Thermodynamic Properties of D$_2$O in the Critical Region

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An analysis is presented of the thermodynamic properties of D₂O in the critical region. It is shown that the data can be represented by the same revised and extended scaled fundamental equation formulated earlier for the thermodynamic properties of H_2O in critical region. The equation is valid in the range 220–465 kg/m³ in density and 638–683 K in temperature. Tabulated values of the thermodynamic properties of D₂O in the critical region are presented. A comparison with a comprehensive analytic fundamental equation, recently formulated by Hill and co-workers, is included in the paper.

Contents

1. Introduction

The modern theory of critical phenomena predicts that the singular behavior of the thermodynamic properties of fluids in the vicinity of the critical point satisfies scaling laws with universal critical exponents and scaling functions.[1,2] A revised and extended scaled fundamental equation that incorporates the theoretical predictions for the asymptotic critical behavior was earlier formulated and shown to represent the thermodynamic properties of H_2O in the critical region.[3] In this paper we use the same fundamental equation to analyze and represent the available experimental information for D₂O in the critical region. We present detailed com-

parisons of the scaled fundamental equation with the experimental data and give tabulated values, derived from our fundamental equation, for the pressure, energy, enthalpy, entropy, specific heats at constant pressure and at constant volume, and velocity of sound.

A global fundamental equation for the thermodynamic properties of D₂O, which is analytic at the critical point, was recently formulated by Hill, MacMillan, and Lee.[4] We include also a comparison between our nonanalytic fundamental equation and the analytic fundamental equation of Hill *et al.*

2. Fundamental Equation

Our fundamental equation involves a relationship between the intensive thermodynamic variables pressure P, chemical potential μ, and temperature T. Specifically we

consider the reduced variables

$$\widetilde{P} = \frac{P}{T} \cdot \frac{T_c}{P_c}, \quad \tilde{\mu} = \frac{\mu}{T} \cdot \frac{\rho_c T_c}{P_c}, \quad \widetilde{T} = -\frac{T_c}{T}, \quad (1)$$

where P_c is the critical pressure, T_c the critical temperature, and ρ_c the critical density. The fundamental equation yields the thermodynamic potential $\widetilde{P}$ as a function of $\tilde{\mu}$ and $\widetilde{T}$ and has the form

$$\widetilde{P} = \widetilde{P}_0(\widetilde{T}) + \Delta\tilde{\mu} + \widetilde{P}_{11}\Delta\tilde{\mu}\Delta\widetilde{T} + \Delta\widetilde{P}, \quad (2)$$

with

$$\Delta\widetilde{T} = \widetilde{T} + 1, \quad (3)$$

$$\Delta\tilde{\mu} = \tilde{\mu} - \tilde{\mu}_0(\widetilde{T}). \quad (4)$$

Here $\widetilde{P}_0(\widetilde{T})$ and $\tilde{\mu}_0(\widetilde{T})$ are analytic functions of $\Delta\widetilde{T}$, while $\Delta\widetilde{P}$ contains the singular, i.e., nonanalytic, contributions to the potential $\widetilde{P}$. The equations for these functions are fully specified in Appendix A. The analytic functions are represented by truncated power series in terms of $\Delta\widetilde{T}$, while the singular part $\Delta\widetilde{P}$ is related to $\Delta\tilde{\mu}$ and $\Delta\widetilde{T}$ with the aid of two auxiliary (parametric) variables r and θ.

The fundamental equation contains the following constants: Three critical parameters P_c, T_c, ρ_c which specify the reduced variables defined in Eq. (2.1), three critical exponents β, δ, Δ_1, and five parameters a, k_0, k_1, c, b^2 in the singular contribution $\Delta\widetilde{P}$, four background parameters $\widetilde{P}_1$, $\widetilde{P}_2$, $\widetilde{P}_3$, $\widetilde{P}_{11}$ that specify the analytic contributions to $\widetilde{P}$ as a function of $\Delta\widetilde{T}$ and $\Delta\tilde{\mu}$, and four background parameters $\tilde{\mu}_c$, $\tilde{\mu}_1$, $\tilde{\mu}_2$, $\tilde{\mu}_3$ that specify the analytic contributions to the caloric properties as a function of temperature. The critical exponents β, δ, Δ_1 and the parameter b^2 in $\Delta\widetilde{P}$ are universal, i.e., independent of the nature of the fluid; hence, for D_2O they have the same values as previously adopted for H_2O.[3] The coefficients a, k_0, k_1, and c in the equations for $\Delta\widetilde{P}$ are adjustable amplitudes that depend in principle on the nature of the fluid; however we find that for D_2O these coefficients have, within currently available experimental accuracy, the same values as found for H_2O. Hence the only constants for D_2O that differ from those for H_2O are the critical parameters P_c, T_c, ρ_c and the analytic background parameters $\widetilde{P}_1$, $\widetilde{P}_2$, $\widetilde{P}_3$, $\widetilde{P}_{11}$ and $\tilde{\mu}_c$, $\tilde{\mu}_1$, $\tilde{\mu}_2$, $\tilde{\mu}_3$ for the pressure and the caloric properties.

The values of the constants in this fundamental equation for D_2O are listed in Appendix B. The equation is valid in a range of temperatures and densities bounded by

$$638 \text{ K} \leqslant T \leqslant 683 \text{ K},$$
$$220 \text{ kg/m}^3 \leqslant \rho \leqslant 465 \text{ kg/m}^3. \quad (5)$$

In terms of reduced variables this range is identical to the range over which our revised and extended fundamental equation was found to be valid for H_2O.[3] All temperatures quoted in this paper correspond to the International Practical Temperature Scale of 1968 (IPTS-68).[5]

3. Data Sources

A survey of the available literature concerning the thermodynamic properties of D_2O is included in the article of Hill et al. in this journal.[4] A list of data sources, that contain relevant experimental information in the range of densities

and temperatures considered here, is given in Table 1. Most of the experimental information in this range originates from research groups in the Soviet Union. In particular PVT data have been reported by Rivkin and Akhundov,[6] Tsederberg et al.,[9] and Aleksandrov et al.,[11] C_p data by Rivkin and Egorov[7] and C_v data by Amirkhanov et al.[10] The PVT data and C_p data of Rivkin and co-workers[6,7] represent the major source of information for determining the thermodynamic surface of D_2O in the vicinity of the critical point, while the PVT data of Tsederberg et al.[9] and of Aleksandrov et al.[11] give valuable supplementary information. An experimental determination of the critical temperature and pressure was made by Blank in the Federal Republic of Germany.[8] A set of high-quality PVT data was recently obtained by Kell at the National Research Council in Canada[12]; most of these data are outside the critical region but a few points at 673.15 K are inside the region considered here. The temperatures T_{48} on IPTS-48 in Refs. 6–10 were converted to temperatures T_{68} on IPTS-68. At temperatures near the critical temperature the correction amounts to[5]

$$T_{68} = T_{48} + 0.077 \text{ K}. \quad (6)$$

The experimental PVT data of Rivkin and Akhundov[6] refer to a sample with 0.13% mole fraction of H_2O. We therefore applied an impurity correction to the data using the method described by Hastings et al.[13] The pseudocritical parameters of the gas with impurity are assumed to vary linearly with the mole fraction x of the impurity

$$T_c(x) = T_c(0)[1 + fx],$$
$$P_c(x) = P_c(0)[1 + gx], \quad (7)$$
$$V_c(x) = V_c(0)[1 + (f - g)x].$$

From an interpolation between the critical parameters of H_2O and D_2O we estimate

$$f = 0.00489, \quad g = 0.01697. \quad (8)$$

The correction can either be entered as a correction δP to the observed pressure P_{obs} at constant mass density ρ and constant temperature T,

$$P_{pure} = P_{obs} + \delta P \quad (9a)$$

with

$$\frac{\delta P}{P} = x\left[g + \left\{\left(1 - \frac{m_{H_2O}}{m_{D_2O}}\right) + (f - g)\right\}\frac{1}{PK_T}\right.$$
$$\left. - f\frac{T}{P}\left(\frac{\partial P}{\partial T}\right)_\rho\right], \quad (9b)$$

Table 1. Data sources.

Property	First author	Ref.	Year
PVT	Rivkin	6	1962–1963
C_p	Rivkin	7	1962–1963
P_c, T_c	Blank	8	1968
PVT	Tsederberg	9	1973
C_v	Amirkhanov	10	1973
PVT	Aleksandrov	11	1976
PVT	Kell	12	1982

or as a correction $\delta\rho$ to the observed density ρ_{obs} at constant pressure P and constant temperature T,

$$\rho_{pure} = \rho_{obs} + \delta\rho \qquad (10a)$$

with

$$\frac{\delta\rho}{\rho} = -x\left[\left(1 - \frac{m_{H_2O}}{m_{D_2O}}\right) + (f - g)\right.$$

$$\left. + PK_T\left\{g - f\frac{T}{P}\left(\frac{\partial P}{\partial T}\right)_\rho\right\}\right]. \qquad (10b)$$

Here $K_T = \rho^{-1}(\partial\rho/\partial P)_T$ is the isothermal compressibility, while m_{H_2O} and m_{D_2O} represent the molar mass of H_2O and D_2O, respectively. The same method for treating the impurity corrections was adopted by Hill and co-workers.[4]

The corrections δP and $\delta\rho$, thus calculated with the aid of a preliminary fit to the uncorrected data, are shown in Figs. 1 and 2. We verified that the final equation of state parameters were the same regardless of whether we applied the corrections to the pressure or the density. In practice, we found it most convenient to correct the pressures at given densities rather than the densities at given pressures. From Fig. 1 we see that the corrections δP are small.

We note that this method for treating impurity corrections assumes that the properties of the fluid with a given amount of impurity are related to those of the pure fluid by a law of corresponding states. This assumption is in disagreement with the theory of Griffiths and Wheeler which asserts that the asymptotic critical behavior of a mixture is analogous to that of a pure fluid only if an intensive variable is kept constant.[14] Hence, our method of correcting for the H_2O impurity cannot be strictly correct close to the critical point. However, since the impurity corrections are small we expect our method of estimating the magnitude of the corrections to be adequate in most of the range.

