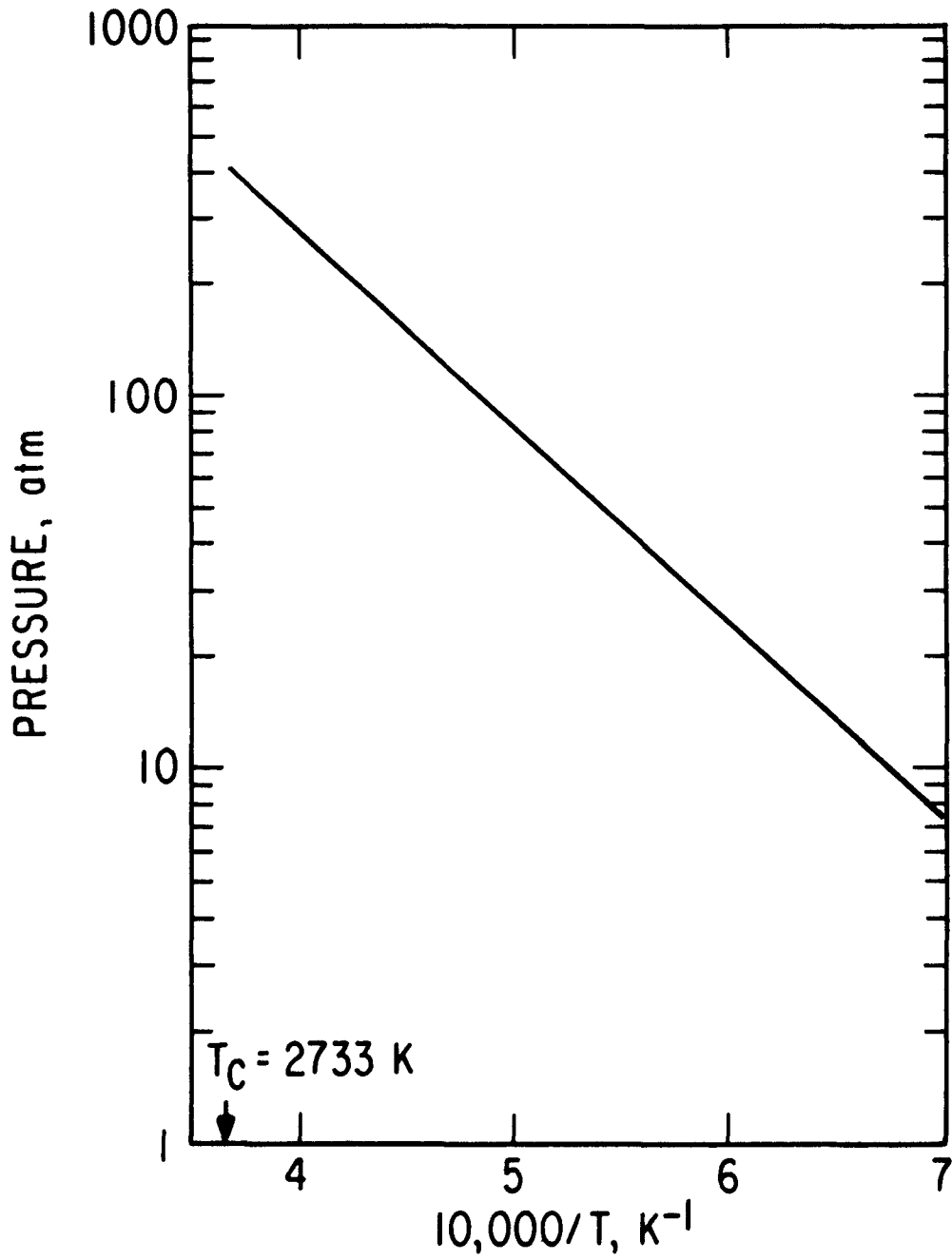
Coolant

Sodium

Saturated Vapor
Pressure

(3303)

Date: 1/76



SATURATED VAPOR PRESSURE OF SODIUM

FUNCTIONMATERIALPROPERTY

Coolant

Sodium

Saturated Vapor Pressure (3303)

Date: 1/76

Data Source

The saturated vapor pressure values came from Reference 1.

Discussion

Golden and Tokar² made a critical analysis of experimental measurements and recommended the equation of Ditchburn and Gilmour³ below 1150K and that of Stone *et al.*⁴ up to 1370K. Padilla used an equation of the same form as Stone *et al.*⁴ to extrapolate vapor pressures to a critical temperature of 2733K and critical pressure of 408 atm (values of Miller *et al.*⁵) while insuring continuity with the lower temperature values. Padilla¹ gives the pertinent equations in English units; Foust⁶ has converted the equations of Refs. 3 and 4 to SI units. These are given below (T in K).

$$\log p(\text{atm}) = 6.354 - \frac{5567}{T} - 0.5 \log T \quad (1)$$

$$T \leq 1150\text{K}$$

$$\log p(\text{atm}) = 6.6808 - \frac{5544.41}{T} - 0.16344 \log T \quad (2)$$

$$1150\text{K} < T \leq 1370\text{K}$$

Padilla's extrapolation equation¹ when converted to SI units, becomes:

$$\log p(\text{atm}) = 1.56182 - \frac{4543.48}{T} + 0.789 \log T \quad (3)$$

$$1370\text{K} \leq T$$

The effect of various estimates of the critical parameters on the vapor pressure extrapolations at high temperatures is shown by Gabelnick.⁷ Current work underway under Bonilla at Columbia University⁸ may provide experimental vapor pressure data up to the critical temperature.

References

1. A. Padilla, "High Temperature Thermodynamic Properties of Sodium," ANL-8095, 1974.
2. G. H. Golden and J. V. Tokar, "Thermophysical Properties of Sodium," ANL-7323, 1967.
3. R. W. Ditchburn and J. C. Gilmour, *Rev. Mod. Phys.* 13, 310 (1941).
4. J. P. Stone, C. T. Ewing, J. R. Spann, E. W. Steinkuller, D. D. Williams, and R. R. Miller, "High Temperature Properties of Sodium," NRL Report 6241, September 24, 1965.

FUNCTION

Coolant

MATERIAL

Sodium

PROPERTY

Saturated Vapor Pressure (3303)

Date: 1/76

References

5. D. Miller, A. B. Cohen, and C. E. Dickerman, "Estimation of Vapor and Liquid Density and Heat of Vaporization of the Alkali Metals to the Critical Point," International Conference on the Safety of Fast Breeder Reactors, Aix-en-Provence, France, September 19-22, 1967.
6. O. J. Foust, Editor, "Sodium-NaK Engineering Handbook Volume 1," Gordon and Breach, New York, 1972.
7. M. G. Chasanov, D. F. Fischer, D. R. Fredrickson, S. D. Gabelnick, R. Kumar, L. Leibowitz, G. T. Reedy, F. A. Cafasso, and L. Burris, "Chemical Engineering Division, Reactor Safety and Physical Property Studies Annual Report, July 1973 - June 1974," ANL-8120.
8. C. F. Bonilla, private communication.

FUNCTIONMATERIALPROPERTY

Coolant

Sodium

Density

(3304)

Date: 1/76

T(K)	ρ_{liquid} (g/cm ³)	ρ_{vapor} (g/cm ³)
400	0.9207	0.00000
500	0.8973	0.00000
600	0.8736	0.00000
700	0.8474	0.00000
800	0.8258	0.00000
900	0.8017	0.00002
1000	0.7775	0.00006
1100	0.7533	0.00017
1200	0.7291	0.00039
1300	0.7048	0.00079
1400	0.6807	0.00145
1500	0.6566	0.00244
1600	0.6327	0.00387
1700	0.6087	0.00584
1800	0.5839	0.00850
1900	0.5579	0.01197
2000	0.5307	0.01642
2100	0.5018	0.02204
2200	0.4710	0.02909
2300	0.4377	0.03794
2400	0.4011	0.04914
2500	0.3595	0.06373
2600	0.3096	0.08402
2700	0.2381	0.1200
2733 (critical temperature)	0.1818	0.1818

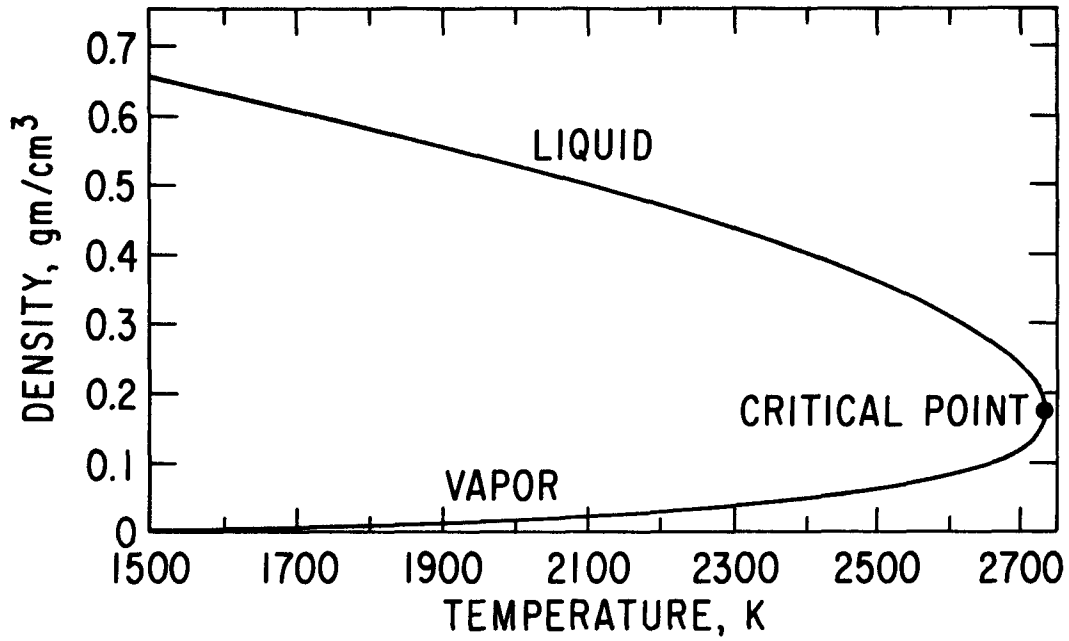
FUNCTION
Coolant

MATERIAL
Sodium

PROPERTY
Density

(3304)

Date: 1/76



DENSITY OF SATURATED SODIUM

FUNCTION
Coolant

MATERIAL
Sodium

PROPERTY
Density

(3304)

Date: 1/76

Data Source

The values for density came from Reference 1.

Discussion

The density of liquid sodium up to 1643K is represented by the density equation of Stone et al.;² in metric units their equation is:³

$$\rho(\text{g/cm}^3) = 0.9501 - 2.2976 \times 10^{-4}(T - 273.15) - 1.460 \times 10^{-8}(T - 273.15)^2 + 5.638 \times 10^{-12}(T - 273.15)^3 \quad (1)$$

where T is in K. Above these temperatures Padilla¹ used a form of equation recommended by Miller et al.⁴ to estimate liquid densities up to the critical point while insuring continuity with lower temperature data (T_c is critical temperature 2733K); T in Kelvin

$$\frac{\rho_{\text{liq}}}{\rho_c} = 1 + 4.163 \left(1 - \frac{T}{T_c}\right)^{0.5885} \quad (2)$$

The vapor densities were obtained via the Clapeyron equation:

$$\rho_{\text{vap}} = \left(\frac{\Delta H_{\text{vap}}}{T \left(\frac{dP}{dT} \right)_{\text{sat}}} + \frac{1}{\rho_{\text{liq}}} \right)^{-1} \quad (3)$$

where the heat of vaporization (ΔH_{vap}), slope of the saturation line $\left(\frac{dP}{dT} \right)_{\text{sat}}$, and liquid density (ρ_{liq}) are those presented previously.

As would be expected, the choice of the critical parameters (Padilla¹ used Miller et al.⁴ values) has a marked effect on the calculated densities. Gabelnick⁵ has discussed this; until more experimental data become available, Padilla's¹ values should be used.

References

1. A. Padilla, "High Temperature Thermodynamic Properties of Sodium," ANL-8095, 1974.
2. J. P. Stone, C. T. Ewing, J. R. Spann, E. W. Steinkuller, D. D. Williams, and R. R. Miller, "High Temperature Properties of Sodium," NRL Report 6241, September 24, 1965.

