

# The Thermodynamic Behavior of the CO<sub>2</sub>-H<sub>2</sub>O System from 400 to 1000 K, up to 100 MPa and 30% Mole Fraction of CO<sub>2</sub>

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Received August 10, 1992; revised manuscript received October 19, 1992

A model is presented for the thermodynamic properties of the aqueous mixture of carbon dioxide, up to 30 mol% composition, in a large range of temperatures (400–1000 K) and pressures (0–100 MPa) around the critical point of water. The model for the Helmholtz free energy of the mixture is based on the principle of generalized corresponding states, with the NBS/NRC Steam Tables as the reference state for pure water. Input to the model are data for the critical line of the mixture, apparent molar volume and  $pVTx$  data in supercritical water, phase boundaries, excess enthalpies and mixture second virial coefficient data. Comparisons are presented with those data, with Henry's constants and with other formulations available for this system. Phase boundaries and tabulated values of molar volumes, enthalpies, and fugacities are presented along 35 isobars from 0.05 to 100 MPa, for four compositions,  $x = 0.05, 0.10, 0.20$  and  $0.30$ , respectively, at 19 temperatures in the range of 400 to 1000 K. For the same pressures and temperatures, we also list the infinite-dilution (standard state) properties: partial molar volume, enthalpy, heat capacity and fugacity coefficient of the solute CO<sub>2</sub>. The Fortran codes for generating these properties are listed in Appendix B.

Keywords: apparent molar volume; carbon dioxide; corresponding states; critical line; equation of state; excess enthalpy; fugacity; Henry's constant; mixture; phase boundaries; steam; virial coefficient; water.

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### List of symbols

$A$	Helmholtz free energy
$B$	second virial coefficient
$B_{ij}$	cross-term second virial coefficient
$H$	enthalpy
$I$	integral occurring in $Q$
$f$	scale factor for temperature
$f_i$	fugacity of component $i$
$G$	Gibbs free energy
$h$	scale factor for volume
$j$	mixing parameter for temperature
$K_T$	isothermal compressibility

$k$	mixing parameter for volume
$k_B$	Boltzman's constant (subscript omitted in combination $kT$ )
$k_H$	Henry's constant
$m$	molecular mass
$N$	number of molecules
$N_\alpha$	number of molecules of type $\alpha$
$n$	number of moles
$n_\alpha$	number of moles of type $\alpha$
$p$	pressure
$Q$	configurational partition function
$S$	entropy
$T$	temperature
$U$	internal energy
$V$	volume
$x$	mole fraction
$Z$	partition function
$z$	compressibility factor

### Greek symbols

$\alpha$	type of molecule
$\theta$	shape factor for temperature
$\theta_0, \theta_V, \theta_T, \theta_{VT}$	constants in temperature shape factor formulation
$\mu$	chemical potential
$\rho$	density
$\varphi$	fugacity coefficient
$\phi$	shape factor for volume
$\phi_0, \phi_V, \phi_T, \phi_{VT}$	constants in volume shape factor formulation

### Subscripts

$\alpha$	molecular species
$i$	component
1	solvent
2	solute
$V, T, x$	on Helmholtz free energy $A$ : differentiation with respect to variable(s) indicated
$s$	solute
$x$	property of binary mixture of mole fraction $x$
$w$	water
liq	liquid, or the denser coexisting phase
vap	vapor, or the less dense coexisting phase

### Superscripts

*	pure solvent
$\infty$	infinite dilution
$c$	critical; pseudocritical
conf	configurational
$F$	excess
mol	molecular
pg	perfect-gas
res	residual
$\varphi$	apparent molar property

## 1. Introduction

The system carbon dioxide-water is of great importance in the natural environment as well as in industrial applications. The interaction of carbon dioxide and water is key to the functioning of living organisms. The solubility of carbon dioxide in water is an order of magnitude larger than that of many other simple gases. As a consequence, dissolved carbon dioxide is an important component and chemical participant in geological hydrothermal systems.<sup>1,2</sup> Large amounts of carbon dioxide are absorbed by the oceans, counterbalancing the greenhouse effect.

Carbon dioxide is becoming an important substance in chemical technology, specifically in its use as a supercritical solvent and reaction medium.<sup>3</sup> The new field of supercritical water oxidation (SCWO)<sup>4,5</sup> has to deal with the thermodynamics and thermochemistry of organic compounds, including carbon dioxide, in supercritical water.

It is to this last application that this paper is meant to contribute. We propose a formulation of the thermodynamic properties of the system carbon dioxide-water in a large region (400-1000 K, 0-100 MPa) around the critical point of water (647 K, 22 MPa), and at carbon dioxide concentrations of up to 30 mol %. By the use of a Helmholtz free energy model we can, for the first time, make consistency tests of the available experimental data for various thermodynamic properties, predict any thermodynamic property desired, and perform extrapolation to infinite dilution safely in ranges where the solute standard state is highly anomalous.

The available experimental data for the critical line, phase equilibria, excess enthalpies, density, second virial coefficient and apparent molar volumes are reviewed in Sec. 2. The formulation is based on a generalized principle of corresponding states that makes use of so-called shape factors and uses the full Helmholtz free energy representation of water and steam as a reference. The model does not incorporate chemical reactivity of CO<sub>2</sub>. The model is described in Sec. 3. The optimization of the parameters in the formulation, and the optimized parameter set are discussed in Sec. 4. The optimized formulation is compared with all experimental sources in Sec. 5.

In Sec. 6, we tabulate the thermodynamic properties of the mixture. We give the critical line data and present a tabulation of molar volume, enthalpy and fugacity coefficients for four different compositions, 20 temperatures and 40 pressures. We also tabulate the infinite-dilution values of the volume, enthalpy and fugacity coefficient of carbon dioxide, which are known as "standard states" for carbon dioxide as a solute in water.

In Sec. 7, we compare with earlier formulations for this mixture. In Sec. 8, we discuss our experience with fitting the model to the data; in particular, we remark on the sensitivity of the various parameters to the different properties. Concluding remarks, in Sec. 9, deal with the potential of this model for describing supercritical aqueous mixtures, and with the minimum amount of ex-

perimental data required to build a reliable model. Appendix B contains the Fortran codes for the calculation of thermodynamic properties and phase boundaries of the mixture.

## 2. Review of the Experimental Data

The system CO<sub>2</sub>-H<sub>2</sub>O has been extensively researched because of its importance in technological and biological fields. Generic bibliographic sources of experimental and correlated thermodynamic data for binary aqueous solutions of industrial importance, including CO<sub>2</sub>, can be found in Ref. 6. In that review the available literature has been covered until the year 1983.

In this section we will consider explicitly only the experimental sources of thermodynamic data that deal with the temperature, pressure and composition range we are interested in.

### 2.1. Supercritical One-Phase Density Data, Phase Boundaries and Critical Line

Supercritical pressure-volume-temperature-composition data for this system have been measured by Franck and Tödheide,<sup>7</sup> Greenwood,<sup>8</sup> Malinin,<sup>1</sup> Chou and Williams,<sup>9</sup> and Zakirov.<sup>10</sup> Some of these authors calculate fugacities and/or excess properties from their experimental data using different equations of state for the system or other data-fitting procedures.

Crovetto, Majer and Wood<sup>11</sup> measured differences in density between supercritical pure water and carbon dioxide solutions; from these data apparent molar volumes for the solute can be calculated.

Subcritical vapor densities were measured by Patel and Eubank<sup>12</sup> in a range that only marginally overlaps with ours.

Liquid-vapor phase boundaries and critical lines were measured by Tödheide and Franck<sup>13</sup> (to be distinguished from the earlier paper by Franck and Tödheide<sup>7</sup> on  $pVTx$ ), by Takenouchi and Kennedy,<sup>14</sup> and by Khitarov and Malinin.<sup>15</sup> The latter authors presented only a graphical critical line. The critical line data of Tödheide and Franck and of Takenouchi and Kennedy do not agree. Recently, Mathier and Franck<sup>16</sup> confirmed the critical line of Tödheide and Franck.

### 2.2. Cross-Term Second Virial Coefficients, $B_{12}$

Cross-term second virial coefficients for this system have been calculated from other measured properties by Coan and King,<sup>17</sup> Patel *et al.*<sup>18</sup> and Wormald *et al.*<sup>19</sup> Agreement among the sources is within the experimental tolerance. This is unusual, since values of  $B_{12}$  obtained from different experimental methods rarely agree.

### 2.3. Excess Enthalpies

Wormald and coworkers<sup>19</sup> measured excess enthalpies for this system in a flow calorimeter for the 50 mol % mixture.

## 2.4. Solubility and Henry's Constant

The existent literature data on solubility of CO<sub>2</sub> in H<sub>2</sub>O have been critically reviewed and evaluated from 273 K to the critical point of water and over a wide range of pressure by Crovetto.<sup>20</sup> In this work, we have not repeated that recent effort, and we refer to Crovetto's paper for references to data sources. Crovetto and Wood<sup>21</sup> recently published new solubility data. An evaluation and review of solubility data for pressures below 1 MPa, and temperatures less than 433 K, has been published by Carroll *et al.*<sup>22</sup> Each review presents formulations for the calculation of Henry's constants as a function of the temperature.

## 2.5. Liquid Densities and the Solute's Apparent Molar Volume

Differences in density between pure water and the carbon dioxide solution have recently been measured by Crovetto *et al.*<sup>11</sup> From the measured differences the apparent molar volume of CO<sub>2</sub> can be calculated. Also Malinin<sup>1</sup> and Zakirov<sup>10</sup> have measured densities for this system.

## 3. The Generalized Corresponding-States Model

### 3.1. The Phase Diagram

The system carbon dioxide-water has a type-III<sub>m</sub> phase diagram according to the classification of van Konynenburg and Scott.<sup>23</sup> The critical line originating at pure CO<sub>2</sub> at 304 K and 7.4 MPa terminates within a few tenths K at a three-phase line, according to Morrison,<sup>24</sup> water being very insoluble in near-critical carbon dioxide. From the measurements of Tödeheide and Franck, we know that the critical line originating at pure water (647 K, 22 MPa) initially moves to lower temperatures and slowly rising pressures. It passes through a minimum temperature at about 30% mole fraction CO<sub>2</sub> and then moves sharply to higher pressures.

### 3.2. Choice of Thermodynamic Potential

Since our purpose is to correlate and calculate the thermodynamic properties in a large range below and above the critical point of water, we decided to use a Helmholtz free energy with derived pressure-explicit equation of state as a starting point. The independent variables are temperature, volume and mole fraction. The alternative, a Gibbs free energy with a volume-explicit equation of state, is not suitable if one of the components is near its critical point.<sup>25</sup>

### 3.3. Configurational and Residual Properties

We follow closely the presentation of Rowlinson and Watson.<sup>26</sup> The Helmholtz free energy  $A(V, T, N_\alpha, \dots)$  fol-

lows from the partition function by the relation

$$A = -kT \ln Z \quad (1)$$

If the partition function  $Z(V, T, V_\alpha, \dots)$  can be factorized into translational, vibrational, rotational and intermolecular contributions, we have

$$Z_N = \prod_\alpha \left( \frac{2\pi m_\alpha kT}{h^2} \right)^{3N_\alpha/2} (\psi_{av})^{N_\alpha} (\psi_{ar})^{N_\alpha} Q \quad (2)$$

$N = \sum N_\alpha$  and  $N_\alpha$  is the number of molecules of type  $\alpha$ . Here  $\alpha$  refers to the species of molecule considered,  $\psi_{av}$  is the vibrational,  $\psi_{ar}$  the rotational partition function of molecules of type  $\alpha$ ,  $Q$  is the configurational partition function

$$Q = \frac{1}{\prod N_\alpha!} \int \dots \int \exp(-U/kT) dr_1 \dots dr_N \\ = \frac{1}{\prod N_\alpha!} [I(T, V, N_\alpha)] \quad (3)$$

Here  $I$  is short-hand for the multidimensional integral and  $U$  is the energy of interaction, depending on the location and type of species. The number of moles of each species is denoted by  $n_\alpha$ , the total number of moles being  $n = \sum n_\alpha$ . Mole fractions  $x_\alpha$  are defined as

$$x_\alpha = \frac{n_\alpha}{n} = \frac{N_\alpha}{N} \quad (4)$$

Then, with  $A = A^{\text{conf}} + A^{\text{mol}}$ , we have

$$A^{\text{conf}} = -kT \ln Q = kT \sum \ln N_\alpha! - kT \ln I \quad (5)$$

$$\frac{A^{\text{conf}}}{NkT} = \sum x_\alpha \ln x_\alpha - 1 - \ln(I/N)$$

while

$$A^{\text{mol}} = -kT \ln(Z/Q) \quad (6)$$

$$= -kT \sum_\alpha \left[ 3 \frac{N_\alpha}{2} \ln \left( \frac{2\pi m_\alpha kT}{h^2} \right) + N_\alpha \ln \psi_{av} + N_\alpha \ln \psi_{ar} \right]$$

The configurational Helmholtz free energy of a perfect gas is obtained by putting  $U = 0$  in Eq. (3). Then  $I = V^N$  and

$$A^{\text{conf, pg}} = NkT \left[ \ln N/V - 1 + \sum_\alpha x_\alpha \ln x_\alpha \right] \quad (7)$$

The residual Helmholtz free energy  $A^{\text{res}}$  is defined as

$$A^{\text{res}} = A(V, T, x_1, \dots) - A^{\text{pg}}(V, T, x_1, \dots) = A^{\text{conf}} - A^{\text{conf, pg}} \quad (8)$$

so that

$$A^{\text{res}} = -kT \ln I(T, V) + NkT \ln V \quad (9)$$

The total Helmholtz free energy is obtained by adding  $A^{\text{mol}}$  to  $A^{\text{conf}}$ , or  $A^{\text{ps}}$  to  $A^{\text{res}}$ . The disadvantage of using the division into  $A^{\text{mol}}$  and  $A^{\text{conf}}$  is that neither  $Q$  nor  $Z/Q$  is dimensionless. Therefore  $A^{\text{conf}}/NkT$  and  $A^{\text{mol}}/NkT$  depend on the units chosen for  $p$ ,  $V$  and  $T$ . This is not so for  $A^{\text{res}}/NkT$  and we find it an advantage to use  $A^{\text{res}}$  as the basis for our corresponding-states treatment.

### 3.4. Corresponding States

The theorem of corresponding states, in the treatment of Rowlinson, Watson and Leland *et al.*,<sup>26-28</sup> maps the Helmholtz free energy  $A$  and the compressibility factor  $z = pV/NkT$  of a substance at temperature  $T$  and volume  $V$  onto those of a reference substance at a different temperature  $T_w$  and volume  $V_w$ . The dependence on  $N$ , the number of molecules, is implicitly assumed though not indicated. Since in our case the reference substance is pure water, we use a subscript  $w$  to indicate its properties.  $V_w$  and  $T_w$  are related to  $V$  and  $T$  by means of two scale factors,  $h^\circ$  and  $f^\circ$ , respectively, which are obtained from the respective critical molar volumes  $V^c$  and temperatures  $T^c$  by means of

$$f^\circ = T^c/T_w^c \quad h^\circ = V^c/V_w^c \quad (10)$$

Because critical pressures are usually better known than critical volumes, it is convenient to introduce a third scale factor  $q^\circ$  involving the critical pressures:

$$q^\circ = p^c/p_w^c \quad (11)$$

The superscript  $o$  is a reminder that  $h^\circ$ ,  $f^\circ$  and  $q^\circ$  are constants, a condition that will be relaxed shortly. The law of corresponding states implies that

$$f^\circ = h^\circ q^\circ \quad (12)$$

In the formulation of Rowlinson and Watson<sup>26</sup> the law of corresponding states takes the form

$$\frac{A^{\text{conf}}(V,T)}{NkT} + \ln V = \frac{A_w^{\text{conf}}(V_w,T_w)}{NkT_w} + \ln V_w \quad (13)$$

from which it follows that

$$z(V,T) = z_w(V_w,T_w) \quad (14)$$

Here

$$V/V^c = V_w/V_w^c \quad \text{or} \quad V/V_w = h^\circ \quad (15)$$

$$T/T^c = T_w/T_w^c \quad \text{or} \quad T/T_w = f^\circ$$

so that

$$A^{\text{conf}}(V,T) = f^\circ A_w^{\text{conf}}(V_w = V/h^\circ, T_w = T/f^\circ) - NkT \ln h^\circ \quad (16)$$

In terms of the residual Helmholtz free energy, we have

$$A^{\text{res}}(V,T) = f^\circ A_w^{\text{res}}(V_w = V/h^\circ, T_w = T/f^\circ) \quad (17)$$

### 3.5. Generalized Corresponding States

Since no two substances obey the law of corresponding states exactly, Rowlinson and Watson,<sup>26</sup> and Leland *et al.*,<sup>27,28</sup> generalized the principle in various ways. We have used the version based on shape factors and on the use of a single reference fluid, pure water.

The shape factors  $\phi(V_w, T_w)$  and  $\theta(V_w, T_w)$  are used to modify the scale factors  $f$  and  $h$ . They are defined as follows

$$f(V_w, T_w) = (T^c/T_w^c) \theta(V_w, T_w)$$

$$h(V_w, T_w) = (T^c/T_w^c) (p_w^c/p_c) \phi(V_w, T_w) \quad (18)$$

In the case of simple corresponding states,  $\theta$  and  $\phi$  would be equal to unity. The generalized shape factors are no longer constants, but functions of volume and temperature of the reference fluid, pure water. If the departures from corresponding states are not large, one may expect that the temperature and volume dependence of these functions is slight and simple to represent. In our present applications, we have assumed that

$$\theta(V_w, T_w) = 1 + \theta_V(V_w/V_w^c - 1) + \theta_T(T_w/T_w^c - 1) + \theta_{VT}(V_w/V_w^c - 1)(T_w/T_w^c - 1)$$

$$\phi(V_w, T_w) = \phi_0 + \phi_V(V_w/V_w^c - 1) + \phi_T(T_w/T_w^c - 1) + \phi_{VT}(V_w/V_w^c - 1)(T_w/T_w^c - 1) \quad (19)$$

with  $\theta_V$ ,  $\theta_T$ ,  $\theta_{VT}$ ,  $\phi_V$ ,  $\phi_T$  and  $\phi_{VT}$  presumably small adjustable coefficients and  $\phi_0$  close to unity. In particular,  $\phi_0$  is very useful in the case that the critical compressibility factor of a fluid differs from that of the reference fluid. The form of Eq. (19) has evolved from earlier, simpler relations, linear in the independent variables, when these were found insufficiently flexible to represent the various data sets for H<sub>2</sub>O-CO<sub>2</sub>. The configurational free energy obeys the relation

$$A^{\text{conf}}(V,T) = f A_w^{\text{conf}}(V_w = V/h, T_w = T/f) - RT \ln h \quad (20)$$

and the residual free energy

$$A^{\text{res}}(VT) = f A_w^{\text{res}}(V_w = V/h, T_w = T/f) \quad (21)$$

but  $f$  and  $h$  are no longer constant and, consequently, the relation (14) is no longer valid. Therefore, the pressure must be obtained by differentiating  $A^{\text{conf}}$  with respect to volume.

When  $V$  and  $T$  are given, it is no longer possible to find the reference values  $V_w$  and  $T_w$  by a simple multiplication such as that in Eq. (16), since  $h$  and  $f$  themselves are functions of  $V_w$  and  $T_w$ . Even when the coefficients in the functional dependence of  $f$  and  $h$  on volume and temper-

been chosen or fixed, every property calculation involves an iteration for obtaining the reference values  $V_w$  and  $T_w$  from the given  $V$  and  $T$ .

### 3.6. Corresponding States for Mixtures

Van der Waals generalized the principle of corresponding states to mixtures by postulating that the Helmholtz free energy of a binary mixture of constant composition  $x$  (denoted by the subscript  $x$ ) can be mapped onto that of the pure components, which are assumed to obey corresponding states. In his footsteps, we perform the mapping of the residual free energy of the mixture onto that of the reference substance, pure water.

$$A^{\text{res}}(V, T, x) = f_x^{\circ} A_w^{\text{res}}(V_w = V_x/h_x^{\circ}, T_w = T_x/f_x^{\circ}) \quad (22)$$

So far, the scale factors  $f_x^{\circ}$  and  $h_x^{\circ}$  are constants for fixed composition. They are related to the so-called pseudocritical parameters of the mixture and to the critical parameters of the reference substances by means of the relations

$$h_x^{\circ} = V_x^c/V_w^c \quad f_x^{\circ} = T_x^c/T_w^c \quad (23)$$

The pseudocritical parameters of the mixture of composition  $x$  are the fictitious critical parameters this mixture would display if it would behave as a pure substance and phase-separate because of mechanical rather than material instability. These pseudocritical parameters can be obtained from those of the pure reference,  $w$ , and of the pure solute,  $s$ , by means of van der Waals-type mixing rules, which for a binary mixture are given by

$$V_x^c = (1-x)^2 V_w^c + 2x(1-x) V_{ws}^c + x^2 V_s^c \quad (24)$$

$$T_x^c = (1-x)^2 T_w^c + 2x(1-x) T_{ws}^c + x^2 T_s^c$$

Lorentz-Berthelot-type combining rules express the constants  $V_{ws}^c$  and  $T_{ws}^c$  in terms of the critical parameters of the two pure substances, thus describing the mixture behavior entirely in terms of that of the two pure components. Some needed flexibility is gained by means of two adjustable empirical constants,  $j$  and  $k$ , which are known as interaction parameters.

$$V_{ws}^c = k \left[ (V_w^c)^{1/3} + (V_s^c)^{1/3} \right]^3 / 2^3 \quad (25)$$

$$T_{ws}^c = j \left[ T_w^c T_s^c \right]^{1/2}$$

### 3.7. Generalized Corresponding States for Mixtures

The principle of corresponding states for mixtures is generalized by defining shape factors  $\theta_x$  and  $\phi_x$  which, for given composition, are assumed to be slowly-varying functions of volume and temperature. Thus we obtain, in analogy with Eq. 18,

$$f_x(V_w, T_w) = (T_x^c/T_w^c) \theta_x(V_w, T_w)$$

$$h_x(V_w, T_w) = (V_x^c/V_w^c) \phi_x(V_w, T_w) \quad (26)$$

Then, in analogy with Eq. (21),

$$A^{\text{res}}(V, T, x) = f_x A_w^{\text{res}}(V_w = V/h_x, T_w = T/f_x) \quad (27)$$

For the functions  $\theta_x$  and  $\phi_x$  we use the following empirical forms

$$\theta_x = (1-x)^2 + 2x(1-x) \theta^{1/2} + x^2 \theta \quad (28)$$

$$\phi_x = (1-x) + x \phi$$

with  $\theta(V_w, T_w)$  and  $\phi(V_w, T_w)$  from Eq. (19).

When the shape factors are volume and temperature dependent, the locus defined by Eq. (24), and from which the scale factors  $f_x$  and  $h_x$  are measured, is no longer a true pseudocritical line; it is now simply a reference curve interpolating smoothly between the solvent critical point, and a state near the critical point of the pure solute. The latter state is far away from our range of application and its precise choice should be irrelevant. In the model presented here,  $V_s^c$  in Eq. (24) is chosen such that  $\phi_0 V_s^c$  equals  $V_{CO_2}^c$ . The reference curve Eq. (24) is used to define  $V_x$  and  $h_x$  in Eq. (26). For given  $V$ ,  $T$  and  $x$  of the mixture, the mapping values  $V_w$  and  $T_w$  are found entering a first estimate for  $f_x$  and  $h_x$  (and therefore  $V_w$  and  $T_w$ ) into equations (19) for  $\theta$  and  $\phi$ , after which  $\theta_x$  and  $\phi_x$  are obtained from Eq. (28). Eq. (26) then gives the next approximation for  $f_x$  and  $h_x$ ,  $V_w$  and  $T_w$ . Iteration proceeds until no further change occurs within preset limits.

The model for the binary aqueous mixture contains, in addition to the complete Helmholtz free energy of the reference substance, water, and the critical parameters of the solute, the following eight adjustable parameters:

In the shape factors:  $\theta_V$ ,  $\theta_T$ ,  $\phi_V$ ,  $\phi_T$ ,  $\theta_{VT}$ ,  $\phi_{VT}$

In the combining rules:  $j$ ,  $k$ .

### 3.8. The Reference Fluid

The NBS/NRC Helmholtz free energy of water and steam<sup>34</sup> in the dimensionless form of Ref. 29 is used as a reference. The equation represents all known thermodynamic properties of water and steam in our range of application to within experimental accuracy. The equation is formulated on the IPTS-68 temperature scale. As a consequence, the present model is also based on this scale. The uncertainties in the data and the model predictions far exceed those resulting from differences between the IPTS-68 and ITS-90 temperature scales. No significant errors will result if the tabulated results are assumed to be stated on ITS-90 instead of IPTS-68.

This equation is analytic at the critical point. It can, therefore, not truly represent the cubic coexistence curve and the weak divergence of the constant-volume heat capacity that characterize real fluids. Four analytic terms in the NBS/NRC equation serve to locally flatten the coexistence curve and enhance the heat capacity. One can therefore consider the NBS/NRC equation a close ana-

lytic approximation to the nonclassical behavior typical of real fluids near critical points.

For a classical description of a mixture, it is legitimate to combine a classical relation for the reference fluid with the classical principle of corresponding states, just expounded. Real mixtures, however, show nonclassical behavior, which can be generated from the nonclassical description of its pure components by means of a nonclassical counterpart of the principle of corresponding states.<sup>30,31</sup> This nonclassical principle maps the mixture properties onto the pure-fluid reference not at constant composition, but at constant field, such as a chemical potential.

By combining a close, albeit analytic, representation of the properties of the reference fluid, water, with the classical principle of corresponding states, as we do here, we set the stage for some distortion of the phase diagram near the reference critical point. For details we refer to the appendix of Ref. 32.

### 3.9. Thermodynamic Properties of the Mixture

All thermodynamic properties of the binary mixture of mole fraction  $x$  of a solute (s) in water (w) are derived from the Helmholtz free energy  $A(V, T, N, x)$ , which is of the following structure

$$\frac{A(V, T, N, x)}{NkT} = (1-x) \frac{A_w^{\text{mol}}(N, T)}{NkT} + x \frac{A_s^{\text{mol}}(N, T)}{NkT} - 1 + \ln N/V + x \ln x + (1-x) \ln(1-x) + \frac{A^{\text{res}}(N, V, T, x)}{NkT} \quad (29)$$

The first line contains the contributions from the internal degrees of freedom of each of the two components, water and solute, cf Eq. (6). The second line contains the perfect-gas part of the configurational free energy, as given by Eq. (7), including the perfect-gas free energy of mixing. The last line contains the residual Helmholtz free energy as defined in Eq. (8) and calculated from Eqs. (26–28). Although the dimensionless form of the NBS/NRC equation is used for all calculations, it is transformed into SI units and separated into perfect-gas and residual parts before the corresponding-states mapping is applied. The perfect-gas free energy of CO<sub>2</sub> is obtained from Ref. 33. We have used a simple quadratic representation for the ideal-gas heat capacity of CO<sub>2</sub> in our range of interest. The absolute value of the tabulated enthalpies has no significance. Only enthalpy differences have meaning.

The properties of the mixture are obtained by means of the following relations

$$p = -(\partial A / \partial V)_{T,x} = -A_V = -A_V^{\text{res}} + \frac{NkT}{V} \quad (30a)$$

$$K_T^{-1} = -V(\partial p / \partial V)_{T,x} = VA_{VV} = V \left[ A_{VV}^{\text{res}} + \frac{NkT}{V^2} \right] \quad (30b)$$

$$S = -(\partial A / \partial T)_{V,x} = -A_T \quad (30c)$$

$$U = A + TS = A - TA_T \quad (30d)$$

$$H = U + pV = A - TA_T - VA_V \quad (30e)$$

$$G = A + pV = A - VA_V \quad (30f)$$

$$N\mu_1 = A - VA_V - xA_x \quad (30g)$$

$$N\mu_2 = A - VA_V + (1-x)A_x \quad (30h)$$

Here the subscripts  $V, T, x$  on  $A$  denote partial differentiation with respect to the subscripted variable, while the other independent variables are kept constant. Some care is needed if the fugacity  $f$  and the fugacity coefficient  $\phi$  are to be derived from the Helmholtz free energy. We will first perform the derivation for a pure fluid, and then for a binary mixture. For our purpose, the best definition to begin with is that of  $\phi$  in terms of  $\mu$ :

$$kT \ln \phi = \mu(p, T) - \mu^{\text{ps}}(p, T) \quad (31)$$

$$\phi = f/p$$

This definition implies that  $f \rightarrow p$  as  $p \rightarrow 0$ . From the definition (30g), applied to a pure fluid, we obtain, with Eq. (29),

$$N\mu(P, T) = A^{\text{mol}}(N, T) + NkT \ln \{N/V(p)\} + G^{\text{res}}(N, V, T) \quad (32)$$

where

$$G^{\text{res}}(N, V, T) = A^{\text{res}}(N, V, T) - V(\partial A^{\text{res}} / \partial V)_T \quad (33)$$

and  $V = V(p)$

Since

$$N\mu^{\text{ps}}(p, T) = A^{\text{mol}}(T) + NkT \ln \{N/V^{\text{ps}}(p)\} \quad (34)$$

it follows that

$$NkT \ln \phi = NkT \ln \{V^{\text{ps}}(p)/V(p)\} + G^{\text{res}}(N, V(p), T) \quad (35)$$

If  $\phi$  is considered a function of  $V$  and  $T$ ,

$$V^{\text{ps}}(p) = NkT/p \quad (36)$$

and

$$\phi(N, V, T) = \frac{\exp(G^{\text{res}}(V, T)/NkT)}{pV/NkT} \quad (37)$$

Thus,  $\phi$  can be directly obtained from the residual Helmholtz free energy, without need for an iteration or integration.

