CALCULATION OF THERMOPHYSICAL PROPERTIES OF SODIUM

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ABSTRACT

The thermodynamic properties of sodium previously recommended by

Padilla have been updated. As much as possible, the approach described by

Padilla has been used.

For sodium in the states of saturated liquid and vapor, subcooled

liquid and superheated vapor, the following thermodynamic properties were

determined: enthalpy, heat capacity (constant pressure and constant volume),

pressure, density, thermal-expansion coefficient, and compressibility (adia-

batic and isothermal). The thermodynamic properties of the superheated

vapor were only calculated to 1600 K for low pressures because of the limi-

tations of the quasi-chemical model of Golden and Tokar which was used in

the determination of these superheated properties. In addition to the

above properties, thermodynamic properties including heat of fusion, heat

of vaporization, surface tension, speed of sound and transport properties

of thermal conductivity, thermal diffusivity, emissivity, and viscosity

were determined for saturated sodium.

INTRODUCTION

Calculations of thermophysical properties of sodium have been made

by Golden and Tokar [1], Padilla [2], Alderson [3], and Breton [4].

Recently, Padilla [5] revised his calculations to include new experimental

data and extended them to include the superheated vapor region.

In this study, modifications to the equations for thermodynamic proper-
ties of sodium recommended by Padilla [5] were made to include recent exper-
imental data and to eliminate discontinuities that existed due to choice of
equations to fit the data. The recent enthalpy data of Fredrickson and
Chasanov [6] along with the data of Ginnings, Douglas, and Ball [7] were
fit to a single enthalpy equation for the entire liquid range instead of
the two separate equations used by Padilla [5]. A single equation derived
by Das Gupta and Bonilla [8] was used for the vapor pressure of saturated
liquid sodium in place of the three vapor equations used by Padilla [5].
The use of this single equation for the vapor pressure plus the requirement
that the critical pressure equal 25.6 MPa (253.0 atm), the value obtained
experimentally by Bhise and Bonilla [9], resulted in a critical temperature
of 2509.46 K. Padilla used 2503 K for the critical temperature. New equa-
tions have also been derived to describe the high-temperature density of
liquid sodium and the thermal pressure coefficient of sodium vapor.

To provide an idea of the uncertainty of calculated values of sodium
properties, errors (1 σ) have been determined. Whenever possible, the
error of the recommended values has been calculated from the experimental
errors and the standard deviations of the fitting functions. Uncertainties
of property values calculated using thermodynamic relations have been
calculated from the uncertainties in the dependent parameters. For the
cases when extrapolation procedures, models, or approximations have been
used to calculate property values, an estimate of the uncertainty of the
calculated values has been made.

Results for the properties of sodium in the saturated, subcooled and superheated regions are summarized below. Additional details on the calculations and tabulations of the property values are given in two reports [10-11].

SATURATED SODIUM PROPERTIES

The assessment of experimental data and the determination of functions for the calculation of properties of saturated sodium have included the determination of errors of values calculated with the recommended functions. Table 1 gives the uncertainties of values of saturated liquid sodium calculated using the equations given below. Uncertainties of calculated values of saturated sodium vapor are given in Table II. Many of the errors given are estimated by comparison of various approximations or by evaluation of a method in a region where experimental data exist. These estimates are indicated by parentheses.

Critical Constants

The main difference in the critical constants used in this study and those used by Padilla is the value of the critical temperature. Padilla used constants recommended by Bhise and Bonilla [9] who gave 2503 K as the critical temperature. The critical temperature of 2509.46 K was obtained by Das Gupta and Bonilla [8] who calculated the temperature at which their vapor-pressure equation equaled the experimental critical pressure of 25.6 MPa [9]. This vapor-pressure equation was derived from a combined fit to all data from the melting point to the critical point. The critical density, 214.1 kg/m^3, is the value calculated by Das Gupta and Bonilla [13] from the density equation of Bhise and Bonilla [9].

Enthalpy

The liquid sodium-enthalpy data of Fredrickson and Chasanov [6] (554 to 1505 K) and Ginnings, Douglas, and Ball [7] (373 to 1173 K) were combined and fit to a function by the method of least squares. The best fit to the data is

$$H_\ell(T) - H_S(298) = -7.1393 \times 10^3 + 35.206\ T - 7.0513 \times 10^{-3}\ T^2$$
$$+ 2.5711 \times 10^{-6}\ T^3 - 1.2428 \times 10^5/T, \tag{1}$$

where T is in kelvins and H is in J/mol. The standard deviation of the experimental data from this fit is 0.14%. This equation is used to calculate the enthalpy of saturated liquid sodium from 371 to 1644.26 K.

To determine the enthalpy of sodium vapor up to 1644.26 K, the heat of vaporization, calculated using the quasi-chemical approach [1], was added to the enthalpy of liquid sodium. Above 1644.26 K, the enthalpy was calculated from the average enthalpy and the heat of vaporization. The average enthalpy, defined as one-half the enthalpies for the liquid plus the vapor, is

$$H(T) - H_S(298) = E + F\ (T - T_\mu), \tag{2}$$

where

$$E = 81678\ \text{J/mol},$$
$$F = 18.55\ \text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1},$$
$$T_\mu = 1644.26\ \text{K},$$

T is in kelvins and enthalpy is in J/mol. The enthalpies for the liquid and vapor were obtained by subtracting and adding one-half the heat of

vaporization [see Eq. (3) below] to the average enthalpy given in Eq. (2).

Tables I and II give the errors of the calculated values of enthalpy of saturated liquid and vapor sodium, respectively. Below 1644.26 K, the errors of the values of the saturated vapor are based on the errors of values of the enthalpy and the heat of vaporization for the liquid. The estimated error in enthalpy values calculated using Eqs. (2-3) is based on comparisons with values calculated by other extrapolation schemes since no experimental data exist.

Figure 1 shows the enthalpies of saturated liquid and vapor sodium from the melting point to the critical point.

Heat of Vaporization

In accordance with Padilla [5,12], the heat of vaporization below 1644.26 K was calculated from the quasi-chemical approach; this property above 1644.26 K was calculated from an empirical equation suggested by Miller, Cohen and Dickerman [13].

$$\Delta H_{VAP} = A_H \, R \, T_c \, (1 - T/T_c)^{B_H} \tag{3}$$

where

$$A_H = 5.2201,$$

$$B_H = 0.32227,$$

$$T_c = 2509.46 \text{ K, the critical temperature.}$$

T is in kelvins and ΔH_{VAP} is in J/mol. The constants E and F in Eq. (2) and A_H and B_H in Eq. (3) were determined by requiring that enthalpies for the liquid and vapor and their partial derivatives with respect to temperature agree at 1644.26 K with those calculated using equations for the

temperature region of 371 to 1644.26 K. This requirement prevents the occurrence of discontinuities in the enthalpy and its derivation at 1644.26 K.

Although Das Gupta [14] obtained a heat of vaporization equation by fitting the heat of vaporization data of Achener and Jouthas [15] (867 - 1202 K) and the density data of Stone et al. [16] (1202 - 1675 K), it has not been used since below 800 K values calculated by the quasi-chemical method produce a curve with a shape closer to the expected behavior for alkali metals than do values calculated with the Das Gupta equation. Above 1644.26 K, an empirical equation was selected because the use of the Das Gupta equation above 1644.26 K and the quasi-chemical method below 1644.26 K would result in a discontinuity at 1644.26 K. While values calculated using the Das Gupta or the quasi-chemical method differ by only 0.6% from the values of experimental data, large differences exist in values calculated by these two methods at high temperatures. This divergence of calculated values with temperature is reflected in the increase in estimated errors with temperature for heat of vaporization in Table I. These large estimated errors indicate the need for experimental data at high temperatures.

Heat Capacity

The heat capacity at constant pressure of the saturated liquid and vapor are calculated from the thermodynamic relation

$$C_P = C_{SAT} + T \, \alpha_P \, \gamma_{SAT}/\rho, \tag{4}$$

where

$$C_{SAT} = \left(\frac{\partial H}{\partial T} \right)_{SAT} - \gamma_{SAT}/\rho \tag{5}$$

and

$$\gamma_{SAT} = \left(\frac{\partial P}{\partial T}\right)_{SAT} . \tag{6}$$

In these equations, T is the temperature in kelvins, P is the vapor pressure given in Eq. (13), ρ is the density given in Eqs. (14-16), and α_P is the volumetric thermal expansion coefficient given in Eqs. (17-21).

The heat capacity at constant volume, C_V, for saturated liquid sodium was calculated from the thermodynamic relation

$$C_V = \frac{C_P \beta_S}{\beta_T} , \tag{7}$$

where β_S and β_T are the adiabatic and isothermal compressibilities defined in Eqs. (21) and (24), respectively.

The heat capacity at contstant volume, C_V, for saturated sodium vapor was calculated from the thermodynamic relation

$$C_V = C_P - \frac{T \alpha_P \gamma_V}{\rho_g} , \tag{8}$$

where C_P, α_P, γ_V, and ρ_g are given by Eq. (4), (19), (27), and (16), respectively.

Figures 2 and 3 show the heat capacities for the saturated liquid and the saturated vapor, respectively, calculated from these equations.