FUNCTION

Coolant

MATERIAL

Sodium

PROPERTY

Density

(3304)

Date: 1/76

References

3. O. J. Foust, Editor, "Sodium-NaK Engineering Handbook, Volume 1," Gordon and Breach, 1972.
4. D. Miller, A. B. Cohen, and C. E. Dickerman, "Estimation of Vapor and Liquid Density and Heat of Vaporization of the Alkali Metals to the Critical Point," International Conference on the Safety of Fast Breeder Reactors, Aix-en-Provence, France, September 19-22, 1967.
5. M. G. Chasanov, D. F. Fischer, D. R. Fredrickson, S. D. Gabelnick, R. Kumar, L. Leibowitz, G. T. Reedy, F. A. Cafasso, and L. Burris, "Chemical Engineering Division, Reactor Safety and Physical Property Studies Annual Report, July 1973 - June 1974," ANL-8120.

<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>	(3307)
Coolant	Sodium	Isothermal Compressibility	
Date: 1/76			
T(K)		$\beta_T(\text{atm}^{-1}) \times 10^5$	
400		1.954	
500		2.167	
600		2.409	
700		2.682	
800		2.991	
900		3.338	
1000		3.726	
1100		4.159	
1200		4.643	
1300		5.185	
1400		5.795	
1500		6.486	
1600		7.277	
1700		8.390	
1800		9.991	
1900		12.13	
2000		15.09	
2100		19.38	
2200		25.95	
2300		36.90	
2400		57.41	
2500		104.2	
2600		263.0	
2700		3128	

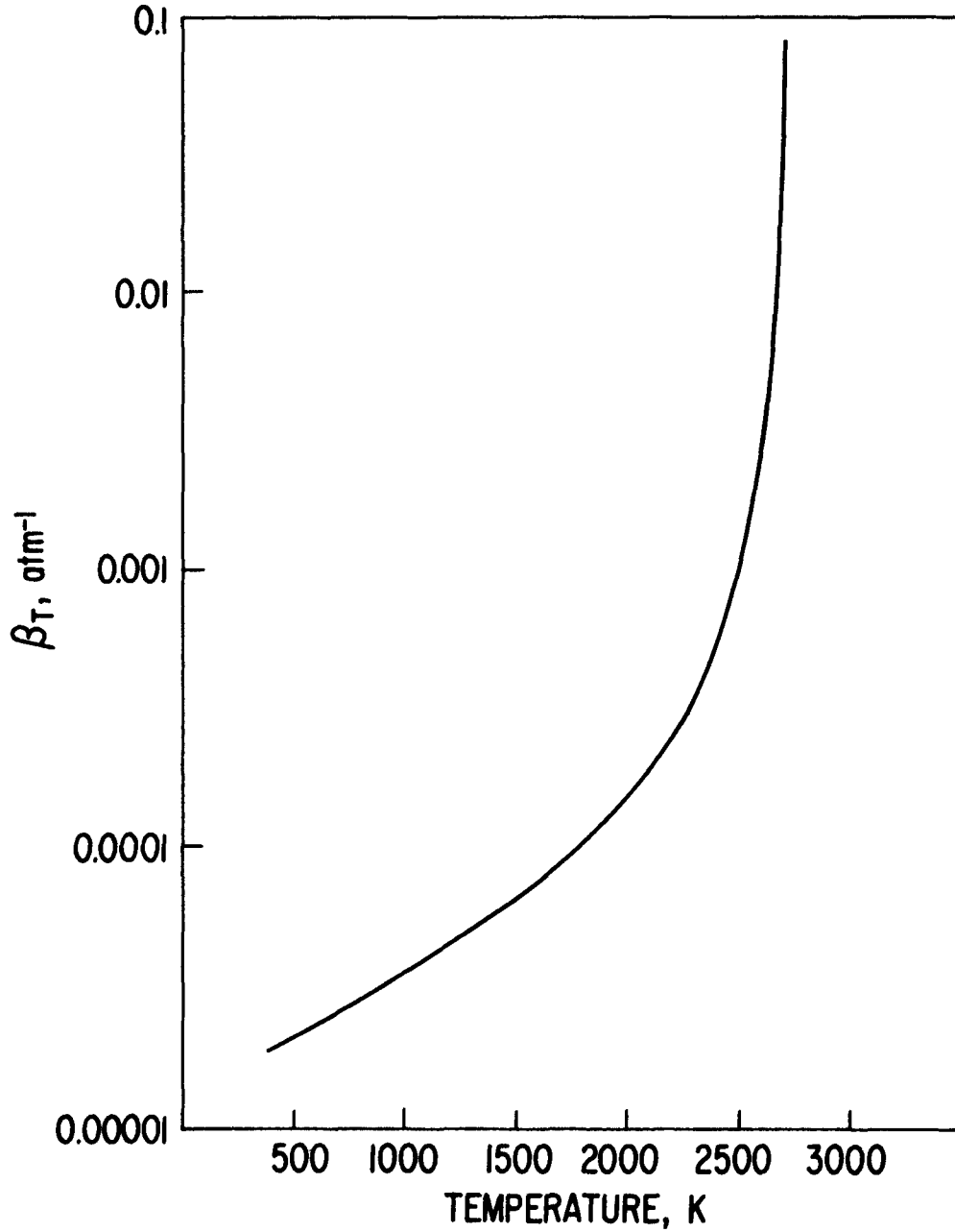
FUNCTION
Coolant

MATERIAL
Sodium

PROPERTY
Isothermal
Compressibility

(3307)

Date: 1/76



ISOTHERMAL COMPRESSIBILITY OF SATURATED SODIUM

FUNCTION

Coolant

MATERIAL

Sodium

PROPERTYIsothermal
Compressibility

(3307)

Date: 1/76

Data Source

The values for the isothermal compressibility of saturated sodium came from Reference 1.

Discussion

In Reference 1, Padilla used the sonic velocity data of Chasanov *et al.*² and saturated liquid sodium density to calculate the adiabatic compressibility, β_S , to 1773K. He then used a method proposed by Grosse³ to extrapolate β_S to higher temperatures. Sonic velocity data, thermal expansion along the saturated-liquid line, saturated density, and the slope of the vapor pressure curve were then employed using an equation from Rowlinson⁴ to obtain the values of isothermal compressibility. This method produces some minor inconsistencies near the critical point and Padilla¹ recommends use of his values only up to within 100K of the critical point.

Of course, the values of isothermal compressibility so obtained are very dependent on estimates of the critical parameters; Gabelnick⁵ has discussed the effect of different choices of critical parameters on β_T . However, until more experimental data become available, the β_T values of Padilla are recommended.

References

1. A. Padilla, "High Temperature Thermodynamic Properties of Sodium," ANL-8095, 1974.
2. M. G. Chasanov, L. Leibowitz, D. F. Fischer, and R. A. Blomquist, J. Appl. Phys. 43, 748 (1972).
3. A. V. Grosse, "Compressibility of Liquid Metals, Particularly Lead, from their Melting Points to their Critical Regions," GL-1970-14, Germantown Laboratories, 1970.
4. J. S. Rowlinson, "Liquids and Liquid Mixtures," 2nd Ed., Plenum Press, New York, 1969.
5. M. G. Chasanov, D. F. Fischer, D. R. Fredrickson, S. D. Gabelnick, R. Kumar, L. Leibowitz, G. T. Reedy, F. A. Cafasso, and L. Burris, "Chemical Engineering Division, Reactor Safety and Physical Property Studies Annual Report, July 1973 - June 1974," ANL-8120.

STRUCTURAL MATERIAL

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
See Below

Date: 1/1976

Melting Point (3103)	1700 K
Heat of Fusion (3104)	3540 cal/mol
Boiling Point (3105)	3080 K
Heat of Vaporization (3106)	98020 cal/mol

	<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Date: 1/1976	Structural	Stainless Steel (Type 304)	Melting Point (3103)

Data Source

References 1 and 2, respectively, give melting ranges of 1673-1723 K and 1670-1730 K.

Data Analysis

Median of the melting range was taken as the melting point.

References

1. A. D. Feith, R. A. Hein, C. P. Johnstone, and P. N. Flagella, "Thermophysical Properties of Low Carbon 304 Stainless Steel to 1350 C," GEMP-643, 1968.
2. T. S. Touloukian, "Recommended Values of the Thermophysical Properties of Eight Alloys, Major Constituents and Their Oxides," NASA-CR-71699, February 1966.

	<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Date: 1/1976	Structural	Stainless Steel (Type 304)	Heat of Fusion (3104)

Data Source

Heat of fusion data for the constituting elements were provided by Reference 1.

Data Analysis

The additivity rule was used in estimation.

Discussion

The use of the additivity rule was based on the ideal solution behavior of liquid Fe-Cr-Ni alloys (Reference 2). In estimating heat of fusion, 304 stainless steel was considered to be composed of 72% Fe, 19% Cr, and 9% Ni.

References

1. R. Hultgren, "Selected Values of Thermodynamic Properties of Metals and Alloys," John Wiley & Sons, N. Y., 1973.
2. G. R. Belton and R. J. Fruehan, "Mass-spectrometric Determination of Activities in Fe-Cr and Fe-Cr-Ni Alloys," Met. Trans., Vol. 1, 781-787, April 1970.

	<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Date:	Structural	Stainless Steel (Type 304)	Boiling Point (3105)
	1/1976		

Data Source

Boiling point was calculated from the vapor pressure data.

Data Analysis

None

Discussion

Temperature with vapor pressure 1 atm was taken as the boiling point.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Heat of Vaporization (3106)

Date: 1/1976

Data Source

Heat of vaporization data for the constituting elements were provided by Reference 1.

Data Analysis

The additivity rule was used in estimation.

Discussion

The use of the additivity rule was based on the ideal solution behavior of liquid Fe-Cr-Ni alloys (Reference 2). In estimating heat of vaporization, 304 stainless steel was considered to be composed of 72% Fe, 19% Cr, and 9% Ni.

References

1. R. Hultgren, "Selected Values of Thermodynamic Properties of Metals and Alloys," John Wiley & Sons, N. Y., 1973.
2. G. R. Belton and R. J. Fruehan, "Mass-spectrometric Determination of Activities in Fe-Cr and Fe-Cr-Ni Alloys," Met. Trans., Vol. 1, 781-787, April 1970.

FUNCTION MATERIAL PROPERTY
 Structural Stainless Steel Specific Heat (3108)
 Date: 1/1976 (Type 304)