The fugacity then follows from

$$f = \frac{NkT}{V} \exp(G^{\text{res}}/NkT) \quad (38a)$$

For a binary mixture, we have, as the equivalent of Eq. (31):

$$kT \ln \varphi_i = \mu_i(p, T, x) - \mu_i^{\text{ps}}(p, T, x) \quad (31a)$$

Here  $N\mu_i = (\partial G / \partial x_i)_{pT}$  is the partial molar Gibbs free energy of component  $i$  in the mixture.

For a binary mixture,  $\mu_1$  and  $\mu_2$  are obtained from the Helmholtz free energy by relations (30g) and (30h). In parallel with the development of Eq. (32), we obtain,

$$\frac{\mu_1(p, T, x) - \mu_1^{\text{ps}}(p, T, x)}{kT} = \ln \frac{V^{\text{ps}}(p)}{V(p)} + \frac{G^{\text{res}}(N, V(p), T, x)}{NkT} - x \left( \frac{\partial A^{\text{res}} / NkT}{\partial x} \right)_{VT} \quad (32a)$$

$$\frac{\mu_2(p, T, x) - \mu_2^{\text{ps}}(p, T, x)}{kT} = \ln \frac{V^{\text{ps}}(p)}{V(p)} + \frac{G^{\text{res}}(N, V(p), T, x)}{NkT} + (1-x) \frac{\partial A^{\text{res}} / NkT}{\partial x}$$

and therefore

$$\varphi_1(V, T, x) = \frac{\exp \left\{ [G^{\text{res}} - x (\partial A^{\text{res}} / \partial x)_{VT}] / NkT \right\}}{pV / NkT} \quad (37a)$$

$$\varphi_2(V, T, x) = \frac{\exp \left\{ [G^{\text{res}} + (1-x) (\partial A^{\text{res}} / \partial x)_{VT}] / NkT \right\}}{pV / NkT}$$

Again, these two fugacity coefficients are derived from the Helmholtz free energy of the mixture by (numerical) differentiation only, without the need for an iteration or integration.

The fugacities  $f_1$  and  $f_2$  are obtained through the relations.

$$f_i = p_i \varphi_i = x_i p \varphi_i \quad (39)$$

with  $p_i$  the partial pressure of component  $i$  in the mixture,  $p_i = x_i p$ .

The mixture critical line is obtained by the following procedures. For a chosen temperature, the locus of points is found for which

$$(\partial^2 G / \partial x^2)_{pT} = A_{xx} - A_{ix}^2 / A_{VV} = 0 \quad (40)$$

The second derivative for  $G$  is calculated from the matrix of second derivatives of the Helmholtz free energy with the subscripts on the Helmholtz free energy denoting consecutive differentiation with respect to the variables indicated. These differentiations are performed numerically. At a chosen temperature, the locus of points is calculated for which the first criticality condition, Eq. (40), is satisfied. Then, the point of maximum pressure is found on this isothermal spinodal (Fig. 1). The procedure

is as follows. At the chosen temperature, an initial estimate is made for the composition. With this temperature and composition, a search is made for the density at which Eq. 40 is satisfied, and the corresponding pressure is calculated. Then  $x$  is incremented and the steps are repeated. The sign of the increment is chosen so that the pressure increases. Then further increments of  $x$  are made until the pressure begins to decrease. Then the process is reversed in smaller steps of  $x$ , and repeated until the maximum pressure is located within a preset tolerance. This search has been automated.

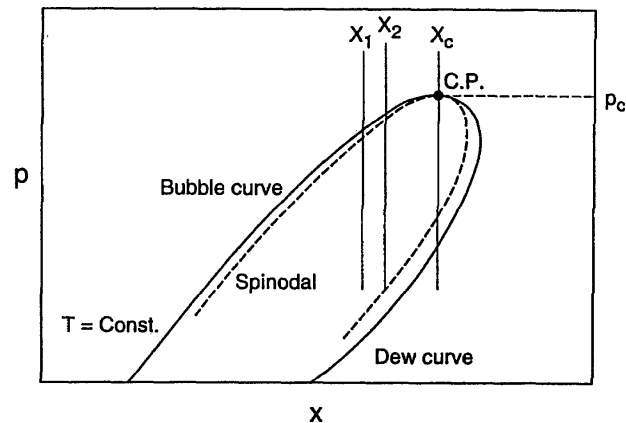


FIG. 1. Schematic diagram showing the method for the determination of a point on the critical line. An isotherm is shown on a  $p$  vs  $x$  plot, with the solid line being the coexistence curve, and the dashed line the "spinodal" — the locus of the zeroes of  $(\partial^2 G / \partial x^2)_{pT}$ .

The phase boundaries are found by equating the fugacities of the two components in the vapor (vap) and liquid (liq) at fixed pressure and temperature. The procedure is usually started far from any critical points, where an initial guess of the compositions of the coexisting phases can be made with some confidence. This initial guess then permits an iteration for the densities of the coexisting phases, and therefore of the fugacities of each of the components. If the conditions

$$f_1(T, \rho_{\text{liq}}, x_{\text{liq}}) = f_1(T, \rho_{\text{vap}}, x_{\text{vap}}) \quad (41)$$

$$f_2(T, \rho_{\text{liq}}, x_{\text{liq}}) = f_2(T, \rho_{\text{vap}}, x_{\text{vap}})$$

are not met, the initial guesses for the composition are modified until Eq. (41) is fulfilled. The final values of these compositions are used as starting values for the next pressure choice on an isothermal  $p$ - $x$  loop. The program uses temperature and pressure as independent variables, but is easily modified for other pairs of independent variables. In general, the calculations became cumbersome within the last few degrees from the critical point, and we had to fill in the curve graphically, helped by the knowledge of the critical point of the mixture.

The virial expansion of the compressibility factor  $pV/RT$  in terms of density is of the following form



$$pV/NkT = 1 + B/V + C/V^2 + \dots \quad (42)$$

where  $B$  is the second,  $C$  the third virial coefficient. The second virial coefficient  $B$  is obtained from the pressure  $p(V, T, x)$  by taking

$$B = \lim_{V \rightarrow \infty} (pV/NkT - 1)V$$

For a binary mixture, the second virial coefficient  $B$  of the mixture with mole fraction  $x$  of the second component can be expressed as follows

$$B(x, T) = B_{11}(1-x)^2 + 2B_{12}x(1-x) + B_{22}x^2 \quad (43)$$

Here  $B_{11}$  is the second virial coefficient of pure component 1 at  $T$ ,  $B_{22}$  that of pure component 2.  $B_{12}$  is the so-called cross-term virial coefficient that is representative of the interactions between unlike pairs. The cross-term virial is obtained from the second virial coefficient  $B$  of the mixture by subtracting the contributions from the two pure components. The second virial coefficient of pure water is that derived from the formulation of Haar, Gallagher and Kell,<sup>34</sup> that of CO<sub>2</sub> is the one obtained from the formulation of Ely *et al.*<sup>33</sup>

Apparent molar properties are defined with  $p$  and  $T$  as independent variables. For any molar property  $F$  of a binary mixture of mole fraction  $x$  of the minority second component dissolved in the first component, a corresponding apparent molar property is defined as

$$x^{\circ}F = F(p, T, x) - F_1^*(p, T) \quad (44)$$

Apparent molar properties measure the change in a molar property as the composition is changed from pure first component (superscript \*) to mole fraction  $x$  of the second component. This change occurs at constant  $p$  and  $T$ . Apparent molar properties are more straightforwardly measured than partial molar properties, and are widely used to characterize the behavior of dilute mixtures. They are less useful for dilute solutions in a large range around the solvent's critical point, because they behave highly anomalously.<sup>25</sup> For calculating apparent molar properties from a Helmholtz free energy, it is necessary to iterate for the volume that corresponds to the chosen pressure.

Excess properties are also defined in terms of the independent variables  $p$  and  $T$ . For any molar property  $F(p, T, x)$ , an excess property  $F^E(p, T, x)$  is defined by

$$F^E(p, T, x) = F(p, T, x) - (1-x)F_1^*(p, T) - xF_2^*(p, T) \quad (45)$$

Calculating excess properties from a Helmholtz free energy involves an iteration for the volume corresponding to the selected pressure. Excess properties behave very anomalously near the pressures and temperatures corresponding to the critical points of the pure components.

Henry's constant  $k_H$  for a gas, component 2, dissolved in a solvent, component 1, in a condition of two-phase equilibrium, is defined in terms of Henry's law

$$k_H = \lim_{x_2 \rightarrow 0} f_2/x_2 \quad (46)$$

with  $f_2$  the fugacity of the gas and  $x_2$  its mole fraction in the liquid phase. With Eq. (39) for the definition of the fugacity, Eq. (46) can be rewritten as

$$k_H = \varphi_2^{\infty} p_{\text{vap}}^* \quad (47)$$

The infinite-dilution value of  $\varphi_2$  is obtained by the same procedure by which we obtain other infinite-dilution or standard-state properties. This procedure is described in Sec. 6.

#### 4. The Optimized Parameter Set

Given the great diversity of data types available for the system H<sub>2</sub>O-CO<sub>2</sub>, a straightforward optimization of the eight adjustable parameters is not feasible for several reasons. First of all, the model is not given in algebraically closed form and the model function does not depend linearly on the adjustable parameters. Secondly, it is not *a priori* obvious how to assign relative weights to very different data sets, such as phase boundaries versus excess enthalpies. Thirdly, not much was known *a priori* about the internal consistency of the various data sets. Which of several alternative representations is the best is to some extent a matter of judgment. For example, for comparison with the most influential input, the critical line data, a parameter set needs to be chosen, after which a lengthy set of calculations must be performed in order to pinpoint the model critical line corresponding to this parameter set. The many aspects of the critical line, its unusual features, and the disparity between the two sets of experimental data make determination of the "best" representation quite subjective. As we narrowed down to an acceptable parameter set, there was no substitute for the preparation of sets of plots comparing the model predictions of many different properties of the system with the experimental data, and with earlier sets, in order to obtain an overall impression of the quality of the representation.

The optimization of the parameter set was achieved in the following way. First, a value of the leading constant  $\phi_0$  in the volume shape factor (Eq. 19) is fixed as the ratio of the critical compressibility factors of CO<sub>2</sub> and H<sub>2</sub>O (about 1.2). Small adjustments to this value were later allowed during the process of fine-tuning. The final value attained, 1.196, is well within the experimental uncertainty of this ratio. Next, values of the interaction parameters  $j$  and  $k$  were obtained by fitting the apparent molar volume and critical-line data. These parameters were not allowed major change after a satisfactory fit was obtained.

Next, a set of "check points" was established consisting of experimentally known target values of various properties at selected values of independent variables. A useful set was found to be: the pressure and composition of the critical line at three temperatures, the temperature of the critical line at its minimum, the value of the second virial

coefficient of the equimolar mixture at three widely separated temperatures, the RMS deviation of a group of values of the compressibility factor at supercritical temperatures, and a selected value of the apparent molar volume near one of the experimental peaks, a total of nine check points.

The six small adjustable parameters in the shape factor equations (Eq. 19) were estimated and adjusted to give a reasonable representation of these check points.

Then, the eight parameters, the above six, plus  $j$  and  $k$  in some cases, were fine-tuned by linearizing the problem around this parameter set. Derivatives of the predicted value at each check point with respect to each of the parameters were calculated numerically. The matrix so obtained was used to calculate a further set of parameter adjustments by means of the method of linear least-squares. At each check point, weights were assigned. The new parameter set was then tested for suitability.

Sometimes, the new set was found to contain one or more parameter values that were unacceptable. Cutting all parameter adjustments down to a fraction of their linearized values often cured this problem. Alternatively, a different weighting scheme was tried.

The actual minimization proceeded through several cycles of the above steps of manual adjustment followed by linearization.

The final parameter set obtained in this fashion is shown in Table 1.

TABLE 1. The values for the parameters in the extended corresponding states model

Parameter	Value	Parameter	Value
$j$	.9044	$\Phi_{VT}$	-0.66
$k$	1.078	$\theta_V$	-0.010
$\Phi_0$	1.196	$\theta_T$	-0.048
$\Phi_V$	-0.22	$\theta_{VT}$	0.08
$\Phi_T$	-0.15		

## 5. Comparison with Experimental Data

In this section, we compare experimental data for the thermodynamic properties of high-temperature  $\text{CO}_2\text{-H}_2\text{O}$  with the experimental data. The data we compare with include the critical line, phase boundaries, compressibility factors, excess enthalpies, second virial coefficients, apparent molar volumes and Henry's constants.

### 5.1. Critical Line

The procedure for obtaining the critical line from the Helmholtz free energy formulation was described in Sec. 3.9. In Fig. 2a-2c we show the predicted critical line in

$T-x$ ,  $p-x$ , and  $p-T$  space, respectively. As explained in Sec. 2, we have preferred to fit the critical line of Tödheide and Franck,<sup>13</sup> from which that of Takenouchi and Kennedy<sup>14</sup> differs sharply at the higher pressures. The critical line data of Tödheide and Franck were not directly measured, but rather were the result of a graphical construction as maxima on the measured isothermal  $P-x$  loops. The critical line was recently reconfirmed by Mather and Franck.<sup>16</sup>

Figure 2a shows that the critical temperature is well predicted by our model at mole fractions up to  $x=0.3$ . The model passes through the minimum sooner and climbs more sharply than the data. It is possible to fit the region around the minimum better, but then the critical line starts bulging at the lower concentrations. Since our principal goal was to represent the lower concentrations well, we chose our parameter set accordingly. Fig. 2b shows a quite respectable representation of the pressure on the critical line, but the model cannot follow the steep rise for  $x$  beyond 0.35. The fit at the low end is somewhat deceptive because of the coarse scale. Our predicted critical curve falls definitely above the data by 5-10% in pressure. This is outside the uncertainty quoted by Tödheide and Franck for their coexistence curve measurements: 1 K and 1% in pressure. It was not possible to obtain a closer fit without doing damage to the agreement with other data. The problem may be due in part to the inherent difficulty a classical corresponding-states model is expected to show if the reference fluid representation is highly accurate, i.e., close to the real nonclassical behavior.<sup>32</sup> In part, we are struggling with inconsistencies between data sets, so that the use of additional adjustable parameters, which might improve the fit, would lead to

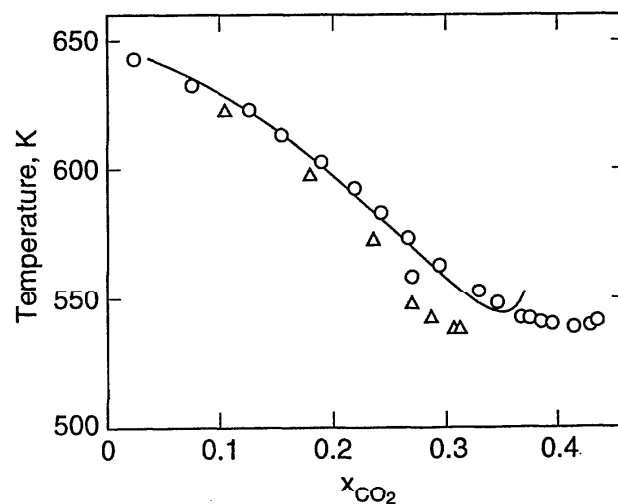


Fig. 2a. View of the critical line:  $T$  vs  $x$ . The solid curve represents the predictions of our model, the dashed curve those of the model of Christoforakos and Franck.<sup>37</sup>  $\circ$ , data of Tödheide and Franck;<sup>13</sup>  $\triangle$ , data of Takenouchi and Kennedy.<sup>14</sup>

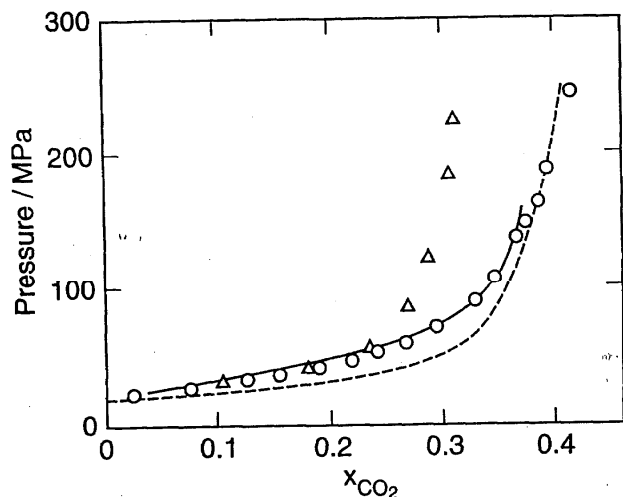


FIG. 2b. View of the critical line:  $p$  vs  $x$ . The solid curve represents the predictions of our model, the dashed curve those of the model of Christoforakos and Franck.<sup>37</sup>  $\circ$ , data of Tödheide and Franck;<sup>13</sup>  $\Delta$ , data of Takenouchi and Kennedy.<sup>14</sup>

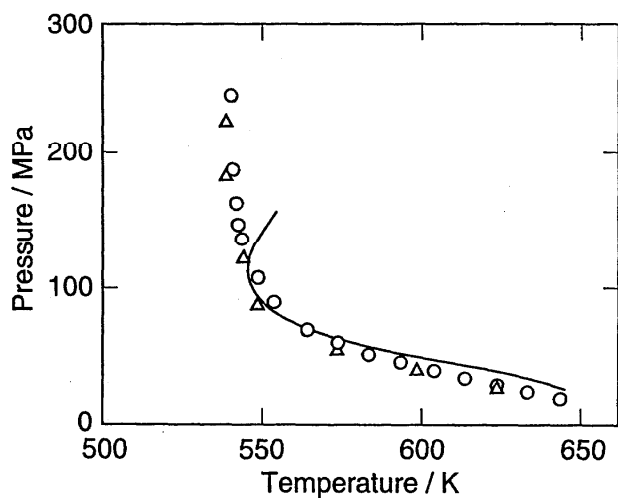


FIG. 2c. View of the critical line:  $p$  vs  $T$ . The solid curve represents the predictions of our model, the dashed curve those of the model of Christoforakos and Franck.<sup>37</sup>  $\circ$ , data of Tödheide and Franck;<sup>13</sup>  $\Delta$ , data of Takenouchi and Kennedy.<sup>14</sup>

overfitting. Fig. 2c is another projection of the data in Figs. 2a and 2b. The model does a reasonable job for temperatures down to the minimum in the critical line.

## 5.2. Coexisting Phases

The coexistent phases follow from the equality of temperature, pressure and fugacities as explained in Sec. 3.9. We compare with the isothermal  $P-x$  loops measured by Tödheide and Franck<sup>13</sup> at temperatures from the critical point of water to below the minimum in the critical curve. In Fig. 3a, we show the comparison at the lowest temperature, 523 K. At this temperature, the loop is no longer closed. We accurately fit the two sides up to 100 MPa in pressure. In Fig. 3b, we show the loop at 573 K. This temperature is above the minimum in the critical line and therefore the loop is closed. The numerical derivatives that we take near the maximum of the loop become quite inaccurate, and we are not able to locate the phase boundary within 10% from the critical pressure. We do, however, know the location of the critical point from our critical-line calculation which proceeds from the one-phase region. Therefore we can be confident about the place where the model closes the loop. One must expect that the experimental loop, being nonclassical, is flatter, but the offset shown in Fig. 3b is due in first instance to our inability to fit the critical pressure closely enough, as

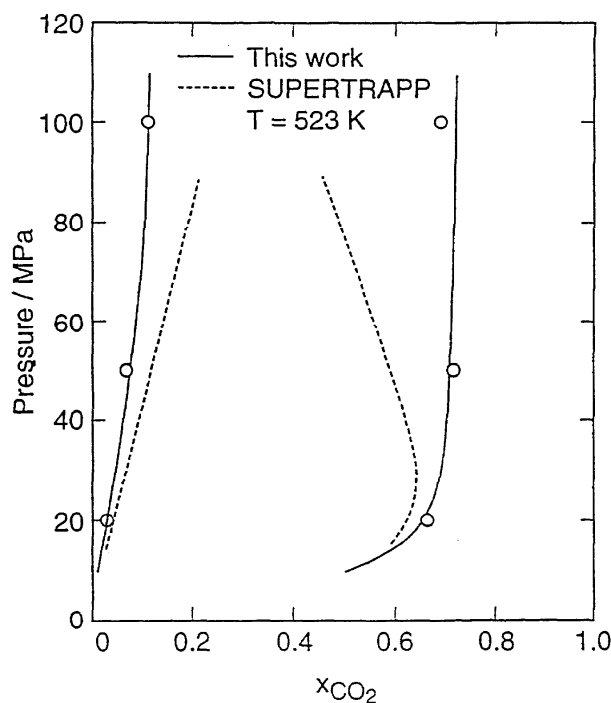


FIG. 3a. The coexistence curve at 523.15 K. The solid line represents the predictions of the model (long-dashed lines in regions where the calculations become uncertain and the values estimated) and the experimental points are from Tödheide and Franck.<sup>13</sup> Also shown, represented by the short-dashed lines, are the predictions of the model SUPERTRAPP.<sup>38</sup>

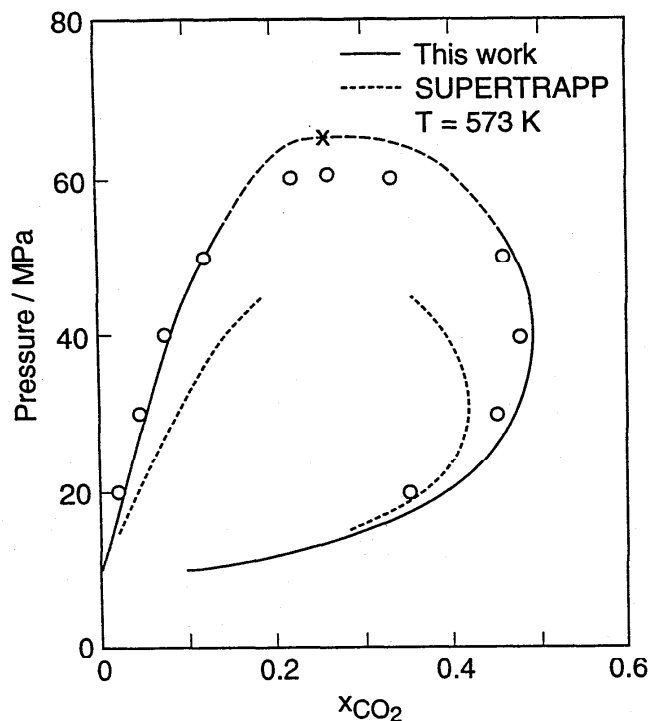


FIG. 3b. The coexistence curve at 573.15 K. The solid line represents the predictions of the model (long-dashed lines in regions where the calculations become uncertain and the values estimated) and the experimental points are from Tödheide and Franck.<sup>13</sup> Also shown, represented by the short-dashed lines, are the predictions of the model SUPERTRAPP.<sup>38</sup>

mentioned earlier. Tödheide and Franck claim 1% in mole fraction for the liquid densities. We fit their data semiquantitatively. The highest-temperature  $p-x$  loop, that at 623 K, is less of a success. We do not do a good job on the liquid side, and we overshoot the experimental curve considerably. This may be a consequence of the fact that our critical pressures are high in this range. We did find that the model predictions away from the critical region were not particularly sensitive to the choice of the parameters.

In Fig. 4, we show the 20 MPa isobar on a logarithmic composition scale, and again compare with Tödheide and Franck. This loop must close on the vapor pressure curve of pure steam. At the lower temperatures, we describe the liquid compositions on the level 0.007 in mole fraction, the claimed uncertainty being 0.15 mol%, a factor of 5 smaller. The differences are systematic. On the vapor side, the deviations are not systematic, and, at the lower temperatures, they are of the order of 0.01 in mole fraction, the claimed uncertainty being 0.75 mol%. This agreement is satisfactory. Close to the pure-water termination point, the differences become larger.

### 5.3. $pVT$ Measurements in the Supercritical Region

Measurements of the compressibility factor  $z = pV/RT$  along isotherms for temperatures near and above critical

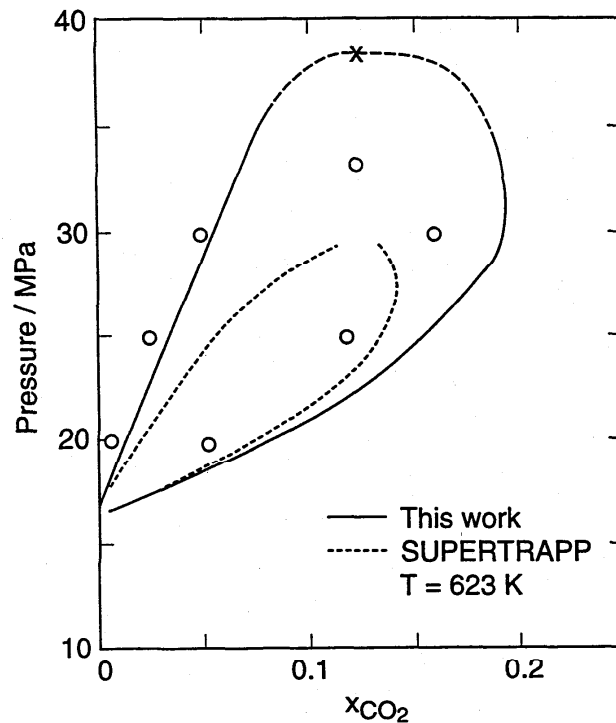


FIG. 3c. The coexistence curve at 623.15 K. The solid line represents the predictions of the model (long-dashed lines in regions where the calculations become uncertain and the values estimated) and the experimental points are from Tödheide and Franck.<sup>13</sup> Also shown, represented by the short-dashed lines, are the predictions of the model SUPERTRAPP.<sup>38</sup>

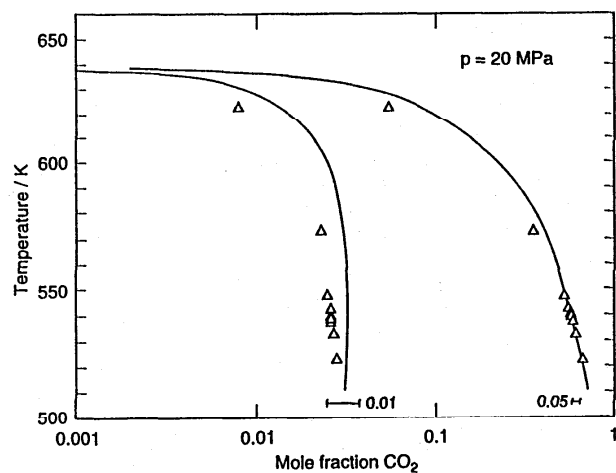


FIG. 4. The coexistence curve at a pressure of 20 MPa. The solid line represents the prediction of the model, and the experimental data of Tödheide and Franck<sup>13</sup> are shown. The horizontal bars represent a mole fraction uncertainty of 0.01, resp. 0.05, as indicated.

point of water are available from several sources: Greenwood<sup>8</sup> for temperatures from 450 to 800 °C and pressures up to 50 MPa; Franck and Tödheide<sup>7</sup> for temperatures from 400 to 750 °C and pressures up to 200 MPa (this paper is to be distinguished from the later, phase equilibria paper.<sup>13</sup>); Zakirov<sup>10</sup> at 300 and 400 °C and pressures up to

100 MPa. All authors cover the entire composition range. Our comparisons are limited to the CO<sub>2</sub> mole fractions up to 0.4.

The data of Greenwood are published in the form of tables generated from a 15-term polynomial in  $p$  and  $x$  determined for each isotherm, and the "data" shown in Fig. 5 are from these tables. We compare our model predictions (full curves; for dashed curves, see Sec. 7) with these data at several temperatures for CO<sub>2</sub> mole fractions 0.2 (Fig. 5a), and 0.4 (Fig. 5b). We consider the agreement very satisfactory, of the order of 1% in  $pV/RT$ .

In the same figures, we show the data points of Franck and Tödheide, which extend to higher pressures than the Greenwood data. These data fall far below our predicted curves, and are in obvious disagreement with the Greenwood data in the range of overlap. In fact, we were not

able to fit these data even when excluding the Greenwood data. The values predicted by the model were robust, being rather insensitive to the shape factor parameters and only marginally sensitive to the mixing parameters.