The PVT data of Tsederberg et al.[9] were similarly corrected for the presence of 0.2% mole fractions of H_2O. For the PVT data of Aleksandrov et al.[11] we used the corrected tables provided to us by Hill et al.[4] The PVT data provided
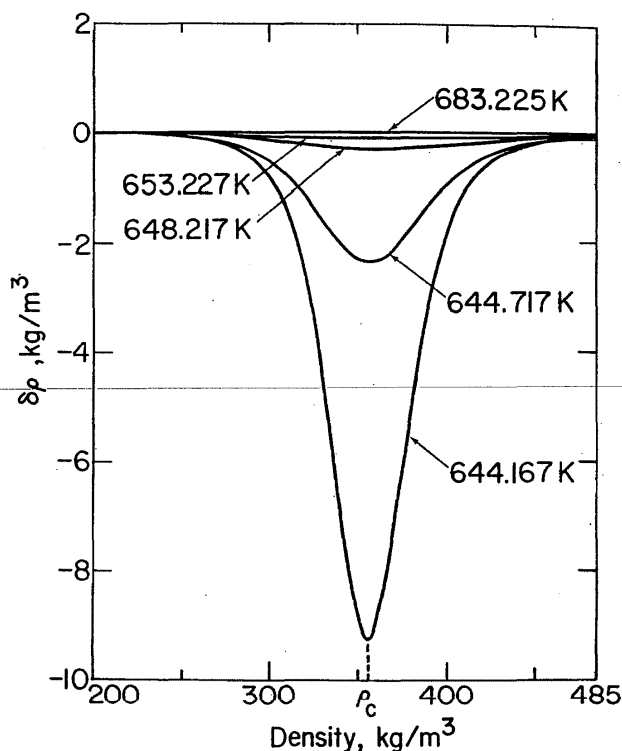
FIGURE 2. Correction $\delta\rho$ to the density at constant pressure and temperature due to 0.13% mole fractions of H_2O.

by Kell[12] correspond to pure D_2O. No attempt was made to correct the experimental specific-heat data for H_2O impurities.

We do not have reliable vapor-pressure data for D_2O near the critical temperature. The only data corresponding to the temperature range considered here are the data reported by Oliver and Grisard.[15] However, the investigators had difficulties in maintaining equilibrium near the critical temperature. Their data appear to yield an infinite slope of the vapor-pressure curve at the critical temperature in disagreement with the well-established principle of continuity of the slopes of the vapor-pressure curve and the critical isochore.[16] The vapor-pressure data of Oliver and Grisard were also omitted by Hill and MacMillan in their attempt to formulate a vapor-pressure equation for D_2O.[17]

4. Critical-Point Parameters

The problems associated with an accurate determination of the critical-point parameters for H_2O and D_2O will be discussed in a separate report.[18] A direct experimental observation of the critical temperature and pressure of D_2O has been reported by Blank[8] who finds $T_c = (643.89 \pm 0.03)$ K and $P_c = (21.659 \pm 0.003)$ MPa and these are the values adopted by Hill et al.[4] With the same apparatus Blank measured also the critical temperature and pressure of H_2O. A problem arises because the critical point of H_2O as reported by Blank is inconsistent with the critical point deduced indirectly from latent heat and PVT data as discussed in our previous paper, while it also differs from a recent direct experimental determination of the critical point reported by
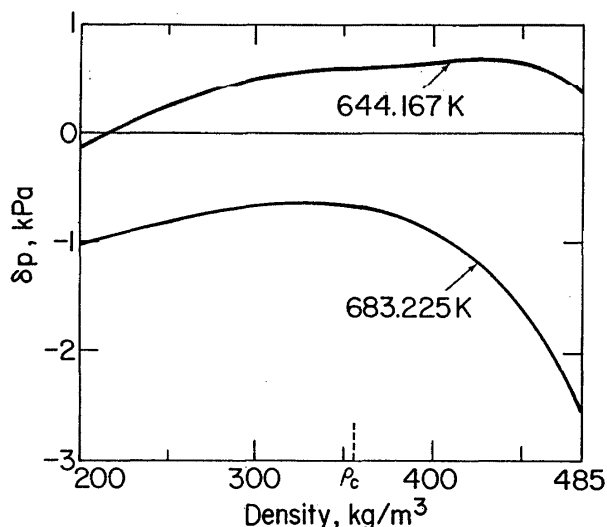

FIGURE 1. Correction δP to the pressure at constant density and temperature due to 0.13% mole fractions of H_2O.

Scheffler and co-workers[19]. As long as we do not know the origin of these discrepancies, we cannot decide whether the critical-point parameters reported by Blank for D_2O should be modified or not.

As an alternative one can attempt to deduce the critical-point parameters indirectly from an analysis of the PVT data in terms of a scaled equation of state, leaving the critical parameters as adjustable constants. However, while PVT data do allow us to determine the relation between pressure and temperature at the phase boundary or along the critical isochore, they do not provide a sensitive criterion for locating the critical temperature on this curve.[3]

As also noted by Hill et al., the critical-point parameters of Blank are reasonably consistent with the PVT data for D_2O. Hence in the absence of other information we adopt the critical temperature of Blank but assign to it an error estimate of ± 0.1 K:

$$T_c = 643.89 \text{ K}. \tag{11}$$

Given this value of T_c, we then determine the critical pressure P_c and the critical density ρ_c from a fit of our scaled equation of state to the experimental PVT data as further discussed in Sec. 5. We thus obtain for P_c,

$$P_c = 21.671 \text{ MPa} \tag{12}$$

with an intrinsic uncertainty of ± 0.005 MPa and an additional uncertainty propagated from the uncertainty δT_c in the critical temperature amounting to $(0.266\,\delta T_c)$ MPa if δT_c is expressed in K. We note that with T_c chosen at Blank's value (11) the critical pressure deduced from the PVT data of Rivkin and Akhundov is 0.01 MPa larger than the critical pressure reported by Blank. (A similar discrepancy between Blank's P_c value and the critical isochore of Rivkin's data was noted for H_2O.[3]) Our fit to the PVT data yields for ρ_c

$$\rho_c = 356.2 \text{ kg/m}^3 \tag{13}$$

with an estimated uncertainty of ± 2.5 kg/m^3.

5. Equation of State

The critical exponents β, δ, Δ_1 and the constant b^2 are expected to be universal, i.e., independent of the nature of the fluid. We therefore fixed these constants at the same values as used in the representation of the thermodynamic properties of H_2O in the critical region. As discussed in the previous paper, these values are in good agreement with the current theoretical predictions.[1-3]

On the other hand, the parameters a, k_0, k_1, c in the scaled contributions depend in principle on the system. Together with the critical parameters P_c, ρ_c and the pressure background parameters $\tilde{P}_1$, $\tilde{P}_2$, $\tilde{P}_3$, $\tilde{P}_{11}$, they can be determined by fitting the equation of state to the experimental PVT data. From this procedure the parameters a, k_0, k_1, c were found to be within error the same as those previously obtained for H_2O. This result indicates that the singular contributions to the thermodynamic properties of H_2O and D_2O in the critical region satisfy a corresponding-states principle to within currently available experimental precision. In our final procedure we therefore fixed all constants in the scaled contributions at the same values as earlier adopted for H_2O

and fitted the equation of state to the experimental PVT data to determine the optimum values of the critical pressure and density and of the pressure background parameters $\tilde{P}_1$, $\tilde{P}_2$, $\tilde{P}_3$, $\tilde{P}_{11}$. In determining $\tilde{P}_{11}$ we actually treated the slope of the coexistence curve diameter at a temperature slightly below the critical temperature as an adjustable parameter and converted this slope into the corresponding value of $\tilde{P}_{11}$. The values of all constants are given in Appendix B. In fitting the equation of state to the experimental PVT data we assigned absolute weights to these data by propagation of error on the basis of the error estimates presented in Table 2. With these error estimates the equation fits the experimental PVT data

Table 2. Error estimates assigned to PVT data.

First author	Ref.	σ_P	σ_T	σ_ρ
Rivkin	6	0.001 MPa	0.02 K	0.05%
Tsederberg	9	0.05%	0.03 K	0.06%
Aleksandrov	11	0.05%	0.03 K	0.06%
Kell	12	0.001 MPa	0.02 K	0.01%

with a statistic chi-square of 1.99 in the range specified by Eq. (5).

A comparison between the experimental PVT data and the values calculated from our equation is presented in Figs. 3 and 4 in the form of pressure deviations as a function of density along various isotherms. The total estimated errors in the pressure propagated from the error estimates in Table 2 are indicated by vertical bars. We conclude that the equation yields a satisfactory representation of the experimental PVT data.
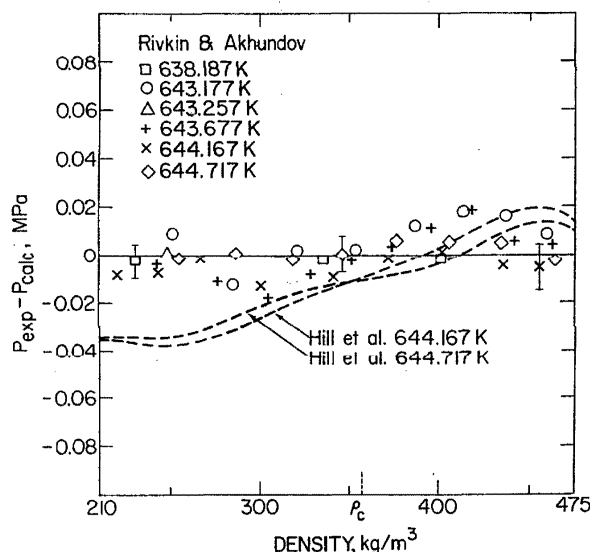
FIGURE 3. Deviations of the experimental pressure data from the calculated values in the temperature range 638.187 K<T<644.717 K. The dashed curves indicate the values calculated from the equation of Hill et al. (Ref. 4).
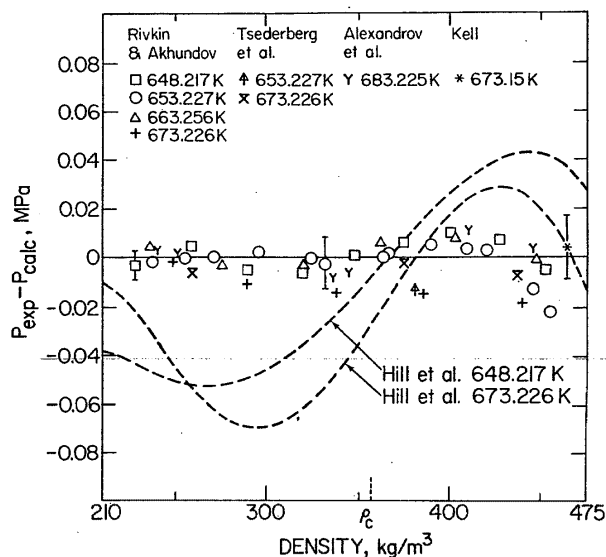
FIGURE 4. Deviations of the experimental pressure data from the calculated values in the temperature range 648.217 K⩽T⩽683.225 K. The dashed curves indicate the values calculated from the equation of Hill *et al.* (Ref. 4).