Temperature (T) (K)	Specific Heat (c_p°) (cal/mol·K)
300	6.748
400	6.927
500	7.105
600	7.283
700	7.462
800	7.640
900	7.819
1000	7.997
1100	8.175
1200	8.354
1300	8.532
1400	8.711
1500	8.889
1600	9.067
1700	9.246
1700(ℓ)	10.52
1800	10.52
1900	10.52
2000	10.52
2100	10.52
2200	10.52
2300	10.52
2400	10.52
2500	10.52
2600	10.52
2700	10.52
2800	10.52
2900	10.52
3000	10.52

$$c_p^\circ = 6.213 + 1.784 \times 10^{-3} T \quad (\text{solid region})$$

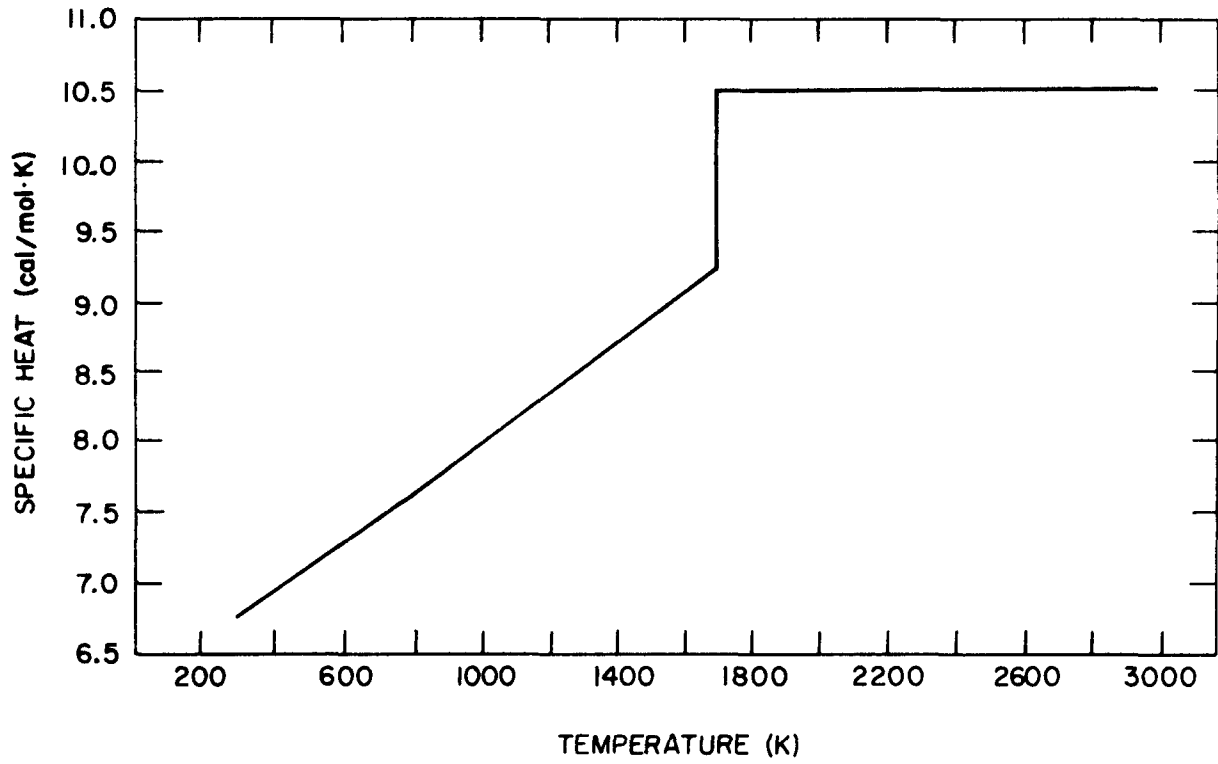
$$c_p^\circ = 10.52 \quad (\text{liquid region})$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Specific Heat (3108)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Specific Heat (3108)

Date: 1/1976

Data Source

Specific heat values were calculated from the enthalpy data.

Analysis

None

Discussion

Specific heat values were obtained by differentiating enthalpy data with respect to temperature.

References

None

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Enthalpy (3109)

Date: 1/1976

Temperature (T) (K)	Enthalpy ($H_T^\circ - H_{298}^\circ$) (cal/mol)
300	12.18
400	695.9
500	1398
600	2117
700	2854
800	3609
900	4382
1000	5174
1100	5982
1200	6808
1300	7652
1400	8515
1500	9395
1600	10290
1700	11210
1700(x)	14750
1800	15800
1900	16850
2000	17910
2100	18960
2200	20010
2300	21060
2400	22110
2500	23170
2600	24220
2700	25270
2800	26320
2900	27370
3000	28430

$$H_T^\circ - H_{298}^\circ = 6.213 T + 8.920 \times 10^{-4} T^2 - 1932 \quad (\text{solid region})$$

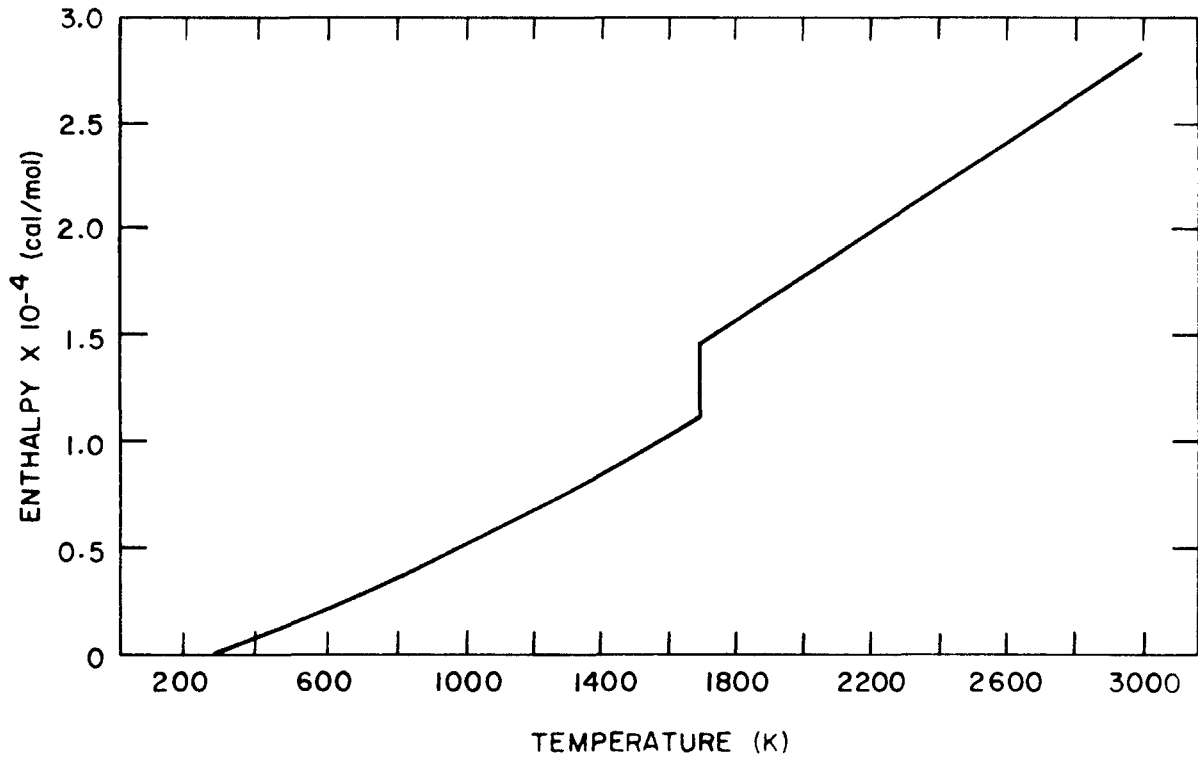
$$H_T^\circ - H_{298}^\circ = 10.52 T - 3134 \quad (\text{liquid region})$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Enthalpy (3109)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Enthalpy (3109)

Date: 1/1976

Data Source

Reference 1 provided enthalpy values in the solid region. Enthalpy data used in the estimation of liquid enthalpy were taken from Reference 2.

Data Analysis

A smooth curve was drawn through the experimental data points and extrapolated to the melting point. Enthalpy in the liquid region was estimated by the additivity rule.

Discussion

The experimental data for enthalpy of 304L stainless steel were taken instead of those of 304 stainless steel. This is because the carbon content of the stainless steel used in the nuclear reactors is 0.05% or less, which is rather closer to that of 304L stainless steel. In estimating liquid enthalpy by the additivity rule, 304 stainless steel was considered to be composed of 72% Fe, 19% Cr, and 9% Ni. The use of the additivity rule was based on the ideal solution behavior of liquid Fe-Cr-Ni alloys reported in Reference 3.

References

1. A. D. Feith, R. A. Hein, C. P. Johnstone, and P. N. Flagella, "Thermophysical Properties of Low Carbon 304 Stainless Steel to 1350 C," GEMP-643, 1968.
2. R. Hultgren, "Selected Values of Thermodynamic Properties of Metals and Alloys," John Wiley & Sons, N. Y., 1973.
3. G. R. Belton and R. J. Fruehan, "Mass-spectrometric Determination of Activities in Fe-Cr and Fe-Cr-Ni Alloys," Met. Trans., Vol. 1, 781-787, April 1970.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Thermal Diffusivity (3110)

Date: 1/1976

Temperature (T) (K)	Thermal Diffusivity (a) $\times 10^2$ (cm ² /sec)
300	3.237
400	3.546
500	3.849
600	4.148
700	4.440
800	4.727
900	5.009
1000	5.285
1100	5.555
1200	5.820
1300	6.080
1400	6.334
1500	6.582
1600	6.852
1700	7.062
1700(x)	3.237
1800	3.323
1900	3.413
2000	3.508
2100	3.608
2200	3.713
2300	3.822
2400	3.936
2500	4.055
2600	4.179
2700	4.307
2800	4.441
2900	4.579
3000	4.721

$$a = 2.276 \times 10^{-2} + 3.285 \times 10^{-5} T - 2.762 \times 10^{-9} T^2 \quad (\text{solid region})$$

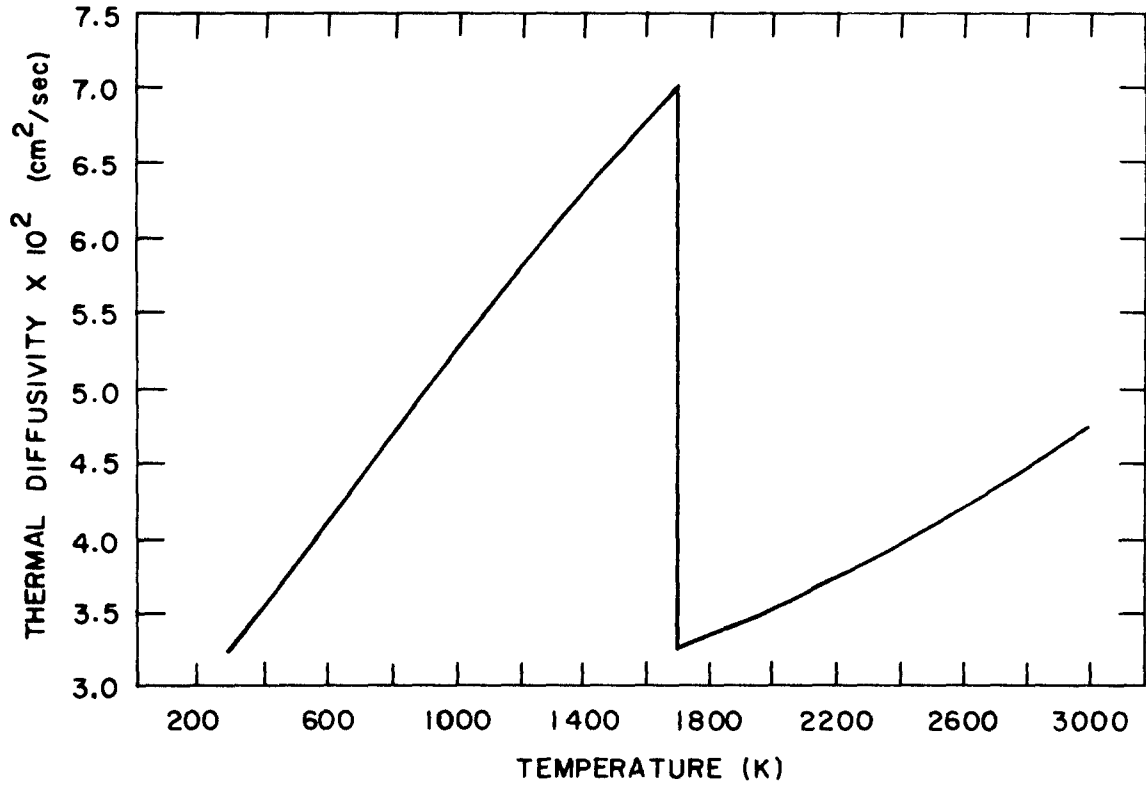
$$a = 2.514 \times 10^{-2} + 1.996 \times 10^{-7} T + 2.386 \times 10^{-9} T^2 \quad (\text{liquid region})$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Thermal Diffusivity (3110)

Date: 1/1976



	<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Date:	Structural 1/1976	Stainless Steel (Type 304)	Thermal Diffusivity (3110)

Data Source

Thermal diffusivity values were calculated from the thermal conductivity, density, and specific heat data.