Entropy

The entropy of saturated liquid sodium was obtained by integrating an equation derived from the second law of thermodynamics. Mathematically, the entropy is expressed as

$$dS_{\ell} = \frac{C_{SAT}}{T} dT, \tag{9}$$

and consequently,

$$S_{\ell} = S_{\ell}(T_m) + \int_{T_m}^{T} \frac{C_{SAT}}{T} dT, \tag{10}$$

where C_{SAT} is defined in Eq. (5) and $S(T_m)$ is the entropy at the melting point of sodium (370.98 K). Below 1644.26 K, the entropy is given by the equation

$$S_{\ell} = -5.90356 + 1.51103 \ln T - 5.73462 \times 10^{-4} T \tag{11}$$
$$+ 1.57165 \times 10^{-7} T^2 - 3425.81/T^2.$$

Equation (11) was obtained by a least-squares fit to the values calculated from Eq. (19) with the upper temperature limit set at 1644.26 K.

The entropy of saturated sodium vapor was obtained by adding the entropy of vaporization to the liquid entropy. Thus,

$$S_g = S_{\ell} + \frac{\Delta H_{VAP}}{T}. \tag{12}$$

Vapor Pressure

The vapor pressure is given by

$$\ln P = 18.832 - 13113/T - 1.0948 \ln T + 1.9777 \times 10^{-4} T, \tag{13}$$

where P is in atmospheres and T is in kelvins. Equation (13) was derived by Das Gupta and Bonilla [8] who fit the vapor pressure data of Bhise and Bonilla [9] (1200 - 2509 K), Stone et al. [16] (1200 - 1644 K), and Ditchburn and Gilmour [17] (371 - 1155 K). The standard deviation for this fit expressed as a percent is 0.96%.

Density

Below 1644.26 K, the density of saturated liquid sodium was calculated from the density equation derived by Stone et al. [16]. In SI units, this equation is

$$\rho_\ell = 1011.8 - 0.22054\ T - 1.9226 \times 10^{-5}\ T^2 + 5.6371 \times 10^{-9}\ T^3 \qquad (14)$$

which has a standard deviation of 0.3% below 866 K and 0.4% from 866 to 1644.26 K.

To prevent discontinuities in the calculated values of subcooled properties, which are a function of the second derivative of the density with respect to temperature, the empirical equation given below has been used instead of the empirical equation of Miller, Cohen, and Dickerman [13] used by Padilla [5,12] or the generalized alkali metal equation derived by Bhise and Bonilla [9]. The empirical equation is

$$\rho_\ell = \rho_c\ [1 + A\ (1 - T/T_c)^B + C\ (T_c - T)^2] \qquad (15)$$

where
$$A = 2.3709,$$
$$B = 0.31645,$$
$$C = 2.8467 \times 10^{-7},$$

and T_c and ρ_c are the critical temperature and critical density, respectively. The constants A, B, and C in Eq. (15) were determined by requiring continuity of the liquid density and its first and second derivatives at 1644.26 K. Estimates of the error of Eq. (15) were determined by comparison of values calculated using Eq. (15) with those calculated using other equations. These are tabulated as a function of temperature in Table I.

The density of saturated sodium vapor was calculated from the Clapeyron equation

$$\rho_g = \left[\frac{\Delta H_{VAP}}{T \left(\frac{\partial P}{\partial T} \right)_{SAT}} + \frac{1}{\rho_P} \right]^{-1}. \tag{16}$$

The calculated liquid and vapor densities are shown in Fig. 4.

Thermal Expansion Coefficient

The volumetric thermal expansion coefficient of saturated liquid sodium was calculated from the thermodynamic relation

$$\alpha_P = \alpha_{SAT} + \beta_T \gamma_{SAT}, \tag{17}$$

where α_{SAT}, the thermal expansion coefficient along the saturation curve, is defined as

$$\alpha_{SAT} = \frac{1}{\rho_\ell} \left(\frac{\partial \rho_\ell}{\partial T} \right)_{SAT}, \tag{18}$$

γ_{SAT} is given in Eq. (6), and β_T is the isothermal compressibility given by Eq. (24).

The volumetric thermal expansion coefficient of the saturated vapor was calculated from the thermal pressure as follows:

$$\alpha_P = \frac{\alpha_{SAT}}{1 - \frac{\alpha_{SAT}}{\gamma_V}}, \tag{19}$$

where

$$\alpha_{SAT} = \frac{-1}{\rho_g} \left(\frac{\partial \rho_g}{\partial T} \right)_{SAT}. \tag{20}$$

Compressibility

In the temperature range of experimental data (370.98 - 1173 K), the adiabatic compressibility of saturated liquid sodium was calculated from the sonic velocity, v, using the relation

$$\beta_S = \frac{1}{\rho v^2} \tag{21}$$

where the speed of sound in m/s is given by

$$v = 2660.7 - 0.37667\ T - 9.0356 \times 10^{-5}\ T^2, \tag{22}$$

which is a least-squares fit to the experimental data of Leibowitz et al. [18] and Chasanov et al. [19]. Above 1173 K, the adiabatic compressibility was calculated with the equilateral hyberbola extrapolation technique of Grosse [20]. Based on the standard deviation in the fit of the speed of sound data, the standard deviation in values of compressibility calculated from Eqs. (21-22) at 371 to 1773 K is 2%. The main contribution to the estimated uncertainty in values calculated with the Grosse extrapolation technique is from uncertainties in the density.

The adiabatic compressibility of the saturated vapor was calculated from the thermodynamic relation

$$\beta_S = \beta_T\ \frac{C_V}{C_P}. \tag{23}$$

The isothermal compressibility of saturated liquid sodium has been experimentally determined in the temperature range of 1155 to 1870 K by Das Gupta [14] from measurements of the slopes of isotherms. Das Gupta fit his experimental data to a seven term equation involving temperature

and pressure and estimates its error as 9%. Although these experimental data could be used to determine isothermal compressibility, they were not used in this study because isothermal compressibility values calculated using Das Gupta's data are thermodynamically inconsistent with adiabatic compressibilities calculated from the speed of sound data. Owing to the greater accuracy of the speed of sound data of Leibowitz et al. [18] (0.2%) and of Chasanov et al. [19] (0.04%) it was decided to determine the adiabatic compressibility from speed of sound experiments and the isothermal compressibility from the thermodynamic relation recommended by Rowlinson [21]

$$\beta_T = \frac{\beta_S \, C_{SAT} + \dfrac{T \, \alpha_{SAT}}{\rho} \, (\alpha_{SAT} + \beta_S \, \gamma_{SAT})}{C_{SAT} - \dfrac{T \, \gamma_{SAT}}{\rho} \, (\alpha_{SAT} + \beta_S \, \gamma_{SAT})} \qquad (24)$$

The isothermal compressibility of the saturated vapor was calculated from the thermal expansion coefficient and the thermal pressure coefficient,

$$\beta_T = \frac{\alpha_P}{\gamma_V} . \qquad (25)$$

Thermal Pressure Coefficient

The thermal pressure coefficient for saturated liquid sodium was calculated from the thermodynamic relation

$$\gamma_V = \frac{\alpha_P}{\beta_T} . \qquad (26)$$

Below 1644.26 K, the thermal pressure coefficient for saturated sodium vapor was calulated using the quasi-chemical approach of Golden and Tokar [1]. Above 1644.26 K, the thermal pressure coefficient was calculated from the empirical equation

$$\gamma_V = \gamma_V^C + A (T_c - T)^{1/2} + B (T_c - T) \qquad (27)$$

where

A = - 0.025165,

$B = 3.4175 \times 10^{-4}$,

and T_c is the critical temperature, 2509.46 K, and γ_V^C is the critical thermal pressure coefficient, 0.46652. The constants A and B in Eq. (27) were evaluated by requiring continuity in the thermal pressure and its temperature derivative at 1644.26 K. The form of Eq. (27) was chosen so that the thermal pressure coefficient has the proper high temperature behavior.

Thermal Conductivity

From the melting point to 1500 K, the values given by Touloukian et al. [22] were used for the thermal conductivity (k) of saturated liquid sodium. Above 1500 K, a semi-empirical method due to Grosse [23] was used to estimate the thermal conductivity. Thermal conductivity was calculated using the Wiedemann-Franz-Lorentz law

$$k = L \ X \ T \qquad (28)$$

where L is the Lorentz constant (2.443×10^{-8} W·Ω·K^{-2}) and X is the electrical conductivity given by the Grosse hyperbolic relation

$$\chi = \chi_m \left[\frac{a}{(\theta + b)} - b \right] , \tag{29}$$

where

$$\chi_m = 1.03734 \times 10^7 \Omega^{-1} \cdot m^{-1},$$

$$\theta = \frac{T - T_m}{T_c - T_m} ,$$

$$a = 0.146,$$

$$b = 0.122,$$

and the subscript m refers to the melting point.

The low-temperature errors given in Table I are those stated by Touloukian et al. [22]. The high-temperature error estimates are based on comparisons of values calculated with the Grosse approach with values recommended by Touloukian et al. [22].

The thermal diffusivity of saturated liquid sodium has been calculated from the thermal conductivity, heat capacity, and density using the relation

$$\kappa = \frac{k}{C_p \, \rho} . \tag{30}$$

Viscosity

Experimental data [23-29] on the viscosity of saturated liquid sodium from the melting point to 1300 K were correlated using a technique of Grosse [30]. These data were fit to an Andrade's II equation [31].

$$\eta \, V^{1/3} = A \, e^{C/(VT)}, \tag{31}$$

where

$A = 0.11259$,

$C = 749.08$,

and η is the viscosity in poise, V is the specific volume in cm^3/g, and T is the temperature in kelvins. The data were fit to Eq. (31) with a standard deviation of 0.36%. The estimated error in viscosity values calculated using Eq. (31) ranges from 1 to 12%.