6. Specific Heat

The constants $\bar{\mu}_c$, $\bar{\mu}_1$, $\bar{\mu}_2$, $\bar{\mu}_3$ in the fundamental equation represent noncritical contributions to the caloric properties. The constants $\bar{\mu}_2$ and $\bar{\mu}_3$ enter into the equations for the specific heat and, hence, can be determined by fitting our fundamental equation to the experimental specific heat data. For this purpose we consider the extensive set of experimental C_p data obtained by Rivkin and Egorov as a function of
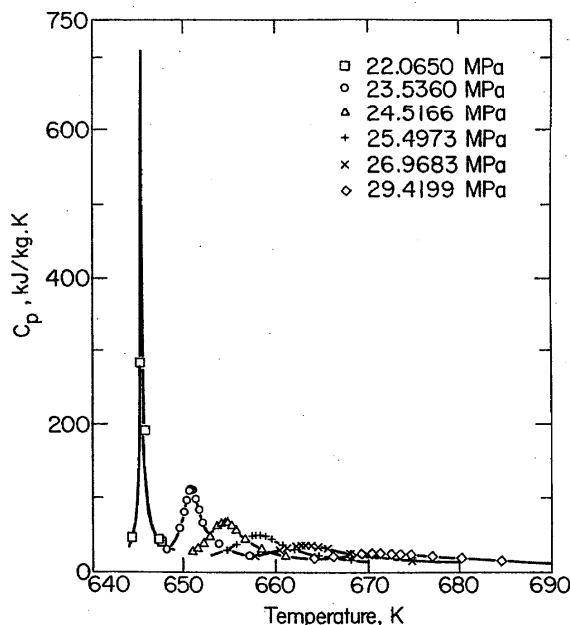
temperature along various isobars.[7] Actually the data were taken at enthalpy increments ΔH in given finite temperature intervals ΔT. When our fundamental equation is fitted to the data for ΔH over the experimental temperature intervals we obtain

$$\bar{\mu}_2 = -19.004, \quad \bar{\mu}_3 = -6.292. \tag{14}$$

A comparison between the experimental and calculated C_p values is presented in Fig. 5. Again the values plotted in this figure are the ratios $\Delta H / \Delta T$; since the temperature intervals ΔT are small and smoothly varying, smooth curves can be drawn through the calculated values of $\Delta H / \Delta T$. Figure 5 confirms that the equation reproduces the experimental maxima in C_p.

In Fig. 6 the comparison is made with the C_p values plotted as functions of density, rather than temperature. Omitting the data at the 22.0650 MPa isobar closest to the critical pressure we make the comparison on an expanded scale in Fig. 7. The plots reveal a small mismatch between the densities calculated for the experimental data points and those corresponding to the predicted C_p values. We do not know the origin of this small lack of consistency between the PVT data and the C_p data, but as discussed in our previous paper,[3] such effects can be explained in part by the fact that data near the critical point become very sensitive to uncertainties in the temperature scale or pressure scale. The mismatch disappears if we lower the temperature scale of the C_p data with respect to that of the PVT data by 0.11 K, a shift somewhat larger than the shift of 0.05 K found between the temperature scales of the C_p data and PVT data for H_2O.[3] If

FIGURE 5. The specific heat at constant pressure at various pressures as a function of temperature. The data points are those of Rivkin and Egorov (Ref. 7). The curves represent the values calculated from our equation.

FIGURE 6. The specific heat at constant pressure at various pressures as a function of density. The data points are those of Rivkin and Egorov (Ref. 7) and the curves represent the values calculated from our equation.

FIGURE 7. The specific heat at constant pressure at various pressures as a function of density. The data points are those of Rivkin and Egorov (Ref. 7) and the curves represent the values calculated from our equation.
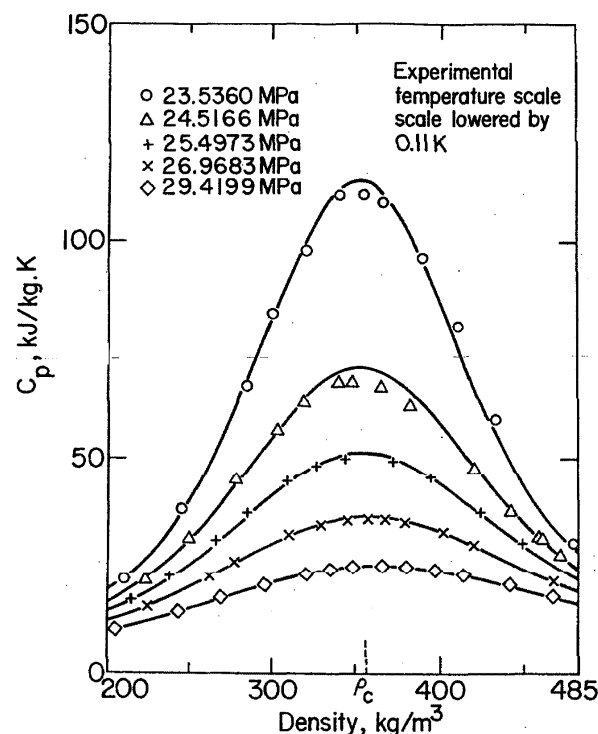
FIGURE 9. The specific heat at constant pressure at various pressures as a function of density. The data points correspond to those of Rivkin and Egorov (Ref. 7) and the curves represent the values calculated from our equation if the temperature scale of the experimental C_p data is lowered by 0.11 K.

FIGURE 8. The specific heat at constant pressure at various pressures as a function of density. The data points correspond to those of Rivkin and Egorov (Ref. 7) and the curves represent the values calculated from our equation, if the temperature scale of the experimental C_p data is lowered by 0.11 K.

we accept such a shift and fit the fundamental equation again to the data we obtain

$$\bar{\mu}_2 = -21.552, \quad \bar{\mu}_3 = +17.308. \tag{15}$$

These are the values adopted in our final fundamental equation. A comparison between the C_p values thus calculated and the data is presented in Figs. 8 and 9. Figure 8 is to be compared with Fig. 6 and Fig. 9 with Fig. 7. The quality of the agreement is comparable to that found earlier for the C_p of H_2O.[3] We emphasize that the coefficients $\bar{\mu}_2$ and $\bar{\mu}_3$ specify only an analytic background behavior and the calculated maxima in C_p are determined by derivatives of the equation of state fitted to the PVT data. Hence, the comparison with the C_p maxima provides a stringent test of the quality of the equation of state.

Experimental data for the specific heat at constant volume C_v for D_2O have been reported by Amirkhanov and co-workers.[10] The data were obtained as a function of temperature at various isochores including two isochores corresponding to $\rho = 344.8$ kg/m^3 and $\rho = 303.0$ kg/m^3 that are within the critical region considered here. A comparison between the C_v data of Amirkhanov et al. and the values calculated from our fundamental equation is presented in Fig. 10. In analyzing the C_v data we encountered some serious problems. In particular the C_v data of Amirkhanov imply a location of the phase boundary at temperatures significantly higher than inferred by us from the PVT data of Rivkin and Akhundov. At $\rho = 344.8$ kg/m^3 the discrepancy is 0.55 K and at $\rho = 303.0$ kg/m^3 as large as 0.92 K. We
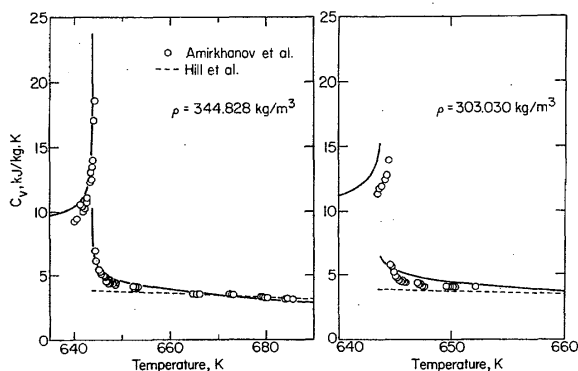
FIGURE 10. The specific heat at constant volume along two different isochores as a function of temperature. The data points are those of Amirkhanov and co-workers (Ref. 10). The solid curves represent the values calculated from our equation and the dashed curves represent values calculated from the equation of Hill et al. (Ref. 4).

conclude that the C_v data of Amirkhanov et al. are inconsistent with the high-quality PVT data of Rivkin and Akhundov.

7. Comparison with Equation of Hill et al.

Recently Hill, MacMillan, and Lee formulated a comprehensive fundamental equation for the thermodynamic properties of D₂O.[4] Their formulation covers pressures up to 100 MPa and temperatures up to 600 °C by a single equation. It represents a major advance in the characterization of the thermodynamic properties of D₂O and supersedes previous formulations. The equation has been submitted to the International Association for the Properties of Steam for possible adoption as an internationally agreed upon formulation for the thermodynamic properties of D₂O.

The formulation of Hill et al. treats the Helmholtz free energy as an analytic function of its variables. As a consequence the formulation does not incorporate the nonanalytic asymptotic scaling behavior of the thermodynamic properties near the critical point predicted by the theory. Having completed an analysis of the behavior of the thermodynamic properties of D₂O in the critical region, we are now in a position to investigate to what extent the formulation of Hill et al. reproduces the observed singular thermodynamic behavior of D₂O in the critical region.