Data Analysis

None

Discussion

Thermal diffusivity was calculated by its definition:

$$\text{thermal diffusivity} = \frac{\text{thermal conductivity}}{\text{density} \times \text{specific heat}}$$

References

None

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Thermal Conductivity (3112)

Date: 1/1976

Temperature (T) (K)	Thermal Conductivity (k) x10 (watt/cm·K)
300	1.297
400	1.459
500	1.620
600	1.782
700	1.944
800	2.106
900	2.267
1000	2.429
1100	2.591
1200	2.753
1300	2.914
1400	3.076
1500	3.238
1600	3.400
1700	3.561
1700(ℓ)	1.781
1800	1.814
1900	1.846
2000	1.879
2100	1.911
2200	1.944
2300	1.976
2400	2.009
2500	2.041
2600	2.073
2700	2.106
2800	2.138
2900	2.171
3000	2.203

$$k = 8.116 \times 10^{-2} + 1.618 \times 10^{-4} T \quad (\text{solid region})$$

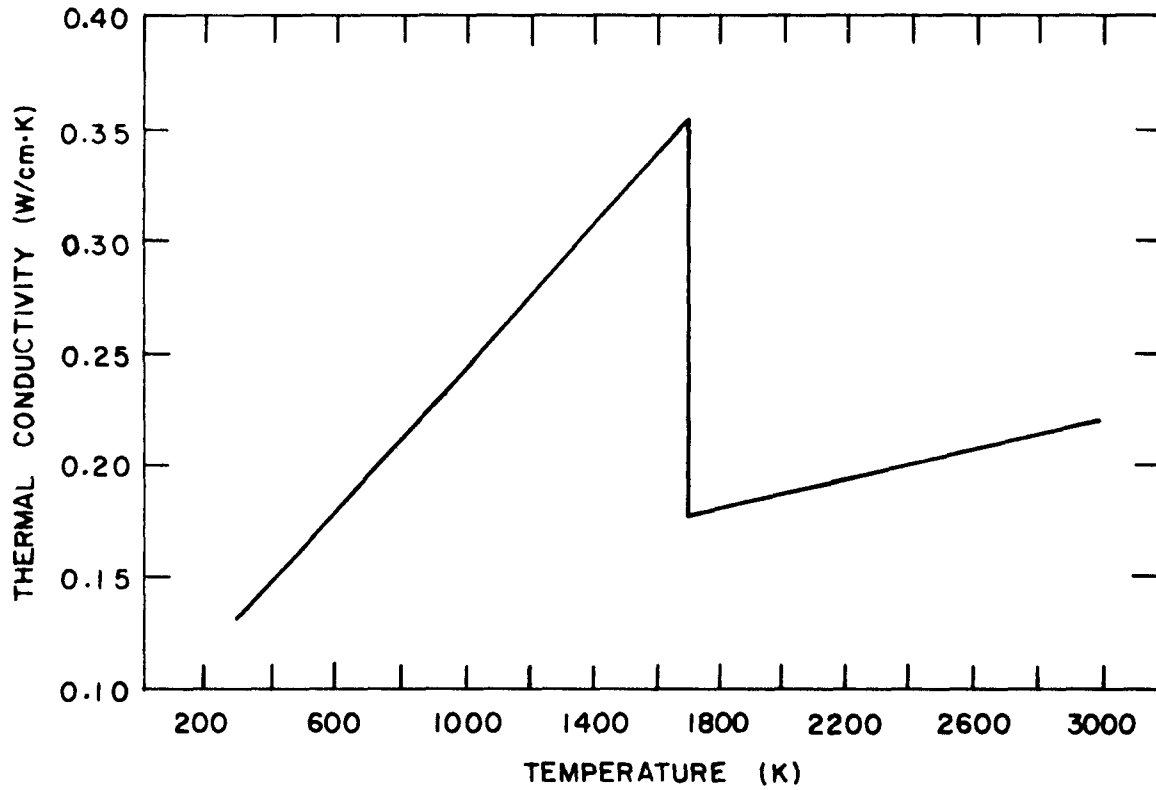
$$k = 1.229 \times 10^{-1} + 3.248 \times 10^{-5} T \quad (\text{liquid region})$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Thermal Conductivity (3112)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Thermal Conductivity (3112)

Date: 1/1976

Data Source

Reference 1 provided the thermal conductivity data to 1600 K. The correlations from Reference 2 were used to estimate liquid thermal conductivity values.

Data Analysis

A straight line was passed through the experimental data points and extended to the melting point. At the melting point, the thermal conductivity of solid stainless steel was divided by two to give the value for the liquid stainless steel. The thermal conductivities in the liquid region were calculated according to

$$k/k_m - 1 = 0.31 (T/T_m - 1)$$

where k = thermal conductivity at the temperature, T
 k_m = thermal conductivity at the melting temperature, T_m .

Discussion

Thermal conductivity data for 304L stainless steel were taken since the carbon content of 304 stainless steels used in nuclear reactors is 0.05% or less and rather closer to that of 304L stainless steel. Derivation of the correlations used in the estimation of liquid thermal conductivity is given in detail in Reference 2.

References

1. A. D. Feith, R. A. Hein, C. P. Johnstone, and P. N. Flagella, "Thermophysical Properties of Low Carbon 304 Stainless Steel to 1350 C," GEMP-643, 1968.
2. C. Kim, "Thermophysical Properties of Stainless Steels," ANL-75-55, September 1975.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Thermal Expansivity (3114)

Date: 1/1976

(a) solid region

Temperature (T) (K)	Thermal Expansivity (B) $\times 10^5$ (1/K)
400	1.469
500	1.524
600	1.581
700	1.638
800	1.693
900	1.759
1000	1.821
1100	1.885
1200	1.950
1300	2.017
1400	2.085
1500	2.154
1600	2.225
1700	2.298

$$B = 1.263 \times 10^{-5} + 4.854 \times 10^{-9} T + 7.238 \times 10^{-13} T^2$$

NOTE:

$$\text{Thermal Expansivity} = \frac{\text{length at } T - \text{length at } 298.15 \text{ K}}{\text{length at } 298.15 \text{ K} (T - 298.15 \text{ K})}$$

<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Structural	Stainless Steel (Type 304)	Thermal Expansivity (3114)

Date: 1/1976

(b) liquid region

Temperature (T) (K)	Thermal Expansivity (B) $\times 10^5$ (1/K)
1800	3.106
1900	3.207
2000	3.313
2100	3.424
2200	3.540
2300	3.662
2400	3.789
2500	3.921
2600	4.057
2700	4.200
2800	4.347
2900	4.499
3000	4.657

$$B = 2.168 \times 10^{-5} + 5.798 \times 10^{-10} T + 2.572 \times 10^{-12} T^2$$

NOTE:

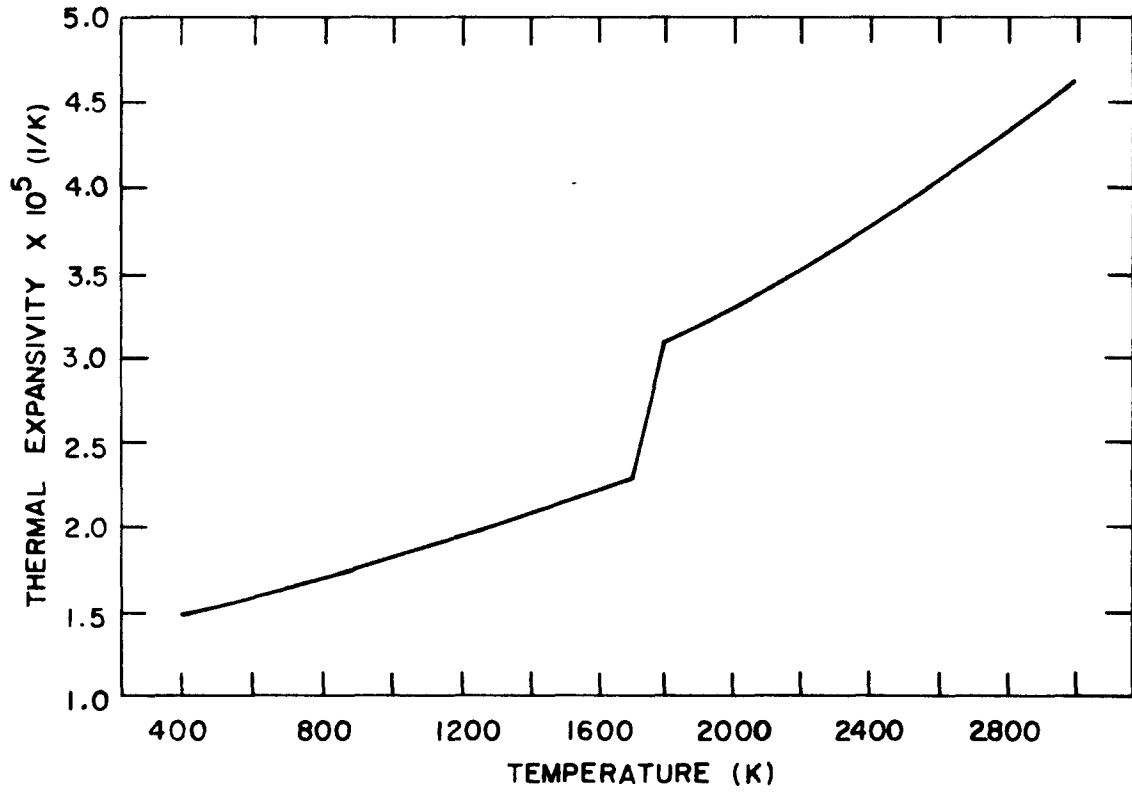
$$\text{Thermal Expansivity} = \frac{\text{length at } T - \text{length at } 1700 \text{ K}}{\text{length at } 1700 \text{ K} (T - 1700 \text{ K})}$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Thermal Expansivity (3114)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Thermal Expansivity (3114)

Date: 1/1976

Data Source

Linear thermal expansion coefficients were calculated from the density data.

Data Analysis

None

Discussion

None

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Viscosity (3301)

Date: 1/1976

Temperature (T) (K)	Viscosity (μ) (cP)
1700	6.416
1800	5.362
1900	4.566
2000	3.952
2100	3.467
2200	3.079
2300	2.762
2400	2.501
2500	2.282
2600	2.097
2700	1.939
2800	1.803
2900	1.685
3000	1.582

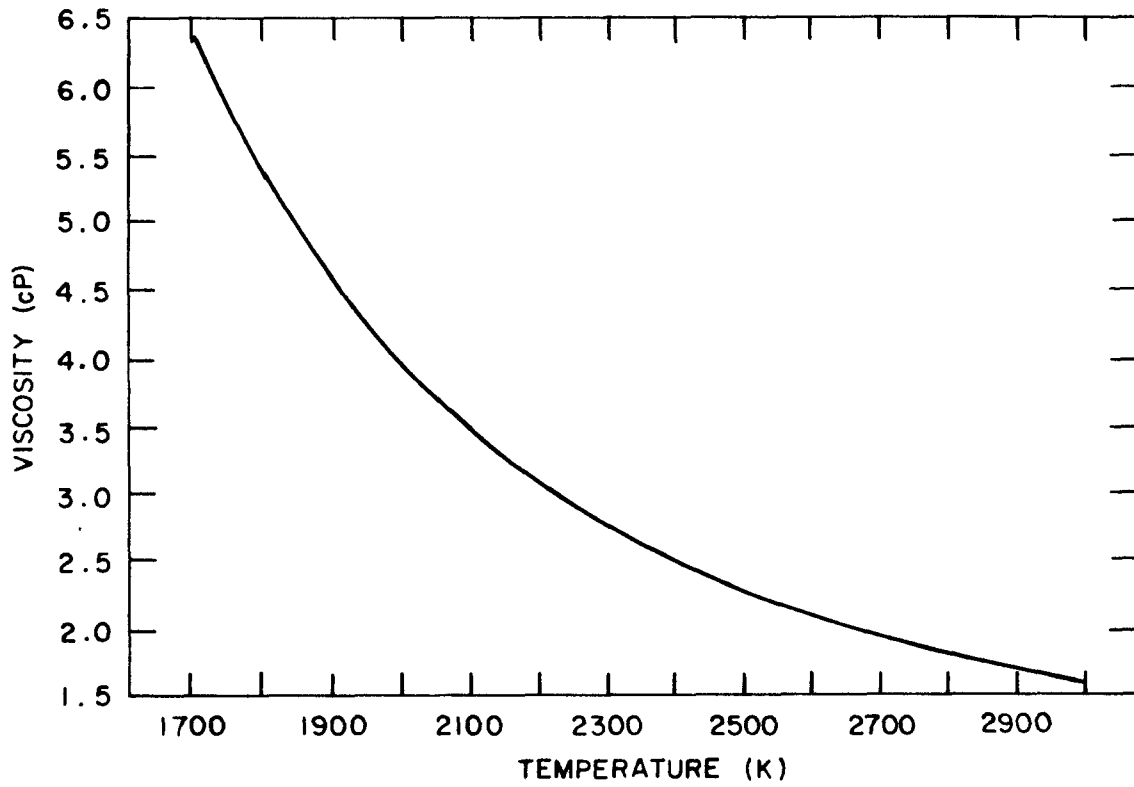
$$\log_{10}\mu = \frac{2385.2}{T} - 0.5958$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Viscosity (3301)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Viscosity (3301)

Date: 1/1976

Data Source

Reference 1 provided the viscosity data for iron to 2200 K.