Subcooled

In the calculation of thermodynamic properties of subcooled sodium, it was assumed that the thermal pressure coefficient is a function of specific volume only. Mathematically, this assumption is

$$\gamma_V = \left(\frac{\partial P}{\partial T} \right)_V = f(V) \tag{32}$$

This assumption, which was also used by Alderson [3] and Padilla [5], is based on the fact, pointed out by Rowlinson [21], that the variation of the thermal pressure coefficient with temperature along isochores is small.

Table III gives the estimated errors of values of subcooled liquid sodium, which were calculated using the equations given below. These error estimates were calculated from the errors of the dependent parameters.

Pressure

By integration of Eq. (32) along a constant volume path starting with the saturation pressure, the following equation-of-state for subcooled liquid sodium was obtained:

$$P(V_{SAT}, T) = P_{SAT}(V_{SAT}) + \gamma_V (T - T_{SAT}), \tag{33}$$

where P_{SAT} is the pressure of the saturated vapor given in Eq. (13) and γ_V is the thermal pressure coefficient given in Eq. (26).

Volumetric Thermal Expansion Coefficient

The volumetric thermal expansion coefficient for subcooled liquid sodium was calculated from the relation

$$\frac{1}{\alpha_P} = \frac{1}{(\alpha_P)_{SAT}} + \frac{(\rho\ell)_{SAT}(P - P_{SAT})}{(\gamma_V{}^2)_{SAT}} \left[\left(\frac{\partial\gamma_V}{\partial\rho}\right)_P\right]_{SAT} \tag{34}$$

where the saturated liquid properties ρ_ℓ, P_{SAT}, α_P and γ_V are given in Eqs. (14, 13, 17, and 26-27), respectively. The derivative of the thermal pressure coefficient with respect to density, $\left(\frac{\partial\gamma_V}{\partial\rho}\right)_P$, was calculated numerically from the derivatives $\left(\frac{\partial\gamma_V}{\partial T}\right)$ and $\left(\frac{\partial T}{\partial\rho}\right)$. In the calculation of $\left(\frac{\partial\gamma_V}{\partial T}\right)$, the second derivative of the density with respect to temperature occurs. Thus, a discontinuity in the second derivative of density with respect to temperature would lead to a discontinuity in α_P and in any subcooled properties calculated from α_P. The use of the empirical equation for the density, Eq. (15), eliminates any discontinuities as is evident from the graph of the volumetric thermal expansion coefficient of subcooled liquid sodium shown in Fig. 5.

Enthalpy

The enthalpy of subcooled liquid sodium may be calculated as a function of pressure and temperature. The effect of pressure on enthalpy of the subcooled liquid at a given temperature is expressed as

$$\left(\frac{\partial H}{\partial P}\right)_T = V - T\left(\frac{\partial V}{\partial T}\right)_P = V(1 - T\alpha_P), \tag{35}$$

where α_p for the subcooled liquid is defined in Eq. (34). By integrating Eq. (35) with respect to pressure along a constant temperature path, one is able to calculate the enthalpy of the subcooled liquid at any temperature, T, and any pressure, P. Thus,

$$H_{SUB} = [H_\ell(T) - H_S(298)]_{SAT} + \int_{P_{SAT}}^{P} V(1 - T\alpha_p) \, dP, \qquad (36)$$

where $[H_\ell(T) - H_S(298)]_{SAT}$ is the enthalpy of the saturated liquid given by Eqs. (1-3). The enthalpy of subcooled liquid sodium as a function of pressure at 500, 1500, and 2500 K is graphed in Fig. 6.

Heat Capacity

The heat capacity at constant volume of subcooled liquid is a function of temperature only

$$C_V = C_V(T)_{SAT} \qquad (37)$$

since the thermal pressure coefficient of the subcooled liquid is assumed to be a function of volume alone. Mathematically this is obvious from consideration of the partial derivatives:

$$\left(\frac{\partial C_V}{\partial V} \right)_T = T \left(\frac{\partial^2 P}{\partial T^2} \right)_V = T \left(\frac{\partial \gamma_V}{\partial T} \right)_V = 0 \qquad (38)$$

The heat capacity of constant pressure of subcooled liquid sodium was calculated from the thermodynamic relation

$$C_P = C_V + \frac{\alpha_P^2}{\rho \beta_T} , \qquad (39)$$

where C_V is given in Eq. (37), α_P is given in Eq. (34) and β_T is defined by Eq. (43).

Entropy

The effect of pressure on the entropy of subcooled liquid sodium at a given temperature is

$$\left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P = -V\alpha_P \quad , \tag{40}$$

where α_P is defined by Eq. (34). The entropy of subcooled liquid sodium at a given temperature, T, and a given pressure, P, is obtained by the integration of Eq. (40) along a constant temperature path beginning with a point on the saturated liquid curve. Thus

$$S = S_{SAT} - \int_{P_{SAT}}^{P} V\alpha_P dP, \tag{41}$$

where S_{SAT} is S_ℓ in Eq. (10).

Compressibility

The adiabatic compressibility of subcooled liquid sodium was calculated using the thermodynamic relation.

$$\beta_S = \beta_T \frac{C_V}{C_P} , \tag{42}$$

where β_T is given in Eq. (43) and the heat capacities, C_V and C_P are given in Eqs. (37) and (39) respectively. The thermodynamic relation

$$\beta_T = \frac{\alpha_P}{\gamma_V} \tag{43}$$

was used to calculate the isothermal compressibility of subcooled liquid sodium. In this equation, α_P is defined in Eq. (34) and γ_V is defined in Eq. (32).

SUPERHEATED SODIUM

For the superheated region, Alderson [3] and Breton [4] assumed that the thermal pressure coefficient is a function of volume only; this same assumption was made for the subcooled region. Padilla [5,12] has shown that this assumption is not valid for superheated sodium because it gives unreasonable values for the constant volume specific heat at low pressures. Padilla [12] evaluated both the virtial equation-of-state and the quasi-chemical approach and chose to use the quasi-chemical approach to calculate properties in this region.

In calculations of thermodynamic properties of superheated sodium, for this study, the quasi-chemical approach as recommended by Padilla [5,12] has been used. Calculations were made only in the temperature range 371 to 1644 K, since evaluations by Padilla have indicated that the quasi-chemical approach is valid only in this temperature region. Since the method of calculation is identical to that described by Padilla [5,12] it is not outlined here. Differences in results are due to the differences in the equations used for the saturated vapor. Figure 7, 8, and 9 show, respectively, the enthalpy, heat capacity, and volumetric thermal expansion coefficient of superheated sodium at 500, 1000, and 1500 K as a function of pressure.

No rigorous error analysis can be made to determine the accuracy of the superheated properties calculated using the quasi-chemical method since no experimental measurements exist. However, based on the standard deviation of values calculated with the quasi-chemical method for the properties of saturated sodium from experimental values, the estimated standard deviation for properties of superheated sodium calculated by this method is 10%.

REFERENCES

1 Golden, G. H. and Tokar, J. V., "Thermodynamic Properties of Sodium," ANL-7323, Argonne National Laboratory, Argonne, IL (1967).

2 Padilla, Jr., A., Nucl. Sci. Eng. 55, 452 (1974).

3 Alderson, M. A. H. G., "An Equation of State for Use with Sodium, Part I - Theory and Computer Program," SRD-R-50 (Pt. 1), United Kingdom Atomic Energy Authority, Wigshaw Lane, Culcheth Warrington (1975).

4 Breton, J. P., "A Simple and Consistent Equation of State for Sodium in the Single Phase and Two Phase Regions," PNC N251 76-12, Proc. of the Third Specialist Meeting on Sodium/Fuel Interaction in Fast Reactors, Tokyo, Japan (March 22-26, 1976).

5 Padilla, Jr., A., "Extrapolation of Thermodynamic Properties of Sodium to the Critical Point," Proc. Seventh Symposium on Thermophysical Properties, National Bureau of Standards Gaithersburg, Maryland (May 10-12, 1977) pp. 887-895.

6 Fredrickson, D. R. and Chasanov, M. G., J. Chem. Thermodynamics 6, 629 (1974).

7 Ginnings, D. C., Douglas, T. B., and Ball, A. F., "Heat Capacity of Sodium between 0 and 900°C, the Triple Point and Heat of Fusion," J. Res. NBS 45, 23-33 (1950).

8 Das Gupta, S. and Bonilla, C. F., private communication (1978).

9 Bhise, V. S. and Bonilla, C. F., "The Experimental Vapor Pressures and Critical Point of Sodium," Proc. International Conf. Liquid Metal Technology in Energy Production, ANS, IAEA, Seven Springs, PA (May 3-6, 1977).

Bhise, V. S., "The Critical Point and High Temperature Thermodynamic Properties of Sodium," Dr. Eng'g. Sci. Dissertation with C. F. Bonilla, Dept. of Chemical Engineering and Applied Chemistry, Columbia University, Xerox-University Microfilm (1976).