In Figs. 3 and 4 we have included curves indicating the differences between the pressures calculated from the formulation of Hill et al. and the pressures calculated from our revised and extended fundamental equation. It is seen that the equation of state of Hill et al. shows systematic departures well outside the accuracy of the experimental PVT data.

A comparison between the equation of Hill et al. and the C_v data of Amirkhanov et al. in the one-phase region above the critical temperature is included in Fig. 10. Since the equation is analytic, it does not accommodate a divergent C_v at the critical point and the calculated C_v remains a slowly varying function of temperature in the critical region. Since Hill et al. did not formulate C_v in the two-phase region, we did not make a comparison of this equation with the C_v data in the two-phase region below the critical temperature.
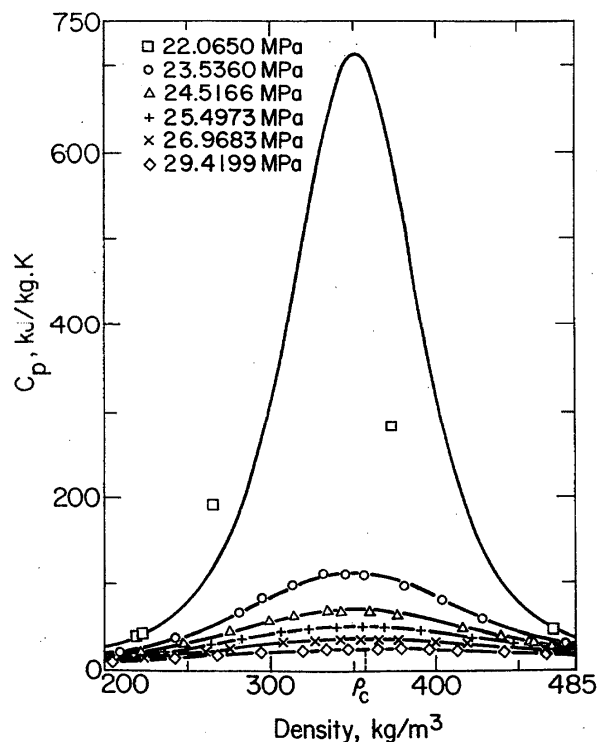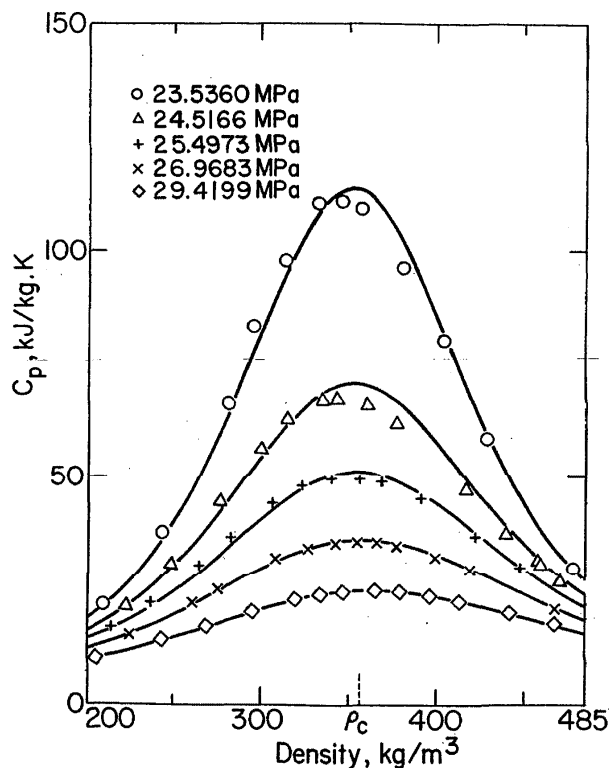

FIGURE 11. The specific heat at constant pressure at various pressures as a function of density. The data points are those of Rivkin and Egorov (Ref. 7) and the curves represent the values calculated from the equation of Hill et al. (Ref. 4)

A comparison between the equation of Hill et al. and the C_p data of Rivkin and Egorov in the critical region is presented in Figs. 11 and 12. It is seen that the equation does not reproduce the experimental maxima of C_p near the criti-
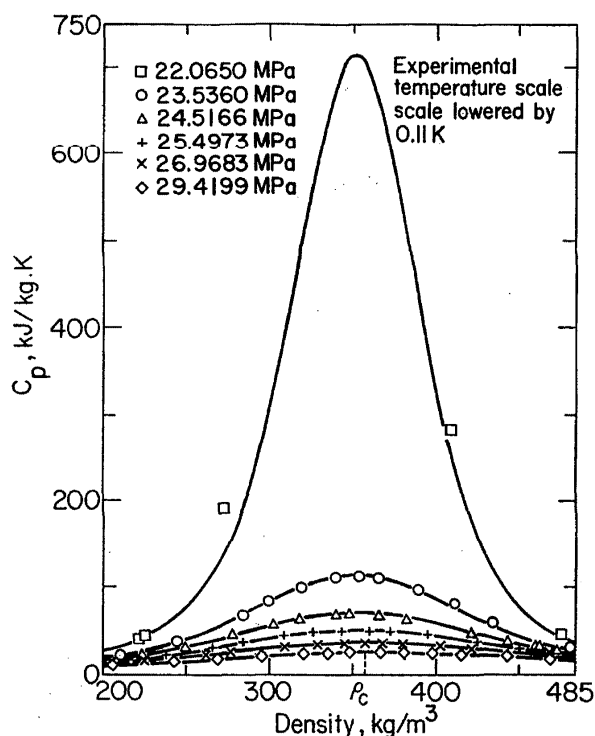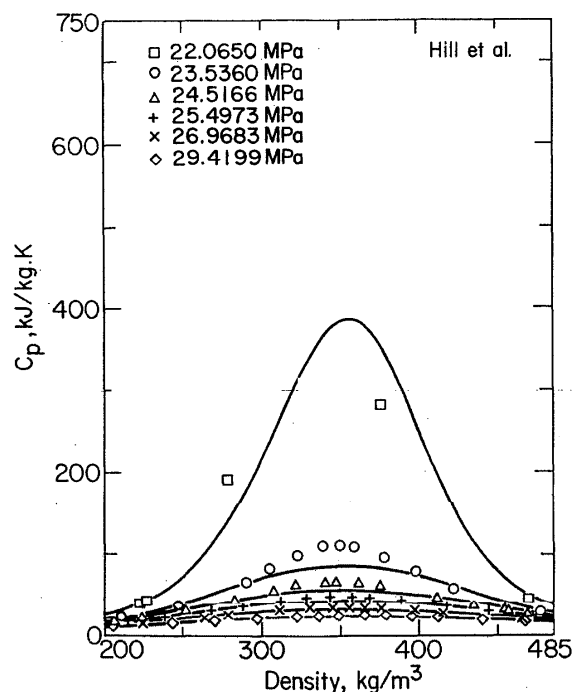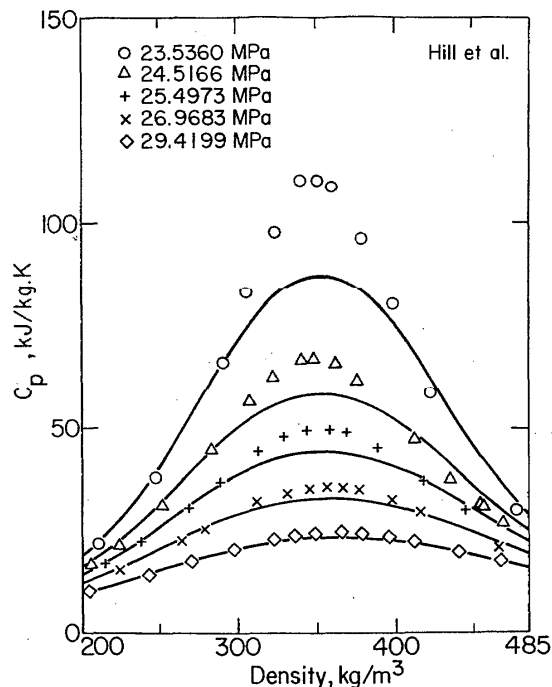

FIGURE 12. The specific heat at constant pressure at various pressures as a function of density. The data points are those of Rivkin and Egorov (Ref. 7) and the curves represent the values calculated from the equation of Hill et al. (Ref. 4).

cal point. On comparing Fig. 11 with Figs. 6 or 8 and on comparing Fig. 12 with Figs. 7 or 9 we conclude that our scaled fundamental equation yields a significantly improved representation of the thermodynamic properties of D_2O in the critical region.

8. Thermodynamic Tables

To make our fundamental equation complete we need to adopt values for $\bar{\mu}_c$ and $\bar{\mu}_1$ which are related to the zero points of energy and entropy. We determine these zero-point constants by identifying the energy and entropy of our surface at $T = 683.15$ K and $\rho = 220$ kg/m³ with the energy and entropy of the global surface of Hill and co-workers.[4] At this point at the edge of our surface the pressures calculated from our equation and from the global surface of Hill et al. agree within 0.02%, while the values of the specific heat at constant pressure differ by 2.8%. The condition that the absolute values of the energy and entropy coincide with those calculated from the global surface of Hill et al. at this point yields

$$\bar{\mu}_c = -11.948, \quad \bar{\mu}_1 = -24.219. \tag{16}$$

Tables of the pressure, enthalpy, entropy, energy, specific heats, and speed of sound at closely spaced densities as a function of temperature, as well as the saturation properties as a function of temperature and as a function of pressure, have been constructed. These tables, derived from our fundamental equation, are presented in Appendix C.