Data Analysis

A smooth curve was drawn through the experimental data points and extrapolated to 3000 K by fitting those data into $(\log \mu)$ vs. $(1/T)$.

Discussion

These values may be used for the viscosity of stainless steel until the experimental viscosity data for stainless steel are available.

References

1. Y. S. Touloukian, "Recommended Values of the Thermophysical Properties of Eight Alloys, Major Constituents and Their Oxides," NASA-CR-71699, February 1966.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Vapor Pressure (3303)

Date: 1/1976

Temperature (T) (K)	Vapor Pressure (P) (atm)
1700	1.099×10^{-5}
1800	4.535×10^{-5}
1900	1.612×10^{-4}
2000	5.047×10^{-4}
2100	1.417×10^{-3}
2200	3.624×10^{-3}
2300	8.540×10^{-3}
2400	1.874×10^{-2}
2500	3.860×10^{-2}
2600	7.523×10^{-2}
2700	1.395×10^{-1}
2800	2.477×10^{-1}
2900	4.225×10^{-1}
3000	6.956×10^{-1}
3100	1.109
3200	1.717
3300	2.589

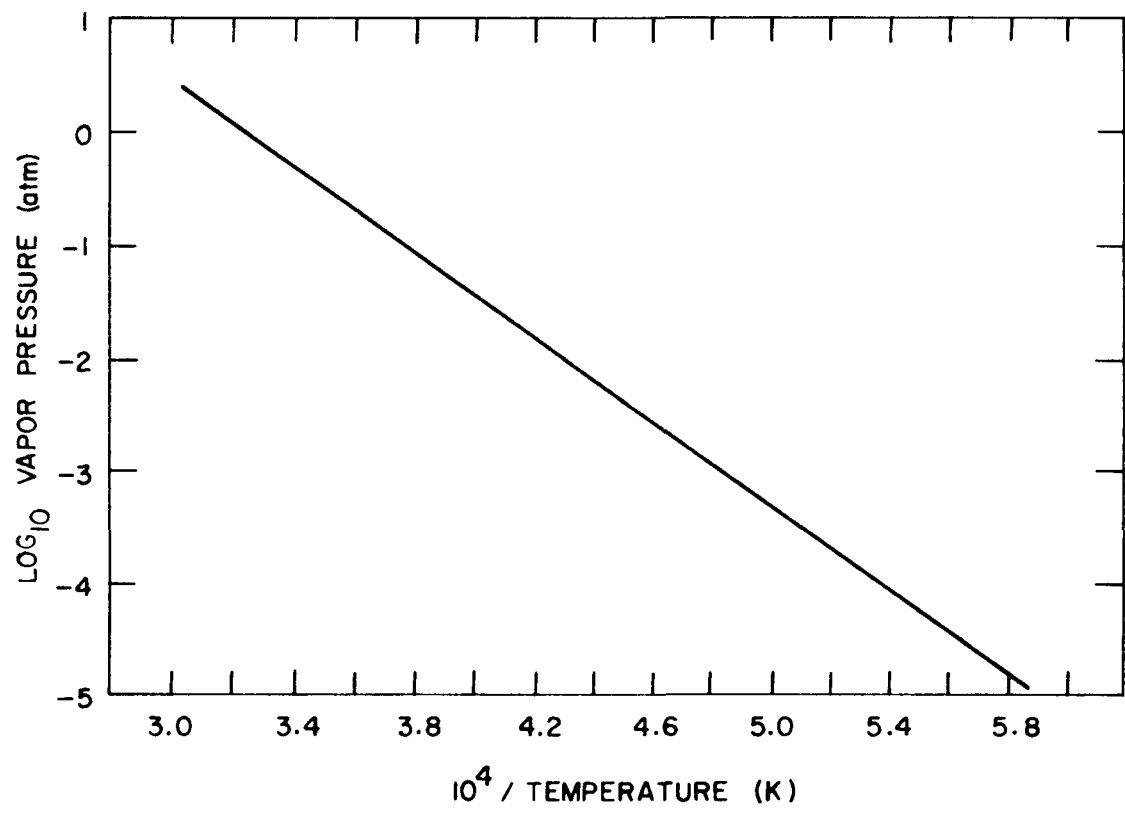
$$\log_{10} P = 6.1210 - \frac{18836}{T}$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Vapor Pressure (3303)

Date: 1/1976



<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Structural	Stainless Steel (Type 304)	Vapor Pressure (3303)

Date: 1/1976

Data Source

Vapor pressure data for the constituting elements were provided by Reference 1.

Data Analysis

The additivity rule was used in estimating the vapor pressure values.

Discussion

The use of additivity rule was based on the ideal solution model (Reference 2). In this estimation, Type 304 stainless steel was considered to be composed of 72% Fe, 19% Cr, and 9% Ni.

References

1. R. Hultgren, "Selected Values of Thermodynamic Properties of Metals and Alloys," John Wiley and Sons, N. Y., 1973.
2. G. R. Belton and R. J. Fruehan, "Mass-spectrometric Determination of Activities in Fe-Cr and Fe-Cr-Ni Alloys," Met. Trans., Vol. 1, 781-787, April 1970.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Density (3304)

Date: 1/1976

Temperature (T) (K)	Density (ρ) (g/cm ³)
300	7.894
400	7.860
500	7.823
600	7.783
700	7.742
800	7.698
900	7.652
1000	7.603
1100	7.552
1200	7.499
1300	7.444
1400	7.386
1500	7.326
1600	7.264
1700	7.199
1700(λ)	6.926
1800	6.862
1900	6.785
2000	6.725
2100	6.652
2200	6.576
2300	6.498
2400	6.416
2500	6.331
2600	6.243
2700	6.152
2800	6.058
2900	5.961
3000	5.861

$$\rho = 7.984 - 2.651 \times 10^{-4} T - 1.158 \times 10^{-7} T^2 \quad (\text{solid region})$$

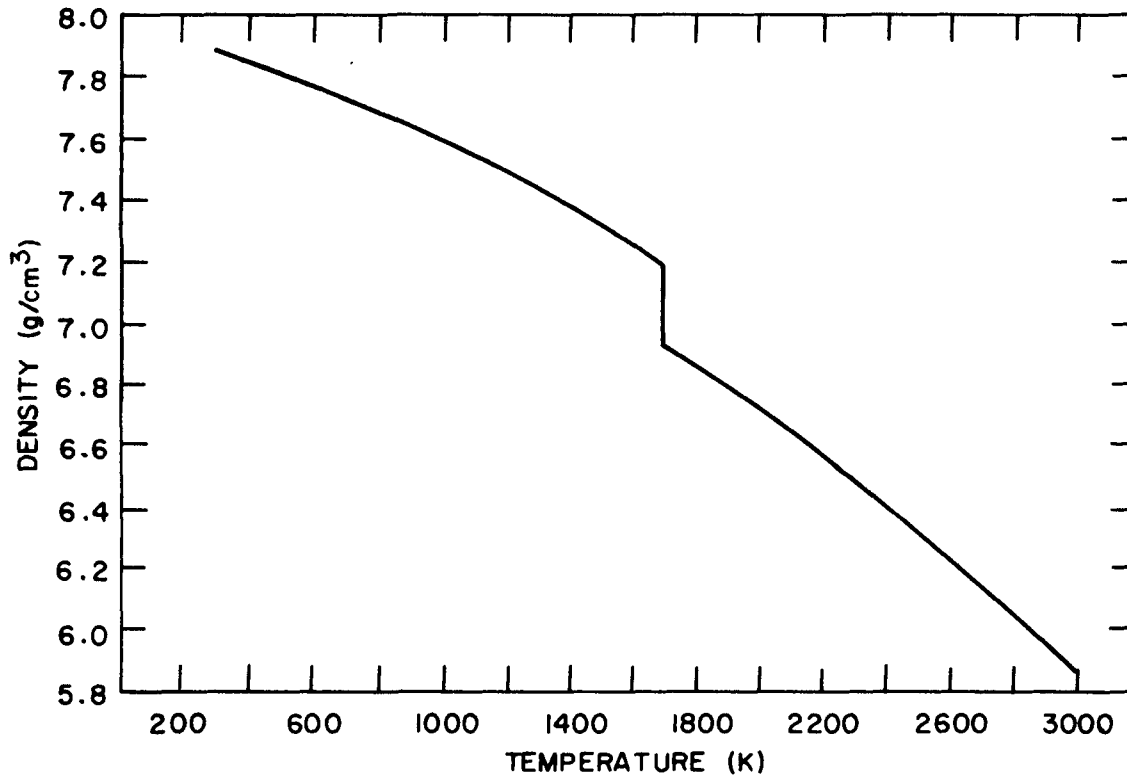
$$\rho = 7.551 - 1.117 \times 10^{-4} T - 1.506 \times 10^{-7} T^2 \quad (\text{liquid region})$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Density (3304)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 304)

PROPERTY
Density (3304)

Date: 1/1976

Data Source

Density data in the solid region were provided by Reference 1. Densities of the constituting elements used in the estimation of liquid density of 304 stainless steel were taken from Reference 2 and 3.

Data Analysis

A smooth curve was drawn through the experimental data and extrapolated to the melting point. In the estimation of liquid density, the following formula suggested by Reference 4 was used.

$$\rho = 1/\sum_i (x_i/\rho_i)$$

where ρ = density of stainless steel

x_i = weight fraction of the i^{th} constituent

ρ_i = density of the i^{th} constituent

Discussion

In the estimation of liquid density, 304 stainless steel was considered to be composed of 72% Fe, 19% Cr, and 9% Ni.

References

1. D. L. Thornburg, E. Thall, and J. Brous, WADD TR-60-325, 1961.
2. Y. S. Touloukian, "Recommended Values of the Thermophysical Properties of Eight Alloys, Major Constituents and Their Oxides," NASA-CR-71699, February 1966.
3. Y. S. Touloukian, editor, "Thermophysical Properties of High Temperature Solid Materials," Vol. 1 Elements, 1967.
4. F. C. Hull, "Estimating Alloy Densities," Metal Progress, Vol. 96, No. 5, 139-140, November 1969.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
See Below

Date: 1/1976

Melting Point (3103)	1700 K
Heat of Fusion (3104)	3610 cal/mol
Boiling Point (3105)	3090 K
Heat of Vaporization (3106)	99720 cal/mol

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Melting Point (3103)

Date: 1/1976

Data Source

Melting point of 304 stainless steel was taken.

Discussion

The melting points of 304 and 316 stainless steels were assumed same.

	<u>FUNCTION</u>	<u>MATERIAL</u>	<u>PROPERTY</u>
Date: 1/1976	Structural	Stainless Steel (Type 316)	Heat of Fusion (3104)

Data Source

Heat of fusion data for the constituting elements were provided by Reference 1.

Data Analysis

The additivity rule was used in estimation.

Discussion

The use of the additivity rule was based on the ideal solution behavior of liquid Fe-Cr-Ni alloys (Reference 2). In estimating heat of fusion, 316 stainless steel was considered to be composed of 69% Fe, 17% Cr, 12% Ni, and 2% Mo.

References

1. R. Hultgren, "Selected Values of Thermodynamic Properties of Metals and Alloys," John Wiley & Sons, N. Y., 1973.
2. G. R. Belton and R. J. Fruehan, "Mass-spectrometric Determination of Activities in Fe-Cr and Fe-Cr-Ni Alloys," Met. Trans., Vol. 1, 781-787, April 1970.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Boiling Point (3105)

Date: 1/1976

Data Source

Boiling point was calculated from the vapor pressure data.