10 Fink, J. K. and Leibowitz, L., "Thermophysical Properties of Sodium," ANL-CEN-RSD-79-1, Argonne National Laboratory, Argonne, IL (May 1979).

11 Fink, J. K., "Computer Codes Used in the Calculation of High-Temperature Thermodynamic Properties of Sodium," ANL-CEN-RSD-79-2, Argonne National Laboratory, Argonne, IL (December 1979).

12 Padilla, Jr., A., "High-Temperature Thermodynamic Properties of Sodium," HEDL-TME 77-27, Hanford Engineering Development Laboratory, Richland, WA (February 1978).

13 Miller, D., Cohen, A. B., and Dickerman, C. E., "Estimation of Vapor and Liquid Density and Heat of Vaporization of Alkali Metals to the Critical Point," Proc. Int. Conf. in Safety of Fast Breeder Reactors, Aix-en-Provence, France (September 1967).

14 Das Gupta, S., "Experimental High-Temperature Coefficient of Compressibility and Expansivity of Liquid Sodium and Other Related Properties," Dr. Eng'g Sci. Dissertation with C. F. Bonilla, Dept. of Chemical Engineering and Applied Chemistry, Columbia University, Xerox-University, Microfilm (1977).

15 Achener, P. Y. and Jouthas, J. T., "The Latent Heat of Vaporization and Vapor Pressure of Sodium," AGN-8191, Vol. 1, Aerojet-General Nucleonics, San Ramon, CA (July 1966).

16 Stone, J. P., Ewing, C. T., Spann, J. R. Steinkuller, E. W. Williams, D. D., and Miller, R. R., "High-Temperature Properties of Sodium," NRL-6241, Naval Research Laboratory (September 24, 1965).

REFERENCES (Cont'd)

17 Ditchburn, R. W. and Gilmour, J. C., Rev. Mod. Phys. 13, 310 (1940).

18 Leibowitz, L. Chasanov, M. G., and Blomquist, R., J. Appl. Phys. 42, 2135 (1971).

19 Chasanov, M. G. Leibowitz, L. Fischer, D. F., and Blomquist, R. A., J. Appl. Phys. 43, 745 (1972).

20 Grosse, A. V., Nature Physical Science 232, 170 (1971).

21 Rowlinson, J. S., "Liquids and Liquid Mixtures, 2nd Ed., Butterworth and Co., Ltd., London (1968).

22 Touloukian, Y. S., ed. "Thermophysical Properties of Matter, Vol. I, Thermal Conductivity Metallic Elements and Alloys," pp. 349-354, Plenum Press, NY (1970).

23 Grosse, A. V., Rev. Hautes Temperature et Refract. 3, 115 (1966).

24 Ewing, C. T., Grand, J. A., and Miller, R. R., J. Am. Chem. Soc. 73, 1168 (1951).

25 Ewing, C. T., Grand, J. A., and Miller, R. R., J. Phys. Chem. Soc. 58, 1068 (1954).

26 Chiang, Y. S., Proc. Roy. Soc. (London) A157, 264 (1936).

27 Godfrey, T., "Physical and Thermodynamic Properties of Sodium, Its Manufacture, Properties, and Uses," M. Sittig, Ed., ACS Monograph Series No. 133, Reinhold Pb. Corp., Chapter 9 (1956).

28 Novikov, I. I., Soloview, A. N., Khabakhnasheva, E. M., Gruzdev, A. V., Pridantzev, A. I., and Vasenina, M. Ya., J. Nuclear Energy 4, 387 (1957).

29 Shpilrain, E. E., Soldatenko, Y. A., Yakimovich, K. A., Fomin, V. A., Savchenko, Belova, A. M. Kaga, D. N., and Krainova, I. F., High Temperature 3, 870 (1965).

30 Grosse, A. V., Science 14, 1438 (1965).

31 da C. Andrade, E. N., Phil. Mag. 17, 698 (1934).

FIGURE CAPTIONS

Fig. 1. The enthalpy of saturated sodium as a function of temperature relative to the enthalpy at 298 K, H(T) − H(298).

Fig. 2. Heat capacity at constant pressure and constant volume for saturated liquid sodium.

Fig. 3. Heat capacity at constant pressure and constant volume for saturated vapor sodium.

Fig. 4. The density of saturated sodium as a function of temperature.

Fig. 5. The volumetric thermal expansion coefficient of subcooled liquid sodium at 500, 1500 and 2500 K and of saturated liquid sodium as functions of pressure.

Fig. 6. The enthalpy, H(T) − H(298), of superheated vapor sodium at 500, 1000, 1500 K and of saturated vapor sodium as functions of pressure.

Fig. 7. The heat capacity at constant pressure of superheated vapor sodium at 500, 1000, and 1500 K and of saturated vapor sodium as functions of pressure.

Fig. 8   The heat capacity at constant pressure of superheated vapor sodium at 500, 1000, and 1500 K and of saturated vapor sodium as functions of pressure.

Fig. 9   The volumetric thermal expansion coefficient of superheated vapor sodium at 500, 1000, and 1500 K and of saturated vapor sodium as functions of pressure.

Fig 1

Fig. 2

HEAT CAPACITY, J/mol·K

TEMPERATURE, K

C_V

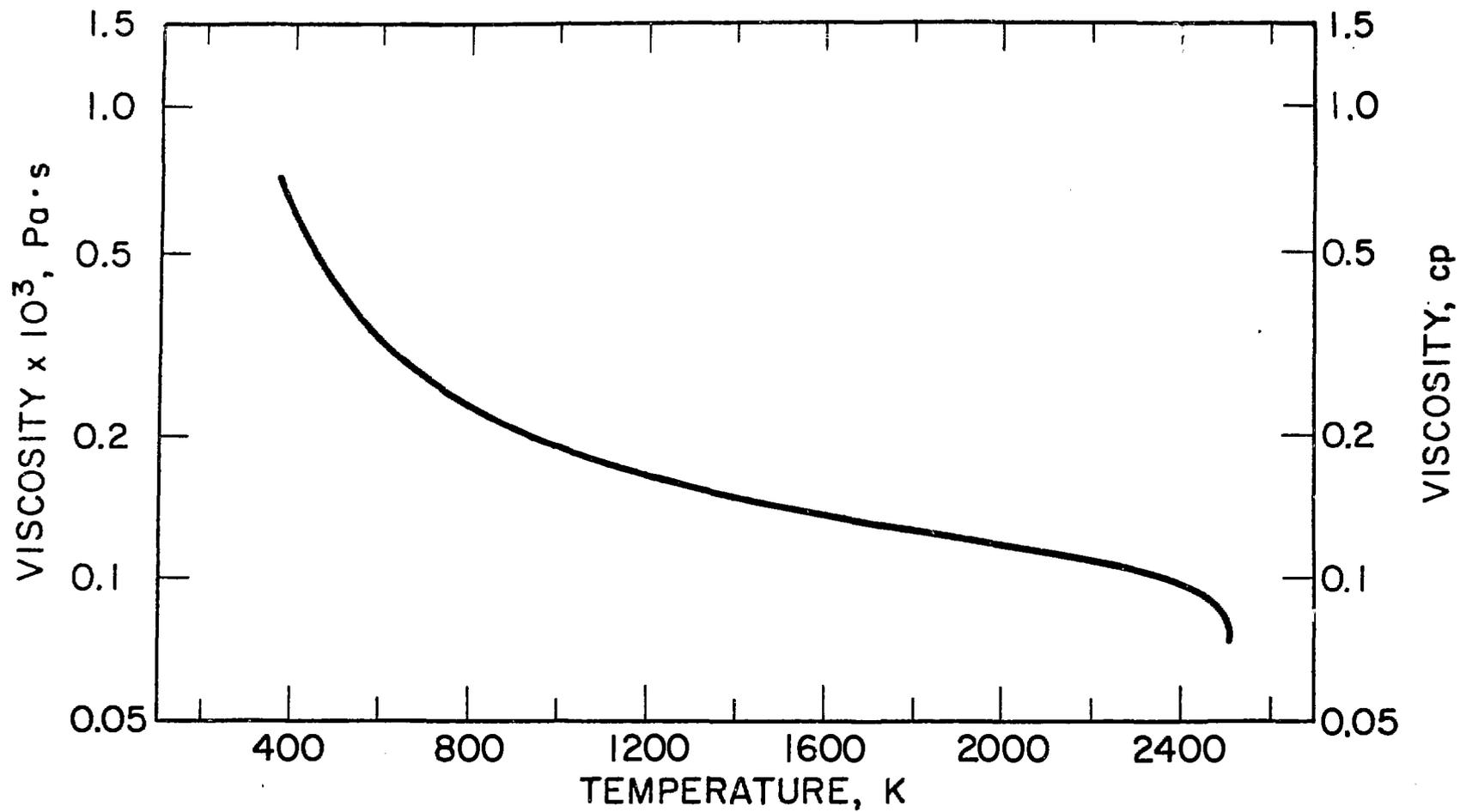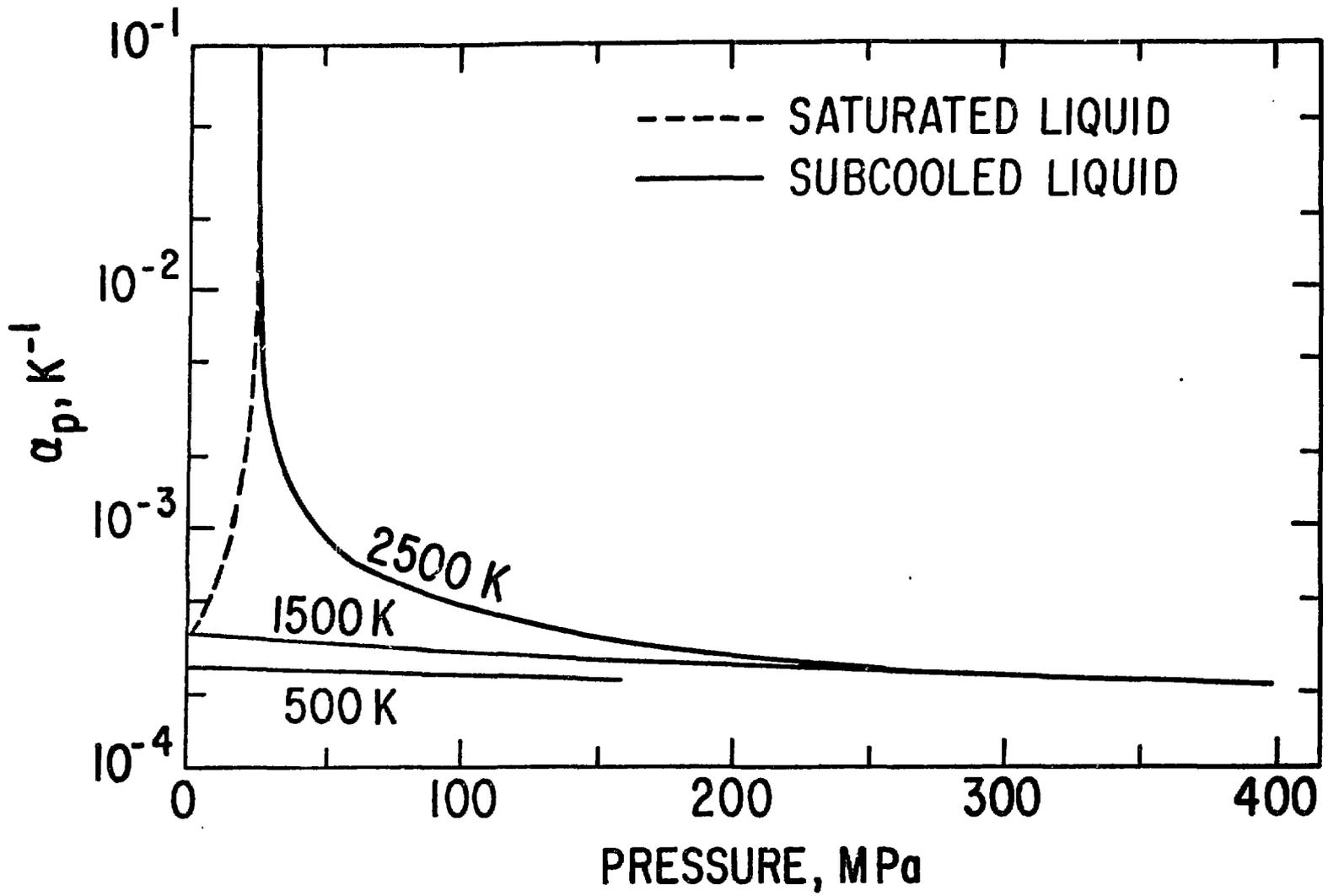C_p