In Fig. 5a, we also compare with Zakirov's data at 400 °C and  $x = 0.2$ . The Zakirov data fall above our prediction by several percents. The comparison at 300 °C and  $x = 0.3$ , not shown, is considerably worse, with our model falling about 10% below Zakirov's data.

In view of the large discrepancies between the different data sets at the lower temperatures and higher pressures, further refining of the model did not seem warranted at this stage.

#### 5.4. The Apparent Molar Volumes

Malinin<sup>1</sup> reported apparent, Eq. (44), and partial molar volumes for the system CO<sub>2</sub> in H<sub>2</sub>O. The evaluation of the apparent molar volumes from the experimental data involved several steps that we could not retrace. His partial molar volumes were assumed to be independent of concentration (which is incorrect),<sup>25</sup> and are reported graphically only. On inspection, his reported partial molar volumes are in reasonable agreement with our predicted infinite-dilution partial molar volumes of CO<sub>2</sub> in H<sub>2</sub>O. We have refrained from more detailed comparison in view of the uncertainties discussed.

The apparent molar volume  ${}^{\circ}V$  was measured for dilute solutions of CO<sub>2</sub> in H<sub>2</sub>O in the supercritical region by Crovetto, Wood and Majer.<sup>11,21</sup> These measurements display striking peaks when the density is near-critical, and these peaks, although diminished, continue to quite high pressures. The measurements are along three supercritical isobars: 28, 33, and 38 MPa, and over a range of temperatures spanning the critical. On each isobar, there were several composition values in the range of 10<sup>-2</sup> to 10<sup>-3</sup> mole fraction. Our model was used for the average composition at the 33 and 38 MPa isobars, and for the lowest (0.0015) and highest (0.012) compositions at 28 MPa. This last isobar is nearest to the critical pressure of steam and therefore most sensitive to composition. The lower composition corresponds to the higher maximum. In Fig. 6, we compare these data with the predictions of the model, and find quite good agreement. The value of the apparent molar volume at the highest peak is quite sensitive to the parameter  $j$  in the mixing rules, and much less sensitive to the other parameters: therefore this extremum was used as the principal determining factor for the parameter  $j$ .

#### 5.5. Excess Enthalpies

Measurements of the excess molar enthalpies of equimolar mixtures of CO<sub>2</sub> and H<sub>2</sub>O at temperatures up to 698 K and pressures up to 13.4 MPa have been made by Wormald *et al.*<sup>19</sup> using a flow mixing calorimeter. Although this composition is outside the range we have established for the model, 0–30% mole fraction of CO<sub>2</sub>, we

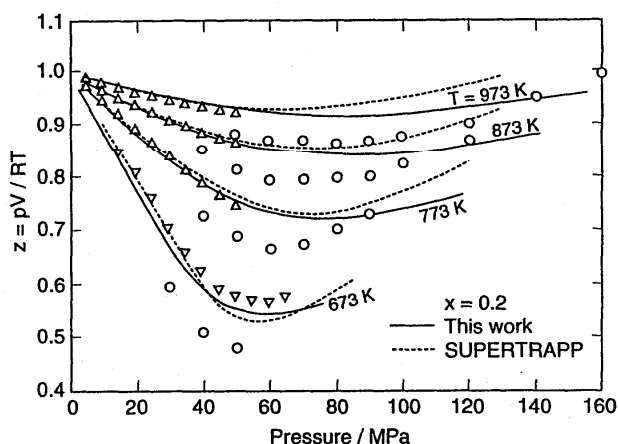


FIG. 5a. Compressibility factors at supercritical temperatures and pressures at  $x = 0.2$ . The data of Greenwood<sup>8</sup> ( $\Delta$ ), of Zakirov<sup>10</sup> ( $\nabla$ ) and of Franck and Tödheide<sup>7</sup> ( $\circ$ ) are shown along with the predictions of our model (solid line) and of the model SUPERTRAPP<sup>38</sup> (dashed line).

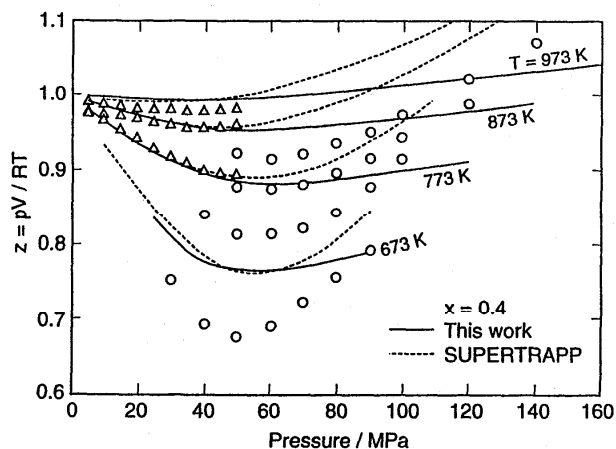


FIG. 5b. Compressibility factors at supercritical temperatures and pressures at  $x = 0.4$ . The data of Greenwood<sup>8</sup> ( $\Delta$ ), of Zakirov<sup>10</sup> ( $\nabla$ ) and of Franck and Tödheide<sup>7</sup> ( $\circ$ ) are shown along with the predictions of our model (solid line) and of the model SUPERTRAPP<sup>38</sup> (dashed line).

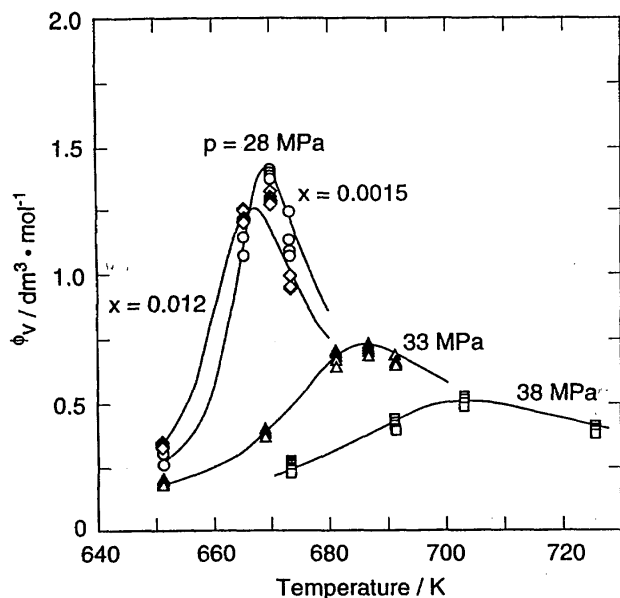


FIG. 6. The apparent molar volumes,  $\phi_V$ , at three supercritical pressures: 28, 33 and 38 MPa, for dilute mixtures. The experimental data are from Crovetto *et al.*<sup>11</sup> They are indicated by the various symbols, and represent a spread of composition from about  $10^{-3}$  to  $10^{-2}$  in mole fraction. The predicted values represented by the solid lines were calculated at an average composition of 0.008 mole fraction for the 33 and 38 MPa lines, and for compositions of 0.0015 and 0.012 for the 28 MPa lines (representing the approximate maximum and minimum compositions of the experimental data).

show the predicted values from the model in comparison with these measured values for four temperatures in Fig. 7. It can be seen that the agreement is quite good at the lower temperatures although at the highest temperatures and pressures the predicted values are a little low, and not within the uncertainties of the measurements.

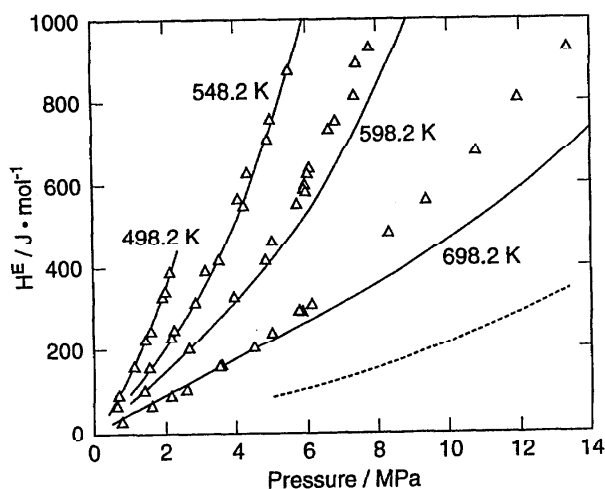


FIG. 7. The excess enthalpies along four isotherms, for the  $x = 0.5$  mole fraction mixture of  $\text{CO}_2$  and  $\text{H}_2\text{O}$ . The experimental data are from Wormald *et al.*,<sup>19</sup> the full curves are from our model and the dashed curve is a SUPERTRAPP prediction at 698.2 K.

Since the excess enthalpies are amongst the most carefully measured data for this mixture, the reader interested in higher concentrations should be pointed not only to the enthalpy data themselves, but also to the properties derived from them by Wormald and collaborators, such as highly accurate  $pV/RT$  values for the equimolar mixture.<sup>19</sup>

### 5.6. The Cross-Term Second Virial Coefficient $B_{12}$

The predicted values for the cross-term virial coefficient  $B_{12}$  from the model can be obtained from the total second virial coefficient  $B$  and the second virial coefficient for pure  $\text{H}_2\text{O}$ ,  $B_{11}$ , by means of the relation

$$B_{12} = B_{11} + \frac{1}{2} \lim_{x \rightarrow 0} \left( \frac{\partial B}{\partial x} \right)_T \quad (48)$$

This derivative at its limit was calculated numerically. The results over a wide range of temperatures are shown in Fig. 8, along with experimental values from several sources. First of all, we show values from a smoothing equation by Vanderzee and Haas<sup>35</sup> correlating several experimental data sets at lower temperatures, with values at higher temperatures resulting from an analysis of the Greenwood<sup>8</sup> compressibility measurements. Secondly, Wormald *et al.*<sup>19</sup> calculated  $B_{12}$  up to about 500 K from their measurement of excess enthalpies. Furthermore, Patel *et al.*<sup>18</sup> calculated  $B_{12}$  values for temperatures up to about 500 K from their  $pVT$  measurements in mixtures from .5 to .98 mole fraction of  $\text{CO}_2$  in  $\text{H}_2\text{O}$ . For temperatures above 400 K the predictions from the model lie within the experimental uncertainties of the

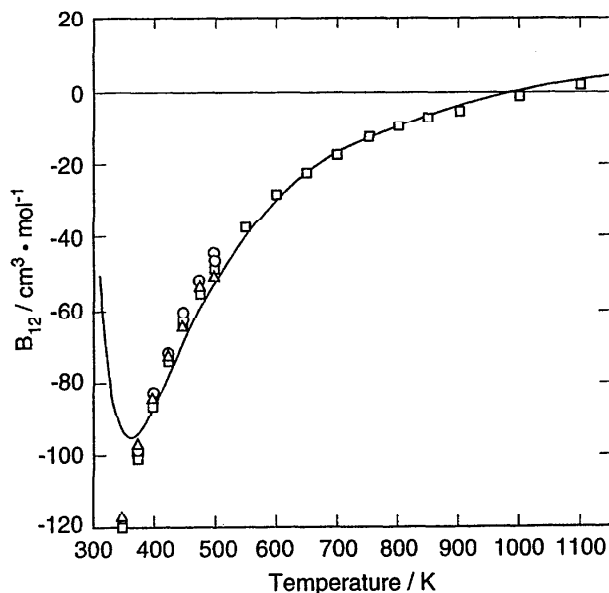


FIG. 8. The cross-term second virial coefficient  $B_{12}$ . The data of Patel *et al.*<sup>18</sup> ( $\circ$ ), Wormald *et al.*<sup>19</sup> ( $\Delta$ ), and Vanderzee and Haas<sup>35</sup> ( $\square$ ) are shown along with the predictions of the model (solid line).

measurements, but the model predicts an unrealistic upturn in the values for  $B_{12}$  at temperatures below 400 K.

### 5.7. Henry's Constant

Crovetto<sup>20</sup> recently analyzed the solubility data for CO<sub>2</sub> in H<sub>2</sub>O, and derived Henry's constants over the whole range from the melting point to the critical point. She used two models, namely the Peng-Robinson equation (PR), and a cubic equation by Wormald (W), to correct the measured data for nonideality and to extrapolate to infinite dilution. She also presented several correlating equations for Henry's constant. The only ones with correct behavior near the critical point of water are those incorporating a term linear in the density of liquid water, or, equivalently, a  $(T - T_c)^{1/3}$  term in temperature. The latter sets are labelled  $T^*(1/3)$  in Ref. 20. In Fig. 9, we compare our predicted curve for Henry's constant with three of Crovetto's models, namely,  $T^*(1/3)$  (W),  $T^*(1/3)$ (PR) and a version of  $T^*(1/3)$  with additional weight given to the higher temperatures,  $T^*(1/3)$  (PR, HT). We also include the data very close to the critical point, from Crovetto *et al.*<sup>11,21</sup> and those of Ellis<sup>36</sup> which seem to be very precise.

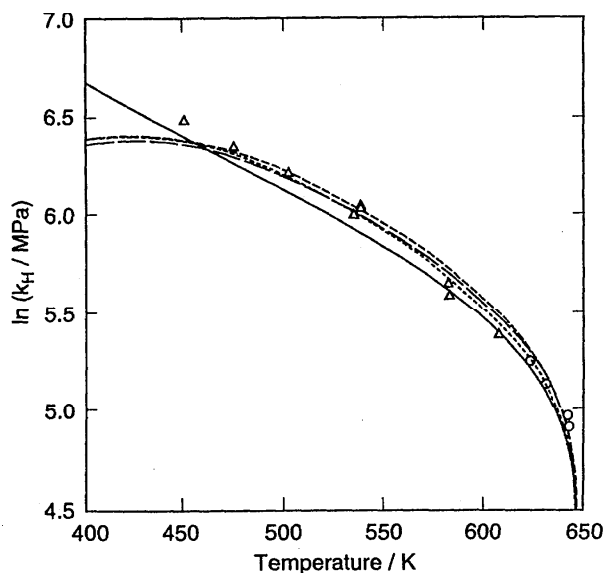


FIG. 9. Crovetto's Henry constant correlation<sup>20</sup> compared to ours. ---  $T^*(1/3)$ (PR); - · -  $T^*(1/3)$ (W); - - -  $T^*(1/3)$ (PR, HT); — this paper. Four data points near  $T_c$  are from Crovetto<sup>20</sup> (O), the other are from Ellis<sup>36</sup> ( $\Delta$ ).

From the comparison in Fig. 9 we draw the following conclusions. Our correlation is best at temperatures near the critical, where we represent the data of Crovetto *et al.* about as well as the other equations do. At temperatures around 500 K, our predictions are 10 to 15% low, about twice the spread between the various correlations of Crovetto. We do believe that our model would have been more appropriate than (PR) and (W) for making the non-ideality corrections preceding the Henry constant calcu-

lations, but we doubt that this would have made an essential difference in the Henry constant values in this middle range of temperatures. At the lower temperatures (420 K) our equation does not display the maximum that is characteristic of aqueous Henry constants. This is near the range where the cross-term second virial coefficient of the model becomes unrealistic as well and where the applicability of the model ends.

## 6. Tabulation of Properties

The predictions of the model for properties of interest are presented as three sets of tables: values of  $x$ ,  $p$ ,  $V$  and  $T$  along the critical line in Table 2; values of  $V$ ,  $H$ ,  $\phi_1$  and  $\phi_2$  along isobars for four values of  $x$  (0.05, 0.10, 0.20 and 0.30) for a range of temperatures from 400 to 1000 K in Table 3; and values of  $V_2$ ,  $H_2$ ,  $C_{p2}$  and  $\phi_2$  at infinite dilution for the same pressure and temperature ranges as the previous table in Table 4. Tables 3 and 4 are presented in Appendix A. As an introduction to these tables we show views of the two-phase surface of this mixture. Fig. 10 shows several isotherms on a  $p$  vs  $x$  plot, and Fig. 11 shows several lines of constant composition on a  $T$  vs  $p$  plot. From these figures it can be seen that if a phase boundary is crossed for the values of pressure and composition chosen for Table 3, the state of the fluid will always progress from the two-phase region at the lower temperatures to a single phase at the higher temperatures, which may be vapor, supercritical or liquid depending upon the pressure. In Table 3 we indicate, in *italics* and at the phase boundary, the temperature, and also the values of the properties and composition of the coexisting phase that coexists with the chosen phase.

TABLE 2. Mole fraction, temperature, pressure and density along the critical line

$x$	$T_c$ K	$P_c$ MPa	$\rho_c$ mol/dm <sup>3</sup>
0.000	647.13	22.06	17.87
0.035	644.0	26.79	17.89
0.058	640.0	29.78	18.27
0.102	630.0	35.65	19.21
0.136	620.0	40.65	20.08
0.167	610.0	45.37	20.88
0.195	600.0	50.10	21.68
0.221	590.0	55.05	22.49
0.247	580.0	60.51	23.38
0.272	570.0	66.92	24.39
0.297	560.0	75.19	25.60
0.310	555.0	80.74	26.35
0.325	550.0	88.38	27.28
0.335	547.0	95.41	28.07
0.343	545.0	103.67	28.92
0.350	544.3	111.26	29.61
0.353	544.3	115.82	29.97
0.358	545.0	124.46	30.65
0.364	547.0	135.72	31.41
0.368	550.0	147.22	32.16
0.372	555.0	162.31	33.03

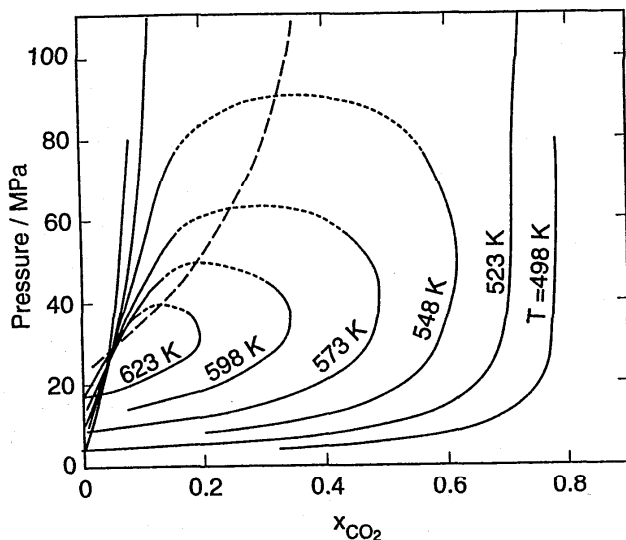


FIG. 10. The coexisting phases of the mixture as predicted by the model. Six isotherms are shown (498.15 K, 523.15 K, 548.15 K, 573.15 K, 598.15 K and 623.15 K). The dashed lines represent regions that have been estimated because of the difficulties with the convergence of the calculations.

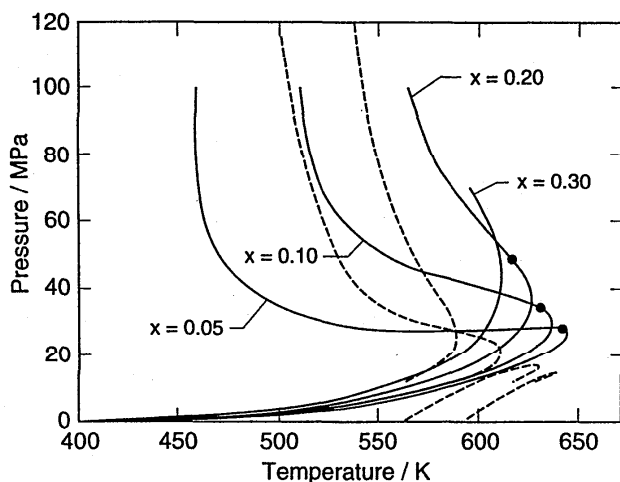


FIG. 11. The phase boundary in  $pT$  space for the compositions chosen in Table 3. The full curves are our model predictions for four isopleths, and the dashed curves those of Christoforakos and Franck<sup>37</sup> for the same isopleths. The black circles are critical points from our model.

For Table 4, the properties at infinite dilution, the phase boundaries are those of pure water, and the table will show values in the liquid at lower temperatures, crossing the phase boundary into the vapor at higher temperatures. For the convenience of the user, values in the liquid phase are indicated by *italics*.

## 7. Comparison with Other Formulations

There are two other Helmholtz free energy formulations available for the system  $\text{CO}_2$  in water in the range of interest. One is the formulation of Christoforakos and Franck,<sup>37</sup> the other that of the computer code

SUPERTRAPP<sup>38</sup> developed at NIST.

The model of Christoforakos and Franck is a van der Waals-Carnahan-Starling model in which the attractive energy is of the van-der-Waals type, proportional to the density, while the repulsions are those of a hard-sphere system. The hard-sphere diameter is slightly temperature-dependent. The molecular attraction is based on a square-well model, incorporating an additional parameter representing the width of the square well. Christoforakos and Franck represented the critical line and the phase equilibria of the  $\text{CO}_2\text{-H}_2\text{O}$  system, as measured by Tödheide and Franck, by means of this model. They used four adjustable parameters for the mixture, and two each for the pure components, not counting the critical parameters. In Fig. 2b, we show the fit to the critical line data of Tödheide and Franck performed by Christoforakos and Franck, compared to ours. It is clear that our model represents these data at least as well as their model.

In the  $p-x$  diagrams, Figs 3a-c, we already showed that we fit the measured phase equilibria data of Tödheide and Franck adequately to well, specifically on isotherms between the water critical point and the temperature minimum on the critical line. In Fig. 10, we showed several isopleths in  $p-T$  space. Similar isopleths were calculated by Christoforakos and Franck, and these are also displayed in Fig. 10. It is obvious that there is serious disagreement about the course of these isopleths at the low concentrations of  $\text{CO}_2$ , 0.1 molar and below. In our model, these isopleths are "flat" on the bubble side, that is, they show only small changes in pressure over a wide temperature range between the critical point and the temperature minimum on the critical line. In the model of Christoforakos and Franck, these isopleths run to considerably lower pressures instead. If we now turn to the measured data of Tödheide and Franck (Fig. 2 in Ref. 13), we note that the bubble parts of the  $p-x$  curves at 573 and 623 K, respectively, intersect at a composition of roughly  $x = 0.05$ , where they have the same pressure, see Fig. 3b and c. This implies that the  $p-T$  isopleth at  $x = 0.05$  must be "flat" in the range 573–623 K, while the  $x = 0.1$  isopleth must move to higher pressures as the temperature falls. Therefore, our model portrays the trends in the Tödheide-Franck coexistence data at low compositions of  $\text{CO}_2$  correctly, while the Christoforakos-Franck model has the wrong trend in that region.

We believe that the principal advantage of our model is at the low concentrations, where the system is close to pure water. Our empirical model must approach the pure-water limit correctly, while one cannot expect that a physically based but relatively simple equation of the type used by Christoforakos and Franck will do a particularly good job of representing near- and supercritical water.

The computer code SUPERTRAPP<sup>38</sup> was developed as a predictive tool for the thermodynamic and transport properties of alkane mixtures. It is based on an earlier NIST model, "TRAPP".<sup>38</sup> The code is based on a generalized corresponding states model of the same philosophy as the one used here. In SUPERTRAPP, however, the



reference substance is propane. A capability for calculating phase equilibria is included. The pressure, temperature and composition at phase equilibrium, however, are not calculated from the model, but from a simpler one, the Peng-Robinson equation, after which all other properties of coexisting phases are calculated from the generalized corresponding states model. Also, many substances other than alkanes were added to the program, including CO<sub>2</sub> and water. Since the program SUPERTRAPP was not specifically designed to describe properties of either aqueous or dilute systems, we cannot expect it to be accurate for pure water or for dilute aqueous systems. In fact, thermophysical properties predicted for water at temperatures near critical (for instance, at 673 K) may be 10% or more in error. On the other hand, at temperatures 773 K and up, SUPERTRAPP predicts steam densities to 1% or better. Nevertheless, we must expect that our model will be superior for the system CO<sub>2</sub>-H<sub>2</sub>O. This is indeed the case for the phase boundaries (Fig. 3a-c), but it is gratifying to see that SUPERTRAPP predicts the phase separation qualitatively in the right place. The comparison with the Greenwood  $pVTx$  data is particularly interesting. At these relatively low densities and high temperatures, it is hard to choose between the two models; at the higher pressures, the predictions of the two models diverge, but given the lack of data it is not possible to decide which model is right. Where SUPERTRAPP fails the test, is in predicting excess enthalpies near the critical temperature of steam. For the 0.5 molar mixture, at 698.2 K, SUPERTRAPP predicts an excess enthalpy only 1/3 of the measured one. This implies that the code cannot predict the heat capacity of a stream of CO<sub>2</sub> in H<sub>2</sub>O at temperatures near the critical temperature of water, that is, at the low end of temperatures in supercritical water reactors. It is obvious that the code could be improved by replacing the propane reference system by one for water, by including interaction parameters different from 1, and by refining the representation of the shape factors. This work is in the planning stage.

### 8. Range and Reliability of the Model and the Sensitivity to the Parameters

The range in which the model may be expected to give reliable results is determined by two factors: the availability of data and the capability of the model to represent the data. Regarding the first factor, only a few of the phase equilibria and  $PVTx$  data extend beyond 100 MPa, so that we have chosen this value as a practical cut-off for the pressure range of the tabulation. Regarding the second factor, since the model is not capable of following the critical line much beyond the temperature minimum, at mole fraction 30% of CO<sub>2</sub>, we have used this number as a cut-off in composition. The temperature cut-off, 400–1000 K, has been arrived at by the following considerations. The model gives unrealistic values of the cross-term second virial coefficient and Henry constant at the low end of this range; the data base extends to 973 K at

the upper end, where behavior should simplify anyway. These considerations have set the bounds on the range as specified in the title and used in the tables.

It is important to record the sensitivity of the adjustable parameters to the various types of property data available. The nine parameters of the model can be divided into two groups. Two parameters,  $j$  and  $k$ , are used in the mixing rules, and modify the shape of the critical line joining the critical points of H<sub>2</sub>O and CO<sub>2</sub>. The remaining seven parameters ( $\phi_0$ ,  $\phi_V$ ,  $\phi_T$ ,  $\phi_{VT}$ ,  $\theta_V$ ,  $\theta_T$  and  $\theta_{VT}$ ) are involved in the representation of the shape factors - the mapping of the target fluid (here CO<sub>2</sub>) surface onto the reference (here pure H<sub>2</sub>O) surface. Of these seven parameters,  $\phi_0$ , which fixes the ratio of the target fluid critical compressibility factor to the critical compressibility factor of the reference fluid, has been fixed close to the experimentally determined value. Although many of the properties are sensitive to this parameter, there seems to be no advantage to allowing it to be adjustable: the experimentally determined value seems to be about optimum. The other six shape factor parameters would normally be used to improve the mapping of the target fluid onto the reference fluid, but in this case, since our goal is to represent H<sub>2</sub>O-rich mixtures at high temperatures, we have not attempted to adjust these parameters to represent pure CO<sub>2</sub>, but instead have used them to better represent the experimental data for mixtures.

Most of the properties at infinite dilution, such as the Henry constant, the infinite dilution fugacity coefficients, and the properties at very low concentrations of CO<sub>2</sub>, such as the apparent molar volumes, depend directly upon the values of  $dp/dx$  and  $dT/dx$ .<sup>32,39,40</sup> These derivatives depend strongly upon the interaction parameters  $j$  and  $k$ , and only weakly upon the shape factors, since at low concentrations of CO<sub>2</sub> the shape factors approach unity and their derivatives with respect to concentration are relatively small. As discussed earlier, we took advantage of this fact by using the apparent molar volume experimental data to fix the value of the  $j$  and  $k$  to within a narrow range; we used the other properties where experimental data exist for less dilute mixtures to fix the parameters in the representation for the shape factors for CO<sub>2</sub>. Although all of the properties depend rather strongly upon  $j$  and  $k$ , most adjustment of the parameters to represent properties at higher CO<sub>2</sub> concentrations took place in the six shape factor parameters. Any further adjustment in  $j$  would be accompanied by a compensatory adjustment in  $k$  so that the apparent molar volumes would still be properly represented.

The model is rather inflexible in the determination of the composition of coexisting phases. Changes in the shape factor parameters of unacceptable size are required to fit the experimental data more accurately. Therefore these data were not given much consideration in the determination of the parameters. The critical line, however, shows a sensitivity to the shape factors as well as to the interaction parameters, and experimental data are available over a wide range of compositions (0 mole% to over 40 mol % CO<sub>2</sub>). These data provided the most

useful guide to the adjustment of the parameters in the shape factors. Although the sharp rise in the critical pressure observed for mole fractions of  $\text{CO}_2$  greater than 0.3 is difficult to reproduce, the representation for smaller concentrations of  $\text{CO}_2$  is quite reasonable, and therefore we can have confidence in the predictions of the model for mole fractions of  $\text{CO}_2$  up to 0.3. The shape factor associated with the temperature,  $\theta$ , has a greater effect on the properties than the  $\phi$ , affecting the densities. For both shape factors, the  $\theta_T$ ,  $\theta_V$ ,  $\phi_T$  and  $\phi_V$  have a greater effect than the  $\theta_{TV}$  and  $\phi_{TV}$ , which were used primarily for "fine-tuning".