Data Analysis

None

Discussion

Temperature with vapor pressure 1 atm was taken as the boiling point.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Heat of Vaporization (3106)

Date: 1/1976

Data Source

Heat of vaporization data for the constituting elements were provided by Reference 1.

Data Analysis

The additivity rule was used in estimation.

Discussion

The use of the additivity rule was based on the ideal solution behavior of liquid Fe-Cr-Ni alloys (Reference 2). In estimating heat of vaporization, 316 stainless steel was considered to be composed of 69% Fe, 17% Cr, 12% Ni, and 2% Mo.

References

1. R. Hultgren, "Selected Values of Thermodynamic Properties of Metals and Alloys," John Wiley & Sons, N. Y., 1973.
2. G. R. Belton and R. J. Fruehan, "Mass-spectrometric Determination of Activities in Fe-Cr and Fe-Cr-Ni Alloys," Met. Trans., Vol. 1, 781-787, April 1970.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Specific Heat (3108)

Date: 1/1976

Temperature (T) (K)	Specific Heat (c_p°) (cal/mol·K)
300	6.717
400	6.896
500	7.075
600	7.254
700	7.433
800	7.611
900	7.790
1000	7.969
1100	8.148
1200	8.327
1300	8.505
1400	8.684
1500	8.863
1600	9.042
1700	9.221
1700(x)	10.37
1800	10.37
1900	10.37
2000	10.37
2100	10.37
2200	10.37
2300	10.37
2400	10.37
2500	10.37
2600	10.37
2700	10.37
2800	10.37
2900	10.37
3000	10.37

$$c_p^\circ = 6.181 + 1.788 \times 10^{-3} T \quad (\text{solid region})$$

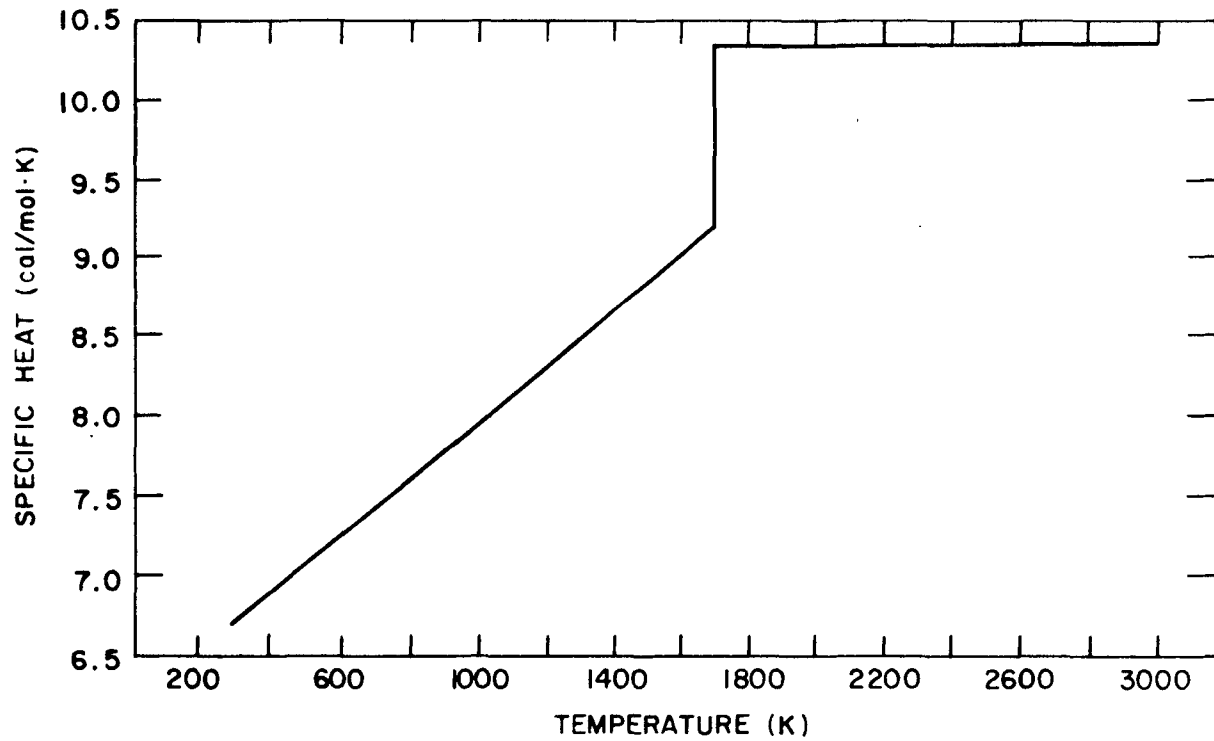
$$c_p^\circ = 10.37 \quad (\text{liquid region})$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Specific Heat (3108)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Specific Heat (3108)

Date: 1/1976

Data Source

Specific heat values were calculated from the enthalpy data.

Data Analysis

None

Discussion

Specific heat values were obtained by differentiating enthalpy data with respect to temperature.

References

None

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Enthalpy (3109)

Date: 1/1976

Temperature (T) (K)	Enthalpy ($H_T^\circ - H_{298}^\circ$) (cal/mol)
300	11.76
400	692.4
500	1391
600	2107
700	2841
800	3594
900	4364
1000	5152
1100	5958
1200	6782
1300	7623
1400	8483
1500	9360
1600	10260
1700	11170
1700(<i>l</i>)	14780
1800	15820
1900	16850
2000	17890
2100	18930
2200	19970
2300	21000
2400	22040
2500	23080
2600	24110
2700	25150
2800	26190
2900	27220
3000	28260

$$H_T^\circ - H_{298}^\circ = 6.181 T + 8.940 \times 10^{-4} T^2 - 1923 \quad (\text{solid region})$$

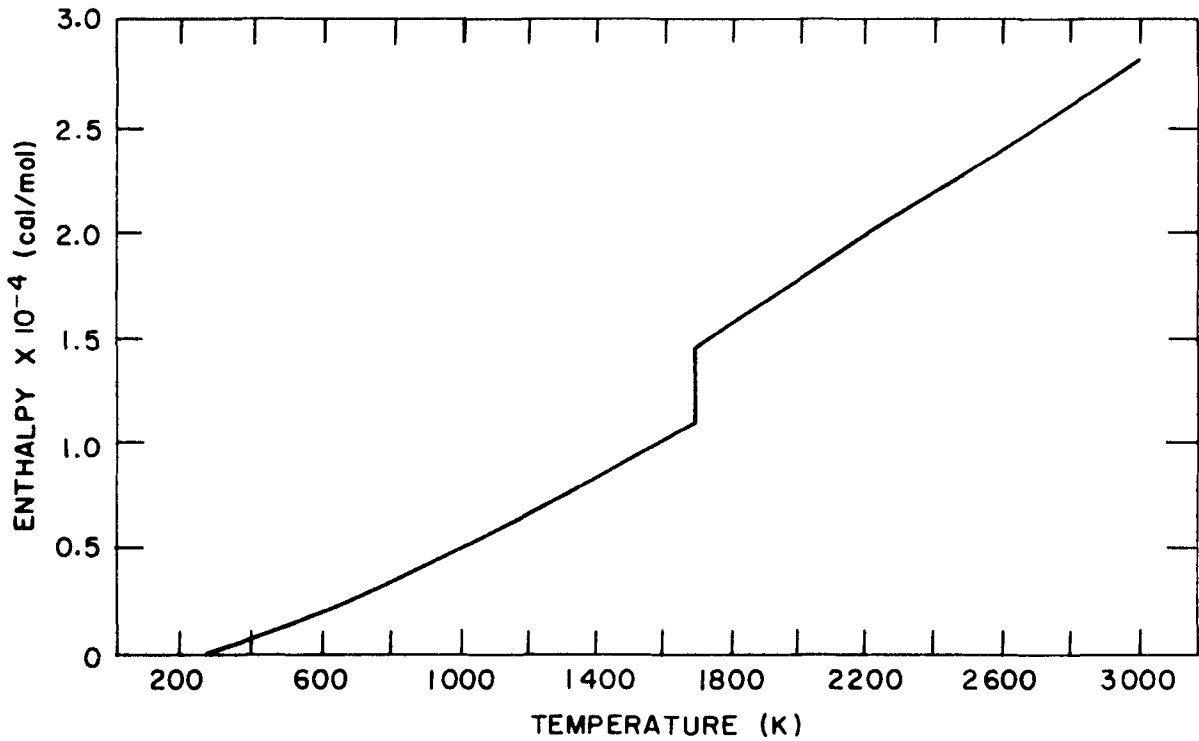
$$H_T^\circ - H_{298}^\circ = 10.37 T - 2849 \quad (\text{liquid region})$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Enthalpy (3109)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Enthalpy (3109)

Date: 1/1976

Data Source

Reference 1 provided enthalpy values in the solid region. Enthalpies of the constituting elements used in the estimation of liquid enthalpy were taken from Reference 2.

Data Analysis

A smooth curve was drawn through the experimental data and extrapolated to the melting point. Enthalpy in the liquid region was estimated by the additivity rule.

Discussion

The use of the additivity rule was based on the ideal solution behavior of liquid Fe-Cr-Ni alloys reported in Reference 3. In estimating liquid enthalpy, 316 stainless steel was considered to be composed of 69% Fe, 17% Cr, 12% Ni, and 2% Mo.

References

1. T. B. Douglas and A. C. Victor, "Physical Properties of High Temperature Materials, Part II," WADC-TR-57-374, August 1957.
2. R. Hultgren, "Selected Values of Thermodynamic Properties of Metals and Alloys," John Wiley & Sons, N. Y., 1973.
3. G. R. Belton and R. J. Fruehan, "Mass-spectrometric Determination of Activities in Fe-Cr and Fe-Cr-Ni Alloys", Met. Trans., Vol. 1, 781-787, April 1970.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Thermal Diffusivity (3110)

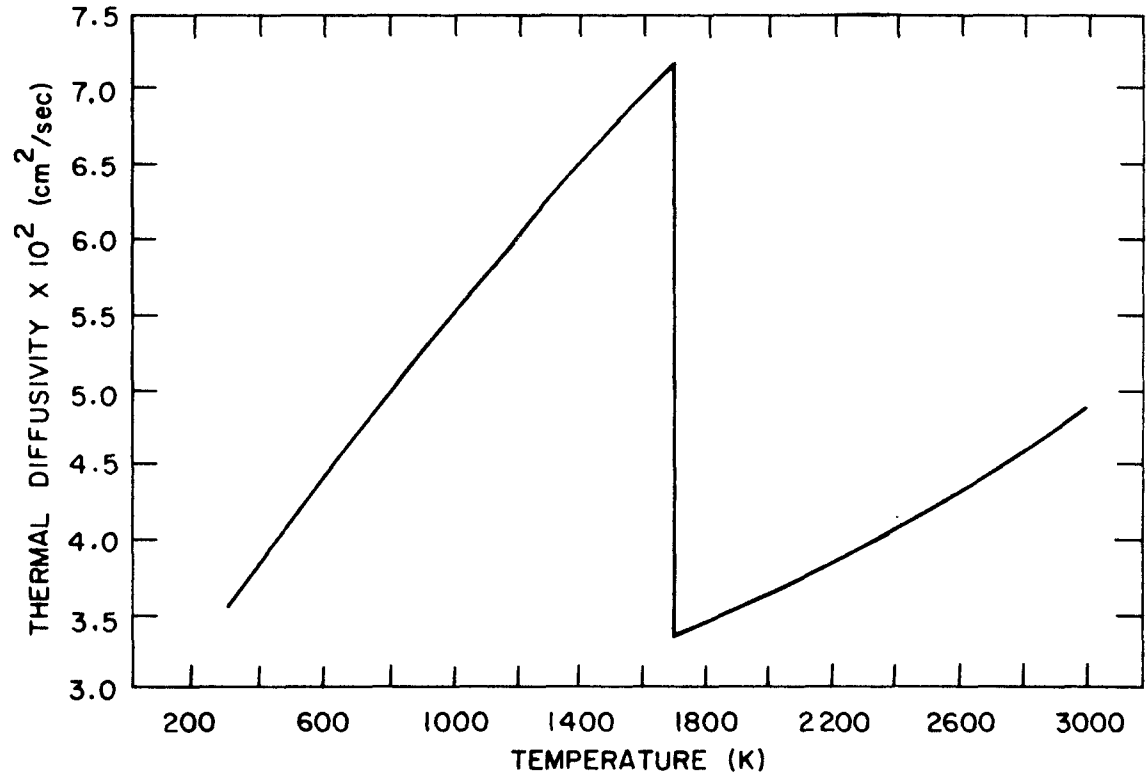
Date: 1/1976

Temperature (T) (K)	Thermal Diffusivity (a) $\times 10^2$ (cm ² /sec)
300	3.529
400	3.834
500	4.132
600	4.424
700	4.710
800	4.989
900	5.262
1000	5.529
1100	5.790
1200	6.044
1300	6.292
1400	6.534
1500	6.769
1600	6.999
1700	7.222
1700(ℓ)	3.350
1800	3.435
1900	3.526
2000	3.622
2100	3.723
2200	3.829
2300	3.940
2400	4.057
2500	4.178
2600	4.305
2700	4.437
2800	4.574
2900	4.716
3000	4.864

$$a = 2.578 \times 10^{-2} + 3.265 \times 10^{-5} T - 3.138 \times 10^{-9} T^2 \quad (\text{solid region})$$

$$a = 2.686 \times 10^{-2} - 4.812 \times 10^{-7} T + 2.580 \times 10^{-9} T^2 \quad (\text{liquid region})$$

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Thermal Diffusivity (3110)

Date: 1/1976

Data Source

Thermal diffusivity values were calculated from the thermal conductivity, density, and specific heat data.