Fig. 3

HEAT CAPACITY, J/mol·K

TEMPERATURE, K

C_p

C_v
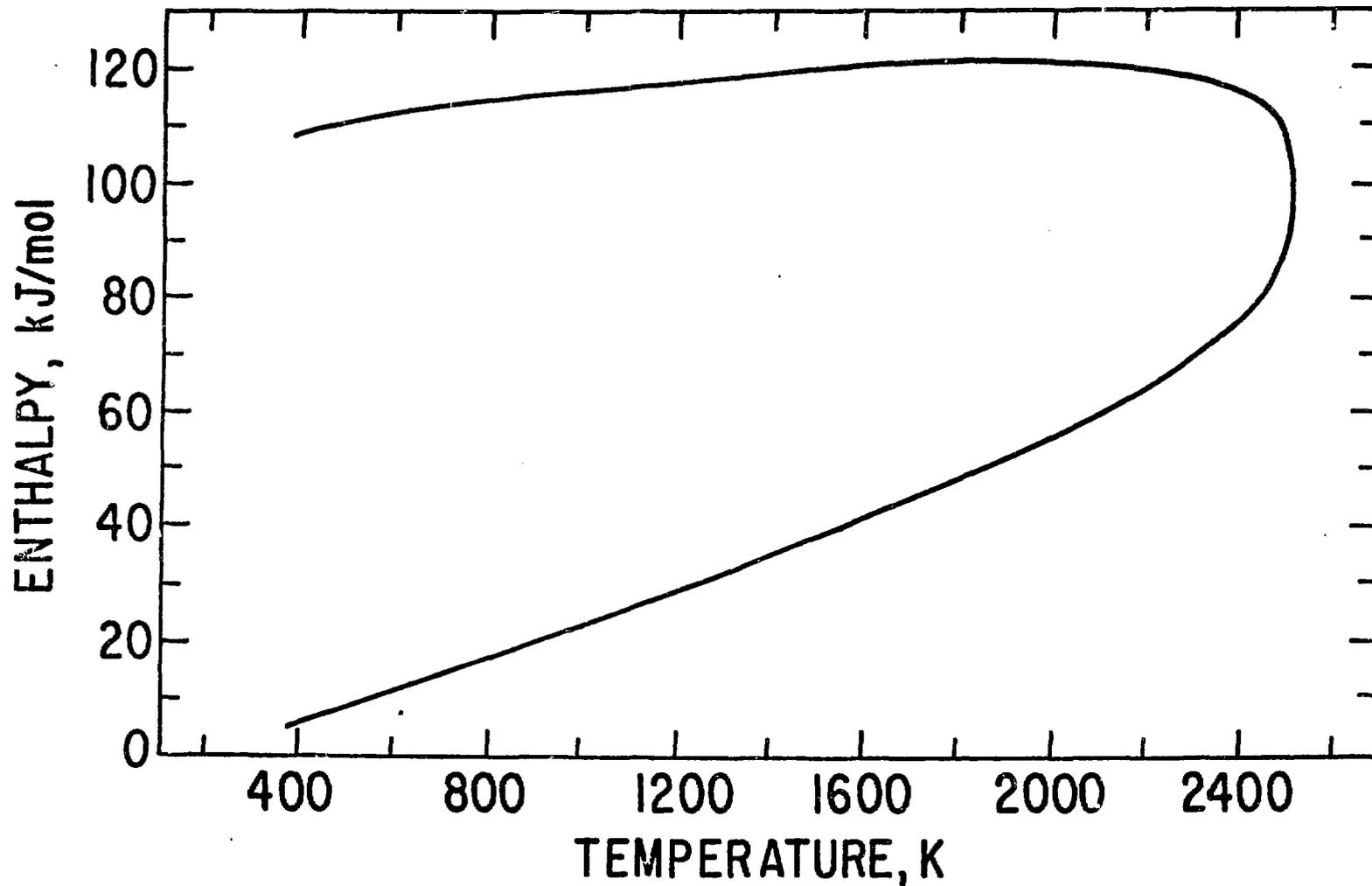