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Appendix A. Definition of the Scaled Fundamental Equation for the Critical Region

Reduced thermodynamic variables

$$\widetilde{T} = -\frac{T_c}{T}, \quad \widetilde{\mu} = \frac{\mu}{T} \cdot \frac{\rho_c T_c}{P_c}, \quad \widetilde{P} = \frac{P}{T} \cdot \frac{T_c}{P_c}. \tag{A1}$$

Fundamental equations

$$\Delta\widetilde{T} = \widetilde{T} + 1, \quad \Delta\widetilde{\mu} = \widetilde{\mu} - \widetilde{\mu}_0(\widetilde{T}), \tag{A2}$$

$$\widetilde{P} = \widetilde{P}_0(\widetilde{T}) + \Delta\widetilde{\mu} + \widetilde{P}_{11}\Delta\widetilde{\mu}\Delta\widetilde{T} + \Delta\widetilde{P}, \tag{A3}$$

with

$$\widetilde{\mu}_0(\widetilde{T}) = \widetilde{\mu}_c + \sum_{j=1}^{3} \widetilde{\mu}_j(\Delta\widetilde{T})^j, \tag{A4}$$

$$\widetilde{P}_0(\widetilde{T}) = 1 + \sum_{j=1}^{3} \widetilde{P}_j(\Delta\widetilde{T})^j. \tag{A5}$$

Critical exponents

$$\alpha_0 = \alpha, \quad \beta_0 = \beta, \quad \gamma_0 = \gamma, \tag{A6a}$$

$$\alpha_1 = \alpha - \Delta_1, \quad \beta_1 = \beta + \Delta_1, \quad \gamma_1 = \gamma - \Delta_1, \tag{A6b}$$

with

$$2 - \alpha = \beta(\delta + 1), \quad \gamma = \beta(\delta - 1). \tag{A7}$$

Parametric equations for singular term $\Delta\widetilde{P}$

$$\Delta\widetilde{\mu} = r^{\beta\delta}a\theta(1 - \theta^2), \tag{A8}$$

$$\Delta\widetilde{T} = r(1 - b^2\theta^2) - c\Delta\widetilde{\mu}, \tag{A9}$$

$$\Delta\widetilde{P} = \sum_{i=0}^{1} r^{2-\alpha_i}ak_i(p_{0i} + p_{2i}\theta^2 + p_{4i}\theta^4) \tag{A10}$$

with

$$p_{0i} = +\frac{\beta\delta - 3\beta_i - b^2\alpha_i\gamma_i}{2b^4(2 - \alpha_i)(1 - \alpha_i)\alpha_i},$$

$$p_{2i} = -\frac{\beta\delta - 3\beta_i - b^2\alpha_i(2\beta\delta - 1)}{2b^2(1 - \alpha_i)\alpha_i}, \tag{A11}$$

$$p_{4i} = +\frac{2\beta\delta - 3}{2\alpha_i}.$$

The resulting equations for the other derived thermodynamic properties are given in Appendix A of Ref. 3.

Appendix B. Parameters for the Thermodynamic Surface of D$_2$O in the Critical Region

Table B1. Parameter values.[g]

Critical parameters:	$T_c = 643.89$ K[a]
	$\rho_c = 356.238$ kg/m^3 [b]
	$P_c = 21.6713$ MPa[b]
Critical exponents:	$\beta = 0.325$[c,d]
	$\delta = 4.82$[c,d]
	$\Delta_1 = 0.50$[c,d]
Parameters in scaling functions:	$a = +23.667$[d]
	$k_0 = +1.4403$[d]
	$k_1 = +0.2942$[d]
	$c = -0.01776$[d]
	$b^2 = +1.3757$[d]
Pressure background parameters:	$\tilde{P}_1 = +6.9107$[b]
	$\tilde{P}_2 = -25.2370$[b]
	$\tilde{P}_3 = +8.6180$[b]
	$\tilde{P}_{11} = +0.54764$[b]
Caloric background parameters:	$\tilde{\mu}_c = -11.948$[e]
	$\tilde{\mu}_1 = -24.219$[e]
	$\tilde{\mu}_2 = -21.552$[f]
	$\tilde{\mu}_3 = +17.308$[f]

[a] From Blank (Ref. 8).
[b] From fit to PVT data.
[c] Fixed from theory.
[d] Same as for H$_2$O.
[e] From identification of our surface with that of Hill et al. (Ref. 4) at $T = 683.15$ K and $\rho = 220$ kg/m^3.
[f] From fit to C_p data.
[g] Note: The number of decimals given exceeds the number of significant decimals so as to retain precision in complex calculations.

Appendix C: Tables of Thermodynamic Properties of D$_2$O in the Critical Region

Table C1. Thermodynamic properties along isochores at regular temperature increments.

Table C2. Properties of coexisting phases at regular temperature increments.

Table C3. Properties of coexisting phases at regular pressure increments.

The uncertainty of the tables is generally a few units in the last decimal given, but in special cases, such as for density values near T_c and P_c and C_p values in the region where this quantity varies rapidly, the uncertainty will be much larger.

Table C1. Thermodynamic properties along isochores at regular temperature increments.

Temp.	Pressure	Density	Internal Energy	Enthalpy	Entropy	C_p	C_v	Velocity	Phase Region
K	MPa	kg/m^3	kJ/kg	kJ/kg	kJ/kg.K	kJ/kg.K		m/s	
638.0	20.173	220.0	2065.8	2157.5	4.4896		13.29		2
639.0	20.419	220.0	2079.2	2172.0	4.5106		13.54		2
640.0	20.656	220.0	2091.2	2185.1	4.5293	84.4	4.91	318.0	1
641.0	20.844	220.0	2096.1	2190.8	4.5369	71.9	4.77	321.5	1
642.0	21.029	220.0	2100.8	2196.4	4.5442	63.1	4.65	324.7	1
643.0	21.214	220.0	2105.4	2201.8	4.5514	56.3	4.55	327.8	1
644.0	21.397	220.0	2109.9	2207.1	4.5584	51.0	4.46	330.7	1
645.0	21.580	220.0	2114.3	2212.4	4.5653	46.7	4.38	333.5	1
650.0	22.481	220.0	2135.4	2237.6	4.5978	33.4	4.07	346.6	1
655.0	23.369	220.0	2155.1	2261.3	4.6280	26.2	3.83	358.9	1
660.0	24.246	220.0	2173.8	2284.0	4.6564	21.8	3.64	370.6	1
665.0	25.116	220.0	2191.5	2305.7	4.6832	18.7	3.47	381.9	1
670.0	25.979	220.0	2208.5	2326.6	4.7086	16.5	3.32	393.0	1
675.0	26.837	220.0	2224.8	2346.7	4.7328	14.8	3.19	403.9	1
680.0	27.691	220.0	2240.4	2366.3	4.7560	13.4	3.07	414.7	1
685.0	28.541	220.0	2255.5	2385.2	4.7781	12.3	2.97	425.4	1
638.0	20.173	240.0	2014.4	2098.5	4.3970		12.54		2
639.0	20.419	240.0	2027.0	2112.1	4.4168		12.77		2
640.0	20.668	240.0	2040.0	2126.1	4.4370		13.07		2
641.0	20.921	240.0	2053.2	2140.4	4.4577		13.49		2
642.0	21.144	240.0	2061.6	2149.7	4.4708	121.8	5.03	309.0	1
643.0	21.347	240.0	2066.5	2155.5	4.4785	98.6	4.86	313.2	1
644.0	21.548	240.0	2071.3	2161.1	4.4859	83.4	4.73	316.9	1
645.0	21.747	240.0	2076.0	2166.6	4.4931	72.6	4.61	320.4	1
650.0	22.731	240.0	2098.0	2192.7	4.5271	44.9	4.21	335.6	1
655.0	23.700	240.0	2118.3	2217.0	4.5582	33.0	3.93	349.1	1
660.0	24.659	240.0	2137.4	2240.1	4.5872	26.3	3.71	361.8	1
665.0	25.609	240.0	2155.5	2262.2	4.6146	22.0	3.53	374.0	1
670.0	26.554	240.0	2172.7	2283.4	4.6404	18.9	3.37	385.9	1
675.0	27.494	240.0	2189.2	2303.8	4.6650	16.7	3.24	397.5	1
680.0	28.430	240.0	2205.1	2323.6	4.6884	15.0	3.11	409.0	1
685.0	29.363	240.0	2220.4	2342.7	4.7107	13.6	2.99	420.2	1
638.0	20.173	260.0	1970.9	2048.5	4.3187		11.90		2
639.0	20.419	260.0	1982.9	2061.4	4.3375		12.11		2
640.0	20.668	260.0	1995.1	2074.6	4.3566		12.39		2
641.0	20.921	260.0	2007.7	2088.2	4.3762		12.77		2
642.0	21.177	260.0	2020.7	2102.2	4.3966		13.38		2
643.0	21.415	260.0	2030.1	2112.5	4.4112	210.8	5.28	297.2	1
644.0	21.633	260.0	2035.3	2118.5	4.4192	152.7	5.04	302.7	1
645.0	21.849	260.0	2040.2	2124.3	4.4269	120.9	4.86	307.3	1
650.0	22.911	260.0	2063.1	2151.2	4.4621	60.8	4.33	325.4	1
655.0	23.957	260.0	2083.9	2176.0	4.4940	41.2	4.01	340.4	1
660.0	24.993	260.0	2103.3	2199.3	4.5236	31.3	3.77	354.2	1
665.0	26.023	260.0	2121.7	2221.8	4.5513	25.4	3.58	367.3	1
670.0	27.047	260.0	2139.2	2243.2	4.5775	21.5	3.41	380.0	1
675.0	28.068	260.0	2155.9	2263.8	4.6023	18.7	3.27	392.3	1
680.0	29.085	260.0	2171.9	2283.7	4.6259	16.5	3.13	404.4	1
685.0	30.100	260.0	2187.2	2303.0	4.6485	14.9	3.01	416.3	1
638.0	20.173	280.0	1933.6	2005.7	4.2515		11.35		2
639.0	20.419	280.0	1945.1	2018.0	4.2695		11.54		2
640.0	20.668	280.0	1956.7	2030.5	4.2877		11.80		2
641.0	20.921	280.0	1968.7	2043.4	4.3064		12.16		2
642.0	21.177	280.0	1981.1	2056.7	4.3257		12.71		2
643.0	21.437	280.0	1994.3	2070.8	4.3463		13.83		2
644.0	21.675	280.0	2001.6	2079.0	4.3577	325.6	5.42	287.3	1
645.0	21.906	280.0	2006.9	2085.1	4.3658	214.7	5.13	294.1	1
650.0	23.039	280.0	2030.5	2112.8	4.4023	81.1	4.44	316.2	1
655.0	24.158	280.0	2051.7	2138.0	4.4349	50.2	4.08	332.9	1
660.0	25.269	280.0	2071.4	2161.7	4.4648	36.5	3.82	347.9	1
665.0	26.375	280.0	2090.0	2184.2	4.4928	28.8	3.61	361.9	1
670.0	27.478	280.0	2107.6	2205.7	4.5192	23.9	3.44	375.4	1
675.0	28.578	280.0	2124.4	2226.5	4.5442	20.4	3.28	388.4	1
680.0	29.676	280.0	2140.5	2246.5	4.5679	17.9	3.15	401.2	1
685.0	30.773	280.0	2155.9	2265.8	4.5905	16.0	3.03	413.7	1

Table C1.   Thermodynamic properties along isochores at regular temperature increments (continued).