Data Analysis

None

Discussion

Thermal diffusivity was calculated by its definition:

$$\text{thermal diffusivity} = \frac{\text{thermal conductivity}}{\text{density} \times \text{specific heat}}$$

References

None

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Thermal Conductivity (3112)

Date: 1/1976

Temperature (T) (K)	Thermal Conductivity (k) x10 (watt/cm·K)
300	1.396
400	1.553
500	1.710
600	1.868
700	2.025
800	2.182
900	2.339
1000	2.496
1100	2.653
1200	2.810
1300	2.967
1400	3.125
1500	3.282
1600	3.439
1700	3.596
1700(x)	1.798
1800	1.831
1900	1.864
2000	1.897
2100	1.930
2200	1.962
2300	1.995
2400	2.028
2500	2.061
2600	2.094
2700	2.126
2800	2.159
2900	2.192
3000	2.225

$$k = 9.248 \times 10^{-2} + 1.571 \times 10^{-4} T \quad (\text{solid region})$$

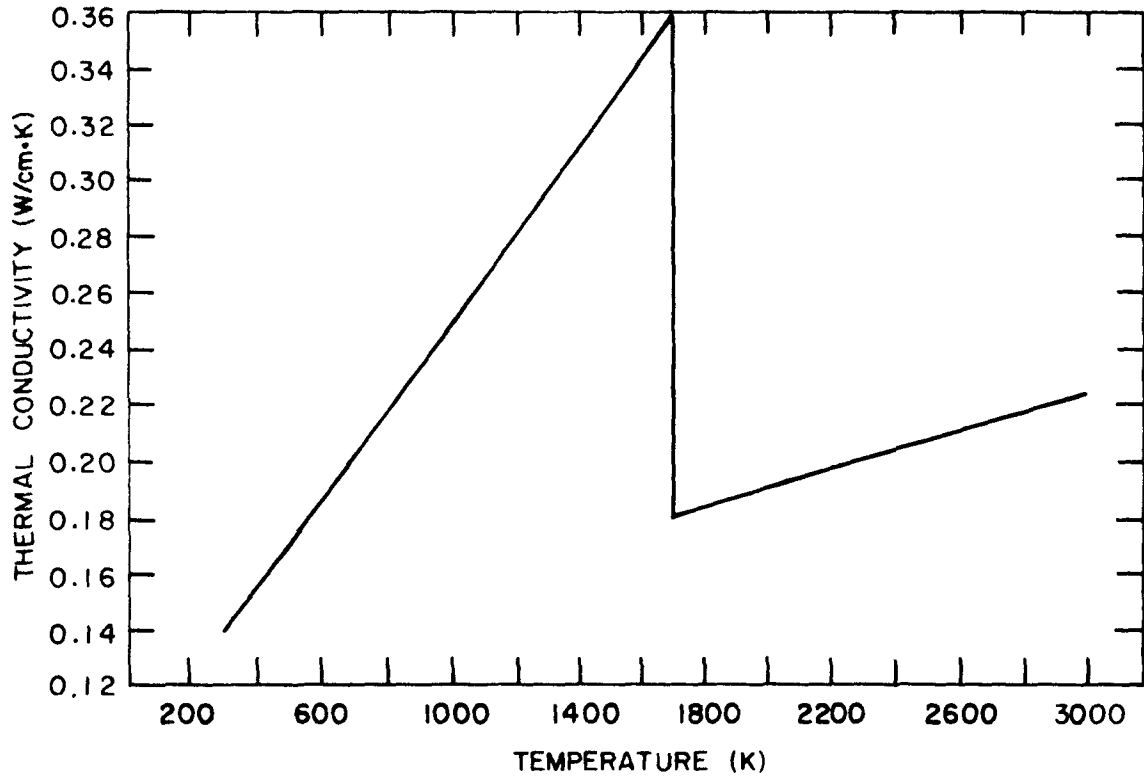
$$k = 1.241 \times 10^{-1} + 3.279 \times 10^{-5} T \quad (\text{liquid region})$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Thermal Conductivity (3112)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Thermal Conductivity (3112)

Date: 1/1976

Data Source

Reference 1 provided the thermal conductivity data to 1600 K. The correlations from Reference 2 were used to estimate liquid thermal conductivity values.

Data Analysis

A straight line was passed through the experimental data points and extended to the melting point. At the melting point, the thermal conductivity of solid stainless steel was divided by two to give the value for the liquid stainless steel. The thermal conductivities in the liquid region were calculated according to

$$k/k_m - 1 = 0.31 (T/T_m - 1)$$

where k = thermal conductivity at the temperature, T

k_m = thermal conductivity at the melting temperature, T_m

Discussion

Derivation of the correlations used in the estimation of liquid thermal conductivity values is given in Reference 2.

References

1. J. Matolich, Jr., "Thermal Conductivity and Electrical Resistivity of Type 316 Stainless Steel from 0 to 1800 F," NASA-CR-54151, 1965.
2. C. Kim, "Thermophysical Properties of Stainless Steels," ANL-75-55, September 1975.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Thermal Expansivity (3114)

Date: 1/1976

(a) solid region

Temperature (T) (K)	Thermal Expansivity (B) $\times 10^5$ (1/K)
400	1.890
500	1.917
600	1.944
700	1.973
800	2.001
900	2.031
1000	2.061
1100	2.092
1200	2.123
1300	2.156
1400	2.188
1500	2.222
1600	2.256
1700	2.291

$$B = 1.789 \times 10^{-5} + 2.398 \times 10^{-9} T + 3.269 \times 10^{-13} T^2$$

NOTE:

$$\text{Thermal Expansivity} = \frac{\text{length at } T - \text{length at } 298.15 \text{ K}}{\text{length at } 298.15 \text{ K} (T - 298.15 \text{ K})}$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Thermal Expansivity (3114)

Date: 1/1976

(b) liquid region

Temperature (T) (K)	Thermal Expansivity (B) $\times 10^5$ (1/K)
1800	2.852
1900	2.961
2000	3.076
2100	3.196
2200	3.321
2300	3.453
2400	3.590
2500	3.733
2600	3.881
2700	4.035
2800	4.195
2900	4.360
3000	4.531

$$B = 1.864 \times 10^{-5} + 3.917 \times 10^{-10} T + 2.833 \times 10^{-12} T^2$$

NOTE:

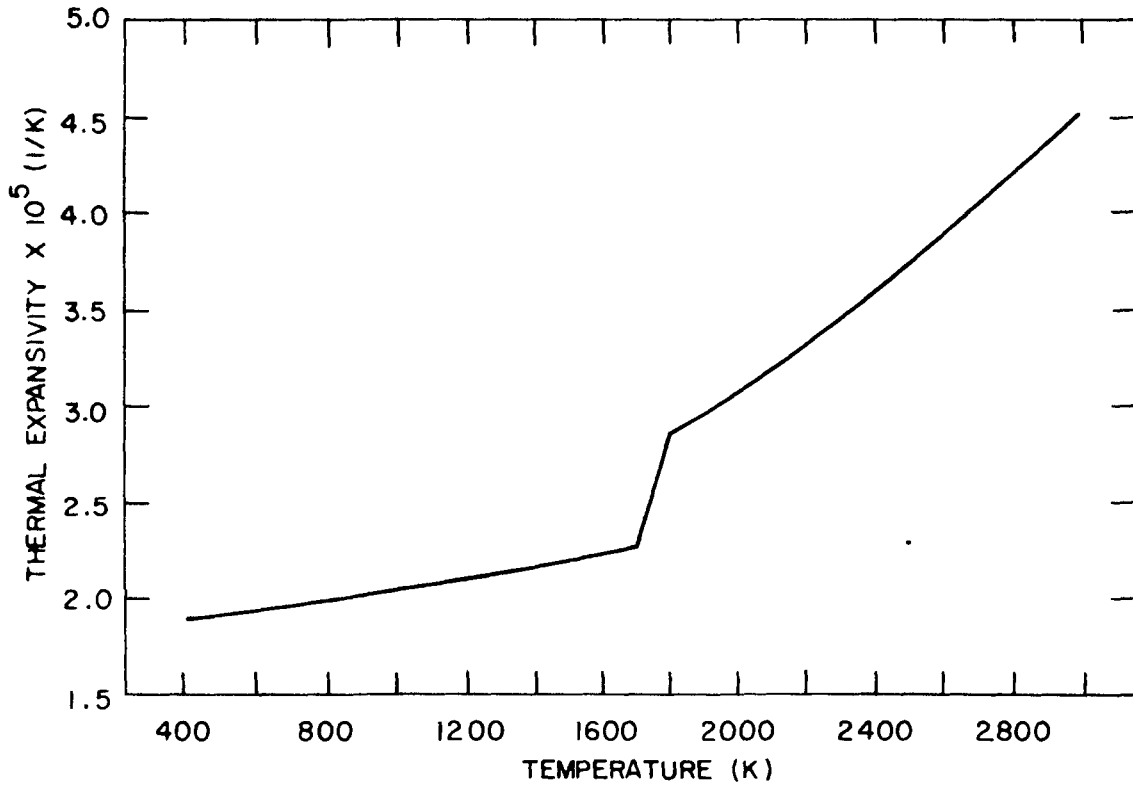
$$\text{Thermal Expansivity} = \frac{\text{length at } T - \text{length at } 1700 \text{ K}}{\text{length at } 1700 \text{ K} (T - 1700 \text{ K})}$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Thermal Expansivity (3114)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Thermal Expansivity (3114)

Date: 1/1976

Data Source

Linear thermal expansion coefficients were calculated from the density data.