The model also is rather inflexible in the representation of the supercritical  $pVT$  data, however the parameters as determined from the other data predict values that agree with the measurements of Greenwood to the level of about 1%. Unacceptable modifications to the parameters in the shape factors would be necessary to fit the measurements of Franck and Tödheide,<sup>7</sup> which seem to be in disagreement with the Greenwood data (see Fig. 5).

Predictions of the model for the excess properties, particularly the excess enthalpies for which very good experimental data exist for this system, are also quite sensitive to all of the parameters, including the shape factor parameters. Since most of these data are at compositions around  $x(\text{CO}_2) = 0.5$ , which is outside the range we have chosen to represent, these data were not used in the adjustment of the parameters, but used as a check to insure the reasonability of the model. The cross-term second virial coefficient,  $B_{12}$ , which is also an excess property, is somewhat sensitive to the shape factor parameters, and strongly sensitive to the mixing parameters. It was used during the adjustment of the shape factor parameters. The model predicts an unphysical minimum in  $B_{12}$  around  $T = 400$  K and we consider the temperature of the minimum to be the lower limit of the useful range of the model. The predictions of the model of the values of Henry's constant reflect this same lower limit, giving values that are within the experimental scatter above about 420 K and departing from the experimental values below this temperature.

Since the reference equation represents pure  $\text{H}_2\text{O}$  very well over a very wide range of pressures and temperatures, the principal uncertainties in the properties of dilute mixtures arise from the behavior of the model as a function of composition, i.e. the mixing rules. The initial slope of the critical line is well represented, as seen from the representation of the apparent molar volumes. We can therefore be confident in the values of the derived properties at infinite dilution, including the Henry's constant and the solute's fugacity coefficient at infinite dilution. Since the critical line is reasonably represented for compositions up to more than 0.3 mole fraction  $\text{CO}_2$ , this value sets an upper limit for the mole fraction range of applicability of the model. As a guide to the accuracy of the predicted values from the model, we can look at the comparisons with the experimental data where available. For the Henry constant, for instance, we agree with the recommended values to within about 5% for tempera-

tures above 420 K, which is about the standard deviation of the recommended fit to the experimental values. Since the infinite-dilution fugacity coefficients are directly related to the Henry constant, we can expect a similar reliability for this property. For  $pVT$  properties at temperatures 673 K and over, an accuracy in the 2% range is expected for pressures up to 60 MPa. The compositions of the coexisting phases can be expected to be reliable to within 1 mole% on the liquid side, and to within 5 mole% for the vapor.

## 9. Conclusions

We have developed a Helmholtz free energy model for the system carbon dioxide in water that is suitable for representing the thermodynamic properties and phase boundaries at the water-rich end in a large temperature and pressure region around the critical point of water. Since the NBS/NRC equation for water and steam is used as the reference in a generalized corresponding-states treatment, the model guarantees accurate representation of the pure-water limit.

The eight adjustable parameters in the model have been chosen so as to represent most known data for the system as closely as possible. The adjustment of these parameters is a time-consuming process that has been only partially automated. In the process, a number of data inconsistencies were noted; in several cases, the model enabled us to decide which of a pair of inconsistent data had to be rejected. Severe inconsistencies in the high-temperature  $PVTx$  data form a practical limit to the reliability of the model in this range.

Data of percent-level uncertainty are generally represented close to their uncertainty. The model cannot approach the reliability of much more accurate data, such as the excess enthalpies, without the introduction of further adjustable parameters.

Though conceptually straightforward, the model is certainly not as simple and transparent, or as easy to use, as engineering equations based on cubic, or even Carnahan-Starling types of equations of state. It has, however, one considerable advantage that is of particular importance in the design of supercritical water reactors: unlike other engineering equations of state for mixtures, it is capable of representing not only phase boundaries and critical lines in  $PTx$  space, but also densities and enthalpies adequately in a regime including the critical point of water and the compressible supercritical state. These are precisely the data needed for reactor design, and this is just the regime of conditions in which supercritical water oxidation (SCWO) will take place.

For the convenience of the user, we have assembled the Fortran subroutines and the main programs for calculation of properties and phase boundaries in Appendix B.

The next phase of our work will be the generalization of our model to multicomponent aqueous mixtures of carbon dioxide, air constituents and prototype organics representative of the classes of hazardous substances under consideration for elimination by SCWO.

## 10. Acknowledgments

This work has been supported in part by the Standard Reference Data Program at NIST.

We have profited from discussions with Professor E.U. Franck regarding the data and computer model originating in his group.

R.F. Kayser, M.R. Moldover, M.L. Huber, and J.A. Given served as careful readers and provided thoughtful criticism.

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### Appendix A. Tables of Thermodynamic Properties for the Mixture

Tables of the volume, enthalpy, and fugacity coefficients for each component along isobars at four composi-

tions and for a range of temperatures are given in Table 3; and tables of  $V_2$ ,  $H_2$ ,  $Cp_2$  and  $\phi_2$  at infinite dilution along the same isobars and range of temperatures are given in Table 4.

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$

$p=0.05 \text{ MPa}$									
$x=0.05$					$x=0.10$				
$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
66.19	48.38	0.9947	1.0027	400	66.21	47.50	0.9947	1.0021	
69.56	49.12	0.9957	1.0019	420	69.58	48.27	0.9958	1.0014	
72.93	49.86	0.9965	1.0013	440	72.94	49.05	0.9965	1.0010	
76.28	50.60	0.9971	1.0009	460	76.30	49.84	0.9971	1.0007	
79.64	51.35	0.9976	1.0007	480	79.65	50.62	0.9976	1.0005	
82.98	52.10	0.9979	1.0005	500	82.99	51.42	0.9979	1.0004	
86.33	52.85	0.9982	1.0004	520	86.34	52.21	0.9982	1.0003	
89.67	53.61	0.9985	1.0003	540	89.68	53.02	0.9985	1.0002	
93.00	54.38	0.9987	1.0002	560	93.01	53.82	0.9987	1.0002	
96.34	55.14	0.9988	1.0002	580	96.35	54.64	0.9988	1.0001	
99.68	55.92	0.9990	1.0001	600	99.68	55.46	0.9990	1.0001	
108.01	57.87	0.9993	1.0001	650	108.02	57.54	0.9993	1.0001	
116.34	59.86	0.9994	1.0001	700	116.34	59.65	0.9994	1.0001	
124.67	61.89	0.9996	1.0001	750	124.67	61.81	0.9996	1.0001	
132.99	63.94	0.9997	1.0001	800	132.99	64.00	0.9997	1.0001	
141.31	66.04	0.9997	1.0001	850	141.31	66.23	0.9997	1.0001	
149.63	68.17	0.9998	1.0001	900	149.63	68.51	0.9998	1.0001	
157.95	70.33	0.9998	1.0001	950	157.95	70.83	0.9998	1.0001	
166.27	72.54	0.9999	1.0001	1000	166.27	73.18	0.9999	1.0001	

$p=0.05 \text{ MPa}$									
$x=0.20$					$x=0.30$				
$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
66.26	45.73	0.9949	1.0010	400	66.30	43.96	0.9952	1.0003	
69.62	46.58	0.9959	1.0007	420	69.65	44.88	0.9961	1.0002	
72.97	47.44	0.9966	1.0005	440	73.00	45.82	0.9967	1.0001	
76.32	48.30	0.9972	1.0003	460	76.35	46.76	0.9973	1.0000	
79.67	49.17	0.9976	1.0002	480	79.69	47.72	0.9977	1.0000	
83.01	50.05	0.9980	1.0002	500	83.03	48.68	0.9980	1.0000	
86.35	50.93	0.9983	1.0001	520	86.37	49.65	0.9983	1.0000	
89.69	51.82	0.9985	1.0001	540	89.70	50.63	0.9985	1.0000	
93.03	52.72	0.9987	1.0001	560	93.04	51.62	0.9987	1.0000	
96.36	53.63	0.9989	1.0001	580	96.37	52.62	0.9989	1.0000	
99.69	54.54	0.9990	1.0001	600	99.70	53.63	0.9990	1.0000	
108.02	56.86	0.9993	1.0001	650	108.03	56.19	0.9993	1.0000	
116.35	59.23	0.9994	1.0001	700	116.36	58.81	0.9994	1.0001	
124.68	61.65	0.9996	1.0001	750	124.68	61.49	0.9996	1.0001	
133.00	64.11	0.9997	1.0001	800	133.00	64.23	0.9997	1.0001	
141.32	66.63	0.9997	1.0001	850	141.32	67.03	0.9997	1.0001	
149.64	69.20	0.9998	1.0001	900	149.64	69.88	0.9998	1.0001	
157.96	71.81	0.9998	1.0001	950	157.96	72.80	0.9998	1.0002	
166.28	74.48	0.9999	1.0001	1000	166.28	75.77	0.9998	1.0002	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O — Continued

$p=0.1$ MPa								
$x=0.05$					$x=0.10$			
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\phi_1$	$\phi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\phi_1$	$\phi_2$
32.92	48.31	0.9893	1.0056	400	32.95	47.43	0.9895	1.0043
34.64	49.06	0.9914	1.0039	420	34.66	48.22	0.9915	1.0029
36.34	49.81	0.9930	1.0027	440	36.36	49.01	0.9930	1.0020
38.04	50.56	0.9942	1.0019	460	38.05	49.80	0.9942	1.0015
39.72	51.31	0.9951	1.0014	480	39.74	50.59	0.9951	1.0011
41.41	52.07	0.9959	1.0010	500	41.42	51.39	0.9959	1.0008
43.09	52.82	0.9965	1.0008	520	43.10	52.19	0.9965	1.0006
44.77	53.59	0.9969	1.0006	540	44.78	52.99	0.9970	1.0004
46.44	54.35	0.9974	1.0005	560	46.45	53.80	0.9974	1.0003
48.12	55.12	0.9977	1.0004	580	48.12	54.62	0.9977	1.0003
49.79	55.90	0.9980	1.0003	600	49.80	55.44	0.9980	1.0002
53.97	57.86	0.9985	1.0002	650	53.97	57.52	0.9985	1.0002
58.14	59.85	0.9989	1.0002	700	58.14	59.64	0.9989	1.0001
62.31	61.88	0.9991	1.0001	750	62.31	61.80	0.9991	1.0001
66.47	63.94	0.9993	1.0001	800	66.48	63.99	0.9993	1.0002
70.64	66.03	0.9995	1.0002	850	70.64	66.23	0.9995	1.0002
74.80	68.16	0.9996	1.0002	900	74.80	68.50	0.9996	1.0002
78.96	70.33	0.9997	1.0002	950	78.96	70.82	0.9997	1.0002
83.12	72.53	0.9997	1.0002	1000	83.13	73.18	0.9997	1.0002
$x=0.20$					$x=0.30$			
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\phi_1$	$\phi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\phi_1$	$\phi_2$
33.00	45.67	0.9898	1.0022	400	33.04	43.91	0.9903	1.0007
34.70	46.53	0.9917	1.0014	420	34.73	44.85	0.9921	1.0004
36.39	47.40	0.9932	1.0010	440	36.42	45.79	0.9935	1.0002
38.08	48.27	0.9943	1.0007	460	38.10	46.73	0.9945	1.0001
39.76	49.14	0.9952	1.0005	480	39.78	47.69	0.9954	1.0000
41.44	50.02	0.9960	1.0003	500	41.46	48.66	0.9961	1.0000
43.12	50.91	0.9965	1.0002	520	43.13	49.63	0.9966	1.0000
44.79	51.80	0.9970	1.0002	540	44.80	50.61	0.9971	1.0000
46.46	52.70	0.9974	1.0001	560	46.48	51.60	0.9975	1.0000
48.14	53.61	0.9977	1.0001	580	48.15	52.60	0.9978	1.0000
49.81	54.53	0.9980	1.0001	600	49.82	53.61	0.9980	1.0000
53.98	56.85	0.9985	1.0001	650	53.99	56.18	0.9985	1.0001
58.15	59.22	0.9989	1.0001	700	58.16	58.80	0.9989	1.0001
62.32	61.64	0.9991	1.0002	750	62.32	61.48	0.9991	1.0002
66.48	64.11	0.9993	1.0002	800	66.49	64.22	0.9993	1.0002
70.65	66.62	0.9995	1.0002	850	70.65	67.02	0.9995	1.0003
74.81	69.19	0.9996	1.0002	900	74.81	69.88	0.9996	1.0003
78.97	71.81	0.9997	1.0003	950	78.98	72.79	0.9996	1.0003
83.13	74.47	0.9997	1.0003	1000	83.14	75.77	0.9997	1.0003

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 0.15 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	
21.84	48.23	0.9840	1.0087	400	21.86	47.36	0.9841	1.0066	
23.00	49.00	0.9871	1.0059	420	23.02	48.16	0.9872	1.0045	
24.15	49.76	0.9894	1.0041	440	24.16	48.96	0.9895	1.0031	
25.29	50.52	0.9912	1.0030	460	25.30	49.76	0.9913	1.0022	
26.42	51.27	0.9927	1.0021	480	26.43	50.55	0.9927	1.0016	
27.55	52.03	0.9938	1.0016	500	27.56	51.35	0.9938	1.0012	
28.68	52.80	0.9947	1.0012	520	28.69	52.16	0.9947	1.0009	
29.80	53.56	0.9954	1.0009	540	29.81	52.97	0.9954	1.0007	
30.92	54.33	0.9960	1.0007	560	30.93	53.78	0.9960	1.0005	
32.04	55.10	0.9965	1.0006	580	32.05	54.60	0.9965	1.0004	
33.16	55.88	0.9970	1.0005	600	33.17	55.42	0.9970	1.0004	
35.95	57.84	0.9978	1.0003	650	35.96	57.51	0.9978	1.0003	
38.74	59.84	0.9983	1.0002	700	38.74	59.63	0.9983	1.0002	
41.52	61.87	0.9987	1.0002	750	41.52	61.79	0.9987	1.0002	
44.30	63.93	0.9990	1.0002	800	44.30	63.98	0.9990	1.0002	
47.08	66.02	0.9992	1.0002	850	47.08	66.22	0.9992	1.0003	
49.86	68.15	0.9994	1.0003	900	49.86	68.50	0.9994	1.0003	
52.63	70.32	0.9995	1.0003	950	52.64	70.82	0.9995	1.0003	
55.41	72.53	0.9996	1.0003	1000	55.41	73.17	0.9996	1.0003	
$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	
21.91	45.62	0.9847	1.0034	400	21.95	43.87	0.9854	1.0011	
23.06	46.49	0.9876	1.0022	420	23.09	44.81	0.9881	1.0006	
24.20	47.36	0.9898	1.0015	440	24.22	45.75	0.9902	1.0003	
25.33	48.23	0.9915	1.0010	460	25.35	46.71	0.9918	1.0001	
26.46	49.11	0.9929	1.0007	480	26.48	47.67	0.9931	1.0000	
27.58	50.00	0.9939	1.0005	500	27.60	48.63	0.9941	1.0000	
28.70	50.89	0.9948	1.0004	520	28.72	49.61	0.9949	1.0000	
29.83	51.78	0.9955	1.0003	540	29.84	50.59	0.9956	1.0000	
30.94	52.69	0.9961	1.0002	560	30.96	51.59	0.9962	1.0000	
32.06	53.60	0.9966	1.0002	580	32.07	52.59	0.9967	1.0000	
33.18	54.51	0.9970	1.0002	600	33.19	53.60	0.9970	1.0000	
35.97	56.84	0.9978	1.0002	650	35.98	56.17	0.9978	1.0001	
38.75	59.21	0.9983	1.0002	700	38.76	58.79	0.9983	1.0002	
41.53	61.63	0.9987	1.0002	750	41.54	61.48	0.9987	1.0003	
44.31	64.10	0.9990	1.0003	800	44.32	64.22	0.9990	1.0003	
47.09	66.62	0.9992	1.0003	850	47.09	67.01	0.9992	1.0004	
49.86	69.19	0.9994	1.0004	900	49.87	69.87	0.9993	1.0004	
52.64	71.80	0.9995	1.0004	950	52.65	72.79	0.9995	1.0005	
55.42	74.47	0.9996	1.0004	1000	55.42	75.76	0.9996	1.0005	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for *x* mole fraction CO<sub>2</sub> in (1-*x*) mole fraction H<sub>2</sub>O - Continued

*p* = 0.2 MPa

<i>x</i> = 0.05					<i>x</i> = 0.10				
<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	
16.29	48.15	0.9785	1.0120	400	16.32	47.29	0.9788	1.0091	
17.17	48.93	0.9827	1.0081	420	17.20	48.11	0.9829	1.0062	
18.05	49.71	0.9859	1.0057	440	18.06	48.91	0.9860	1.0043	
18.91	50.47	0.9883	1.0040	460	18.93	49.72	0.9884	1.0030	
19.77	51.24	0.9902	1.0029	480	19.78	50.52	0.9903	1.0022	
20.62	52.00	0.9917	1.0021	500	20.63	51.32	0.9917	1.0016	
21.47	52.77	0.9929	1.0016	520	21.48	52.13	0.9929	1.0012	
22.32	53.54	0.9939	1.0012	540	22.33	52.94	0.9939	1.0009	
23.16	54.31	0.9947	1.0009	560	23.17	53.76	0.9947	1.0007	
24.01	55.08	0.9954	1.0008	580	24.01	54.58	0.9954	1.0006	
24.85	55.86	0.9960	1.0006	600	24.85	55.41	0.9960	1.0005	
26.95	57.83	0.9970	1.0004	650	26.95	57.50	0.9970	1.0003	
29.04	59.83	0.9978	1.0003	700	29.04	59.62	0.9978	1.0003	
31.13	61.86	0.9983	1.0003	750	31.13	61.78	0.9983	1.0003	
33.22	63.92	0.9987	1.0003	800	33.219	63.98	0.9987	1.0003	
35.30	66.02	0.9990	1.0003	850	35.304	66.21	0.9990	1.0003	
37.39	68.15	0.9992	1.0003	900	37.388	68.49	0.9992	1.0004	
39.47	70.32	0.9993	1.0004	950	39.472	70.81	0.9993	1.0004	
41.55	72.52	0.9995	1.0004	1000	41.554	73.17	0.9995	1.0004	

<i>x</i> = 0.20					<i>x</i> = 0.30				
<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	
16.37	45.56	0.9795	1.0046	400	16.40	43.82	0.9805	1.0015	
17.24	46.44	0.9834	1.0031	420	17.27	44.77	0.9842	1.0008	
18.10	47.32	0.9864	1.0021	440	18.12	45.72	0.9869	1.0004	
18.95	48.20	0.9887	1.0014	460	18.98	46.68	0.9891	1.0002	
19.80	49.08	0.9905	1.0010	480	19.82	47.64	0.9908	1.0000	
20.65	49.97	0.9919	1.0007	500	20.67	48.61	0.9921	1.0000	
21.50	50.86	0.9931	1.0005	520	21.51	49.59	0.9932	1.0000	
22.34	51.76	0.9940	1.0004	540	22.36	50.58	0.9941	1.0000	
23.18	52.67	0.9948	1.0003	560	23.20	51.57	0.9949	1.0000	
24.02	53.58	0.9955	1.0003	580	24.04	52.58	0.9955	1.0000	
24.86	54.50	0.9960	1.0002	600	24.88	53.59	0.9961	1.0001	
26.96	56.83	0.9971	1.0002	650	26.97	56.16	0.9971	1.0002	
29.05	59.20	0.9978	1.0003	700	29.06	58.78	0.9978	1.0003	
31.14	61.62	0.9983	1.0003	750	31.14	61.47	0.9983	1.0004	
33.22	64.09	0.9987	1.0004	800	33.23	64.21	0.9986	1.0004	
35.31	66.61	0.9989	1.0004	850	35.32	67.01	0.9989	1.0005	
37.39	69.18	0.9992	1.0005	900	37.40	69.87	0.9991	1.0006	
39.48	71.80	0.9993	1.0005	950	39.48	72.78	0.9993	1.0006	
41.56	74.46	0.9995	1.0006	1000	41.56	75.76	0.9994	1.0007	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 0.25 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	
12.96	48.08	0.9731	1.0154	400	12.99	47.22	0.9734	1.0117	
13.68	48.87	0.9784	1.0104	420	13.70	48.05	0.9786	1.0079	
14.39	49.65	0.9823	1.0072	440	14.41	48.86	0.9825	1.0055	
15.09	50.43	0.9854	1.0051	460	15.10	49.67	0.9855	1.0039	
15.78	51.20	0.9877	1.0037	480	15.79	50.48	0.9878	1.0028	
16.46	51.97	0.9896	1.0027	500	16.48	51.29	0.9897	1.0020	
17.15	52.74	0.9911	1.0020	520	17.16	52.11	0.9912	1.0015	
17.83	53.51	0.9924	1.0015	540	17.84	52.92	0.9924	1.0012	
18.51	54.28	0.9934	1.0012	560	18.52	53.74	0.9934	1.0009	
19.18	55.06	0.9942	1.0009	580	19.19	54.56	0.9942	1.0007	
19.86	55.84	0.9949	1.0008	600	19.86	55.39	0.9950	1.0006	
21.54	57.81	0.9963	1.0005	650	21.55	57.48	0.9963	1.0004	
23.22	59.81	0.9972	1.0004	700	23.22	59.61	0.9972	1.0004	
24.89	61.85	0.9979	1.0004	750	24.90	61.77	0.9979	1.0004	
26.56	63.91	0.9983	1.0004	800	26.57	63.97	0.9983	1.0004	
28.24	66.01	0.9987	1.0004	850	28.24	66.21	0.9987	1.0004	
29.90	68.14	0.9990	1.0004	900	29.90	68.49	0.9990	1.0005	
31.57	70.31	0.9992	1.0005	950	31.57	70.81	0.9992	1.0005	
33.24	72.52	0.9993	1.0005	1000	33.24	73.16	0.9993	1.0006	

$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	
13.04	45.51	0.9744	1.0060	400	13.08	43.77	0.9756	1.0020	
13.74	46.39	0.9793	1.0039	420	13.78	44.73	0.9802	1.0011	
14.44	47.28	0.9830	1.0026	440	14.47	45.69	0.9836	1.0006	
15.13	48.16	0.9858	1.0018	460	15.15	46.65	0.9863	1.0002	
15.81	49.05	0.9881	1.0012	480	15.83	47.62	0.9885	1.0001	
16.50	49.94	0.9899	1.0009	500	16.51	48.59	0.9902	1.0000	
17.18	50.84	0.9913	1.0006	520	17.19	49.57	0.9916	1.0000	
17.85	51.74	0.9925	1.0005	540	17.87	50.56	0.9927	1.0000	
18.53	52.65	0.9935	1.0004	560	18.54	51.56	0.9936	1.0000	
19.20	53.56	0.9943	1.0003	580	19.21	52.56	0.9944	1.0000	
19.88	54.48	0.9950	1.0003	600	19.89	53.57	0.9951	1.0001	
21.56	56.81	0.9963	1.0003	650	21.56	56.15	0.9963	1.0002	
23.23	59.19	0.9972	1.0003	700	23.24	58.78	0.9972	1.0003	
24.90	61.61	0.9979	1.0004	750	24.91	61.46	0.9978	1.0004	
26.57	64.09	0.9983	1.0005	800	26.58	64.20	0.9983	1.0006	
28.24	66.61	0.9987	1.0005	850	28.25	67.00	0.9986	1.0006	
29.91	69.17	0.9989	1.0006	900	29.92	69.86	0.9989	1.0007	
31.58	71.79	0.9992	1.0007	950	31.58	72.78	0.9991	1.0008	
33.24	74.46	0.9993	1.0007	1000	33.25	75.76	0.9993	1.0009	



TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O - Continued

$p=0.3$ MPa								
$x=0.05$				$x=0.10$				
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\phi_1$	$\phi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\phi_1$	$\phi_2$
				403.04	0.0193	9.84	<i>coexisting phase</i> 0.9837	<i>x = .000039</i> 2619.
				403.04	10.86	47.28	0.9690	1.0136
		<i>coexisting phase</i>	<i>x = .000021</i>					
0.0193	9.98	0.9209	2590.	404.91				
10.89	48.20	0.9694	1.0173	404.91				
11.35	48.81	0.9740	1.0129	420	11.37	47.99	0.9742	1.0097
11.95	49.60	0.9788	1.0089	440	11.97	48.82	0.9789	1.0067
12.54	50.38	0.9824	1.0063	460	12.55	49.63	0.9825	1.0047
13.12	51.16	0.9853	1.0045	480	13.13	50.45	0.9854	1.0034
13.69	51.93	0.9875	1.0033	500	13.70	51.26	0.9876	1.0025
14.27	52.71	0.9894	1.0025	520	14.28	52.08	0.9894	1.0019
14.84	53.48	0.9908	1.0019	540	14.84	52.90	0.9909	1.0014
15.40	54.26	0.9921	1.0015	560	15.41	53.72	0.9921	1.0011
15.97	55.04	0.9931	1.0011	580	15.98	54.54	0.9931	1.0009
16.53	55.82	0.9939	1.0009	600	16.54	55.37	0.9939	1.0007
17.94	57.80	0.9955	1.0006	650	17.94	57.47	0.9956	1.0005
19.34	59.80	0.9966	1.0005	700	19.34	59.60	0.9967	1.0005
20.74	61.84	0.9974	1.0004	750	20.74	61.76	0.9974	1.0005
22.13	63.90	0.9980	1.0004	800	22.13	63.96	0.9980	1.0005
23.52	66.00	0.9984	1.0005	850	23.53	66.20	0.9984	1.0005
24.92	68.14	0.9988	1.0005	900	24.92	68.48	0.9988	1.0006
26.30	70.31	0.9990	1.0006	950	26.31	70.80	0.9990	1.0006
27.70	72.51	0.9992	1.0006	1000	27.70	73.16	0.9992	1.0007
$x=0.20$				$x=0.30$				
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\phi_1$	$\phi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\phi_1$	$\phi_2$
10.82	45.45	0.9691	1.0074	400	10.86	43.73	0.9707	1.0025
11.41	46.35	0.9751	1.0049	420	11.45	44.69	0.9762	1.0014
12.00	47.24	0.9795	1.0032	440	12.03	45.65	0.9804	1.0007
12.58	48.13	0.9830	1.0022	460	12.60	46.62	0.9836	1.0003
13.15	49.02	0.9857	1.0015	480	13.17	47.59	0.9862	1.0001
13.72	49.92	0.9878	1.0011	500	13.74	48.57	0.9882	1.0000
14.29	50.82	0.9896	1.0008	520	14.31	49.55	0.9899	1.0000
14.86	51.72	0.9910	1.0006	540	14.87	50.54	0.9912	1.0000
15.42	52.63	0.9922	1.0005	560	15.44	51.54	0.9924	1.0000
15.99	53.55	0.9932	1.0004	580	16.00	52.55	0.9933	1.0000
16.55	54.47	0.9940	1.0004	600	16.56	53.56	0.9941	1.0001
17.95	56.80	0.9956	1.0004	650	17.96	56.14	0.9956	1.0002
19.35	59.18	0.9967	1.0004	700	19.36	58.77	0.9967	1.0004
20.74	61.61	0.9974	1.0005	750	20.75	61.45	0.9974	1.0005
22.14	64.08	0.9980	1.0006	800	22.14	64.20	0.9980	1.0007
23.53	66.60	0.9984	1.0006	850	23.54	67.00	0.9984	1.0008
24.92	69.17	0.9987	1.0007	900	24.93	69.86	0.9987	1.0009
26.31	71.79	0.9990	1.0008	950	26.32	72.78	0.9989	1.0010
27.70	74.46	0.9992	1.0008	1000	27.71	75.75	0.9991	1.0010





TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 0.6 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
				427.74	0.0197	11.75			<i>coexisting phase</i> $x = .000090$
				427.74	5.666	47.96	0.8568	1136.6	
							0.9519	1.0195	
									<i>coexisting phase</i> $x = .000046$
0.0198	11.92	0.9049	1122.9	429.92					
5.677	48.82	0.9525	1.0247	429.92					
5.840	49.26	0.9571	1.0203	440	5.861	48.51	0.9575	1.0154	
6.154	50.10	0.9646	1.0141	460	6.171	49.38	0.9649	1.0106	
6.461	50.92	0.9704	1.0100	480	6.474	50.23	0.9706	1.0075	
6.762	51.73	0.9750	1.0072	500	6.773	51.07	0.9751	1.0054	
7.058	52.53	0.9787	1.0053	520	7.068	51.91	0.9788	1.0040	
7.351	53.33	0.9816	1.0040	540	7.360	52.75	0.9817	1.0030	
7.642	54.12	0.9841	1.0031	560	7.650	53.59	0.9842	1.0023	
7.931	54.92	0.9861	1.0024	580	7.937	54.43	0.9862	1.0019	
8.218	55.71	0.9879	1.0019	600	8.224	55.27	0.9879	1.0015	
8.931	57.71	0.9911	1.0013	650	8.936	57.38	0.9911	1.0011	
9.639	59.73	0.9933	1.0010	700	9.642	59.53	0.9933	1.0009	
10.343	61.78	0.9949	1.0009	750	10.346	61.70	0.9949	1.0009	
11.044	63.85	0.9960	1.0009	800	11.047	63.91	0.9960	1.0010	
11.744	65.96	0.9969	1.0010	850	11.747	66.16	0.9969	1.0011	
12.443	68.10	0.9975	1.0010	900	12.445	68.45	0.9975	1.0012	
13.141	70.27	0.9980	1.0011	950	13.143	70.77	0.9980	1.0013	
13.838	72.48	0.9984	1.0012	1000	13.840	73.13	0.9984	1.0013	
$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
				418.08	0.0195	11.01			<i>coexisting phase</i> $x = .000251$
				418.08	5.592	44.35	0.6659	1200.5	
							0.9511	1.0039	
									<i>coexisting phase</i> $x = .000173$
0.0196	11.40	0.7611	1166.5	423.14					
5.635	46.20	0.9512	1.0107	423.14					
5.896	46.99	0.9588	1.0075	420	5.622	44.45	0.9521	1.0036	
6.200	47.92	0.9658	1.0051	440	5.926	45.45	0.9606	1.0020	
6.499	48.84	0.9713	1.0035	460	6.225	46.44	0.9671	1.0010	
6.794	49.76	0.9756	1.0024	480	6.520	47.44	0.9723	1.0004	
7.086	50.68	0.9792	1.0017	500	6.812	48.43	0.9764	1.0001	
7.376	51.60	0.9820	1.0013	520	7.102	49.43	0.9797	1.0000	
7.663	52.52	0.9844	1.0010	540	7.390	50.43	0.9824	1.0000	
7.950	53.44	0.9864	1.0009	560	7.676	51.44	0.9847	1.0000	
8.235	54.38	0.9880	1.0009	580	7.961	52.46	0.9866	1.0001	
8.944	56.73	0.9912	1.0007	600	8.246	53.48	0.9882	1.0002	
9.650	59.12	0.9933	1.0008	650	8.953	56.07	0.9912	1.0005	
10.352	61.56	0.9949	1.0010	700	9.657	58.71	0.9933	1.0008	
11.053	64.04	0.9960	1.0011	750	10.359	61.41	0.9948	1.0011	
11.752	66.56	0.9968	1.0013	800	11.059	64.16	0.9959	1.0014	
12.450	69.14	0.9975	1.0014	850	11.757	66.96	0.9967	1.0016	
13.147	71.76	0.9980	1.0016	900	12.455	69.83	0.9974	1.0018	
13.844	74.43	0.9984	1.0017	950	13.152	72.75	0.9978	1.0019	
				1000	13.849	75.73	0.9982	1.0021	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O - Continued

$p = 0.7 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	
				433.71	0.0199	12.22	<i>coexisting phase</i>		$x = .000108$
				433.71	4.8993	48.12	0.8524	0.9470	942.2
									1.0212
		<i>coexisting phase</i>							$x = .000055$
0.0199	12.39	0.9003	930.5	435.96					
4.908	48.96	0.9477	1.0269	435.96					
4.965	49.14	0.9498	1.0248	440	4.987	48.40	0.9502		1.0187
5.242	50.00	0.9586	1.0171	460	5.259	49.29	0.9589		1.0129
5.509	50.84	0.9654	1.0121	480	5.523	50.16	0.9656		1.0091
5.771	51.66	0.9708	1.0087	500	5.782	51.01	0.9710		1.0065
6.028	52.47	0.9751	1.0064	520	6.038	51.86	0.9752		1.0048
6.282	53.27	0.9786	1.0048	540	6.290	52.70	0.9787		1.0036
6.533	54.07	0.9814	1.0037	560	6.541	53.54	0.9815		1.0028
6.782	54.87	0.9838	1.0029	580	6.789	54.39	0.9839		1.0022
7.030	55.67	0.9858	1.0023	600	7.036	55.23	0.9859		1.0018
7.644	57.68	0.9896	1.0015	650	7.649	57.36	0.9896		1.0013
8.253	59.71	0.9922	1.0012	700	8.256	59.50	0.9922		1.0011
8.858	61.76	0.9940	1.0011	750	8.861	61.68	0.9940		1.0011
9.461	63.83	0.9954	1.0011	800	9.463	63.90	0.9954		1.0012
10.062	65.94	0.9964	1.0011	850	10.064	66.15	0.9963		1.0013
10.661	68.09	0.9971	1.0012	900	10.664	68.43	0.9971		1.0014
11.260	70.26	0.9977	1.0013	950	11.262	70.76	0.9977		1.0015
11.858	72.47	0.9982	1.0014	1000	11.860	73.12	0.9982		1.0016
$x = 0.20$					$x = 0.30$				
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	
				423.70	0.0197	11.45	<i>coexisting phase</i>		$x = .000302$
				423.70	4.838	44.55	0.6624	0.9460	996.5
									1.0041
		<i>coexisting phase</i>							$x = .000209$
0.0198	11.85	0.7571	967.7	428.93					
4.874	46.37	0.9462	1.0117	428.93					
5.024	46.90	0.9518	1.0092	440	5.054	45.38	0.9539		1.0025
5.288	47.85	0.9600	1.0062	460	5.314	46.38	0.9616		1.0013
5.548	48.78	0.9665	1.0042	480	5.569	47.38	0.9676		1.0006
5.803	49.70	0.9716	1.0029	500	5.822	48.39	0.9724		1.0002
6.056	50.63	0.9757	1.0021	520	6.072	49.39	0.9763		1.0001
6.306	51.55	0.9790	1.0016	540	6.320	50.40	0.9795		1.0000
6.555	52.48	0.9818	1.0012	560	6.567	51.41	0.9822		1.0001
6.802	53.41	0.9841	1.0010	580	6.813	52.43	0.9844		1.0001
7.047	54.35	0.9860	1.0009	600	7.058	53.45	0.9862		1.0003
7.658	56.70	0.9897	1.0009	650	7.666	56.05	0.9898		1.0006
8.264	59.10	0.9922	1.0010	700	8.271	58.69	0.9922		1.0010
8.867	61.54	0.9940	1.0012	750	8.874	61.39	0.9940		1.0013
9.469	64.02	0.9953	1.0013	800	9.475	64.14	0.9952		1.0016
10.069	66.55	0.9963	1.0015	850	10.075	66.95	0.9962		1.0018
10.668	69.13	0.9970	1.0017	900	10.674	69.82	0.9969		1.0021
11.267	71.75	0.9976	1.0018	950	11.272	72.74	0.9975		1.0023
11.864	74.42	0.9981	1.0020	1000	11.869	75.72	0.9979		1.0024

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p=0.8$ MPa								
$x=0.05$				$x=0.10$				
$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$
				439.02	0.0200	12.64	<i>coexisting phase</i> $x=.000128$	
				439.02	4.318	48.24	0.8483	800.4
							0.9424	1.0228
		<i>coexisting phase</i> $x=.000065$						
0.0200	12.82	0.8961	790.2	441.34				
4.326	49.07	0.9432	1.0289	441.34				
4.556	49.90	0.9526	1.0203	460	4.574	49.20	0.9529	1.0153
4.795	50.75	0.9604	1.0142	480	4.809	50.08	0.9607	1.0107
5.027	51.59	0.9666	1.0102	500	5.039	50.95	0.9668	1.0077
5.255	52.41	0.9715	1.0075	520	5.265	51.80	0.9716	1.0056
5.480	53.22	0.9755	1.0056	540	5.488	52.65	0.9756	1.0042
5.701	54.03	0.9788	1.0043	560	5.709	53.50	0.9789	1.0032
5.921	54.83	0.9815	1.0033	580	5.928	54.35	0.9816	1.0026
6.139	55.64	0.9838	1.0027	600	6.145	55.20	0.9838	1.0021
6.679	57.65	0.9881	1.0017	650	6.684	57.33	0.9881	1.0015
7.213	59.68	0.9911	1.0013	700	7.217	59.48	0.9911	1.0013
7.744	61.74	0.9932	1.0012	750	7.748	61.67	0.9932	1.0012
8.273	63.82	0.9947	1.0012	800	8.276	63.88	0.9947	1.0013
8.800	65.93	0.9958	1.0013	850	8.802	66.13	0.9958	1.0014
9.325	68.07	0.9967	1.0014	900	9.327	68.42	0.9967	1.0016
9.850	70.25	0.9974	1.0015	950	9.852	70.75	0.9974	1.0017
10.373	72.46	0.9979	1.0016	1000	10.375	73.11	0.9979	1.0018
$x=0.20$				$x=0.30$				
$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$
				428.70	0.0198	11.84	<i>coexisting phase</i> $x=.000355$	
				428.70	4.267	44.72	0.6590	847.6
							0.9412	1.0044
		<i>coexisting phase</i> $x=.000246$						
0.0199	12.26	0.7534	822.5	434.09				
4.298	46.53	0.9415	1.0125	434.09				
4.369	46.81	0.9448	1.0111	440	4.400	45.30	0.9472	1.0031
4.604	47.77	0.9543	1.0073	460	4.630	46.32	0.9561	1.0016
4.835	48.71	0.9616	1.0050	480	4.856	47.33	0.9630	1.0008
5.061	49.65	0.9675	1.0035	500	5.079	48.34	0.9685	1.0003
5.284	50.58	0.9722	1.0025	520	5.300	49.35	0.9729	1.0001
5.504	51.51	0.9760	1.0019	540	5.519	50.36	0.9766	1.0001
5.723	52.44	0.9792	1.0015	560	5.736	51.38	0.9796	1.0001
5.940	53.38	0.9818	1.0012	580	5.952	52.40	0.9821	1.0002
6.156	54.31	0.9840	1.0011	600	6.167	53.43	0.9843	1.0003
6.693	56.68	0.9882	1.0010	650	6.701	56.03	0.9883	1.0007
7.225	59.08	0.9911	1.0011	700	7.232	58.68	0.9911	1.0011
7.754	61.52	0.9931	1.0013	750	7.760	61.38	0.9931	1.0015
8.281	64.01	0.9946	1.0015	800	8.287	64.13	0.9946	1.0018
8.807	66.54	0.9958	1.0018	850	8.813	66.94	0.9956	1.0021
9.332	69.12	0.9966	1.0019	900	9.337	69.81	0.9965	1.0024
9.856	71.74	0.9973	1.0021	950	9.861	72.73	0.9971	1.0026
10.380	74.41	0.9978	1.0023	1000	10.385	75.71	0.9976	1.0028

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O - Continued

$p = 0.9 \text{ MPa}$								
$x = 0.05$				$x = 0.10$				
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$
				443.83	0.0201	13.02	coexisting phase $x = .000148$	
				443.83	3.863	48.36	0.8443	692.8
							0.9380	1.0244
		coexisting phase $x = .000075$						
0.0201	13.20	0.8920	683.8	446.22				
3.868	49.17	0.9389	1.0309	446.22				
4.023	49.80	0.9465	1.0237	460	4.041	49.10	0.9469	1.0179
4.239	50.67	0.9554	1.0166	480	4.254	50.00	0.9557	1.0124
4.449	51.51	0.9623	1.0118	500	4.461	50.88	0.9626	1.0089
4.654	52.35	0.9679	1.0086	520	4.664	51.74	0.9681	1.0065
4.855	53.17	0.9724	1.0064	540	4.864	52.60	0.9725	1.0048
5.054	53.98	0.9761	1.0049	560	5.062	53.46	0.9762	1.0037
5.251	54.79	0.9792	1.0038	580	5.258	54.31	0.9793	1.0029
5.446	55.60	0.9818	1.0031	600	5.452	55.16	0.9818	1.0024
5.928	57.62	0.9866	1.0020	650	5.933	57.30	0.9867	1.0017
6.405	59.66	0.9900	1.0015	700	6.409	59.46	0.9900	1.0014
6.878	61.72	0.9923	1.0014	750	6.881	61.65	0.9923	1.0014
7.349	63.80	0.9940	1.0014	800	7.352	63.87	0.9940	1.0015
7.818	65.92	0.9953	1.0015	850	7.821	66.12	0.9953	1.0016
8.286	68.06	0.9963	1.0016	900	8.288	68.41	0.9963	1.0018
8.753	70.24	0.9971	1.0017	950	8.755	70.74	0.9970	1.0019
9.219	72.45	0.9977	1.0018	1000	9.221	73.11	0.9976	1.0020
$x = 0.20$				$x = 0.30$				
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$
				433.22	0.0199	12.19	coexisting phase $x = .000410$	
				433.22	3.819	44.88	0.6559	734.6
							0.9366	1.0047
		coexisting phase $x = .000284$						
0.0200	12.62	0.7498	712.3	438.76				
3.845	46.66	0.9370	1.0134	438.76				
3.859	46.72	0.9377	1.0130	440	3.890	45.23	0.9406	1.0038
4.072	47.70	0.9485	1.0086	460	4.098	46.26	0.9505	1.0020
4.279	48.65	0.9568	1.0058	480	4.301	47.28	0.9583	1.0010
4.483	49.59	0.9634	1.0040	500	4.501	48.29	0.9645	1.0004
4.683	50.53	0.9687	1.0029	520	4.699	49.31	0.9696	1.0002
4.880	51.47	0.9730	1.0021	540	4.895	50.32	0.9737	1.0001
5.076	52.40	0.9766	1.0017	560	5.089	51.34	0.9771	1.0001
5.270	53.34	0.9795	1.0014	580	5.282	52.37	0.9799	1.0002
5.463	54.28	0.9820	1.0012	600	5.474	53.40	0.9823	1.0004
5.942	56.65	0.9867	1.0012	650	5.951	56.01	0.9869	1.0008
6.416	59.06	0.9900	1.0013	700	6.424	58.66	0.9900	1.0013
6.888	61.50	0.9923	1.0015	750	6.894	61.36	0.9922	1.0017
7.357	63.99	0.9940	1.0017	800	7.363	64.12	0.9939	1.0021
7.826	66.53	0.9952	1.0020	850	7.831	66.93	0.9951	1.0024
8.293	69.10	0.9962	1.0022	900	8.298	69.80	0.9960	1.0027
8.759	71.73	0.9970	1.0024	950	8.764	72.72	0.9968	1.0029
9.225	74.41	0.9975	1.0026	1000	9.230	75.71	0.9973	1.0031

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 1.0 \text{ MPa}$									
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$x = 0.05$		$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$x = 0.10$		$\varphi_2$
		$\varphi_1$	$\varphi_2$				$\varphi_1$	$\varphi_2$	
				448.22	0.0202	13.36	<i>coexisting phase</i> $x = .000170$		
				448.22	3.495	48.46	0.8405	606.6	
							0.9338	1.0259	
		<i>coexisting phase</i> $x = .000089$							
0.0203	13.56	0.8881	589.8	450.68					
3.500	49.26	0.9348	1.0328	450.68					
3.595	49.69	0.9404	1.0274	460	3.614	49.01	0.9409	1.0206	
3.794	50.58	0.9503	1.0190	480	3.809	49.92	0.9507	1.0143	
3.986	51.44	0.9581	1.0135	500	3.998	50.81	0.9584	1.0102	
4.173	52.28	0.9643	1.0099	520	4.183	51.69	0.9645	1.0074	
4.356	53.11	0.9693	1.0073	540	4.365	52.55	0.9695	1.0055	
4.537	53.93	0.9735	1.0056	560	4.544	53.41	0.9736	1.0042	
4.715	54.75	0.9769	1.0043	580	4.722	54.27	0.9770	1.0033	
4.891	55.56	0.9797	1.0034	600	4.898	55.13	0.9798	1.0027	
5.328	57.59	0.9851	1.0022	650	5.332	57.27	0.9852	1.0019	
5.758	59.63	0.9888	1.0017	700	5.762	59.44	0.9888	1.0016	
6.185	61.70	0.9915	1.0015	750	6.188	61.63	0.9915	1.0016	
6.610	63.78	0.9934	1.0016	800	6.613	63.85	0.9934	1.0017	
7.033	65.90	0.9948	1.0016	850	7.035	66.11	0.9948	1.0018	
7.454	68.05	0.9959	1.0018	900	7.457	68.40	0.9959	1.0020	
7.875	70.23	0.9967	1.0019	950	7.877	70.73	0.9967	1.0021	
8.295	72.45	0.9974	1.0020	1000	8.297	73.10	0.9974	1.0023	
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$x = 0.20$		$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$x = 0.30$		$\varphi_2$
		$\varphi_1$	$\varphi_2$				$\varphi_1$	$\varphi_2$	
				437.34	0.0199	12.52	<i>coexisting phase</i> $x = .000467$		
				437.34	3.457	45.02	0.6527	646.4	
							0.9321	1.0049	
		<i>coexisting phase</i> $x = .000324$							
0.0201	12.96	0.7464	626.2	443.03					
3.481	46.78	0.9327	1.0142	443.03					
3.646	47.62	0.9426	1.0100	440	3.483	45.16	0.9339	1.0046	
3.835	48.59	0.9519	1.0067	460	3.672	46.20	0.9450	1.0024	
4.020	49.54	0.9593	1.0046	480	3.857	47.22	0.9537	1.0012	
4.202	50.48	0.9652	1.0033	500	4.039	48.25	0.9606	1.0006	
4.381	51.43	0.9700	1.0025	520	4.218	49.27	0.9662	1.0003	
4.559	52.37	0.9740	1.0019	540	4.396	50.29	0.9707	1.0001	
4.734	53.31	0.9773	1.0016	560	4.572	51.31	0.9745	1.0002	
4.909	54.25	0.9800	1.0014	580	4.746	52.34	0.9777	1.0003	
5.341	56.63	0.9853	1.0013	600	4.920	53.37	0.9803	1.0004	
5.770	59.04	0.9889	1.0014	650	5.350	55.98	0.9854	1.0009	
6.195	61.49	0.9914	1.0017	700	5.777	58.64	0.9889	1.0014	
6.618	63.98	0.9933	1.0019	750	6.202	61.35	0.9914	1.0019	
7.040	66.51	0.9947	1.0022	800	6.624	64.11	0.9932	1.0023	
7.461	69.09	0.9958	1.0024	850	7.046	66.92	0.9946	1.0027	
7.882	71.72	0.9966	1.0027	900	7.467	69.79	0.9956	1.0030	
8.301	74.40	0.9973	1.0028	950	7.887	72.71	0.9964	1.0033	
				1000	8.306	75.70	0.9971	1.0035	



TABLE 3. Molar volume, enthalpy, and fugacity coefficients for x mole fraction CO<sub>2</sub> in (1-x) mole fraction H<sub>2</sub>O - Continued

<i>p</i> = 1.5 MPa									
<i>x</i> = 0.05					<i>x</i> = 0.10				
<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	
				466.08	0.0206	14.80			<i>coexisting phase</i> <i>x</i> = .000281
				466.08	2.373	48.81	0.8240	367.9	
							0.9153	1.0329	
									<i>coexisting phase</i> <i>x</i> = .000145
0.0207	15.01	0.8710	362.6	468.82					
2.374	49.56	0.9167	1.0416	468.82					
2.456	50.12	0.9248	1.0336	480	2.472	49.51	0.9254	1.0251	
2.595	51.06	0.9368	1.0234	500	2.608	50.46	0.9372	1.0175	
2.728	51.96	0.9462	1.0167	520	2.739	51.39	0.9466	1.0125	
2.857	52.83	0.9539	1.0122	540	2.866	52.29	0.9541	1.0092	
2.983	53.68	0.9601	1.0092	560	2.991	53.18	0.9603	1.0069	
3.106	54.53	0.9653	1.0070	580	3.113	54.07	0.9654	1.0054	
3.228	55.36	0.9696	1.0056	600	3.234	54.94	0.9697	1.0043	
3.526	57.44	0.9777	1.0035	650	3.530	57.13	0.9778	1.0030	
3.818	59.51	0.9833	1.0027	700	3.822	59.32	0.9833	1.0025	
4.106	61.60	0.9872	1.0024	750	4.110	61.53	0.9872	1.0024	
4.393	63.70	0.9901	1.0024	800	4.395	63.77	0.9900	1.0026	
4.677	65.83	0.9922	1.0025	850	4.679	66.04	0.9922	1.0028	
4.960	67.99	0.9938	1.0027	900	4.962	68.34	0.9938	1.0030	
5.242	70.18	0.9951	1.0029	950	5.244	70.68	0.9951	1.0032	
5.523	72.40	0.9961	1.0030	1000	5.525	73.05	0.9961	1.0034	
<i>x</i> = 0.20					<i>x</i> = 0.30				
<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	
				454.03	0.0203	13.85			<i>coexisting phase</i> <i>x</i> = .000768
				454.03	2.354	45.55	0.6391	392.9	
							0.9124	1.0063	
									<i>coexisting phase</i> <i>x</i> = .000536
0.0205	14.34	0.7311	379.5	460.31					
2.367	47.23	0.9134	1.0180	460.31					
2.501	48.25	0.9275	1.0120	460	2.394	45.87	0.9171	1.0053	
2.632	49.25	0.9387	1.0082	480	2.525	46.95	0.9303	1.0028	
2.759	50.24	0.9477	1.0058	500	2.652	48.01	0.9408	1.0015	
2.883	51.21	0.9549	1.0042	520	2.776	49.06	0.9492	1.0008	
3.005	52.17	0.9609	1.0032	540	2.898	50.10	0.9561	1.0005	
3.126	53.13	0.9659	1.0027	560	3.019	51.14	0.9618	1.0005	
3.245	54.10	0.9700	1.0023	580	3.138	52.19	0.9665	1.0006	
3.540	56.50	0.9779	1.0021	600	3.256	53.24	0.9705	1.0008	
3.829	58.94	0.9833	1.0023	650	3.548	55.87	0.9781	1.0015	
4.116	61.40	0.9872	1.0026	700	3.837	58.55	0.9833	1.0022	
4.401	63.91	0.9900	1.0030	750	4.123	61.27	0.9871	1.0029	
4.685	66.45	0.9921	1.0034	800	4.407	64.04	0.9898	1.0035	
4.967	69.04	0.9937	1.0037	850	4.690	66.86	0.9918	1.0041	
5.249	71.67	0.9949	1.0040	900	4.972	69.74	0.9934	1.0045	
5.530	74.36	0.9959	1.0043	950	5.254	72.67	0.9946	1.0049	
				1000	5.535	75.66	0.9956	1.0053	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 2.0 \text{ MPa}$									
$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$x = 0.05$		$T$ K	$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$x = 0.10$		$\varphi_2$
		$\varphi_1$	$\varphi_2$				$\varphi_1$	$\varphi_2$	
				479.69	0.0210	15.90	<i>coexisting phase</i>		$x = .00041$
				479.69	1.798	49.04	0.8097	0.8994	256.2
									1.0394
		<i>coexisting phase</i>							$x = .000202$
0.0211	16140.	0.8603	252.7	482.67					
1.797	49743.	0.9011	1.0499	482.67					
1.896	50.64	0.9151	1.0357	500	1.911	50.09	0.9158		1.0267
2.003	51.61	0.9280	1.0251	520	2.015	51.08	0.9285		1.0188
2.106	52.53	0.9383	1.0181	540	2.116	52.02	0.9387		1.0136
2.205	53.43	0.9467	1.0134	560	2.213	52.95	0.9470		1.0102
2.301	54.30	0.9536	1.0102	580	2.308	53.86	0.9538		1.0078
2.395	55.16	0.9594	1.0080	600	2.401	54.76	0.9596		1.0062
2.624	57.28	0.9703	1.0049	650	2.629	56.98	0.9703		1.0042
2.848	59.39	0.9777	1.0037	700	2.851	59.20	0.9777		1.0035
3.067	61.49	0.9829	1.0033	750	3.070	61.44	0.9829		1.0034
3.284	63.62	0.9867	1.0033	800	3.287	63.69	0.9867		1.0035
3.499	65.76	0.9896	1.0034	850	3.502	65.97	0.9896		1.0038
3.713	67.92	0.9918	1.0036	900	3.715	68.28	0.9917		1.0041
3.926	70.12	0.9935	1.0039	950	3.928	70.62	0.9934		1.0044
4.138	72.35	0.9948	1.0041	1000	4.140	73.00	0.9948		1.0046
$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$x = 0.20$		$T$ K	$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$x = 0.30$		$\varphi_2$
		$\varphi_1$	$\varphi_2$				$\varphi_1$	$\varphi_2$	
				446.68	0.0207	14.87	<i>coexisting phase</i>		$x = .00110$
				466.68	1.788	45.91	0.6267	0.8953	275.0
									1.0077
		<i>coexisting phase</i>							$x = .00077$
0.0209	15.41	0.7180	265.0	473.45					
1.796	47.53	0.8969	1.0217	473.45					
1.831	47.89	0.9027	1.0189	480	1.857	46.66	0.9068		1.0052
1.936	48.95	0.9180	1.0127	500	1.957	47.76	0.9209		1.0030
2.036	49.98	0.9301	1.0088	520	2.054	48.84	0.9322		1.0017
2.133	50.98	0.9398	1.0064	540	2.149	49.91	0.9414		1.0012
2.228	51.97	0.9478	1.0049	560	2.242	50.97	0.9490		1.0010
2.322	52.96	0.9545	1.0039	580	2.334	52.03	0.9554		1.0011
2.413	53.93	0.9600	1.0034	600	2.425	53.10	0.9607		1.0013
2.639	56.38	0.9705	1.0029	650	2.648	55.76	0.9708		1.0021
2.859	58.83	0.9777	1.0031	700	2.867	58.46	0.9778		1.0031
3.077	61.32	0.9829	1.0036	750	3.084	61.19	0.9827		1.0040
3.293	63.83	0.9866	1.0041	800	3.299	63.97	0.9864		1.0048
3.507	66.39	0.9894	1.0046	850	3.513	66.81	0.9891		1.0055
3.720	68.99	0.9916	1.0050	900	3.725	69.69	0.9912		1.0061
3.932	71.63	0.9932	1.0054	950	3.938	72.63	0.9928		1.0066
4.144	74.31	0.9946	1.0058	1000	4.149	75.62	0.9941		1.0071