Temp.	Pressure	Density	Internal Energy	Enthalpy	Entropy	C_p	C_v	Velocity of sound	Phase Region
K	MPa	kg/m³	kJ/kg	kJ/kg	kJ/kg.K	kJ/kg.K		m/s	
638.0	20.173	300.0	1901.3	1968.5	4.1934		10.88		2
639.0	20.419	300.0	1912.3	1980.3	4.2105		11.06		2
640.0	20.668	300.0	1923.4	1992.3	4.2280		11.29		2
641.0	20.921	300.0	1934.9	2004.6	4.2459		11.62		2
642.0	21.177	300.0	1946.7	2017.3	4.2644		12.14		2
643.0	21.437	300.0	1959.3	2030.8	4.2839		13.18		2
644.0	21.693	300.0	1970.3	2042.6	4.3010	860.5	5.93	269.6	1
645.0	21.936	300.0	1975.9	2049.0	4.3097	392.8	5.39	281.0	1
650.0	23.134	300.0	2000.2	2077.3	4.3472	103.7	4.51	308.3	1
655.0	24.322	300.0	2021.7	2102.7	4.3801	58.9	4.11	326.8	1
660.0	25.504	300.0	2041.5	2126.5	4.4103	41.1	3.84	343.0	1
665.0	26.685	300.0	2060.2	2149.1	4.4385	31.7	3.63	358.0	1
670.0	27.865	300.0	2077.8	2170.7	4.4650	25.8	3.45	372.2	1
675.0	29.043	300.0	2094.7	2191.5	4.4900	21.9	3.29	386.0	1
680.0	30.222	300.0	2110.8	2211.5	4.5138	19.0	3.15	399.4	1
685.0	31.400	300.0	2126.2	2230.9	4.5364	16.9	3.03	412.5	1
638.0	20.173	320.0	1873.0	1936.1	4.1424		10.46		2
639.0	20.419	320.0	1883.6	1947.4	4.1590		10.63		2
640.0	20.668	320.0	1894.3	1958.9	4.1757		10.85		2
641.0	20.921	320.0	1905.3	1970.7	4.1929		11.16		2
642.0	21.177	320.0	1916.7	1982.8	4.2106		11.64		2
643.0	21.437	320.0	1928.7	1995.7	4.2294		12.61		2
644.0	21.699	320.0	1941.3	2009.1	4.2489	2994.1	6.61	249.1	1
645.0	21.952	320.0	1947.3	2015.9	4.2582	678.5	5.60	269.0	1
650.0	23.208	320.0	1971.9	2044.5	4.2963	123.4	4.54	301.9	1
655.0	24.461	320.0	1993.5	2070.0	4.3294	65.4	4.12	322.3	1
660.0	25.714	320.0	2013.4	2093.7	4.3596	44.3	3.84	339.7	1
665.0	26.968	320.0	2032.0	2116.3	4.3878	33.5	3.63	355.7	1
670.0	28.223	320.0	2049.7	2137.9	4.4143	27.1	3.45	370.7	1
675.0	29.481	320.0	2066.5	2158.7	4.4393	22.8	3.29	385.2	1
680.0	30.740	320.0	2082.4	2178.7	4.4630	19.7	3.15	399.2	1
685.0	32.001	320.0	2098.1	2198.1	4.4856	17.4	3.02	412.9	1
638.0	20.173	340.0	1848.1	1907.4	4.0975		10.10		2
639.0	20.419	340.0	1858.2	1918.3	4.1135		10.25		2
640.0	20.668	340.0	1868.6	1929.4	4.1296		10.46		2
641.0	20.921	340.0	1879.2	1940.7	4.1462		10.74		2
642.0	21.177	340.0	1890.1	1952.4	4.1632		11.20		2
643.0	21.437	340.0	1901.7	1964.8	4.1813		12.11		2
644.0	21.700	340.0	1914.6	1978.4	4.2013	11182.9	7.33	228.9	1
645.0	21.962	340.0	1920.8	1985.4	4.2110	960.4	5.69	259.6	1
650.0	23.271	340.0	1945.6	2014.0	4.2492	133.3	4.53	297.6	1
655.0	24.587	340.0	1967.1	2039.4	4.2821	67.9	4.11	319.7	1
660.0	25.909	340.0	1986.9	2063.1	4.3123	45.3	3.83	338.3	1
665.0	27.237	340.0	2005.4	2085.6	4.3403	34.1	3.61	355.2	1
670.0	28.570	340.0	2023.0	2107.1	4.3667	27.4	3.43	371.0	1
675.0	29.907	340.0	2039.8	2127.8	4.3916	23.0	3.28	386.1	1
680.0	31.247	340.0	2055.8	2147.7	4.4152	19.8	3.14	400.8	1
685.0	32.591	340.0	2071.2	2167.0	4.4377	17.5	3.01	415.0	1
638.0	20.173	360.0	1825.9	1881.9	4.0576		9.77		2
639.0	20.419	360.0	1835.7	1892.4	4.0730		9.92		2
640.0	20.668	360.0	1845.7	1903.1	4.0887		10.11		2
641.0	20.921	360.0	1856.0	1914.1	4.1046		10.38		2
642.0	21.177	360.0	1866.5	1925.4	4.1211		10.81		2
643.0	21.437	360.0	1877.7	1937.3	4.1385		11.66		2
644.0	21.701	360.0	1890.3	1950.5	4.1580	16268.4	7.41	219.0	1
645.0	21.969	360.0	1896.4	1957.5	4.1676	974.1	5.62	254.4	1
650.0	23.331	360.0	1920.9	1985.7	4.2054	128.7	4.48	295.7	1
655.0	24.711	360.0	1942.2	2010.8	4.2380	65.7	4.07	319.4	1
660.0	26.104	360.0	1961.8	2034.3	4.2678	43.9	3.79	339.0	1
665.0	27.507	360.0	1980.2	2056.6	4.2956	33.1	3.58	356.7	1
670.0	28.919	360.0	1997.7	2078.0	4.3218	26.7	3.41	373.3	1
675.0	30.337	360.0	2014.3	2098.6	4.3465	22.4	3.25	389.1	1
680.0	31.762	360.0	2030.2	2118.4	4.3700	19.4	3.12	404.3	1
685.0	33.192	360.0	2045.5	2137.7	4.3924	17.2	2.99	419.1	1

Table C1. Thermodynamic properties along isochores at regular temperature increments (continued).