Data Analysis

None

Discussion

None

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Viscosity (3301)

Date: 1/1976

Temperature (T) (K)	Viscosity (μ) (cP)
1700	6.416
1800	5.362
1900	4.566
2000	3.952
2100	3.467
2200	3.079
2300	2.762
2400	2.501
2500	2.282
2600	2.097
2700	1.939
2800	1.803
2900	1.685
3000	1.582

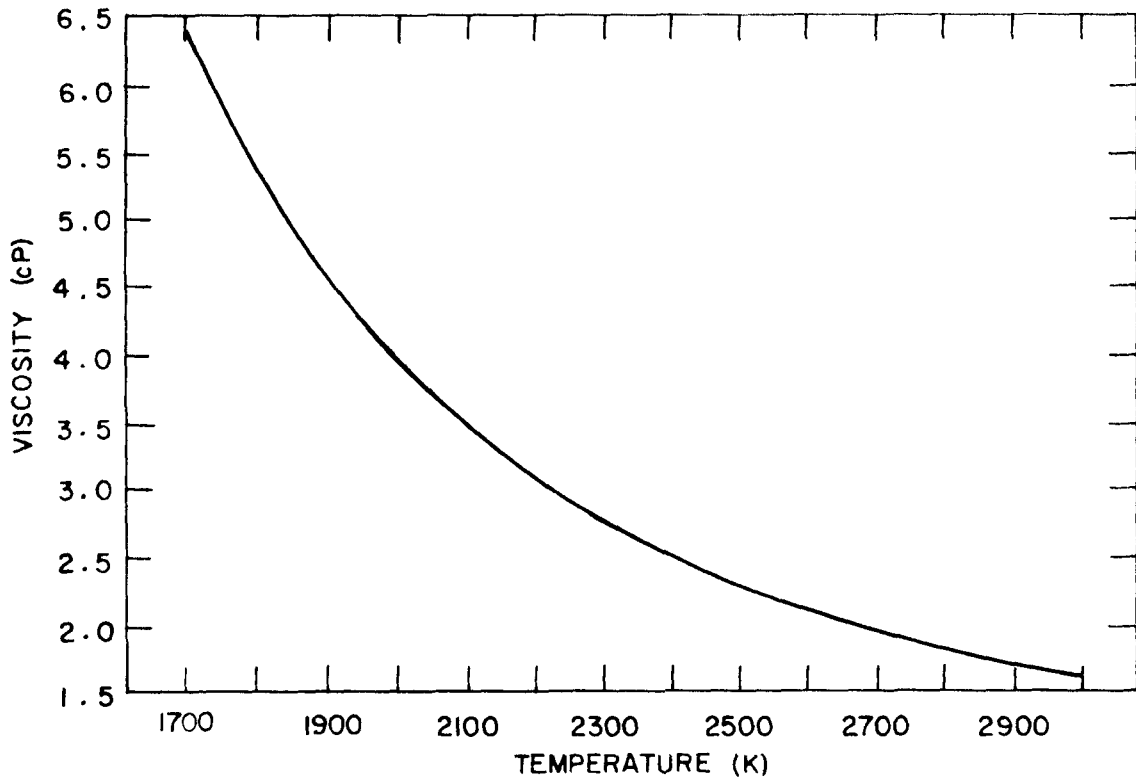
$$\log_{10}\mu = \frac{2385.2}{T} - 0.5958$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Viscosity (3301)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Viscosity (3301)

Date: 1/1976

Data Source

Reference 1 provided the viscosity data for iron to 2200 K.

Data Analysis

A smooth curve was drawn through the experimental data points and extrapolated to 3000 K by fitting those data into $(\log \mu)$ vs. $(1/T)$.

Discussion

These values may be used for the viscosity of stainless steel until the experimental viscosity data for stainless steel are available.

References

1. Y. S. Touloukian, "Recommended Values of the Thermophysical Properties of Eight Alloys, Major Constituents and Their Oxides," NASA-CR-71699, February 1966.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Vapor Pressure (3303)

Date: 1/1976

Temperature (T) (K)	Vapor Pressure (P) (atm)
1700	1.032×10^{-5}
1800	4.270×10^{-5}
1900	1.521×10^{-4}
2000	4.772×10^{-4}
2100	1.343×10^{-3}
2200	3.438×10^{-3}
2300	8.114×10^{-3}
2400	1.783×10^{-2}
2500	3.677×10^{-2}
2600	7.174×10^{-2}
2700	1.332×10^{-1}
2800	2.367×10^{-1}
2900	4.041×10^{-1}
3000	6.658×10^{-1}
3100	1.062
3200	1.646
3300	2.484

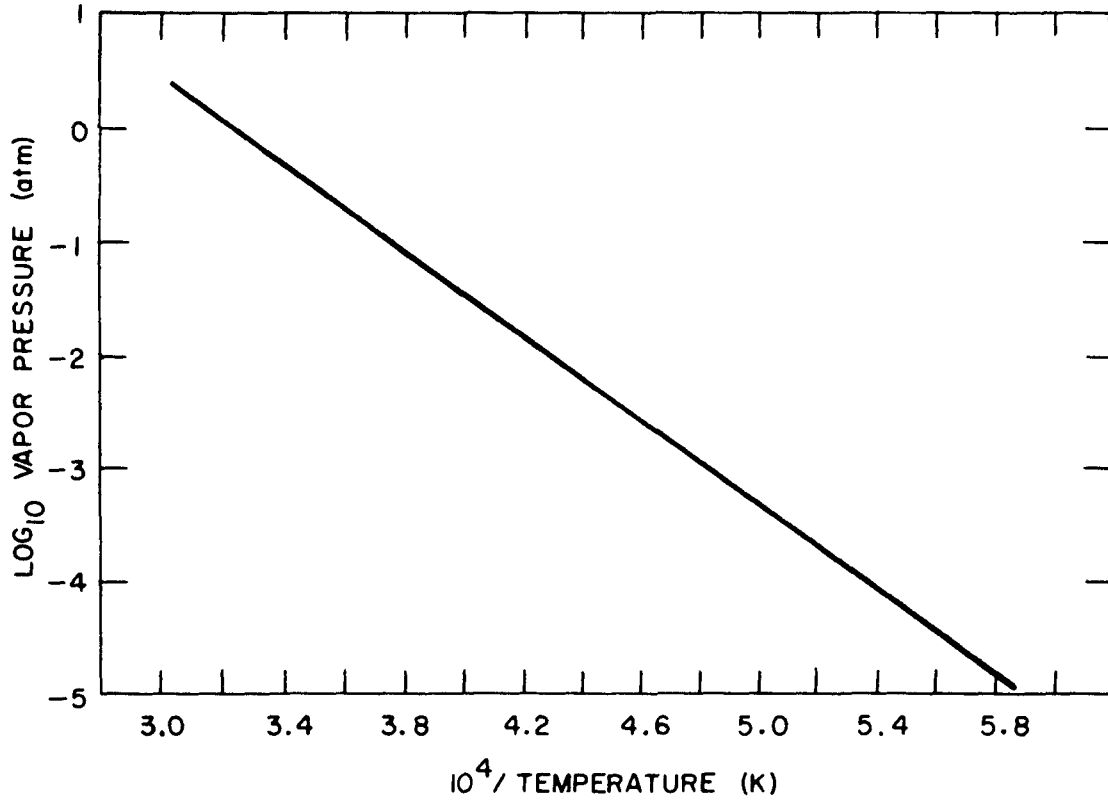
$$\log_{10} P = 6.1127 - \frac{18868}{T}$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Vapor Pressure (3303)

Date: 1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Vapor Pressure (3303)

Date: 1/1976

Data Source

Vapor pressure data for the constituting elements were provided by Reference 1.

Data Analysis

The additivity rule was used in estimating the vapor pressure values.

Discussion

The use of additivity rule was based on the ideal solution model (Reference 2). In this estimation, 316 stainless steel was considered to be composed of 69% Fe, 17% Cr, 12% Ni, and 2% Mo.

References

1. R. Hultgren, "Selected Values of Thermodynamic Properties of Metals and Alloys," John Wiley & Sons, N. Y., 1973.
2. G. R. Belton and R. J. Fruehan, "Mass-spectrometric Determination of Activities in Fe-Cr and Fe-Cr-Ni Alloys," Met. Trans., Vol. 1, 781-787, April 1970.

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Density (3304)

Date: 1/1976

Temperature (T) (K)	Density (ρ) (g/cm ³)
300	7.954
400	7.910
500	7.864
600	7.818
700	7.771
800	7.723
900	7.674
1000	7.624
1100	7.574
1200	7.523
1300	7.471
1400	7.419
1500	7.365
1600	7.311
1700	7.256
1700(l)	6.979
1800	6.920
1900	6.857
2000	6.791
2100	6.721
2200	6.648
2300	6.571
2400	6.490
2500	6.406
2600	6.318
2700	6.226
2800	6.131
2900	6.032
3000	5.930

$$\rho = 8.084 - 4.209 \times 10^{-4} T - 3.894 \times 10^{-8} T^2 \quad (\text{solid region})$$

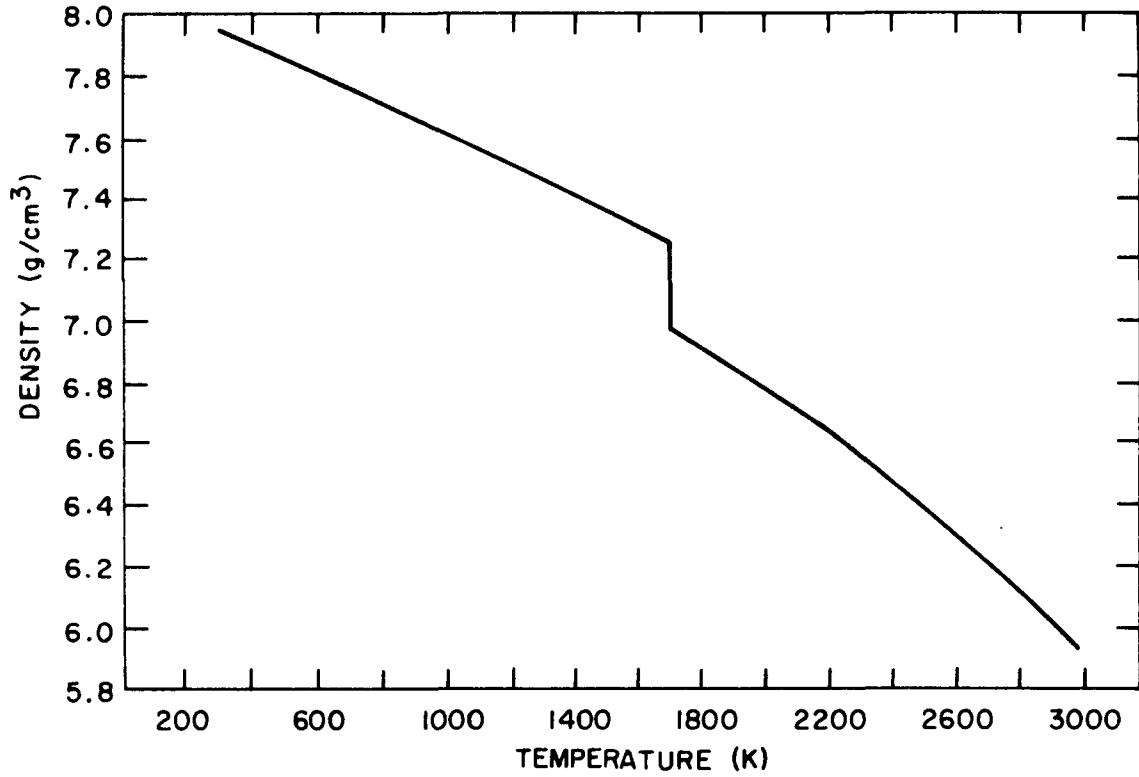
$$\rho = 7.433 + 3.934 \times 10^{-5} T - 1.801 \times 10^{-7} T^2 \quad (\text{liquid region})$$

FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Density (3304)

Date:1/1976



FUNCTION
Structural

MATERIAL
Stainless Steel
(Type 316)

PROPERTY
Density (3304)

Date: 1/1976

Data Source

Density data in the solid region were provided by Reference 1. Densities of the constituting elements used in the estimation of liquid density of 316 stainless steel were taken from Reference 2 and 3.

Data Analysis

A smooth curve was drawn through the experimental data and extrapolated to the melting point. In the estimation of liquid density, the following formula suggested by Reference 4 was used.

$$\rho = 1/\sum_i (x_i/\rho_i)$$

where ρ = density of stainless steel

x_i = weight fraction of the i^{th} constituent

ρ_i = density of the i^{th} constituent

Discussion

In the estimation of liquid density, 316 stainless steel was considered to be composed of 69% Fe, 17% Cr, 12% Ni, and 2% Mo.

References

1. I. B. Fieldhouse, J. C. Hedge, and J. I. Lang, "Measurements of Thermal Properties," WADC-TR-58-274, 1958.
2. Y. S. Touloukian, "Recommended Values of the Thermophysical Properties of Eight Alloys, Major Constituents and Their Oxides," NASA-CR-71699, February 1966.
3. Y. S. Touloukian, editor, "Thermophysical Properties of High Temperature Solid Materials," Vol. 1 Elements, 1967.
4. F. C. Hull, "Estimating Alloy Densities," Metal Progress, Vol. 96, No. 5, 139-140, November 1969.