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O — Continued

$p = 2.5 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	
				490.84	0.0214	16.83	coexisting phase $x = .000542$		
				490.84	1.4463	49.18	0.7971	192.80	
							0.8852	1.0457	
		coexisting phase $x = .000279$							
0.0215	17.08	0.8432	189.57	494.03					
1.4440	49.85	0.8874	1.0578	494.03					
1.473	50.18	0.8931	1.0513	500	1.490	49.69	0.8940	1.0381	
1.567	51.24	0.9096	1.0353	520	1.579	50.74	0.9102	1.0263	
1.654	52.22	0.9226	1.0250	540	1.664	51.74	0.9231	1.0188	
1.737	53.16	0.9332	1.0183	560	1.746	52.71	0.9336	1.0139	
1.817	54.07	0.9420	1.0138	580	1.825	53.65	0.9422	1.0106	
1.895	54.96	0.9492	1.0107	600	1.902	54.57	0.9494	1.0084	
1.971	55.83	0.9553	1.0085	620	1.977	55.48	0.9555	1.0069	
2.046	56.70	0.9605	1.0070	640	2.051	56.39	0.9606	1.0059	
2.120	57.56	0.9650	1.0060	660	2.125	57.29	0.9650	1.0052	
2.193	58.41	0.9688	1.0053	680	2.197	58.19	0.9688	1.0047	
2.265	59.26	0.9721	1.0048	700	2.269	59.09	0.9721	1.0045	
2.443	61.39	0.9786	1.0042	750	2.447	61.34	0.9786	1.0043	
2.619	63.53	0.9834	1.0042	800	2.622	63.61	0.9834	1.0045	
2.792	65.68	0.9870	1.0043	850	2.795	65.90	0.9870	1.0048	
2.964	67.86	0.9897	1.0046	900	2.967	68.22	0.9897	1.0052	
3.136	70.07	0.9918	1.0049	950	3.138	70.57	0.9918	1.0055	
3.306	72.30	0.9935	1.0052	1000	3.308	72.96	0.9935	1.0059	
$x = 0.20$					$x = 0.30$				
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	
				476.99	0.0210	15.72	coexisting phase $x = .00146$		
				476.99	1.4418	46.18	0.6169	207.82	
							0.8800	1.0093	
		coexisting phase $x = .00103$							
0.0212	16.29	0.7064	199.92	484.18					
1.4467	47.75	0.8821	1.0253	484.18					
1.517	48.63	0.8970	1.0183	480	1.455	46.35	0.8831	1.0086	
1.602	49.71	0.9123	1.0126	500	1.539	47.50	0.9010	1.0049	
1.683	50.75	0.9247	1.0090	520	1.621	48.62	0.9152	1.0030	
1.762	51.77	0.9347	1.0068	540	1.699	49.71	0.9268	1.0021	
1.839	52.77	0.9431	1.0054	560	1.776	50.80	0.9363	1.0017	
1.914	53.77	0.9500	1.0046	580	1.851	51.88	0.9442	1.0017	
1.988	54.76	0.9559	1.0041	600	1.925	52.95	0.9509	1.0019	
2.061	55.75	0.9609	1.0039	620	1.999	54.03	0.9565	1.0022	
2.134	56.75	0.9652	1.0039	640	2.071	55.11	0.9613	1.0026	
2.206	57.74	0.9690	1.0039	660	2.143	56.19	0.9655	1.0031	
2.277	58.73	0.9722	1.0041	680	2.214	57.27	0.9691	1.0035	
2.453	61.23	0.9786	1.0046	700	2.285	58.36	0.9722	1.0040	
2.627	63.76	0.9833	1.0052	750	2.460	61.12	0.9784	1.0051	
2.800	66.33	0.9868	1.0058	800	2.634	63.91	0.9830	1.0061	
2.972	68.93	0.9895	1.0063	850	2.806	66.75	0.9864	1.0069	
3.143	71.58	0.9916	1.0069	900	2.977	69.64	0.9890	1.0077	
3.313	74.27	0.9932	1.0073	950	3.148	72.58	0.9911	1.0084	
				1000	3.318	75.58	0.9927	1.0089	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 3.0 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
				500.36	0.0217	17.62	coexisting phase $x = .00069$		
				500.36	1.208	49.28	0.7856	152.53	
							0.8723	1.0519	
		coexisting phase $x = .000356$							
0.0218	17.90	0.8314	149.73	503.73					
1.205	49.91	0.8749	1.0656	503.73					
1.274	50.84	0.8909	1.0476	520	1.288	50.39	0.8917	1.0354	
1.351	51.89	0.9069	1.0333	540	1.363	51.45	0.9074	1.0249	
1.424	52.88	0.9197	1.0240	560	1.434	52.45	0.9201	1.0182	
1.494	53.83	0.9303	1.0179	580	1.502	53.43	0.9306	1.0137	
1.561	54.75	0.9390	1.0137	600	1.568	54.38	0.9392	1.0108	
1.627	55.65	0.9464	1.0109	620	1.633	55.31	0.9465	1.0088	
1.691	56.53	0.9526	1.0089	640	1.696	56.23	0.9527	1.0074	
1.754	57.41	0.9579	1.0076	660	1.759	57.15	0.9580	1.0065	
1.816	58.27	0.9625	1.0066	680	1.820	58.06	0.9626	1.0059	
1.877	59.14	0.9665	1.0060	700	1.881	58.97	0.9665	1.0056	
2.027	61.29	0.9744	1.0052	750	2.031	61.24	0.9744	1.0053	
2.175	63.44	0.9801	1.0051	800	2.178	63.53	0.9801	1.0055	
2.321	65.61	0.9844	1.0053	850	2.324	65.83	0.9844	1.0059	
2.466	67.80	0.9877	1.0056	900	2.468	68.16	0.9876	1.0063	
2.609	70.01	0.9902	1.0059	950	2.611	70.52	0.9902	1.0067	
2.752	72.25	0.9922	1.0063	1000	2.754	72.91	0.9922	1.0071	
$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
				485.72	0.0212	16.45	coexisting phase $x = .00184$		
				485.72	1.208	46.38	0.6072	165.07	
							0.8660	1.0110	
		coexisting phase $x = .00130$							
0.0215	17058.	0.6958	158.44	493.31					
1.210	47903.	0.8686	1.0289	493.31					
1.237	48.30	0.8759	1.0252	500	1.260	47.23	0.8809	1.0076	
1.311	49.42	0.8945	1.0170	520	1.331	48.39	0.8982	1.0047	
1.382	50.51	0.9095	1.0121	540	1.399	49.51	0.9121	1.0032	
1.450	51.56	0.9216	1.0090	560	1.465	50.62	0.9236	1.0026	
1.516	52.59	0.9316	1.0071	580	1.529	51.72	0.9331	1.0024	
1.581	53.61	0.9400	1.0060	600	1.592	52.81	0.9411	1.0026	
1.644	54.62	0.9471	1.0053	620	1.655	53.90	0.9478	1.0030	
1.706	55.62	0.9531	1.0050	640	1.716	54.99	0.9536	1.0034	
1.768	56.62	0.9583	1.0049	660	1.777	56.08	0.9586	1.0039	
1.829	57.62	0.9628	1.0049	680	1.837	57.17	0.9629	1.0044	
1.889	58.63	0.9666	1.0051	700	1.897	58.27	0.9667	1.0050	
2.038	61.14	0.9743	1.0057	750	2.044	61.04	0.9741	1.0063	
2.184	63.69	0.9799	1.0064	800	2.190	63.84	0.9796	1.0074	
2.329	66.26	0.9842	1.0071	850	2.335	66.69	0.9837	1.0084	
2.473	68.88	0.9874	1.0077	900	2.478	69.59	0.9868	1.0093	
2.616	71.53	0.9899	1.0083	950	2.621	72.54	0.9893	1.0101	
2.758	74.23	0.9918	1.0088	1000	2.764	75.54	0.9912	1.0108	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for *x* mole fraction CO<sub>2</sub> in (1-*x*) mole fraction H<sub>2</sub>O - Continued

<i>p</i> = 4.0 MPa									
<i>x</i> = 0.05					<i>x</i> = 0.10				
<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	
				516.14	0.0223	18.98	coexisting phase		<i>x</i> = .00102
				516.14	0.906	49.37	0.7652	104.71	
							0.8494	1.0642	
		coexisting phase							<i>x</i> = .000527
0.0224	19286.	0.8104	102.54	519.87					
0.902	49934.	0.8526	1.0811	519.87					
0.902	49.94	0.8528	1.0809	520	0.919	49.62	0.8542	1.0593	
0.970	51.18	0.8749	1.0543	540	0.983	50.81	0.8758	1.0404	
1.032	52.29	0.8924	1.0381	560	1.042	51.92	0.8931	1.0288	
1.089	53.32	0.9067	1.0278	580	1.097	52.97	0.9072	1.0213	
1.143	54.31	0.9185	1.0210	600	1.150	53.97	0.9189	1.0164	
1.195	55.26	0.9284	1.0164	620	1.202	54.95	0.9287	1.0132	
1.246	56.19	0.9368	1.0132	640	1.252	55.91	0.9369	1.0110	
1.295	57.10	0.9439	1.0111	660	1.300	56.86	0.9440	1.0096	
1.344	57.99	0.9500	1.0096	680	1.348	57.80	0.9501	1.0086	
1.391	58.88	0.9553	1.0086	700	1.395	58.73	0.9554	1.0080	
1.507	61.08	0.9658	1.0074	750	1.511	61.04	0.9658	1.0075	
1.621	63.27	0.9735	1.0071	800	1.624	63.36	0.9735	1.0077	
1.732	65.46	0.9792	1.0073	850	1.735	65.69	0.9792	1.0081	
1.842	67.67	0.9836	1.0077	900	1.844	68.04	0.9835	1.0086	
1.951	69.90	0.9870	1.0081	950	1.953	70.42	0.9869	1.0091	
2.059	72.16	0.9896	1.0086	1000	2.061	72.82	0.9896	1.0096	
<i>x</i> = 0.20					<i>x</i> = 0.30				
<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	
				500.13	0.0217	17.68	coexisting phase		<i>x</i> = .00266
				500.13	0.910	46.67	0.5901	114.28	
							0.8407	1.0149	
		coexisting phase							<i>x</i> = .00190
0.0220	18.35	0.6768	109.23	508.41					
0.910	48.10	0.8444	1.0364	508.41					
0.946	48.82	0.8585	1.0287	520	0.968	47.90	0.8639	1.0094	
1.005	50.00	0.8788	1.0199	540	1.023	49.10	0.8827	1.0064	
1.060	51.12	0.8953	1.0146	560	1.075	50.26	0.8981	1.0050	
1.113	52.20	0.9088	1.0113	580	1.126	51.40	0.9108	1.0044	
1.164	53.26	0.9200	1.0093	600	1.176	52.52	0.9215	1.0044	
1.214	54.31	0.9295	1.0081	620	1.225	53.64	0.9305	1.0047	
1.262	55.34	0.9375	1.0075	640	1.272	54.75	0.9382	1.0052	
1.310	56.37	0.9444	1.0072	660	1.319	55.86	0.9448	1.0058	
1.357	57.39	0.9503	1.0072	680	1.366	56.97	0.9506	1.0064	
1.404	58.41	0.9555	1.0073	700	1.412	58.08	0.9556	1.0071	
1.518	60.97	0.9658	1.0079	750	1.525	60.88	0.9655	1.0087	
1.630	63.54	0.9733	1.0088	800	1.636	63.71	0.9728	1.0102	
1.740	66.14	0.9789	1.0097	850	1.746	66.58	0.9783	1.0115	
1.849	68.77	0.9832	1.0105	900	1.855	69.49	0.9825	1.0127	
1.958	71.44	0.9865	1.0113	950	1.963	72.45	0.9857	1.0137	
2.066	74.14	0.9891	1.0120	1000	2.071	75.47	0.9883	1.0145	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 5.0 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
				529.06	0.0228	20.12	coexisting phase $x = .00138$		
				529.06	0.721	49.37	0.7472	77.74	
							0.8291	1.0769	
		coexisting phase $x = .00072$							
0.0230	20.46	0.7920	75.99	533.06					
0.716	49.88	0.8331	1.0969	533.06					
0.737	50.36	0.8422	1.0837	540	0.752	50.11	0.8436	1.0615	
0.794	51.64	0.8648	1.0568	560	0.805	51.34	0.8657	1.0425	
0.844	52.78	0.8830	1.0404	580	0.853	52.48	0.8837	1.0309	
0.891	53.84	0.8979	1.0299	600	0.899	53.55	0.8984	1.0234	
0.936	54.85	0.9104	1.0230	620	0.943	54.58	0.9107	1.0185	
0.979	55.83	0.9209	1.0184	640	0.984	55.58	0.9211	1.0152	
1.020	56.77	0.9298	1.0152	660	1.025	56.56	0.9300	1.0131	
1.060	57.70	0.9375	1.0131	680	1.065	57.53	0.9376	1.0117	
1.100	58.62	0.9442	1.0116	700	1.104	58.48	0.9442	1.0108	
1.195	60.87	0.9573	1.0098	750	1.199	60.84	0.9573	1.0099	
1.288	63.09	0.9669	1.0093	800	1.291	63.19	0.9668	1.0100	
1.379	65.32	0.9740	1.0095	850	1.381	65.55	0.9740	1.0104	
1.468	67.54	0.9795	1.0099	900	1.470	67.92	0.9794	1.0110	
1.556	69.79	0.9837	1.0104	950	1.558	70.31	0.9836	1.0117	
1.643	72.06	0.9871	1.0109	1000	1.645	72.73	0.9870	1.0123	
$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
				511.78	0.0222	18.70	coexisting phase $x = .00357$		
				511.78	0.728	46.85	0.5746	85.58	
							0.8181	1.0195	
		coexisting phase $x = .000021$							
0.0225	19.43	0.6600	81.46	520.70					
0.727	48.21	0.8229	1.0443	520.70					
				520	0.749	47.39	0.8295	1.0162	
0.777	49.46	0.8479	1.0304	540	0.796	48.66	0.8533	1.0110	
0.825	50.66	0.8688	1.0218	560	0.841	49.88	0.8726	1.0084	
0.870	51.80	0.8858	1.0166	580	0.884	51.06	0.8885	1.0071	
0.913	52.91	0.8999	1.0134	600	0.926	52.22	0.9019	1.0068	
0.955	54.00	0.9118	1.0115	620	0.966	53.37	0.9132	1.0069	
0.996	55.06	0.9219	1.0104	640	1.006	54.50	0.9228	1.0074	
1.035	56.11	0.9305	1.0099	660	1.045	55.64	0.9311	1.0080	
1.074	57.16	0.9380	1.0097	680	1.083	56.77	0.9383	1.0087	
1.112	58.20	0.9444	1.0098	700	1.121	57.90	0.9445	1.0095	
1.206	60.79	0.9572	1.0104	750	1.213	60.72	0.9569	1.0114	
1.297	63.39	0.9666	1.0114	800	1.304	63.58	0.9660	1.0132	
1.387	66.01	0.9736	1.0125	850	1.393	66.46	0.9729	1.0147	
1.475	68.66	0.9790	1.0135	900	1.481	69.39	0.9781	1.0161	
1.563	71.34	0.9832	1.0144	950	1.569	72.37	0.9822	1.0173	
1.650	74.06	0.9865	1.0152	1000	1.655	75.39	0.9854	1.0184	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O — Continued

$p = 6.0 \text{ MPa}$								
$x = 0.05$					$x = 0.10$			
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$
				540.07	0.0234	21.12	coexisting phase $x = .00180$	
				540.07	0.596	49.32	0.7310	60.65
							0.8107	1.0901
		coexisting phase $x = .00094$						
0.0236	21.49	0.7754	59.14	544.43				
0.591	49.77	0.8154	1.1134	544.43				
0.632	50.91	0.8367	1.0816	560	0.645	50.71	0.8380	1.0604
0.679	52.19	0.8590	1.0564	580	0.690	51.96	0.8599	1.0428
0.722	53.35	0.8772	1.0409	600	0.731	53.10	0.8779	1.0319
0.762	54.43	0.8923	1.0310	620	0.769	54.19	0.8928	1.0248
0.800	55.45	0.9050	1.0244	640	0.806	55.24	0.9053	1.0202
0.836	56.44	0.9158	1.0200	660	0.841	56.26	0.9160	1.0172
0.871	57.40	0.9250	1.0170	680	0.876	57.25	0.9252	1.0152
0.905	58.35	0.9330	1.0150	700	0.909	58.23	0.9331	1.0139
0.987	60.65	0.9488	1.0124	750	0.991	60.64	0.9488	1.0125
1.066	62.92	0.9603	1.0117	800	1.069	63.03	0.9602	1.0125
1.143	65.16	0.9689	1.0118	850	1.146	65.40	0.9688	1.0129
1.218	67.42	0.9754	1.0122	900	1.221	67.80	0.9753	1.0136
1.293	69.68	0.9805	1.0128	950	1.295	70.20	0.9804	1.0143
1.366	71.96	0.9845	1.0133	1000	1.368	72.64	0.9844	1.0150
$x = 0.20$					$x = 0.30$			
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$
				521.64	0.0226	19.58	coexisting phase $x = .00456$	
				521.64	0.605	46.96	0.5608	67.35
							0.7974	1.0246
		coexisting phase $x = .00330$						
0.0230	20.38	0.6448	63.84	531.13				
0.602	48.25	0.8034	1.0527	531.13				
0.623	48.87	0.8167	1.0441	540	0.645	48.20	0.8237	1.0172
0.667	50.17	0.8421	1.0310	560	0.685	49.48	0.8471	1.0128
0.708	51.38	0.8628	1.0231	580	0.723	50.72	0.8663	1.0106
0.746	52.55	0.8799	1.0184	600	0.759	51.92	0.8824	1.0097
0.782	53.67	0.8942	1.0156	620	0.794	53.09	0.8959	1.0096
0.818	54.77	0.9063	1.0139	640	0.828	54.26	0.9075	1.0099
0.852	55.85	0.9167	1.0130	660	0.862	55.41	0.9174	1.0105
0.885	56.92	0.9256	1.0126	680	0.894	56.56	0.9260	1.0112
0.918	57.98	0.9333	1.0125	700	0.927	57.70	0.9335	1.0121
0.998	60.61	0.9487	1.0131	750	1.005	60.56	0.9483	1.0142
1.075	63.24	0.9599	1.0142	800	1.082	63.44	0.9593	1.0162
1.151	65.88	0.9684	1.0154	850	1.157	66.35	0.9675	1.0181
1.226	68.55	0.9748	1.0165	900	1.232	69.29	0.9738	1.0197
1.300	71.24	0.9798	1.0175	950	1.305	72.28	0.9787	1.0210
1.373	73.98	0.9838	1.0185	1000	1.378	75.31	0.9826	1.0222

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 7.0 \text{ MPa}$									
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$x = 0.05$		$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$x = 0.10$		$\varphi_2$
		$\varphi_1$	$\varphi_2$				$\varphi_1$	$\varphi_2$	
<i>coexisting phase</i> $x = .001187$									
0.0241	22.43	0.7602	47.63	554.36					
0.500	49.61	0.7992	1.1307	554.36					
<i>coexisting phase</i> $x = .00225$									
				549.70	0.0239	22.03	0.7161	48.97	
				549.70	0.505	49.22	0.7938	1.1041	
0.514	50.08	0.8080	1.1150	560	0.529	50.02	0.8099	1.0837	
0.560	51.55	0.8348	1.0768	580	0.572	51.39	0.8360	1.0577	
0.600	52.82	0.8564	1.0545	600	0.610	52.64	0.8572	1.0422	
0.637	53.98	0.8742	1.0405	620	0.645	53.79	0.8748	1.0324	
0.672	55.07	0.8891	1.0315	640	0.678	54.89	0.8895	1.0260	
0.704	56.10	0.9017	1.0255	660	0.710	55.94	0.9020	1.0219	
0.735	57.10	0.9125	1.0215	680	0.741	56.97	0.9127	1.0192	
0.766	58.07	0.9219	1.0188	700	0.770	57.98	0.9220	1.0174	
0.795	59.03	0.9300	1.0169	720	0.799	58.97	0.9300	1.0163	
0.824	59.97	0.9371	1.0157	740	0.828	59.95	0.9371	1.0156	
0.852	60.90	0.9433	1.0149	760	0.856	60.92	0.9433	1.0152	
0.880	61.82	0.9488	1.0145	780	0.883	61.89	0.9488	1.0151	
0.907	62.73	0.9537	1.0142	800	0.911	62.86	0.9536	1.0151	
0.975	65.01	0.9637	1.0142	850	0.977	65.26	0.9636	1.0155	
1.040	67.29	0.9714	1.0146	900	1.043	67.67	0.9712	1.0162	
1.105	69.57	0.9773	1.0152	950	1.107	70.10	0.9771	1.0170	
1.168	71.87	0.9820	1.0159	1000	1.170	72.54	0.9818	1.0178	
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$x = 0.20$		$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$x = 0.30$		$\varphi_2$
		$\varphi_1$	$\varphi_2$				$\varphi_1$	$\varphi_2$	
<i>coexisting phase</i> $x = .00410$									
0.0234	21.22	0.6308	51.78	540.19					
0.513	48.24	0.7853	1.0618	540.19					
<i>coexisting phase</i> $x = .00563$									
				530.15	0.0230	20.37	0.5479	54.87	
				530.15	0.517	47.01	0.7782	1.0305	
0.554	49.65	0.8153	1.0425	560	0.536	47.72	0.7941	1.0252	
0.591	50.95	0.8397	1.0312	580	0.573	49.07	0.8216	1.0184	
0.626	52.17	0.8598	1.0244	600	0.607	50.36	0.8441	1.0149	
0.659	53.34	0.8765	1.0203	620	0.640	51.60	0.8629	1.0132	
0.690	54.47	0.8907	1.0179	640	0.671	52.81	0.8787	1.0127	
0.721	55.58	0.9028	1.0165	660	0.701	54.00	0.8922	1.0128	
0.750	56.68	0.9132	1.0158	680	0.731	55.18	0.9037	1.0133	
0.779	57.76	0.9223	1.0156	700	0.760	56.35	0.9137	1.0141	
0.808	58.83	0.9301	1.0156	720	0.788	57.51	0.9224	1.0149	
0.836	59.90	0.9370	1.0158	740	0.816	58.67	0.9301	1.0158	
0.863	60.96	0.9431	1.0162	760	0.843	59.83	0.9367	1.0168	
0.890	62.03	0.9485	1.0166	780	0.870	60.99	0.9427	1.0177	
0.917	63.09	0.9533	1.0171	800	0.897	62.15	0.9479	1.0186	
0.983	65.75	0.9631	1.0184	850	0.924	63.31	0.9526	1.0195	
1.048	68.44	0.9707	1.0196	900	0.989	66.24	0.9621	1.0215	
1.112	71.15	0.9765	1.0208	950	1.054	69.19	0.9695	1.0233	
1.175	73.89	0.9811	1.0218	1000	1.117	72.19	0.9752	1.0248	
					1.181	75.24	0.9797	1.0262	



TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O — Continued

$p = 8.0 \text{ MPa}$								
$x = 0.05$				$x = 0.10$				
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$
				558.26	0.0244	22.86	coexisting phase $x = .00276$	
				558.26	0.436	49.09	0.7022	40.53
							0.7781	1.1190
		coexisting phase $x = .00146$						
0.0247	23.28	0.7461	39.31	563.22				
0.431	49.43	0.7842	1.1493	563.22				
				560	0.441	49.24	0.7811	1.1144
0.469	50.83	0.8102	1.1030	580	0.482	50.79	0.8118	1.0764
0.508	52.25	0.8354	1.0711	600	0.518	52.14	0.8365	1.0546
0.543	53.51	0.8560	1.0520	620	0.551	53.37	0.8567	1.0413
0.575	54.66	0.8731	1.0398	640	0.582	54.52	0.8736	1.0328
0.605	55.75	0.8876	1.0319	660	0.611	55.62	0.8880	1.0272
0.634	56.79	0.9000	1.0266	680	0.639	56.68	0.9002	1.0236
0.661	57.79	0.9107	1.0230	700	0.666	57.71	0.9108	1.0213
0.688	58.77	0.9200	1.0206	720	0.692	58.73	0.9201	1.0198
0.714	59.73	0.9281	1.0190	740	0.718	59.73	0.9281	1.0188
0.739	60.68	0.9352	1.0180	760	0.743	60.72	0.9352	1.0183
0.764	61.62	0.9415	1.0173	780	0.767	61.71	0.9415	1.0180
0.788	62.55	0.9471	1.0169	800	0.792	62.68	0.9470	1.0179
0.848	64.86	0.9586	1.0168	850	0.851	65.12	0.9584	1.0183
0.906	67.16	0.9673	1.0172	900	0.909	67.55	0.9672	1.0190
0.964	69.46	0.9741	1.0178	950	0.966	69.99	0.9739	1.0198
1.020	71.77	0.9794	1.0185	1000	1.022	72.45	0.9792	1.0207
$x = 0.20$				$x = 0.30$				
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$
				537.64	0.0234	21.09	coexisting phase $x = .00678$	
				537.64	0.449	47.02	0.5358	45.85
							0.7602	1.0370
		coexisting phase $x = .00498$						
0.0239	21.99	0.6178	43.08	548.21				
0.445	48.19	0.7683	1.0716	548.21				
				540	0.454	47.20	0.7644	1.0353
0.468	49.09	0.7882	1.0570	560	0.488	48.64	0.7961	1.0253
0.503	50.48	0.8165	1.0410	580	0.520	49.99	0.8220	1.0201
0.535	51.77	0.8397	1.0315	600	0.550	51.28	0.8435	1.0174
0.566	52.99	0.8589	1.0259	620	0.579	52.53	0.8616	1.0163
0.595	54.17	0.8751	1.0225	640	0.606	53.75	0.8769	1.0161
0.622	55.31	0.8890	1.0205	660	0.633	54.95	0.8901	1.0165
0.649	56.43	0.9009	1.0194	680	0.659	56.14	0.9015	1.0171
0.675	57.53	0.9112	1.0189	700	0.684	57.31	0.9115	1.0180
0.701	58.62	0.9202	1.0188	720	0.709	58.49	0.9202	1.0189
0.726	59.71	0.9281	1.0190	740	0.733	59.66	0.9278	1.0199
0.750	60.79	0.9350	1.0193	760	0.758	60.83	0.9345	1.0209
0.774	61.86	0.9412	1.0197	780	0.782	62.00	0.9405	1.0219
0.798	62.94	0.9467	1.0202	800	0.805	63.17	0.9458	1.0228
0.857	65.62	0.9579	1.0215	850	0.863	66.12	0.9568	1.0250
0.914	68.33	0.9665	1.0229	900	0.920	69.10	0.9652	1.0270
0.971	71.05	0.9732	1.0241	950	0.977	72.11	0.9717	1.0286
1.027	73.81	0.9785	1.0252	1000	1.032	75.16	0.9769	1.0301

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  - Continued

$p = 9.0 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
				565.99	0.0249	23.62			<i>coexisting phase</i> $x = .00332$
				565.99	0.383	48.93			34.19
									1.1350
									<i>coexisting phase</i> $x = .00177$
0.0252	24.09	0.7329	33.07	571.23					
0.376	49.21	0.7701	1.1693	571.23					
0.396	50.04	0.7852	1.1374	580	0.411	50.13	0.7873	1.0999	
0.435	51.64	0.8142	1.0917	600	0.446	51.61	0.8155	1.0696	
0.469	53.01	0.8377	1.0656	620	0.478	52.92	0.8386	1.0517	
0.499	54.24	0.8571	1.0495	640	0.507	54.14	0.8577	1.0405	
0.528	55.38	0.8735	1.0392	660	0.534	55.28	0.8739	1.0333	
0.554	56.46	0.8875	1.0323	680	0.560	56.38	0.8878	1.0286	
0.580	57.50	0.8996	1.0278	700	0.585	57.45	0.8997	1.0256	
0.604	58.51	0.9100	1.0247	720	0.609	58.49	0.9101	1.0236	
0.628	59.50	0.9192	1.0226	740	0.632	59.51	0.9192	1.0223	
0.651	60.46	0.9272	1.0212	760	0.655	60.52	0.9272	1.0215	
0.674	61.42	0.9343	1.0204	780	0.677	61.52	0.9342	1.0211	
0.696	62.37	0.9405	1.0198	800	0.699	62.51	0.9405	1.0210	
0.750	64.71	0.9534	1.0195	850	0.753	64.97	0.9533	1.0212	
0.803	67.03	0.9632	1.0198	900	0.805	67.42	0.9631	1.0219	
0.854	69.34	0.9709	1.0204	950	0.856	69.88	0.9707	1.0227	
0.904	71.67	0.9769	1.0211	1000	0.907	72.36	0.9767	1.0236	
$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
				555.40					<i>coexisting phase</i> $x = .00592$
0.0243	22.70	0.6054	36.53	555.40					
0.392	48.11	0.7523	1.0823	555.40					
									<i>coexisting phase</i> $x = .00801$
				544.32	0.0237	21.74	0.5243	39.07	
				544.32	0.397	47.01	0.7431	1.0442	
0.400	48.49	0.7609	1.0750	560	0.422	48.20	0.7707	1.0338	
0.434	50.00	0.7933	1.0528	580	0.452	49.61	0.7999	1.0263	
0.465	51.36	0.8195	1.0400	600	0.480	50.95	0.8241	1.0223	
0.493	52.64	0.8413	1.0323	620	0.507	52.23	0.8445	1.0205	
0.520	53.86	0.8596	1.0277	640	0.532	53.49	0.8618	1.0199	
0.546	55.03	0.8752	1.0250	660	0.556	54.71	0.8766	1.0200	
0.570	56.18	0.8886	1.0234	680	0.580	55.92	0.8894	1.0205	
0.594	57.30	0.9002	1.0226	700	0.603	57.12	0.9006	1.0213	
0.617	58.41	0.9103	1.0223	720	0.626	58.31	0.9103	1.0222	
0.640	59.52	0.9192	1.0223	740	0.648	59.49	0.9189	1.0232	
0.662	60.61	0.9270	1.0226	760	0.670	60.68	0.9265	1.0242	
0.684	61.70	0.9339	1.0229	780	0.692	61.86	0.9332	1.0253	
0.706	62.78	0.9401	1.0234	800	0.713	63.04	0.9392	1.0263	
0.759	65.49	0.9527	1.0248	850	0.765	66.01	0.9515	1.0286	
0.811	68.22	0.9624	1.0262	900	0.817	69.00	0.9609	1.0307	
0.861	70.96	0.9699	1.0275	950	0.867	72.02	0.9683	1.0325	
0.912	73.73	0.9758	1.0287	1000	0.917	75.09	0.9741	1.0341	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for x mole fraction CO<sub>2</sub> in (1-x) mole fraction H<sub>2</sub>O - Continued