Temp.	Pressure	Density	Internal Energy	Enthalpy	Entropy	C_p	C_v	Velocity of sound	Phase region
K	MPa	kg/m³	kJ/kg	kJ/kg	kJ/kg.K	kJ/kg.K		m/s	
630.0	20.173	380.0	1806.0	1859.1	4.0219		9.48		2
639.0	20.419	380.0	1815.6	1869.3	4.0368		9.62		2
640.0	20.668	380.0	1825.3	1879.7	4.0520		9.79		2
641.0	20.921	380.0	1835.2	1890.3	4.0675		10.05		2
642.0	21.177	380.0	1845.4	1901.2	4.0834		10.45		2
643.0	21.437	380.0	1856.2	1912.6	4.1002		11.27		2
644.0	21.701	380.0	1868.0	1925.1	4.1185	5312.8	6.65	224.1	1
545.0	21.978	380.0	1873.8	1931.7	4.1276	688.6	5.40	254.3	1
550.0	23.395	380.0	1897.6	1959.2	4.1643	111.4	4.39	296.7	1
655.0	24.843	380.0	1918.5	1983.9	4.1964	59.2	4.01	321.5	1
660.0	26.310	380.0	1937.9	2007.1	4.2258	40.5	3.75	342.1	1
665.0	27.793	380.0	1956.1	2029.2	4.2533	30.9	3.54	360.6	1
670.0	29.286	380.0	1973.4	2050.5	4.2792	25.2	3.37	377.8	1
675.0	30.790	380.0	1989.9	2070.9	4.3037	21.3	3.22	394.2	1
680.0	32.302	380.0	2005.7	2090.7	4.3270	18.6	3.09	409.9	1
685.0	33.822	380.0	2020.8	2109.8	4.3492	16.5	2.97	425.2	1
638.0	20.173	400.0	1788.2	1838.6	3.9897		9.22		2
639.0	20.419	400.0	1797.5	1848.5	4.0043		9.34		2
640.0	20.668	400.0	1806.9	1858.6	4.0190		9.51		2
641.0	20.921	400.0	1816.5	1868.8	4.0340		9.76		2
642.0	21.177	400.0	1826.4	1879.4	4.0495		10.14		2
643.0	21.437	400.0	1836.9	1890.5	4.0658		10.91		2
644.0	21.704	400.0	1847.3	1901.6	4.0819	1162.0	5.74	238.2	1
645.0	21.991	400.0	1852.6	1907.6	4.0902	379.3	5.09	259.5	1
650.0	23.473	400.0	1875.6	1934.3	4.1257	88.2	4.28	300.9	1
655.0	24.995	400.0	1896.0	1958.5	4.1570	50.5	3.93	326.5	1
660.0	26.542	400.0	1915.1	1981.4	4.1859	35.7	3.69	347.9	1
665.0	28.109	400.0	1933.0	2003.3	4.2130	27.9	3.50	367.0	1
670.0	29.690	400.0	1950.1	2024.3	4.2386	23.1	3.33	384.8	1
675.0	31.284	400.0	1966.4	2044.6	4.2628	19.8	3.19	401.7	1
680.0	32.888	400.0	1982.0	2064.2	4.2859	17.4	3.06	417.9	1
685.0	34.502	400.0	1997.0	2083.3	4.3079	15.5	2.94	433.6	1
638.0	20.173	420.0	1772.0	1820.1	3.9606		8.98		2
639.0	20.419	420.0	1781.1	1829.7	3.9748		9.10		2
640.0	20.668	420.0	1790.2	1839.4	3.9891		9.26		2
641.0	20.921	420.0	1799.6	1849.4	4.0038		9.49		2
642.0	21.177	420.0	1809.3	1859.7	4.0188		9.85		2
643.0	21.437	420.0	1819.4	1870.5	4.0346		10.58		2
644.0	21.716	420.0	1827.6	1879.3	4.0473	339.8	5.08	255.1	1
645.0	22.017	420.0	1832.5	1884.9	4.0549	191.9	4.76	270.0	1
650.0	23.576	420.0	1854.5	1910.6	4.0889	65.9	4.15	308.9	1
655.0	25.181	420.0	1874.4	1934.4	4.1194	41.3	3.84	334.8	1
660.0	26.816	420.0	1893.1	1956.9	4.1478	30.6	3.62	356.6	1
665.0	28.474	420.0	1910.7	1978.5	4.1745	24.5	3.45	376.2	1
670.0	30.149	420.0	1927.6	1999.3	4.1997	20.7	3.29	394.4	1
675.0	31.840	420.0	1943.7	2019.5	4.2236	18.0	3.15	411.7	1
680.0	33.542	420.0	1959.1	2039.0	4.2464	15.9	3.03	428.3	1
685.0	35.256	420.0	1974.0	2057.9	4.2682	14.4	2.91	444.4	1
638.0	20.173	440.0	1757.3	1803.2	3.9342		8.77		2
639.0	20.419	440.0	1766.2	1812.6	3.9480		8.88		2
640.0	20.668	440.0	1775.1	1822.1	3.9620		9.03		2
641.0	20.921	440.0	1784.2	1831.8	3.9762		9.25		2
642.0	21.177	440.0	1793.6	1841.8	3.9909		9.59		2
643.0	21.437	440.0	1803.5	1852.2	4.0063		10.29		2
644.0	21.749	440.0	1808.5	1857.9	4.0140	136.1	4.63	274.1	1
645.0	22.069	440.0	1813.0	1863.2	4.0211	100.7	4.46	285.1	1
650.0	23.720	440.0	1834.1	1888.0	4.0536	48.0	4.02	320.8	1
655.0	25.420	440.0	1853.5	1911.3	4.0833	33.0	3.76	346.5	1
660.0	27.153	440.0	1871.8	1933.5	4.1111	25.6	3.56	368.5	1
665.0	28.911	440.0	1889.1	1954.8	4.1373	21.2	3.39	388.3	1
670.0	30.687	440.0	1905.7	1975.5	4.1622	18.3	3.23	406.9	1
675.0	32.483	440.0	1921.6	1995.4	4.1858	16.1	3.11	424.5	1
680.0	34.291	440.0	1936.9	2014.8	4.2083	14.5	2.99	441.3	1
685.0	36.111	440.0	1951.6	2033.6	4.2299	13.2	2.88	457.7	1

Table C1. Thermodynamic properties along isochores at regular temperature increments (continued).

Temp.	Pressure	Density	Internal Energy	Enthalpy	Entropy	C_p	C_v	Velocity of sound	Phase Region
K	MPa	kg/m^3	kJ/kg	kJ/kg	kJ/kg.K	kJ/kg.K		m/s	
638.0	20.173	460.0	1743.9	1787.8	3.9100		8.57		2
639.0	20.419	460.0	1752.5	1796.9	3.9235		8.68		2
640.0	20.668	460.0	1761.3	1806.2	3.9372		8.82		2
641.0	20.921	460.0	1770.2	1815.7	3.9511		9.03		2
642.0	21.177	460.0	1779.4	1825.4	3.9654		9.35		2
643.0	21.489	460.0	1785.3	1832.0	3.9747	85.6	4.45	285.2	1
644.0	21.827	460.0	1789.7	1837.2	3.9815	68.6	4.32	295.6	1
645.0	22.170	460.0	1794.0	1842.2	3.9882	58.1	4.22	304.2	1
650.0	23.929	460.0	1814.2	1866.2	4.0194	35.1	3.89	336.7	1
655.0	25.737	460.0	1833.1	1889.0	4.0483	26.2	3.67	361.8	1
660.0	27.580	460.0	1851.0	1910.9	4.0755	21.4	3.49	383.7	1
665.0	29.448	460.0	1868.1	1932.1	4.1013	18.2	3.34	403.6	1
670.0	31.337	460.0	1884.4	1952.5	4.1258	16.0	3.20	422.3	1
675.0	33.244	460.0	1900.1	1972.4	4.1491	14.3	3.08	440.0	1
680.0	35.166	460.0	1915.2	1991.6	4.1714	13.0	2.96	457.0	1
685.0	37.100	460.0	1929.7	2010.4	4.1927	12.0	2.85	473.5	1
638.0	20.173	465.0	1740.7	1784.1	3.9043		8.52		2
639.0	20.419	465.0	1749.3	1793.2	3.9178		8.63		2
640.0	20.668	465.0	1758.0	1802.5	3.9313		8.77		2
641.0	20.921	465.0	1766.9	1811.9	3.9452		8.97		2
642.0	21.177	465.0	1776.0	1821.5	3.9594		9.30		2
643.0	21.512	465.0	1780.7	1827.0	3.9668	71.6	4.37	291.8	1
644.0	21.857	465.0	1785.0	1832.1	3.9735	59.4	4.26	301.4	1
645.0	22.206	465.0	1789.3	1837.0	3.9800	51.4	4.17	309.6	1
650.0	23.995	465.0	1809.3	1860.9	4.0110	32.6	3.86	341.3	1
655.0	25.832	465.0	1828.1	1883.6	4.0397	24.8	3.65	366.2	1
660.0	27.704	465.0	1845.9	1905.4	4.0668	20.4	3.48	388.0	1
665.0	29.602	465.0	1862.9	1926.5	4.0925	17.5	3.33	407.9	1
670.0	31.520	465.0	1879.1	1946.9	4.1168	15.5	3.19	426.6	1
675.0	33.457	465.0	1894.8	1966.7	4.1401	13.9	3.07	444.3	1
680.0	35.408	465.0	1909.8	1986.0	4.1623	12.7	2.95	461.4	1
685.0	37.372	465.0	1924.3	2004.7	4.1835	11.7	2.85	477.9	1

Table C2. Properties of coexisting phases at regular temperature increments.

vapor

Temp.	Pressure	Density	Latent Heat	Internal Energy	Enthalpy	Entropy	C_p	C_v	Velocity of sound
K	MPa	kg/m³	kJ/kg	kJ/kg	kJ/kg	kJ/kg.K	kJ/kg.K		m/s
639.80	20.618	219.90	407.8	2090.5	2184.2	4.5282	87.2	4.94	317.4
640.00	20.668	222.10	400.2	2086.9	2180.0	4.5212	91.6	4.96	316.2
640.20	20.719	224.38	392.3	2083.3	2175.6	4.5140	96.6	4.98	315.0
640.40	20.769	226.75	384.2	2079.5	2171.1	4.5066	102.2	5.01	313.7
640.60	20.819	229.21	375.8	2075.5	2166.4	4.4989	108.5	5.04	312.3
640.80	20.870	231.78	367.1	2071.5	2161.5	4.4910	115.7	5.07	310.9
641.00	20.921	234.45	358.1	2067.2	2156.5	4.4828	123.5	5.10	309.3
641.20	20.972	237.26	348.8	2062.8	2151.2	4.4742	133.5	5.13	307.7
641.40	21.023	240.21	339.0	2058.1	2145.7	4.4652	144.6	5.17	306.0
641.60	21.074	243.33	328.8	2053.2	2139.9	4.4559	157.9	5.21	304.2
641.80	21.125	246.63	318.0	2048.1	2133.7	4.4460	173.8	5.26	302.2
642.00	21.177	250.16	306.6	2042.6	2127.2	4.4356	193.3	5.31	300.0
642.20	21.228	253.94	294.5	2036.7	2120.3	4.4245	217.8	5.36	297.6
642.40	21.280	258.05	281.6	2030.4	2112.9	4.4126	249.3	5.43	294.9
642.60	21.332	262.54	267.5	2023.5	2104.8	4.3996	291.2	5.50	291.9
642.80	21.384	267.53	252.0	2015.9	2095.8	4.3854	349.8	5.59	288.4
643.00	21.437	273.19	234.7	2007.4	2085.8	4.3696	436.8	5.71	284.2
643.20	21.489	279.78	214.8	1997.5	2074.3	4.3514	578.7	5.85	279.1
643.40	21.542	287.83	190.9	1985.6	2060.4	4.3295	847.9	6.05	272.3
643.60	21.594	298.56	159.7	1970.0	2042.4	4.3012	1533.8	6.38	262.2
643.80	21.647	316.81	107.9	1944.4	2012.7	4.2548	5902.7	7.20	241.4
643.890	21.6713	356.238	.0	1893.7	1954.6	4.1644			.0

liquid

Temp.	Pressure	Density	Latent Heat	Internal Heat	Enthalpy	Entropy	C_p	C_v	Velocity of sound
K	MPa	kg/m³	kJ/kg	kJ/kg	kJ/kg	kJ/kg.K	kJ/kg.K		m/s
642.00	21.177	466.22	306.6	1775.2	1820.6	3.9580	88.5	4.50	281.5
642.20	21.228	462.07	294.5	1779.8	1825.8	3.9658	100.3	4.55	277.7
642.40	21.280	457.60	281.6	1784.8	1831.3	3.9743	115.6	4.61	273.7
642.60	21.332	452.73	267.5	1790.2	1837.3	3.9834	136.4	4.69	269.5
642.80	21.384	447.36	252.0	1796.0	1843.8	3.9934	166.0	4.77	264.8
643.00	21.437	441.31	234.7	1802.5	1851.1	4.0045	210.9	4.88	259.7
643.20	21.489	434.32	214.8	1810.0	1859.5	4.0173	286.3	5.03	254.0
643.40	21.542	425.85	190.9	1818.9	1869.5	4.0328	434.9	5.24	247.1
643.60	21.594	414.68	159.7	1830.6	1882.7	4.0530	834.7	5.59	238.0
643.80	21.647	395.95	107.9	1850.2	1904.8	4.0873	3673.4	6.47	221.8
643.890	21.6713	356.238	.0	1893.7	1954.6	4.1644			.0