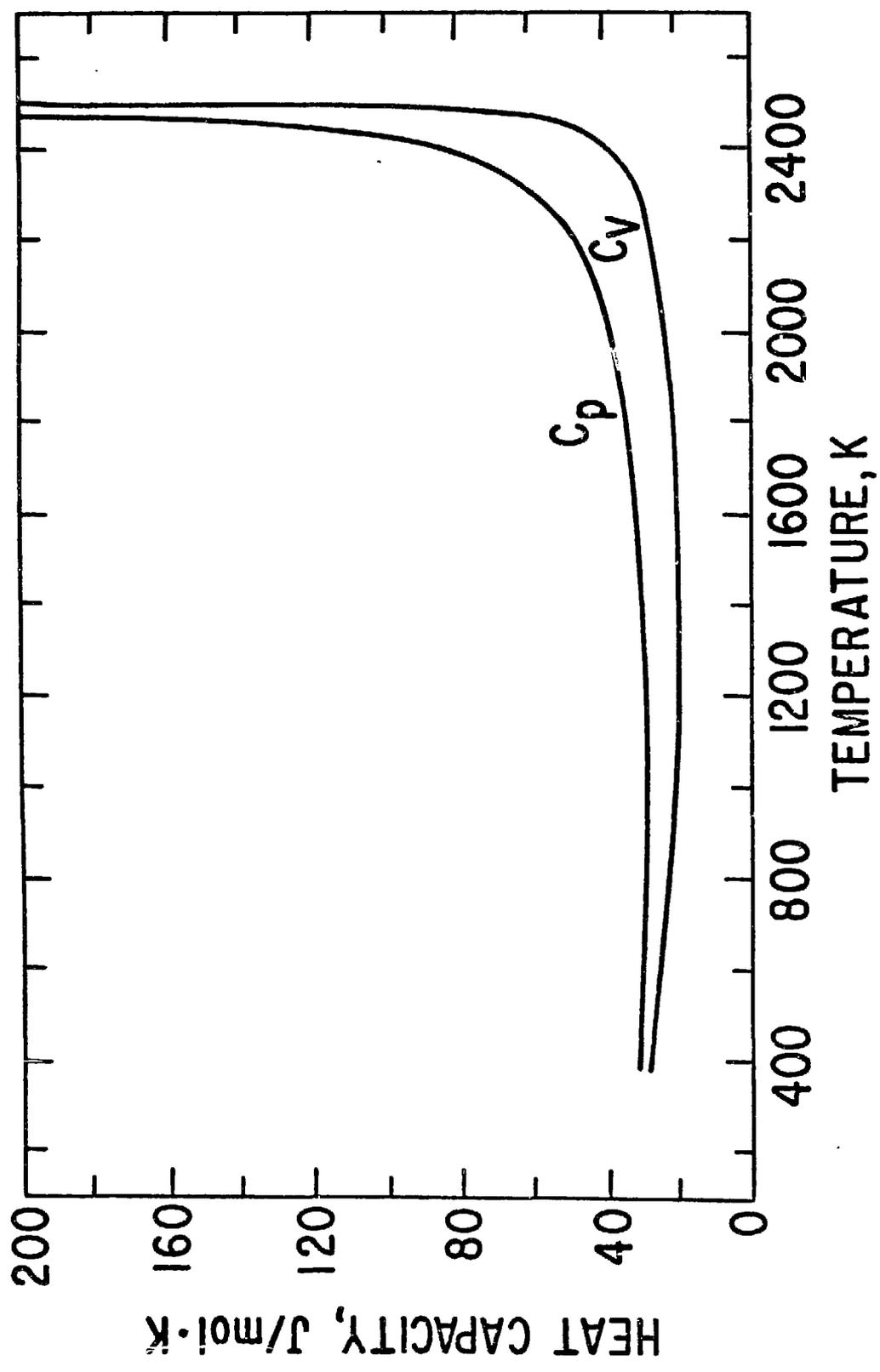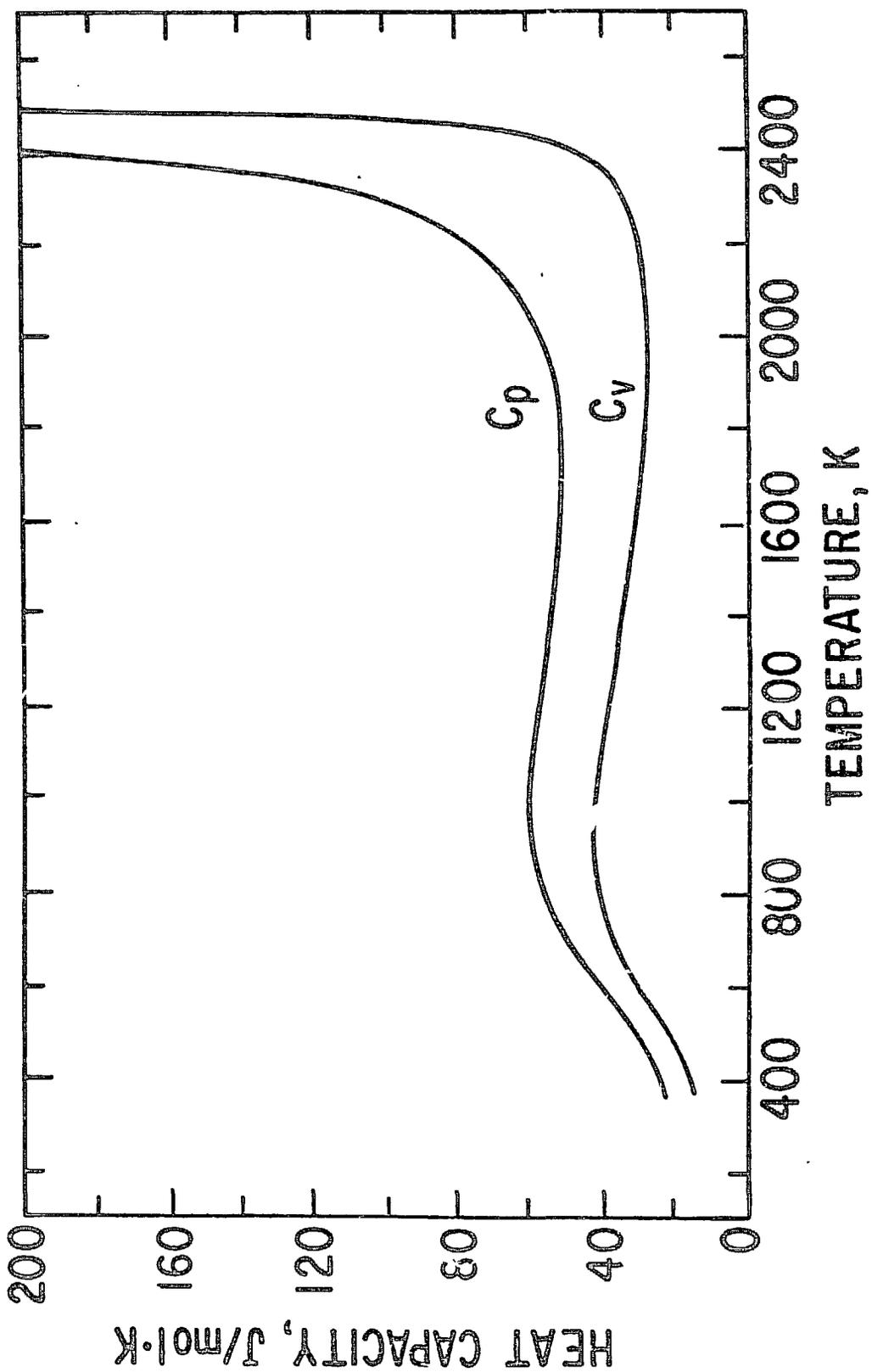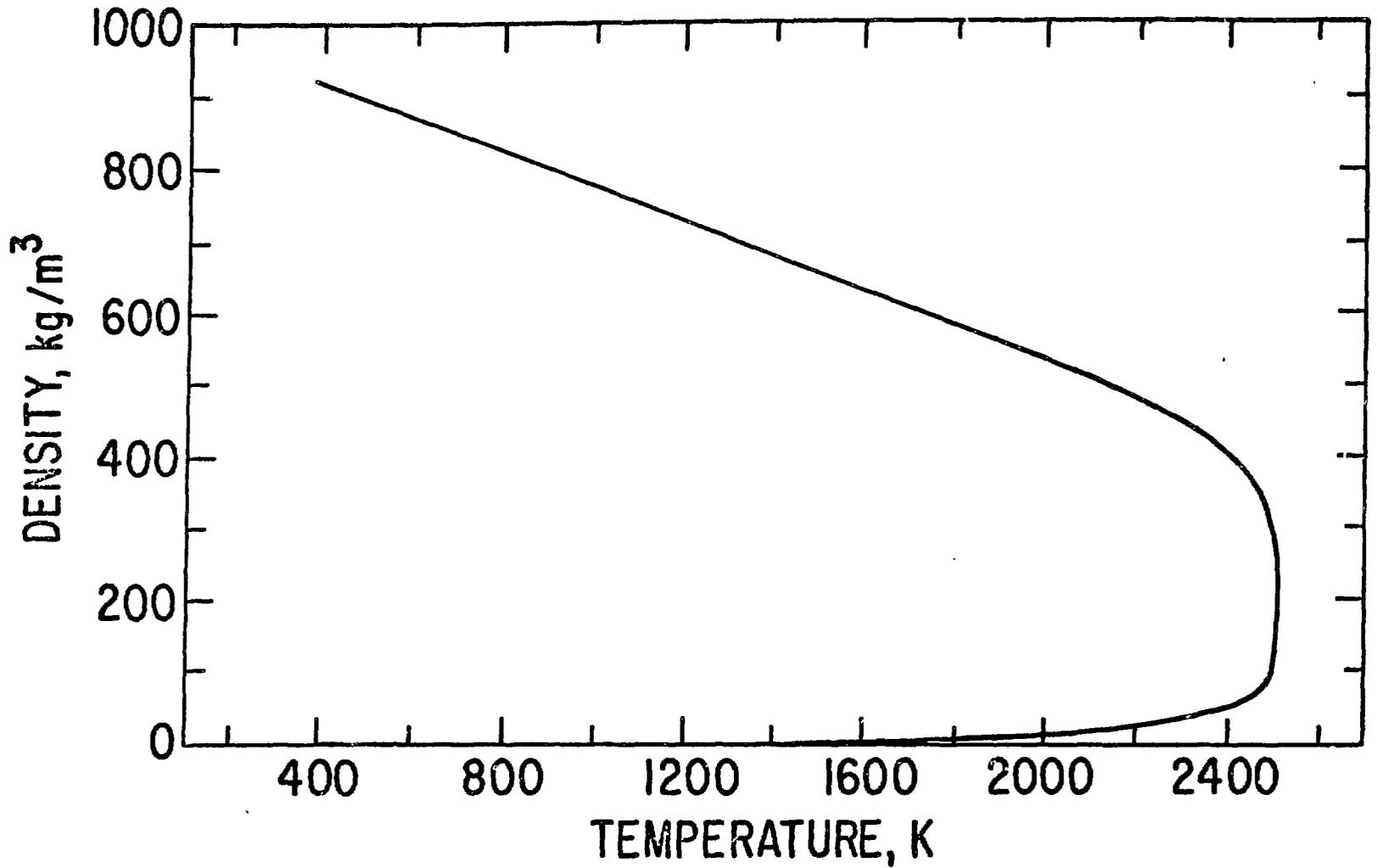
Fig 4