<i>p</i> = 10.0 MPa									
<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	<i>x</i> = 0.05		<i>T</i> K	<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	<i>x</i> = 0.10		
		$\phi_1$	$\phi_2$				$\phi_1$	$\phi_2$	
				573.00	0.0254	24.35	coexisting phase <i>x</i> = .00394		
				573.00	0.339	48.74	0.6768	29.28	
							0.7491	1.1523	
		coexisting phase <i>x</i> = .00211							
0.0258	24.84	0.7204	28.22	578.55					
0.333	48.96	0.7567	1.1910	578.55					
0.336	49.12	0.7595	1.1839	580	0.353	49.40	0.7623	1.1298	
0.376	50.97	0.7927	1.1174	600	0.388	51.04	0.7945	1.0879	
0.409	52.47	0.8193	1.0819	620	0.419	52.46	0.8204	1.0640	
0.439	53.79	0.8411	1.0608	640	0.446	53.74	0.8418	1.0495	
0.465	55.00	0.8594	1.0475	660	0.472	54.94	0.8599	1.0402	
0.491	56.13	0.8750	1.0388	680	0.496	56.08	0.8754	1.0342	
0.514	57.21	0.8884	1.0330	700	0.519	57.18	0.8886	1.0303	
0.537	58.24	0.9001	1.0291	720	0.542	58.24	0.9002	1.0277	
0.559	59.26	0.9102	1.0265	740	0.563	59.29	0.9103	1.0260	
0.581	60.24	0.9191	1.0248	760	0.584	60.31	0.9191	1.0250	
0.601	61.22	0.9270	1.0236	780	0.605	61.33	0.9269	1.0244	
0.622	62.18	0.9340	1.0229	800	0.625	62.34	0.9339	1.0241	
0.671	64.55	0.9483	1.0223	850	0.674	64.83	0.9481	1.0242	
0.719	66.89	0.9592	1.0225	900	0.722	67.30	0.9590	1.0249	
0.766	69.23	0.9677	1.0231	950	0.769	69.78	0.9675	1.0257	
0.812	71.57	0.9743	1.0239	1000	0.814	72.26	0.9741	1.0266	
<i>p</i> = 10.0 MPa									
<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	<i>x</i> = 0.20		<i>T</i> K	<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	<i>x</i> = 0.30		
		$\phi_1$	$\phi_2$				$\phi_1$	$\phi_2$	
				550.32	0.0241	22.34	coexisting phase <i>x</i> = .00933		
				550.32	0.354	46.96	0.5134	33.81	
							0.7268	1.0520	
		coexisting phase <i>x</i> = .00695							
0.0247	23.36	0.5937	31.46	561.91					
0.348	48.01	0.7371	1.0937	561.91					
0.379	49.49	0.7699	1.0669	560	0.369	47.73	0.7452	1.0440	
0.408	50.94	0.7993	1.0498	580	0.398	49.22	0.7779	1.0336	
0.435	52.27	0.8237	1.0397	600	0.424	50.61	0.8049	1.0280	
0.460	53.54	0.8441	1.0336	620	0.449	51.94	0.8275	1.0252	
0.484	54.75	0.8614	1.0299	640	0.473	53.22	0.8467	1.0240	
0.507	55.92	0.8763	1.0278	660	0.495	54.47	0.8631	1.0238	
0.529	57.07	0.8892	1.0266	680	0.517	55.70	0.8773	1.0241	
0.551	58.20	0.9004	1.0260	700	0.539	56.92	0.8897	1.0248	
0.572	59.32	0.9103	1.0259	720	0.559	58.13	0.9005	1.0257	
0.592	60.43	0.9190	1.0260	740	0.580	59.33	0.9100	1.0267	
0.612	61.53	0.9266	1.0264	760	0.600	60.52	0.9184	1.0278	
0.632	62.63	0.9335	1.0268	780	0.620	61.71	0.9259	1.0288	
0.680	65.36	0.9475	1.0282	800	0.639	62.90	0.9325	1.0298	
0.728	68.10	0.9582	1.0296	850	0.687	65.89	0.9462	1.0323	
0.774	70.86	0.9666	1.0310	900	0.733	68.90	0.9567	1.0345	
0.819	73.64	0.9732	1.0323	950	0.779	71.94	0.9649	1.0365	
				1000	0.825	75.01	0.9713	1.0382	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  - Continued

$p = 15 \text{ MPa}$									
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$x = 0.05$		$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$x = 0.10$		$\varphi_2$
		$\varphi_1$	$\varphi_2$				$\varphi_1$	$\varphi_2$	
				600.85	0.0282	27.53	<i>coexisting phase</i> $x = .00815$		
				600.85	0.206	47.49	0.6228	15.50	
							0.6863	1.2631	
		<i>coexisting phase</i> $x = .00457$							
0.0289	28.24	0.6659	14.61	607.88					
0.197	47.37	0.6978	1.3660	607.88					
0.221	49.09	0.7245	1.2358	620	0.237	49.71	0.7277	1.1676	
0.251	51.18	0.7599	1.1533	640	0.262	51.51	0.7618	1.1181	
0.276	52.85	0.7886	1.1104	660	0.285	53.06	0.7898	1.0900	
0.298	54.30	0.8126	1.0851	680	0.305	54.45	0.8133	1.0727	
0.317	55.61	0.8330	1.0691	700	0.323	55.73	0.8334	1.0617	
0.335	56.83	0.8505	1.0587	720	0.341	56.95	0.8508	1.0544	
0.352	57.99	0.8658	1.0517	740	0.357	58.12	0.8659	1.0496	
0.369	59.10	0.8792	1.0469	760	0.373	59.25	0.8792	1.0464	
0.384	60.17	0.8909	1.0437	780	0.388	60.36	0.8909	1.0442	
0.399	61.22	0.9014	1.0414	800	0.403	61.44	0.9013	1.0428	
0.436	63.75	0.9228	1.0386	850	0.439	64.08	0.9226	1.0413	
0.470	66.22	0.9391	1.0379	900	0.473	66.67	0.9389	1.0413	
0.503	68.66	0.9518	1.0381	950	0.506	69.23	0.9515	1.0419	
0.535	71.08	0.9618	1.0387	1000	0.537	71.79	0.9615	1.0427	
$p = 15 \text{ MPa}$									
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$x = 0.20$		$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$x = 0.30$		$\varphi_2$
		$\varphi_1$	$\varphi_2$				$\varphi_1$	$\varphi_2$	
				573.39	0.0258	24.88	<i>coexisting phase</i> $x = .01730$		
				573.39	0.226	46.47	0.4658	19.08	
							0.6539	1.1003	
		<i>coexisting phase</i> $x = .01350$							
0.0269	26.19	0.5423	17.26	587.22					
0.218	47.22	0.6687	1.1646	587.22					
				580	0.234	47.09	0.6693	1.0901	
0.235	48.52	0.6978	1.1285	600	0.256	48.82	0.7102	1.0694	
0.259	50.27	0.7358	1.0946	620	0.276	50.38	0.7440	1.0580	
0.280	51.82	0.7670	1.0752	640	0.295	51.85	0.7726	1.0517	
0.300	53.25	0.7932	1.0635	660	0.312	53.25	0.7969	1.0483	
0.318	54.59	0.8155	1.0562	680	0.329	54.60	0.8180	1.0466	
0.335	55.88	0.8348	1.0517	700	0.345	55.92	0.8363	1.0460	
0.351	57.12	0.8516	1.0489	720	0.360	57.21	0.8523	1.0461	
0.366	58.33	0.8663	1.0473	740	0.375	58.48	0.8664	1.0466	
0.382	59.52	0.8792	1.0464	760	0.390	59.74	0.8789	1.0474	
0.396	60.69	0.8906	1.0460	780	0.404	60.99	0.8900	1.0483	
0.411	61.85	0.9008	1.0459	800	0.418	62.23	0.8998	1.0493	
0.445	64.71	0.9218	1.0467	850	0.452	65.32	0.9202	1.0519	
0.479	67.55	0.9378	1.0479	900	0.485	68.41	0.9359	1.0544	
0.511	70.38	0.9503	1.0494	950	0.517	71.51	0.9481	1.0566	
0.543	73.22	0.9602	1.0507	1000	0.548	74.64	0.9578	1.0587	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for x mole fraction CO<sub>2</sub> in (1-x) mole fraction H<sub>2</sub>O — Continued

<i>p</i> = 20 MPa									
<i>x</i> = 0.05					<i>x</i> = 0.10				
<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	
									<i>coexisting phase</i> <i>x</i> = .01548
				620.32	0.0317	30.36	0.5757	9.275	
				620.32	0.136	45.75	0.6297	1.4359	
									<i>coexisting phase</i> <i>x</i> = .00957
0.0335	31.44	0.6185	8.340	628.90					
0.125	45.05	0.6449	1.5961	628.90					
				620	0.1357	45.69	0.6288	1.4407	
0.1480	47.42	0.6750	1.3872	640	0.1660	48.69	0.6802	1.2572	
0.1766	50.14	0.7169	1.2357	660	0.1886	50.83	0.7196	1.1782	
0.1983	52.14	0.7501	1.1664	680	0.2075	52.60	0.7518	1.1354	
0.2167	53.80	0.7779	1.1276	700	0.2242	54.15	0.7789	1.1097	
0.233	55.27	0.8015	1.1037	720	0.239	55.56	0.8021	1.0933	
0.248	56.61	0.8219	1.0882	740	0.254	56.88	0.8222	1.0824	
0.262	57.87	0.8397	1.0778	760	0.267	58.13	0.8399	1.0751	
0.275	59.06	0.8554	1.0706	780	0.280	59.34	0.8554	1.0700	
0.288	60.21	0.8692	1.0657	800	0.292	60.51	0.8692	1.0665	
0.318	62.93	0.8976	1.0588	850	0.321	63.32	0.8974	1.0619	
0.345	65.54	0.9193	1.0560	900	0.348	66.03	0.9190	1.0602	
0.371	68.07	0.9362	1.0551	950	0.374	68.69	0.9358	1.0600	
0.397	70.57	0.9494	1.0551	1000	0.399	71.32	0.9491	1.0603	
<i>x</i> = 0.20					<i>x</i> = 0.30				
<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> kJ·mol <sup>-1</sup>	φ <sub>1</sub>	φ <sub>2</sub>	
									<i>coexisting phase</i> <i>x</i> = .0279
				588.69	0.0275	26.89	0.4251	12.516	
				588.69	0.161	45.70	0.5904	1.1628	
									<i>coexisting phase</i> <i>x</i> = .0231
0.0292	28.54	0.4980	10.919	604.42					
0.152	46.11	0.6081	1.2617	604.42					
				600	0.1725	46.87	0.6197	1.1371	
0.1698	47.95	0.6486	1.1927	620	0.1904	48.74	0.6643	1.1083	
0.1896	49.91	0.6912	1.1431	640	0.2066	50.43	0.7017	1.0918	
0.2070	51.62	0.7264	1.1148	660	0.2215	51.99	0.7335	1.0821	
0.223	53.18	0.7562	1.0975	680	0.235	53.47	0.7610	1.0763	
0.237	54.62	0.7817	1.0865	700	0.249	54.90	0.7849	1.0730	
0.251	55.99	0.8039	1.0794	720	0.261	56.28	0.8059	1.0712	
0.264	57.31	0.8232	1.0748	740	0.273	57.63	0.8244	1.0704	
0.276	58.59	0.8403	1.0718	760	0.285	58.96	0.8407	1.0703	
0.288	59.83	0.8554	1.0698	780	0.297	60.26	0.8552	1.0705	
0.300	61.06	0.8689	1.0687	800	0.308	61.56	0.8682	1.0711	
0.328	64.05	0.8966	1.0677	850	0.335	64.75	0.8951	1.0730	
0.354	66.99	0.9178	1.0681	900	0.360	67.93	0.9158	1.0753	
0.380	69.90	0.9344	1.0691	950	0.385	71.10	0.9320	1.0775	
0.404	72.81	0.9475	1.0702	1000	0.410	74.28	0.9448	1.0795	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 25 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
<i>coexisting phase</i>				$x = .0251$					
0.0436	35.50	0.5710	4.427	642.4					
0.749	41.28	0.5860	2.226	642.4					
<i>coexisting phase calculation unreliable and not included</i>									
				640	0.1041	44.95	0.5953	1.5655	
0.1112	46.42	0.6424	1.5227	660	0.1291	48.18	0.6490	1.3356	
0.1363	49.51	0.6874	1.3138	680	0.1483	50.51	0.6908	1.2351	
0.1552	51.73	0.7232	1.2217	700	0.1644	52.41	0.7252	1.1806	
0.1711	53.54	0.7531	1.1710	720	0.1786	54.07	0.7543	1.1477	
0.1852	55.13	0.7787	1.1399	740	0.1915	55.57	0.7794	1.1265	
0.1980	56.56	0.8009	1.1197	760	0.2035	56.97	0.8014	1.1124	
0.2098	57.90	0.8204	1.1061	780	0.2148	58.29	0.8206	1.1026	
0.2210	59.15	0.8377	1.0965	800	0.2255	59.55	0.8377	1.0957	
0.247	62.09	0.8729	1.0830	850	0.250	62.54	0.8727	1.0859	
0.270	64.84	0.8998	1.0770	900	0.274	65.38	0.8995	1.0816	
0.293	67.48	0.9208	1.0743	950	0.295	68.14	0.9204	1.0798	
0.314	70.07	0.9373	1.0732	1000	0.316	70.85	0.9369	1.0793	
$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
				598.9	0.0292	28.57	<i>coexisting phase</i>		$x = .0415$
				598.9	0.1232	44.76	0.3895	8.937	
							0.5334	1.2377	
<i>coexisting phase</i>				$x = .0373$					
0.0319	30.63	0.4581	7.460	616.0					
0.1121	44.76	0.5513	1.3898	616.0					
0.0929	42.01	0.4942	1.5963	600	0.1241	44.88	0.5365	1.2337	
0.1164	45.34	0.5638	1.3565	620	0.1402	47.07	0.5901	1.1774	
0.1356	47.84	0.6179	1.2469	640	0.1547	48.99	0.6352	1.1450	
0.1518	49.90	0.6619	1.1884	660	0.1678	50.73	0.6738	1.1255	
0.1662	51.70	0.6988	1.1539	680	0.1801	52.35	0.7071	1.1133	
0.1793	53.33	0.7304	1.1323	700	0.1915	53.89	0.7361	1.1056	
0.1915	54.84	0.7577	1.1183	720	0.2024	55.37	0.7616	1.1008	
0.2029	56.27	0.7816	1.1088	740	0.2129	56.79	0.7841	1.0979	
0.2137	57.65	0.8026	1.1024	760	0.2229	58.19	0.8041	1.0961	
0.224	58.97	0.8212	1.0980	780	0.233	59.55	0.8219	1.0952	
0.234	60.27	0.8378	1.0950	800	0.242	60.90	0.8378	1.0949	
0.258	63.40	0.8720	1.0911	850	0.265	64.20	0.8709	1.0954	
0.280	66.44	0.8983	1.0899	900	0.286	67.46	0.8964	1.0969	
0.301	69.43	0.9189	1.0900	950	0.307	70.69	0.9165	1.0986	
0.322	72.40	0.9352	1.0905	1000	0.327	73.93	0.9323	1.1004	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O – Continued

$p=30$ MPa								
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x=0.05$		$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x=0.10$	
		$\varphi_1$	$\varphi_2$				$\varphi_1$	$\varphi_2$
<i>coexisting phase <math>y=.6906</math></i>								
0.1117	38.45	0.4026	0.9570	523.3				
0.0234	21.32	0.1311	13.217	523.3				
<i>coexisting phase calculation unreliable and not included</i>								
0.0242	22.80	0.1665	12.028	540				
0.0254	24.65	0.2160	10.614	560				
0.0269	26.65	0.2731	9.186	580				
0.0291	28.86	0.3376	7.700	600				
0.0327	31.50	0.4085	6.080	620	0.0447	35.57	0.4280	3.461
0.0410	35.25	0.4855	4.149	640	0.0655	40.73	0.5109	2.177
0.0653	41.38	0.5641	2.267	660	0.0895	45.12	0.5790	1.6119
0.0932	46.27	0.6242	1.5952	680	0.1088	48.19	0.6309	1.3901
0.1134	49.35	0.6692	1.3698	700	0.1246	50.54	0.6727	1.2826
0.1294	51.64	0.7056	1.2702	720	0.1382	52.50	0.7078	1.2219
0.1431	53.53	0.7364	1.2118	740	0.1503	54.21	0.7378	1.1843
0.1552	55.18	0.7630	1.1755	760	0.1614	55.77	0.7638	1.1596
0.1662	56.68	0.7863	1.1516	780	0.1717	57.21	0.7867	1.1427
0.1764	58.07	0.8068	1.1351	800	0.1813	58.58	0.8070	1.1309
0.1997	61.23	0.8487	1.1117	850	0.2036	61.76	0.8486	1.1136
0.2206	64.13	0.8807	1.1008	900	0.2239	64.73	0.8804	1.1055
0.2401	66.89	0.9057	1.0955	950	0.2430	67.59	0.9053	1.1015
0.2585	69.56	0.9254	1.0928	1000	0.2611	70.38	0.9249	1.0995
$x=0.20$								
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\varphi_1$	$\varphi_2$
$x=0.30$								
<i>coexisting phase <math>x=.0586</math></i>								
				605.5	0.0308	30.01	0.3580	6.764
				605.5	0.0985	43.74	0.4815	1.3221
<i>coexisting phase <math>x=.0579</math></i>								
0.0349	32.53	0.4215	5.357	623.0				
0.0865	43.24	0.4964	1.5512	623.0				
0.1010	45.73	0.5492	1.3918	620	0.1086	45.47	0.5236	1.2626
0.1161	48.15	0.6009	1.2874	640	0.1214	47.60	0.5746	1.2100
0.1294	50.20	0.6443	1.2273	660	0.1331	49.51	0.6186	1.1776
0.1414	52.02	0.6814	1.1900	680	0.1440	51.26	0.6568	1.1569
0.1524	53.69	0.7135	1.1658	700	0.1542	52.91	0.6903	1.1435
0.1626	55.24	0.7415	1.1497	720	0.1638	54.48	0.7199	1.1346
0.1723	56.71	0.7663	1.1384	740	0.1730	55.98	0.7461	1.1286
0.1815	58.12	0.7882	1.1305	760	0.1818	57.44	0.7694	1.1247
0.1904	59.48	0.8078	1.1249	780	0.1903	58.86	0.7902	1.1221
0.2111	62.75	0.8482	1.1168	800	0.1986	60.26	0.8088	1.1205
0.2305	65.89	0.8794	1.1133	850	0.2182	63.67	0.8477	1.1189
0.2488	68.96	0.9038	1.1119	900	0.2367	67.00	0.8778	1.1191
0.2665	71.99	0.9231	1.1115	950	0.2545	70.30	0.9016	1.1201
				1000	0.2717	73.59	0.9204	1.1213

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 40 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$\varphi_1$	$\varphi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$\varphi_1$	$\varphi_2$	
<i>coexisting phase <math>y = .816</math></i>									
0.0789	33.29	0.2783	0.8371	484.1					
0.0218	18.11	0.0540	13.655	484.1					
				606.1	0.0720	41.77	0.3894	1.4363	
				606.1	0.0325	31.54	0.2910	4.700	
<i>coexisting phase <math>y = .327</math></i>									
0.0223	19.40	0.0714	12.630	500					
0.0230	21.06	0.0983	11.429	520					
0.0238	22.77	0.1312	10.286	540					
0.0248	24.56	0.1702	9.180	560					
0.0261	26.45	0.2152	8.094	580					
0.0278	28.47	0.2661	7.011	600					
0.0300	30.70	0.3221	5.914	620	0.0355	33.40	0.3321	4.065	
0.0335	33.26	0.3825	4.787	640	0.0419	36.53	0.3956	3.159	
0.0394	36.39	0.4458	3.638	660	0.0520	40.10	0.4610	2.392	
0.0499	40.24	0.5090	2.610	680	0.0647	43.66	0.5222	1.8849	
0.0643	44.21	0.5666	1.946	700	0.0777	46.72	0.5753	1.6002	
0.0787	47.50	0.6151	1.6105	720	0.0895	49.27	0.6204	1.4419	
0.0913	50.11	0.6558	1.4385	740	0.1002	51.43	0.6592	1.3479	
0.1024	52.28	0.6906	1.3407	760	0.1098	53.33	0.6928	1.2884	
0.1123	54.15	0.7209	1.2799	780	0.1187	55.05	0.7224	1.2486	
0.1213	55.83	0.7476	1.2397	800	0.1269	56.63	0.7485	1.2209	
0.1413	59.49	0.8021	1.1841	850	0.1456	60.20	0.8023	1.1806	
0.1588	62.72	0.8438	1.1579	900	0.1624	63.45	0.8436	1.1607	
0.1748	65.71	0.8764	1.1442	950	0.1779	66.50	0.8760	1.1499	
0.1897	68.55	0.9022	1.1365	1000	0.1925	69.45	0.9017	1.1437	
$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$\varphi_1$	$\varphi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\text{-mol}^{-1}$	$\varphi_1$	$\varphi_2$	
				610.9	0.0338	32.33	0.3057	4.373	
				610.9	0.0696	41.63	0.3915	1.507	
<i>coexisting phase calculation unreliable and not included</i>									
				620	0.0740	42.79	0.4185	1.4516	
0.0649	42.17	0.4373	1.7460	640	0.0835	45.15	0.4741	1.3604	
0.0759	44.94	0.4958	1.5441	660	0.0926	47.30	0.5242	1.2998	
0.0864	47.38	0.5475	1.4184	680	0.1012	49.27	0.5691	1.2592	
0.0962	49.53	0.5928	1.3387	700	0.1094	51.10	0.6092	1.2314	
0.1053	51.46	0.6326	1.2863	720	0.1172	52.82	0.6450	1.2121	
0.1139	53.24	0.6676	1.2507	740	0.1246	54.46	0.6771	1.1984	
0.1219	54.90	0.6988	1.2258	760	0.1316	56.04	0.7059	1.1885	
0.1295	56.47	0.7265	1.2079	780	0.1385	57.57	0.7319	1.1814	
0.1367	57.96	0.7513	1.1948	800	0.1451	59.06	0.7553	1.1762	
0.1536	61.50	0.8030	1.1746	850	0.1607	62.65	0.8045	1.1684	
0.1692	64.83	0.8432	1.1641	900	0.1754	66.13	0.8431	1.1649	
0.1839	68.06	0.8749	1.1584	950	0.1895	69.55	0.8737	1.1634	
0.1979	71.21	0.9002	1.1552	1000	0.2030	72.94	0.8982	1.1630	



TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O - Continued

$p = 50 \text{ MPa}$								
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x = 0.05$		$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x = 0.10$	
		$\phi_1$	$\phi_2$				$\phi_1$	$\phi_2$
<i>coexisting phase <math>y = .846</math></i>								
0.0617	30.98	0.2125	0.7772	469.4				
0.0212	17.04	0.0344	13.154	469.4				
<i>coexisting phase <math>y = .596</math></i>								
				553.8	0.0682	38.81	0.3023	1.0745
				553.8	0.0259	25.70	0.1356	6.402
0.0215	17.87	0.0421	12.502	480				
0.0220	19.47	0.0601	11.347	500				
0.0227	21.10	0.0826	10.294	520				
0.0234	22.78	0.1102	9.308	540				
0.0243	24.51	0.1429	8.371	560	0.0263	26.27	0.1465	6.199
0.0254	26.33	0.1808	7.469	580	0.0278	28.22	0.1852	5.535
0.0268	28.23	0.2236	6.591	600	0.0297	30.30	0.2292	4.863
0.0285	30.27	0.2708	5.729	620	0.0323	32.56	0.2778	4.187
0.0309	32.49	0.3219	4.881	640	0.0358	35.06	0.3305	3.522
0.0341	34.96	0.3758	4.050	660	0.0409	37.81	0.3861	2.903
0.0389	37.74	0.4312	3.266	680	0.0476	40.76	0.4422	2.382
0.0458	40.83	0.4860	2.592	700	0.0557	43.70	0.4962	1.996
0.0686	48.22	0.6052	1.6707	750	0.0770	49.98	0.6100	1.5107
0.0896	53.61	0.6929	1.3853	800	0.0957	54.76	0.6949	1.3376
0.1071	57.78	0.7585	1.2780	850	0.1118	58.71	0.7592	1.2631
0.1223	61.33	0.8089	1.2281	900	0.1261	62.21	0.8090	1.2258
0.1361	64.55	0.8485	1.2017	950	0.1393	65.46	0.8484	1.2050
0.1488	67.56	0.8801	1.1863	1000	0.1516	68.55	0.8797	1.1925
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x = 0.20$		$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x = 0.30$	
		$\phi_1$	$\phi_2$				$\phi_1$	$\phi_2$
<i>coexisting phase <math>x = .1593</math></i>								
				609.4	0.0361	34.00	0.2652	3.188
				609.4	0.0540	39.62	0.3186	1.6934
<i>coexisting phase calculation unreliable and not included</i>								
0.0436	37.23	0.3071	2.361	620	0.0575	40.92	0.3473	1.6207
0.0500	39.95	0.3630	2.048	640	0.0644	43.30	0.4009	1.5098
0.0572	42.60	0.4186	1.807	660	0.0713	45.53	0.4518	1.4288
0.0647	45.10	0.4713	1.6343	680	0.0780	47.61	0.4991	1.3705
0.0723	47.40	0.5198	1.5141	700	0.0846	49.55	0.5425	1.3285
0.0900	52.36	0.6219	1.3493	750	0.0999	53.97	0.6350	1.2664
0.1057	56.56	0.7005	1.2763	800	0.1139	57.98	0.7080	1.2363
0.1199	60.33	0.7617	1.2398	850	0.1269	61.73	0.7656	1.2206
0.1331	63.85	0.8098	1.2198	900	0.1392	65.34	0.8115	1.2121
0.1454	67.21	0.8496	1.1991	950	0.1508	68.87	0.8483	1.2072
0.1570	70.48	0.8787	1.2009	1000	0.1620	72.34	0.8817	1.1922

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 60 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	$T$ K	$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	
<i>coexisting phase</i> $y = .858$									
0.0515	29.70	0.1747	0.7404	462.2					
0.0209	16.58	0.0261	12.707	462.2					
					<i>coexisting phase</i> $y = .00225$				
				531.8	0.0580	36.45	0.2513	0.9804	
				531.8	0.0243	23.71	0.0881	6.706	
0.0213	17.96	0.0369	11.656	480					
0.0218	19.54	0.0526	10.580	500					
0.0224	21.15	0.0723	9.612	520					
0.0231	22.80	0.0964	8.719	540	0.0247	24.42	0.0988	6.469	
0.0239	24.49	0.1250	7.882	560	0.0257	26.20	0.1279	5.899	
0.0249	26.25	0.1581	7.089	580	0.0269	28.05	0.1618	5.335	
0.0261	28.08	0.1955	6.331	600	0.0285	30.01	0.2000	4.776	
0.0275	30.00	0.2369	5.602	620	0.0304	32.08	0.2425	4.223	
0.0293	32.04	0.2819	4.899	640	0.0329	34.30	0.2885	3.686	
0.0316	34.23	0.3296	4.224	660	0.0362	36.67	0.3372	3.177	
0.0347	36.59	0.3791	3.587	680	0.0403	39.18	0.3877	2.719	
0.0387	39.14	0.4293	3.010	700	0.0455	41.78	0.4381	2.335	
0.0534	45.84	0.5478	1.999	750	0.0608	47.95	0.5540	1.7339	
0.0702	51.59	0.6440	1.5674	800	0.0762	53.06	0.6471	1.4759	
0.0854	56.15	0.7184	1.3931	850	0.0901	57.31	0.7198	1.3595	
0.0987	60.00	0.7764	1.3114	900	0.1026	61.04	0.7770	1.3001	
0.1108	63.43	0.8224	1.2678	950	0.1141	64.47	0.8224	1.2664	
0.1219	66.61	0.8591	1.2422	1000	0.1248	67.70	0.8590	1.2458	
$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	$T$ K	$V$ $\text{dm}^3\cdot\text{mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	
<i>coexisting phase calculation</i> <i>unreliable and not included</i>					<i>coexisting phase calculation</i> <i>unreliable and not included</i>				
0.0350	33.84	0.2191	2.848	600	0.0439	37.32	0.2508	1.892	
0.0385	36.19	0.2651	2.539	620	0.0486	39.67	0.2995	1.754	
0.0427	38.62	0.3142	2.260	640	0.0536	41.97	0.3490	1.6395	
0.0476	41.06	0.3646	2.023	660	0.0588	44.18	0.3979	1.5490	
0.0530	43.46	0.4147	1.834	680	0.0642	46.29	0.4449	1.4793	
0.0587	45.75	0.4629	1.6899	700	0.0694	48.28	0.4893	1.4262	
0.0729	50.89	0.5697	1.4712	750	0.0821	52.87	0.5871	1.3426	
0.0861	55.32	0.6558	1.3659	800	0.0939	57.03	0.6668	1.2988	
0.0983	59.27	0.7244	1.3108	850	0.1050	60.91	0.7312	1.2744	
0.1095	62.94	0.7792	1.2796	900	0.1154	64.63	0.7832	1.2600	
0.1201	66.42	0.8232	1.2605	950	0.1253	68.24	0.8253	1.2511	
0.1301	69.79	0.8587	1.2483	1000	0.1349	71.79	0.8594	1.2453	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O — Continued