Table C3. Properties of coexisting phases at regular pressure increments.

vapor

Temp.	Pressure	Density	Latent Heat	Internal Energy	Enthalpy	Entropy	C_p	C_v	Velocity of sound
K	MPa	kg/m^3	kJ/kg	kJ/kg	kJ/kg	kJ/kg.K	kJ/kg.K		m/s
639.73	20.600	219.11	410.6	2091.7	2185.7	4.5307	85.6	4.93	317.8
639.93	20.650	221.29	403.0	2088.2	2181.5	4.5238	89.9	4.95	316.6
640.13	20.700	223.53	395.2	2084.6	2177.2	4.5167	94.7	4.97	315.4
640.33	20.750	225.85	387.2	2080.9	2172.8	4.5094	100.0	5.00	314.1
640.52	20.800	228.26	379.0	2077.1	2168.2	4.5019	106.0	5.03	312.8
640.72	20.850	230.75	370.6	2073.1	2163.5	4.4942	112.8	5.05	311.4
640.92	20.900	233.34	361.8	2069.0	2158.5	4.4862	120.4	5.09	310.0
641.11	20.950	236.05	352.8	2064.7	2153.5	4.4779	129.2	5.12	308.4
641.31	21.000	238.88	343.4	2060.2	2148.1	4.4693	139.4	5.15	306.8
641.51	21.050	241.85	333.6	2055.6	2142.6	4.4603	151.4	5.19	305.0
641.70	21.100	244.98	323.4	2050.7	2136.8	4.4509	165.6	5.23	303.2
641.90	21.150	248.30	312.6	2045.5	2130.7	4.4411	182.7	5.28	301.1
642.09	21.200	251.83	301.3	2040.0	2124.2	4.4307	203.6	5.33	298.9
642.28	21.250	255.61	289.2	2034.1	2117.3	4.4196	229.9	5.39	296.5
642.48	21.300	259.71	276.3	2027.8	2109.9	4.4078	263.8	5.46	293.8
642.67	21.350	264.19	262.4	2021.0	2101.8	4.3949	309.0	5.53	290.7
642.86	21.400	269.16	247.0	2013.4	2093.0	4.3809	372.2	5.63	287.2
643.05	21.450	274.78	229.9	2005.0	2083.0	4.3651	466.4	5.74	283.0
643.24	21.500	281.33	210.2	1995.2	2071.6	4.3471	620.5	5.89	277.8
643.43	21.550	289.32	186.6	1983.4	2057.9	4.3255	914.6	6.09	271.0
643.62	21.600	299.96	155.6	1968.0	2040.0	4.2975	1672.5	6.43	260.8
643.81	21.650	318.26	103.8	1942.4	2010.4	4.2513	6753.3	7.28	239.4
643.890	21.6713	356.238	.0	1893.7	1954.6	4.1644			.0

liquid

Temp.	Pressure	Density	Latent Heat	Internal Energy	Enthalpy	Entropy	C_p	C_v	Velocity of sound
K	MPa	kg/m^3	kJ/kg	kJ/kg	kJ/kg	kJ/kg.K	kJ/kg.K		m/s
641.90	21.150	468.27	312.6	1772.9	1818.0	3.9540	83.4	4.48	283.4
642.09	21.200	464.39	301.3	1777.2	1822.9	3.9614	93.4	4.52	279.8
642.28	21.250	460.25	289.2	1781.9	1828.0	3.9693	106.1	4.58	276.1
642.48	21.300	455.80	276.3	1786.8	1833.5	3.9777	122.8	4.64	272.1
642.67	21.350	450.96	262.4	1792.1	1839.5	3.9867	145.3	4.71	267.9
642.86	21.400	445.62	247.0	1797.9	1845.9	3.9966	177.4	4.80	263.4
643.05	21.450	439.62	229.9	1804.3	1853.1	4.0076	226.4	4.92	258.3
643.24	21.500	432.69	210.2	1811.7	1861.4	4.0203	309.0	5.07	252.6
643.43	21.550	424.30	186.6	1820.6	1871.3	4.0356	472.6	5.28	245.8
643.62	21.600	413.23	155.6	1832.1	1884.4	4.0557	918.2	5.64	236.8
643.81	21.650	394.47	103.8	1851.7	1906.6	4.0900	4256.3	6.57	220.3
643.890	21.6713	356.238	.0	1893.7	1954.6	4.1644			.0

Appendix D: Computer Program for Table Generation

The thermodynamic properties of D_2O in the critical region can be calculated with the computer program for the properties of H_2O published in Appendix D of Ref. 3 except for the BLOCKDATA routine which specifies the parameter values of the fundamental equation and the subroutine RANGE which checks whether the entry point lies within the range of validity of the equation. These routines for D_2O are given below.

```
-----------------------------------------------------------------------
        BLOCKDATA
C
C  THIS SUBROUTINE SUPPLIES THE PARAMETERS USED IN THE EQUATION OF STATE.
C
        DOUBLE PRECISION A,Q
        COMMON /COEFS/A(20),Q(20),ANAMES(20),QNAMES(20)
        DATA A/-.01776247D0,8.61797D0,0.D0,-25.23705D0,6.910737D0,.325D0,
       11.440299D0,0.D0,1.3757D0,23.66659D0,4.82D0,.294184D0,-11.948D0,
       2-24.219D0,-21.55221D0,17.30764D0,4*0.D0/
        DATA Q/-.006D0,-.003D0,0.D0,643.89D0,356.2382D0,21.671324D0
       1,.267D0,-1.54369D0,12*0.D0/
        DATA ANAMES/6HC      ,6HCOT3   ,6HDELROC,6HCOT2   ,6HDPDT   ,6HBETA
       1,6HKO    ,6HDELTC  ,6HB*B    ,6HA     ,6HDELTA  ,6HK1     ,6HMUC
       2,6HMU1   ,6HMU2    ,6HMU3    ,6HS00   ,6HS20    ,6HS01    ,6HS21    /
        DATA QNAMES/6HPOINTA,6HPOINTB,6HDELPC ,6HTC      ,6HRHOC   ,6HPC
       1,6HDPCDTC,6HSLOPDI,6HP11    ,6HALPHA ,6HPOO     ,6HP20    ,6HP40
       2,6HDELTAI,6HALPHAI,6HBETA I,6HGAMMAI,6HPO1      ,6HP21    ,6HP41    /
        END
-----------------------------------------------------------------------
        SUBROUTINE RANGE(IRANGE,IOPT,T,D,P)
C
C  THIS ROUTINE DETERMINES WHETHER THE ENTRY POINT IS WITHIN THE RANGE
C  OF VALIDITY OF THE EQUATION OF STATE (IRANGE=1), OR NOT (IRANGE=0).
C
        IMPLICIT REAL*8(A-H,O-Z)
        COMMON/SATUR/ISAT
        COMMON/CRITS/TC,RHOC,PC
        DATA TMIN,TMAX/638.D0,685.D0/,DMIN,DMAX/220.D0,465.D0/
C
        IRANGE=1
        IF(ISAT.NE.0) GO TO 10
        IF(T.LT.TMIN .OR. T.GT.TMAX) GO TO 99
        IF(IOPT.EQ.2) GO TO 20
        IF(D.LT.DMIN .OR. D.GT.DMAX) GO TO 99
        RETURN
20      CALL THERMO(1,T,DMIN,PMIN,R,THETA)
        CALL THERMO(1,T,DMAX,PMAX,R,THETA)
        IF(P.LT.PMIN .OR. P.GT.PMAX) GO TO 99
        RETURN
10      IF(IOPT.EQ.2) GO TO 30
        IF(T.GE.TC) GO TO 99
        IF(ISAT.EQ.-1 .AND. T.LT.639.D0) GO TO 99
        IF(ISAT.EQ. 1 .AND. T.LT.642.D0) GO TO 99
        RETURN
30      IF(P.GE.PC) GO TO 99
        IF(ISAT.EQ.-1 .AND. P.LT.20.60D0) GO TO 99
        IF(ISAT.EQ. 1 .AND. P.LT.21.15D0) GO TO 99
        RETURN
99      IRANGE=0
        WRITE(6,2)
2       FORMAT(2X,'THIS POINT IS OUTSIDE THE RANGE!'/)
        RETURN
        END
-----------------------------------------------------------------------
```

Appendix E: Units and Conversion Factors

Units used in the tables

Pressure MPa
Temperature K
Density kg/m^3
Energy, enthalpy, latent heat kJ/kg
Entropy, specific heats kJ/kg·K
Sound velocity m/s

Conversion factors

Pressure
MPa to	multiply table values by
Pa	10^6
bar	10
atmosphere	9.869 233
lbf/in^2	145.037 738

Density
kg/m^3 to	multiply table values by
mol/dm^3	0.049 931 1
lbm/ft^3	0.062 428 0

Energy, enthalpy
kJ/kg to	multiply table values
J/mol	20.027 6
BTU/lbm	0.429 922 6

Entropy, specific heats
kJ/kg·K to	multiply table values by
J/mol·K	20.027 6
BTU/lbm·R	0.238 845 9

Sound velocity
m/s to	multiply table value by
ft/s	3.280 83

Temperature
K to	transform table value by
°C	$(T,°C) = (T,K) - 273.15$
°F	$(T,°F) = \frac{9}{5}[(T,K) - 273.15] + 32$
R	$(T,R) = \frac{9}{5}(T,K)$