Fig 5
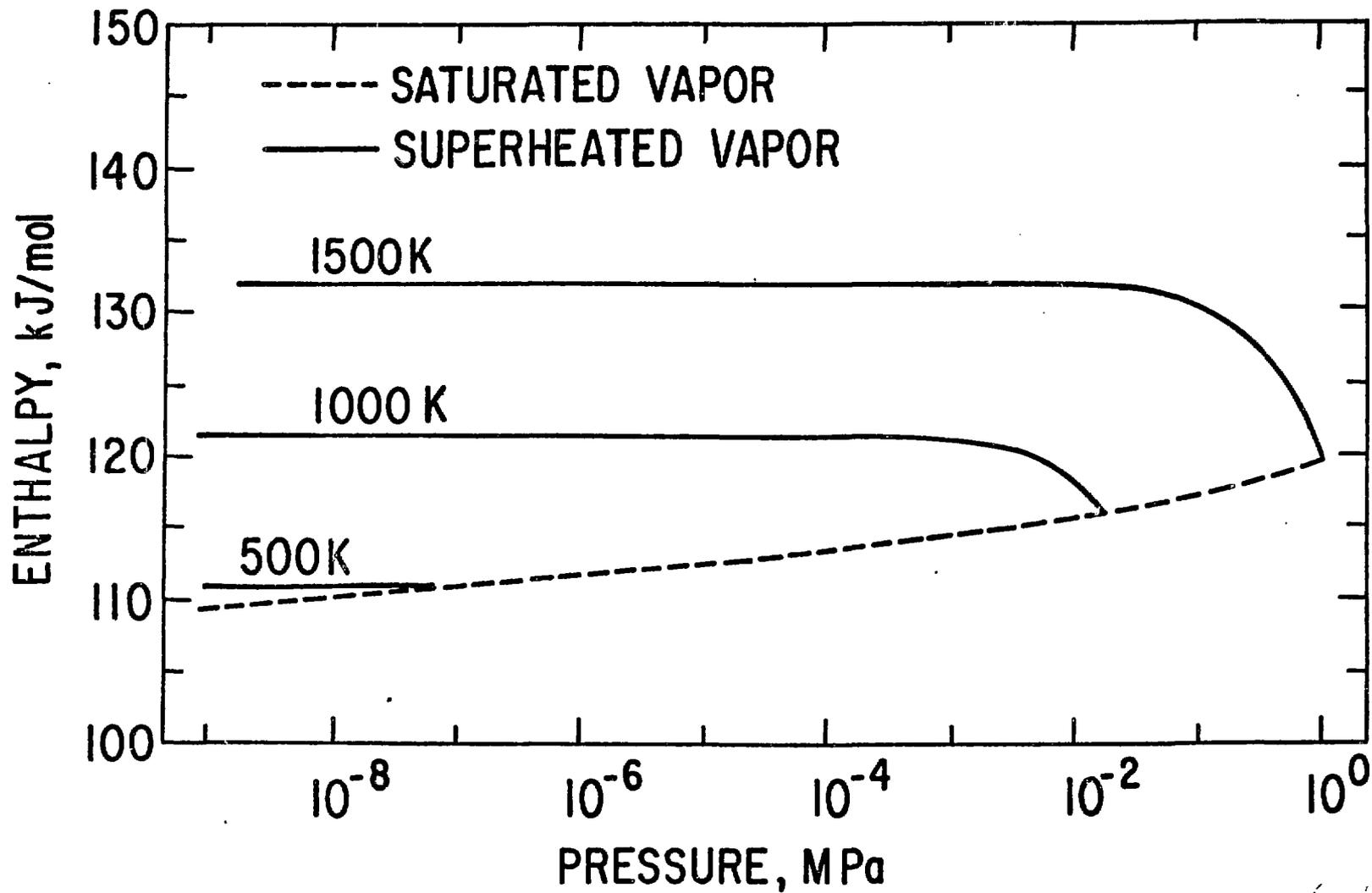
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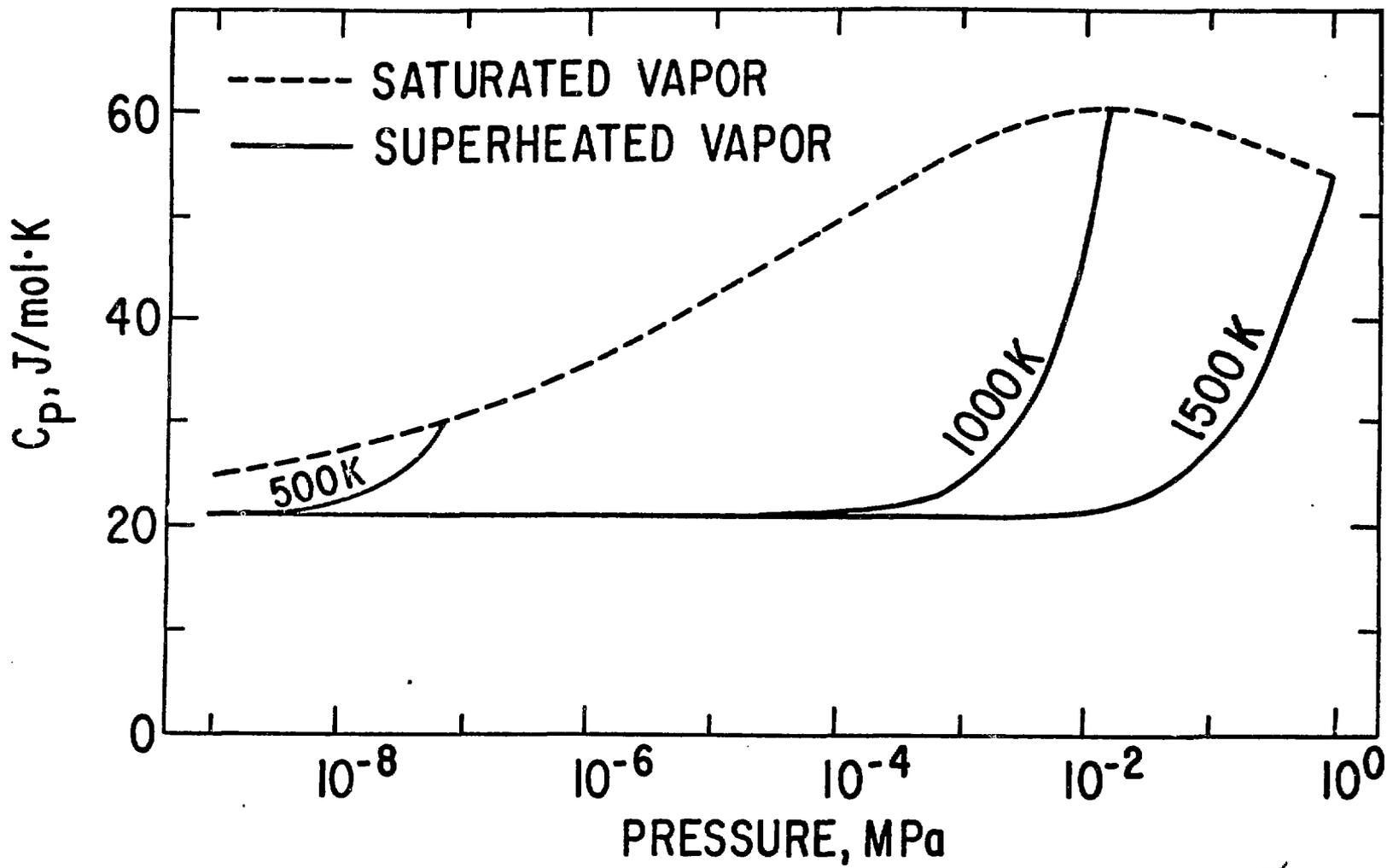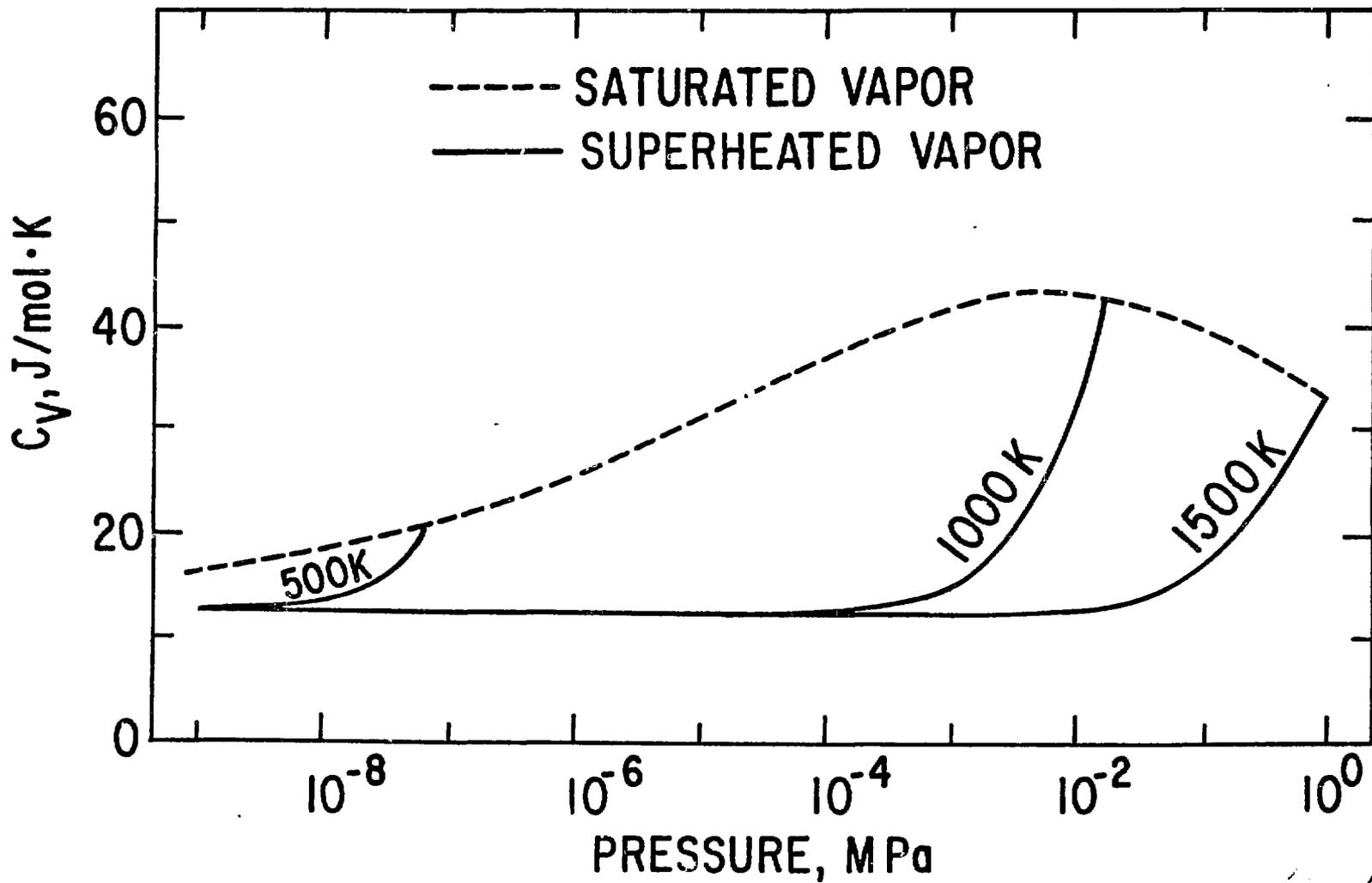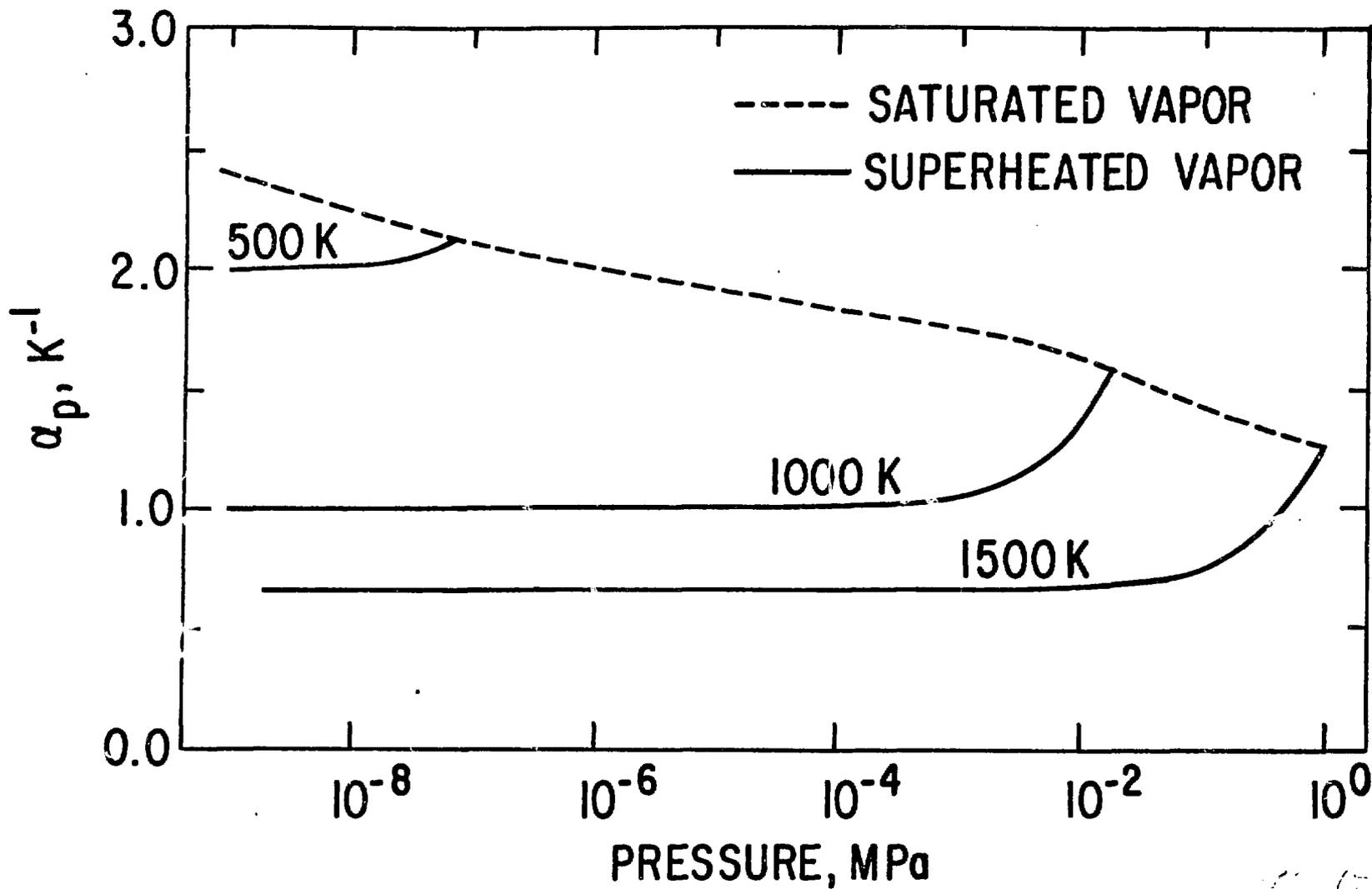
Fig. 1

Fig. 8

Fig. 1

Table I. Errors (1σ) of values of properties of saturated liquid sodium

Error, %

Property Temperature K	Enthalpy H	Heat Capacity		Heat of Vaporization ΔH_{vap}	Entropy S	Density ρ	Thermal Expansion α_p	Compressibility		Thermal Pressure Coef. γ_V	Conductivity k	Diffusivity κ	Viscosity η
		C_p	C_v					β_S	β_T				
371 – 1644	0.14	2	4	(2)[a]	(0.5)	0.4	(2)	2	2	3	5–10	10	1
1644 – 2000	(12)	(27)	(36)	(12)	(17)	(3)	(24)	(20)	(24)	(34)	(15)	(28)	(12)
2000 – 2400	(20)	(36)	(50)	($\gtrsim$20)	(50)	(7)	(30)	(20)	(30)	(40)	(15)	(40)	(12)
2400 – 2509	($\gtrsim$50)	(80)	(100)[b]	($\gtrsim$50)	(70)	(15)	(60)	(20)	(60)	(80)	(15)	(80)	(12)

[a] Parentheses indicates estimated error.

[b] A 100% error is a factor of a uncertainty in the value.

Table II. Errors (1σ) of values of properties of saturated sodium vapor.

Error, %

Property Temperature K	Enthalpy H	Heat Capacity C_p	C_V	Entropy S	Pressure P	Density ρ	Thermal Expansion α ρ	Compressibility $β_S$	$β_T$	Pressure Coef. $γ_V$
371 – 1644	(2)[a]	(16)	(28)	(4)	0.96	2	(15)	(38)	(20)	(14)
1644 – 2000	(12)	(36)	(40)	(20)	0.96	(12)	(30)	(60)	(33)	(14)
2000 – 2400	(20)	(50)	(60)	(50)	0.96	(20)	(38)	(200)[c]	(40)	(14)
2400 – 2509	(50)	(100)[b]	(100)	(85)	0.96	≳(50)	(80)	(200)	(80)	(14)

[a] Parenthesis indicates estimated error.

[b] A 100% error is a factor of 2 uncertainty in the value.

[c] A 200% error is a factor of 4 uncertainty in the value.

Table III. Estimated errors (1σ) of values of properties of subcooled liquid sodium.

Property Temperature K	Enthalpy H	Heat Capacity C_p	Heat Capacity C_v	Entropy S	Density ρ	Thermal Expansion α_p	Compressibility β_S	Compressibility β_T	Thermal Pressure Coef. α_v
					Error, %				
371 – 1644	3	6	4	2	0.4	2	8	4	5
1644 – 2300	36	60	36	30	3	24	24	42	50
2300 – 2400	52	75	50	60	7	31	100	46	55
2400 – 2509	95	100[a]	97	90	15	60	100	100	100

[a] A 100% error is a factor of 2 uncertainty in the value.

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