$p = 70 \text{ MPa}$									
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x = 0.05$		$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x = 0.10$		$\phi_2$
		$\phi_1$	$\phi_2$				$\phi_1$	$\phi_2$	
<i>coexisting phase <math>y = .8630</math></i>									
0.0449	28.97	0.1521	0.7178	458.8					
0.0207	16.43	0.0219	12.378	458.8					
<i>coexisting phase <math>y = .7237</math></i>									
				520.4	0.0504	35.01	0.2187	0.9333	
				520.4	0.0235	22.79	0.0671	6.750	
0.0207	16.52	0.0225	12.303	460					
0.0211	18.06	0.0333	11.146	480					
0.0216	19.62	0.0474	10.112	500					
0.0222	21.21	0.0651	9.194	520					
0.0228	22.83	0.0867	8.356	540	0.0243	24.43	0.0888	6.230	
0.0236	24.50	0.1123	7.582	560	0.0252	26.16	0.1150	5.715	
0.0245	26.21	0.1421	6.858	580	0.0262	27.95	0.1453	5.213	
0.0255	27.98	0.1757	6.175	600	0.0275	29.82	0.1796	4.723	
0.0290	32.75	0.2749	4.615	650	0.0322	34.89	0.2808	3.562	
0.0351	38.18	0.3883	3.276	700	0.0400	40.58	0.3957	2.589	
0.0452	44.18	0.5021	2.298	750	0.0512	46.40	0.5087	1.953	
0.0581	49.88	0.6018	1.7692	800	0.0637	51.60	0.6058	1.6266	
0.0708	54.69	0.6824	1.5254	850	0.0755	56.06	0.6846	1.4666	
0.0825	58.76	0.7466	1.4065	900	0.0864	59.97	0.7477	1.3821	
0.0932	62.38	0.7980	1.3421	950	0.0965	63.55	0.7985	1.3334	
0.1030	65.71	0.8395	1.3038	1000	0.1059	66.90	0.8396	1.3031	
$x = 0.20$									
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\phi_1$	$\phi_2$	$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$\phi_1$	$\phi_2$	
<i>coexisting phase <math>y = .4311</math></i>									
0.0464	38.26	0.2371	1.4425	585.7					
0.0312	31.88	0.1686	3.109	585.7					
<i>coexisting phase calculation unreliable and not included</i>									
0.0328	33.37	0.1955	2.918	600	0.0395	36.59	0.2222	1.982	
0.0353	35.54	0.2364	2.656	620	0.0430	38.81	0.2660	1.856	
0.0384	37.77	0.2803	2.410	640	0.0469	41.02	0.3117	1.7468	
0.0420	40.04	0.3263	2.190	660	0.0510	43.17	0.3578	1.6544	
0.0460	42.31	0.3731	2.002	680	0.0552	45.26	0.4033	1.5792	
0.0504	44.52	0.4193	1.849	700	0.0595	47.27	0.4472	1.5191	
0.0617	49.68	0.5266	1.5946	750	0.0701	51.93	0.5472	1.4184	
0.0729	54.23	0.6172	1.4598	800	0.0802	56.20	0.6315	1.3618	
0.0834	58.33	0.6914	1.3856	850	0.0897	60.19	0.7011	1.3286	
0.0932	62.12	0.7515	1.3421	900	0.0988	63.99	0.7580	1.3080	
0.1024	65.70	0.8005	1.3149	950	0.1074	67.68	0.8047	1.2946	
0.1112	69.16	0.8403	1.2969	1000	0.1157	71.29	0.8429	1.2856	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  - Continued

$p = 80 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	
<i>coexisting phase</i> $y = .8654$									
0.0401	28.55	0.1382	0.7037	457.3					
0.0205	16.43	0.0196	12.172	457.3					
					<i>coexisting phase</i> $y = .7439$				
				514.3	0.0448	34.13	0.1975	0.9064	
				514.3	0.0230	22.35	0.0562	6.738	
0.0206	16.63	0.0207	12.004	460					
0.0210	18.16	0.0306	10.854	480					
0.0215	19.71	0.0435	9.838	500					
0.0220	21.28	0.0597	8.946	520	0.0232	22.81	0.0612	6.590	
0.0226	22.88	0.0795	8.140	540	0.0239	24.46	0.0814	6.088	
0.0233	24.51	0.1031	7.404	560	0.0247	26.15	0.1054	5.608	
0.0241	26.19	0.1303	6.724	580	0.0257	27.89	0.1332	5.146	
0.0250	27.92	0.1612	6.090	600	0.0268	29.70	0.1646	4.701	
0.0280	32.50	0.2524	4.668	650	0.0306	34.51	0.2574	3.663	
0.0328	37.55	0.3577	3.466	700	0.0366	39.78	0.3641	2.782	
0.0403	43.06	0.4662	2.546	750	0.0452	45.26	0.4726	2.151	
0.0502	48.53	0.5662	1.9706	800	0.0552	50.40	0.5708	1.7796	
0.0608	53.41	0.6506	1.6681	850	0.0652	54.96	0.6535	1.5801	
0.0710	57.65	0.7196	1.5108	900	0.0748	59.01	0.7212	1.4699	
0.0804	61.41	0.7757	1.4233	950	0.0837	62.70	0.7765	1.4048	
0.0892	64.87	0.8213	1.3706	1000	0.0921	66.15	0.8217	1.3637	
$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\varphi_1$	$\varphi_2$	
<i>coexisting phase</i> $y = .4961$									
0.0438	37.75	0.2167	1.3159	574.7					
0.0290	30.58	0.1365	3.263	574.7					
					<i>coexisting phase calculation unreliable and not included</i>				
0.0294	31.09	0.1448	3.202	580	0.0341	34.00	0.1648	2.165	
0.0312	33.06	0.1784	2.970	600	0.0366	36.09	0.2018	2.049	
0.0369	38.27	0.2768	2.419	650	0.0440	41.37	0.3057	1.789	
0.0449	43.61	0.3859	1.988	700	0.0526	46.45	0.4140	1.6050	
0.0541	48.69	0.4914	1.7134	750	0.0616	51.15	0.5143	1.4917	
0.0636	53.30	0.5843	1.5544	800	0.0703	55.49	0.6014	1.4239	
0.0727	57.50	0.6623	1.4623	850	0.0786	59.55	0.6748	1.3823	
0.0813	61.38	0.7268	1.4063	900	0.0865	63.43	0.7358	1.3555	
0.0894	65.05	0.7799	1.3705	950	0.0941	67.18	0.7863	1.3375	
0.0972	68.58	0.8236	1.3463	1000	0.1015	70.85	0.8281	1.3249	

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction CO<sub>2</sub> in  $(1-x)$  mole fraction H<sub>2</sub>O — Continued

$p = 90 \text{ MPa}$								
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x = 0.05$		$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x = 0.10$	
		$\phi_1$	$\phi_2$				$\phi_1$	$\phi_2$
<i>coexisting phase <math>y = .8666</math></i>								
0.0365	28.35	0.1298	0.6959	457.1				
0.0204	16.53	0.0182	12.059	457.1				
<i>coexisting phase <math>y = .7552</math></i>								
				511.2	0.0407	33.59	0.1835	0.8902
				511.2	0.0227	22.18	0.0499	6.7237
0.0204	16.75	0.0194	11.875	460				
0.0208	18.27	0.0286	10.714	480				
0.0213	19.80	0.0406	9.698	500				
0.0218	21.36	0.0557	8.814	520	0.0230	22.88	0.0571	6.499
0.0223	22.94	0.0741	8.025	540	0.0236	24.50	0.0759	6.012
0.0230	24.55	0.0960	7.311	560	0.0243	26.16	0.0982	5.554
0.0237	26.19	0.1213	6.657	580	0.0252	27.86	0.1239	5.118
0.0246	27.88	0.1500	6.054	600	0.0262	29.62	0.1531	4.703
0.0273	32.32	0.2351	4.726	650	0.0295	34.24	0.2396	3.748
0.0312	37.12	0.3340	3.618	700	0.0343	39.23	0.3397	2.937
0.0371	42.27	0.4378	2.750	750	0.0411	44.41	0.4438	2.324
0.0449	47.48	0.5365	2.160	800	0.0492	49.43	0.5414	1.928
0.0537	52.33	0.6230	1.8139	850	0.0578	54.01	0.6264	1.6959
0.0626	56.66	0.6955	1.6210	900	0.0662	58.15	0.6977	1.5613
0.0709	60.53	0.7554	1.5099	950	0.0741	61.93	0.7566	1.4795
0.0788	64.09	0.8046	1.4417	1000	0.0816	65.47	0.8053	1.4270
$p = 90 \text{ MPa}$								
$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x = 0.20$		$T$ K	$V$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H$ kJ·mol <sup>-1</sup>	$x = 0.30$	
		$\phi_1$	$\phi_2$				$\phi_1$	$\phi_2$
<i>coexisting phase <math>x = .5384</math></i>								
0.0410	37.30	0.2030	1.2400	567.6				
0.0277	29.82	0.1169	3.3504	567.6				
<i>coexisting phase calculation unreliable and not included</i>								
0.0285	30.96	0.1345	3.223	580				
0.0299	32.86	0.1656	3.016	600	0.0344	35.74	0.1866	2.104
0.0316	34.80	0.2001	2.811	620	0.0366	37.77	0.2238	2.004
0.0336	36.80	0.2374	2.613	640	0.0391	39.81	0.2633	1.910
0.0358	38.83	0.2769	2.427	660	0.0418	41.84	0.3043	1.824
0.0383	40.88	0.3180	2.258	680	0.0446	43.84	0.3460	1.7482
0.0411	42.93	0.3599	2.108	700	0.0476	45.81	0.3876	1.6830
0.0440	44.95	0.4017	1.980	720	0.0506	47.72	0.4284	1.6277
0.0471	46.93	0.4427	1.872	740	0.0537	49.59	0.4679	1.5815
0.0503	48.86	0.4824	1.7817	760	0.0567	51.40	0.5058	1.5430
0.0535	50.72	0.5204	1.7078	780	0.0598	53.16	0.5418	1.5109
0.0567	52.52	0.5563	1.6472	800	0.0628	54.87	0.5758	1.4842
0.0647	56.77	0.6371	1.5390	850	0.0701	58.99	0.6520	1.4348
0.0723	60.73	0.7050	1.4711	900	0.0772	62.92	0.7163	1.4020
0.0796	64.47	0.7615	1.4266	950	0.0840	66.73	0.7701	1.3795
0.0865	68.06	0.8085	1.3960	1000	0.0905	70.44	0.8150	1.3633

TABLE 3. Molar volume, enthalpy, and fugacity coefficients for  $x$  mole fraction  $\text{CO}_2$  in  $(1-x)$  mole fraction  $\text{H}_2\text{O}$  — Continued

$p = 100 \text{ MPa}$									
$x = 0.05$					$x = 0.10$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
<i>coexisting phase</i> $y = .8666$									
0.0338	28.30	0.1251	0.6929	457.9					
0.0203	16.71	0.0176	12.009	457.9					
					<i>coexisting phase</i> $y = .7621$				
				509.9	0.0374	33.31	0.1748	0.8821	
				509.9	0.0224	22.16	0.0462	6.7227	
0.0203	16.87	0.0183	11.8733	460					
0.0207	18.38	0.0270	10.6753	480					
0.0211	19.90	0.0384	9.6573	500					
0.0216	21.44	0.0526	8.7696	520	0.0227	22.96	0.0539	6.4663	
0.0221	23.00	0.0699	7.9844	540	0.0233	24.56	0.0716	5.9870	
0.0227	24.59	0.0905	7.2808	560	0.0240	26.19	0.0925	5.5407	
0.0234	26.21	0.1143	6.6431	580	0.0248	27.86	0.1168	5.1216	
0.0242	27.87	0.1414	6.0598	600	0.0257	29.57	0.1443	4.7258	
0.0266	32.19	0.2216	4.7910	650	0.0285	34.05	0.2257	3.8276	
0.0300	36.81	0.3154	3.7480	700	0.0326	38.82	0.3206	3.0675	
0.0349	41.70	0.4150	2.9239	750	0.0382	43.77	0.4206	2.4759	
0.0412	46.68	0.5119	2.3335	800	0.0449	48.65	0.5169	2.0674	
0.0486	51.44	0.5993	1.9580	850	0.0523	53.21	0.6030	1.8109	
0.0562	55.79	0.6742	1.7343	900	0.0596	57.39	0.6768	1.6542	
0.0637	59.74	0.7371	1.6002	950	0.0667	61.25	0.7388	1.5562	
0.0707	63.38	0.7894	1.5161	1000	0.0735	64.86	0.7904	1.4921	
$x = 0.20$					$x = 0.30$				
$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	$T$ K	$V$ $\text{dm}^3\text{-mol}^{-1}$	$H$ $\text{kJ}\cdot\text{mol}^{-1}$	$\phi_1$	$\phi_2$	
<i>coexisting phase</i> $y = .5686$									
0.0384	36.98	0.1937	1.1996	563.2					
0.0268	29.39	0.1045	3.408	563.2					
					<i>coexisting phase calculation unreliable and not included</i>				
0.0277	30.89	0.1265	3.2493	580					
0.0289	32.72	0.1557	3.0594	600	0.0326	35.50	0.1751	2.1498	
0.0329	37.49	0.2415	2.6019	650	0.0377	40.42	0.2665	1.9320	
0.0383	42.41	0.3393	2.2132	700	0.0438	45.29	0.3665	1.7534	
0.0447	47.27	0.4393	1.9269	750	0.0504	49.95	0.4646	1.6267	
0.0516	51.86	0.5328	1.7366	800	0.0570	54.35	0.5541	1.5420	
0.0585	56.14	0.6152	1.6147	850	0.0635	58.50	0.6324	1.4856	
0.0653	60.15	0.6857	1.5356	900	0.0698	62.48	0.6993	1.4472	
0.0718	63.94	0.7451	1.4826	950	0.0759	66.33	0.7559	1.4201	
0.0781	67.59	0.7949	1.4456	1000	0.0818	70.08	0.8034	1.4004	

TABLE 4. Solute properties at infinite dilution

$p = 0.05$ MPa					$p = 0.10$ MPa				
$V_2$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H_2$ kJ·mol <sup>-1</sup>	$C_{p2}$ kJ mol <sup>-1</sup> K <sup>-1</sup>	$\varphi_2$	$T$ K	$V_2$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H_2$ kJ·mol <sup>-1</sup>	$C_{p2}$ kJ mol <sup>-1</sup> K <sup>-1</sup>	$\varphi_2$	
66.8	31.62	0.045	1.0034	400	33.5	31.72	0.042	1.0071	
70.1	33.06	0.047	1.0024	420	35.1	33.13	0.045	1.0049	
73.3	34.53	0.049	1.0017	440	36.7	34.58	0.047	1.0034	
76.6	36.03	0.049	1.0012	460	38.3	36.07	0.048	1.0024	
79.9	37.56	0.050	1.0009	480	40.0	37.59	0.049	1.0018	
83.2	39.12	0.051	1.0006	500	41.6	39.14	0.051	1.0013	
86.5	40.69	0.053	1.0005	520	43.3	40.71	0.052	1.0010	
89.8	42.29	0.053	1.0004	540	44.9	42.30	0.053	1.0007	
93.1	43.91	0.054	1.0003	560	46.6	43.92	0.054	1.0006	
96.5	45.56	0.055	1.0002	580	48.2	45.57	0.054	1.0005	
99.8	47.22	0.055	1.0002	600	49.9	47.23	0.055	1.0004	
108.1	51.48	0.057	1.0001	650	54.1	51.49	0.057	1.0002	
116.4	55.87	0.059	1.0001	700	58.2	55.87	0.059	1.0002	
124.7	60.39	0.061	1.0001	750	62.4	60.39	0.061	1.0001	
133.0	65.03	0.062	1.0001	800	66.5	65.03	0.063	1.0001	
141.4	69.80	0.065	1.0001	850	70.7	69.80	0.064	1.0001	
149.7	74.69	0.066	1.0001	900	74.8	74.69	0.066	1.0001	
158.0	79.70	0.068	1.0001	950	79.0	79.70	0.068	1.0002	
166.3	84.83	0.069	1.0001	1000	83.2	84.83	0.069	1.0002	

$p = 0.15$ MPa					$p = 0.20$ MPa				
$V_2$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H_2$ kJ·mol <sup>-1</sup>	$C_{p2}$ kJ mol <sup>-1</sup> K <sup>-1</sup>	$\varphi_2$	$T$ K	$V_2$ dm <sup>3</sup> ·mol <sup>-1</sup>	$H_2$ kJ·mol <sup>-1</sup>	$C_{p2}$ kJ mol <sup>-1</sup> K <sup>-1</sup>	$\varphi_2$	
22.45	31.82	0.040	1.0110	400	16.92	31.94	0.036	1.0151	
23.48	33.20	0.043	1.0075	420	17.67	33.28	0.041	1.0103	
24.54	34.64	0.045	1.0052	440	18.44	34.69	0.044	1.0071	
25.60	36.11	0.047	1.0037	460	19.23	36.15	0.046	1.0051	
26.7	37.62	0.049	1.0027	480	20.0	37.65	0.048	1.0037	
27.8	39.16	0.050	1.0020	500	20.8	39.18	0.050	1.0027	
28.9	40.72	0.051	1.0015	520	21.7	40.74	0.051	1.0020	
30.0	42.32	0.053	1.0011	540	22.5	42.33	0.052	1.0015	
31.1	43.93	0.053	1.0009	560	23.3	43.94	0.053	1.0012	
32.2	45.57	0.054	1.0007	580	24.1	45.58	0.054	1.0009	
33.3	47.24	0.055	1.0005	600	25.0	47.24	0.055	1.0007	
36.0	51.49	0.057	1.0003	650	27.0	51.49	0.057	1.0005	
38.8	55.87	0.059	1.0002	700	29.1	55.88	0.059	1.0003	
41.6	60.39	0.061	1.0002	750	31.2	60.39	0.061	1.0003	
44.4	65.03	0.062	1.0002	800	33.3	65.03	0.063	1.0003	
47.1	69.80	0.064	1.0002	850	35.3	69.80	0.064	1.0003	
49.9	74.69	0.066	1.0002	900	37.4	74.68	0.066	1.0003	
52.7	79.70	0.067	1.0002	950	39.5	79.70	0.068	1.0003	
55.4	84.83	0.069	1.0003	1000	41.6	84.83	0.069	1.0003	

TABLE 4. Solute properties at infinite dilution — Continued

<i>p</i> = 0.25 MPa					<i>p</i> = 0.30 MPa				
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	
0.044	39.49	0.061	3178.	400	0.044	39.49	0.063	2650.	
0.044	39.55	0.063	3167.	400.59					
13.63	32.10	0.032	1.0193	400.59					
				406.70	0.044	40.18	0.062	2547.	
				406.70	11.55	32.61	0.031	1.0211	
14.19	33.37	0.039	1.0132	420	11.87	33.46	0.035	1.0162	
14.79	34.75	0.042	1.0091	440	12.36	34.81	0.040	1.0112	
15.41	36.19	0.045	1.0065	460	12.86	36.24	0.044	1.0079	
16.05	37.68	0.047	1.0047	480	13.39	37.71	0.046	1.0057	
16.69	39.20	0.049	1.0034	500	13.92	39.23	0.048	1.0042	
17.34	40.76	0.050	1.0026	520	14.46	40.78	0.050	1.0031	
18.00	42.34	0.052	1.0019	540	15.00	42.36	0.051	1.0023	
18.65	43.95	0.053	1.0015	560	15.55	43.97	0.053	1.0018	
19.31	45.59	0.054	1.0012	580	16.10	45.60	0.053	1.0014	
19.97	47.25	0.054	1.0009	600	16.65	47.26	0.054	1.0011	
21.63	51.50	0.057	1.0006	650	18.03	51.50	0.056	1.0007	
23.29	55.88	0.059	1.0004	700	19.41	55.88	0.059	1.0005	
25.0	60.39	0.060	1.0004	750	20.8	60.39	0.061	1.0004	
26.6	65.03	0.063	1.0003	800	22.2	65.03	0.062	1.0004	
28.3	69.80	0.064	1.0003	850	23.6	69.79	0.064	1.0004	
29.9	74.68	0.066	1.0004	900	25.0	74.68	0.066	1.0004	
31.6	79.70	0.068	1.0004	950	26.3	79.69	0.067	1.0005	
33.3	84.83	0.069	1.0004	1000	27.7	84.83	0.068	1.0005	

<i>p</i> = 0.40 MPa					<i>p</i> = 0.50 MPa				
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	
0.044	39.49	0.061	1990.	400	0.044	39.50	0.064	1594.	
				420	0.045	41.57	0.058	1418.	
0.045	41.23	0.062	1804.	416.79					
8.92	33.46	0.028	1.0244	416.79					
				425.02	0.045	42.11	0.061	1377.	
				425.02	7.31	34.17	0.025	1.0273	
9.32	34.95	0.036	1.0156	440	7.50	35.10	0.031	1.0205	
9.68	36.33	0.041	1.0110	460	7.78	36.44	0.038	1.0143	
10.07	37.78	0.044	1.0079	480	8.08	37.86	0.042	1.0102	
10.46	39.28	0.047	1.0057	500	8.39	39.34	0.045	1.0074	
10.86	40.82	0.049	1.0042	520	8.70	40.86	0.047	1.0055	
11.26	42.39	0.050	1.0032	540	9.02	42.42	0.049	1.0041	
11.67	43.99	0.052	1.0025	560	9.34	44.01	0.051	1.0031	
12.08	45.62	0.053	1.0019	580	9.67	45.64	0.052	1.0024	
12.49	47.27	0.054	1.0015	600	10.00	47.28	0.053	1.0019	
13.52	51.51	0.056	1.0009	650	10.82	51.51	0.056	1.0012	
14.56	55.88	0.058	1.0007	700	11.65	55.89	0.058	1.0009	
15.60	60.39	0.060	1.0006	750	12.48	60.39	0.060	1.0007	
16.64	65.03	0.062	1.0005	800	13.31	65.03	0.062	1.0007	
17.68	69.79	0.064	1.0006	850	14.14	69.79	0.064	1.0007	
18.72	74.68	0.066	1.0006	900	14.98	74.68	0.066	1.0008	
19.76	79.69	0.068	1.0006	950	15.81	79.69	0.067	1.0008	
20.80	84.83	0.069	1.0007	1000	16.64	84.82	0.069	1.0009	



TABLE 4. Solute properties at infinite dilution – Continued

<i>p</i> = 0.60 MPa					<i>p</i> = 0.70 MPa				
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	
0.044	39.50	0.063	1330.	400	0.044	39.50	0.064	1142.	
0.045	41.58	0.062	1183.	420	0.045	41.58	0.060	1016.	
0.046	42.88	0.062	1104.	432.01					
6.22	34.80	0.022	1.0301	432.01					
				438.13	0.046	43.57	0.060	915.	
				438.13	5.43	35.36	0.019	1.0327	
6.30	35.27	0.026	1.0258	440	5.44	35.46	0.020	1.0315	
6.52	36.56	0.034	1.0178	460	5.61	36.69	0.030	1.0216	
6.75	37.94	0.040	1.0126	480	5.81	38.03	0.036	1.0152	
7.00	39.40	0.043	1.0091	500	6.02	39.46	0.041	1.0110	
7.26	40.90	0.046	1.0067	520	6.24	40.95	0.045	1.0080	
7.53	42.45	0.048	1.0050	540	6.46	42.49	0.047	1.0060	
7.79	44.04	0.050	1.0038	560	6.69	44.06	0.049	1.0046	
8.06	45.65	0.052	1.0030	580	6.92	45.67	0.051	1.0035	
8.34	47.30	0.053	1.0024	600	7.15	47.31	0.052	1.0028	
9.02	51.52	0.055	1.0014	650	7.74	51.53	0.055	1.0017	
9.71	55.89	0.058	1.0010	700	8.33	55.90	0.058	1.0012	
10.40	60.40	0.060	1.0009	750	8.92	60.40	0.060	1.0010	
11.10	65.03	0.062	1.0008	800	9.51	65.03	0.062	1.0010	
11.79	69.79	0.064	1.0009	850	10.11	69.79	0.064	1.0010	
12.48	74.68	0.065	1.0009	900	10.70	74.68	0.065	1.0011	
13.18	79.69	0.067	1.0010	950	11.30	79.69	0.067	1.0011	
13.87	84.82	0.069	1.0010	1000	11.89	84.82	0.069	1.0012	

<i>p</i> = 0.80 MPa					<i>p</i> = 0.90 MPa				
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	
0.044	39.50	0.063	1000.5	400	0.044	39.51	0.059	890.5	
0.045	41.58	0.061	889.8	420	0.045	41.58	0.060	791.9	
0.047	43.78	0.063	792.9	440	0.047	43.78	0.064	705.7	
0.047	44.20	0.064	776.7	443.59					
4.83	35.87	0.016	1.0351	443.59					
				448.54	0.047	44.78	0.062	671.9	
				448.54	4.36	36.34	0.013	1.0375	
4.94	36.83	0.026	1.0257	460	4.42	36.98	0.020	1.0301	
5.10	38.13	0.034	1.0180	480	4.56	38.24	0.030	1.0210	
5.28	39.53	0.039	1.0129	500	4.71	39.61	0.037	1.0150	
5.47	41.00	0.043	1.0094	520	4.87	41.06	0.041	1.0109	
5.66	42.53	0.046	1.0070	540	5.04	42.57	0.044	1.0081	
5.86	44.09	0.048	1.0053	560	5.21	44.12	0.048	1.0061	
6.06	45.70	0.050	1.0041	580	5.39	45.72	0.049	1.0047	
6.26	47.33	0.052	1.0032	600	5.57	47.35	0.051	1.0037	
6.77	51.54	0.055	1.0020	650	6.02	51.55	0.055	1.0022	
7.29	55.90	0.057	1.0014	700	6.48	55.90	0.057	1.0016	
7.80	60.40	0.059	1.0012	750	6.94	60.40	0.060	1.0013	
8.32	65.03	0.062	1.0011	800	7.40	65.03	0.062	1.0013	
8.84	69.79	0.064	1.0012	850	7.86	69.79	0.063	1.0013	
9.37	74.68	0.065	1.0012	900	8.33	74.68	0.065	1.0014	
9.89	79.69	0.067	1.0013	950	8.79	79.69	0.067	1.0015	
10.41	84.82	0.069	1.0014	1000	9.25	84.82	0.069	1.0016	

TABLE 4. Solute properties at infinite dilution — Continued

$p = 1.0 \text{ MPa}$					$p = 1.5 \text{ MPa}$			
$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$	$T$ K	$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$
0.044	39.51	0.060	802.5	400	0.044	39.52	0.062	538.6
0.045	41.58	0.060	713.7	420	0.045	41.60	0.065	478.9
0.047	43.78	0.062	635.9	440	0.046	43.79	0.059	426.7
				460	0.048	46.18	0.066	380.4
0.048 <sup>a</sup>	45.32	0.066	590.0	453.07				
3.98	36.78	0.010	1.0398	453.07				
				471.48	0.050	47.67	0.068	356.0
				471.48	2.81	38.68	-0.007	1.0506
4.01	37.15	0.015	1.0348	460				
4.12	38.35	0.027	1.0241	480	2.83	39.07	0.003	1.0429
4.25	39.69	0.034	1.0171	500	2.89	40.17	0.019	1.0297
4.39	41.11	0.040	1.0124	520	2.97	41.45	0.030	1.0211
4.54	42.61	0.043	1.0092	540	3.05	42.85	0.035	1.0154
4.70	44.15	0.046	1.0069	560	3.15	44.33	0.040	1.0115
4.85	45.74	0.048	1.0053	580	3.25	45.88	0.044	1.0087
5.01	47.37	0.050	1.0042	600	3.35	47.47	0.047	1.0068
5.42	51.56	0.054	1.0025	650	3.62	51.61	0.052	1.0040
5.83	55.91	0.057	1.0018	700	3.89	55.93	0.056	1.0028
6.25	60.40	0.059	1.0015	750	4.17	60.41	0.058	1.0023
6.66	65.03	0.061	1.0014	800	4.44	65.03	0.060	1.0022
7.08	69.79	0.063	1.0015	850	4.72	69.79	0.063	1.0022
7.49	74.67	0.065	1.0015	900	5.00	74.67	0.065	1.0023
7.91	79.68	0.067	1.0016	950	5.28	79.68	0.066	1.0025
8.33	84.82	0.069	1.0017	1000	5.56	84.81	0.068	1.0026

$p = 2.0 \text{ MPa}$				$p = 2.5 \text{ MPa}$				
$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$	$T$ K	$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$
0.044	39.54	0.062	406.6	400	0.044	39.55	0.064	327.4
0.045	41.61	0.062	361.5	420	0.045	41.62	0.061	291.0
0.046	43.80	0.062	322.0	440	0.046	43.80	0.060	259.3
0.048	46.18	0.065	287.1	460	0.048	46.18	0.066	231.1
0.051	48.84	0.077	255.6	480	0.051	48.83	0.074	205.8
0.052	49.65	0.081	247.3	485.57				
2.21	40.27	-0.024	1.0607	485.57				
				497.14	0.054	51.42	0.085	185.8
				497.14	1.849	41.70	-0.043	1.0704
2.23	40.84	-0.003	1.0458	500	1.847	41.76	-0.037	1.0664
2.26	41.90	0.014	1.0319	520	1.853	42.49	-0.005	1.0452
2.32	43.16	0.026	1.0229	540	1.882	43.56	0.013	1.0318
2.38	44.56	0.034	1.0168	560	1.925	44.83	0.025	1.0230
2.45	46.04	0.039	1.0126	580	1.975	46.23	0.033	1.0171
2.53	47.59	0.043	1.0097	600	2.03	47.73	0.038	1.0131
2.72	51.66	0.049	1.0056	650	2.18	51.73	0.047	1.0074
2.92	55.96	0.054	1.0039	700	2.34	55.99	0.052	1.0051
3.13	60.43	0.057	1.0032	750	2.51	60.44	0.056	1.0041
3.34	65.04	0.059	1.0030	800	2.67	65.04	0.059	1.0038
3.55	69.79	0.062	1.0030	850	2.84	69.78	0.061	1.0039
3.75	74.66	0.064	1.0032	900	3.01	74.66	0.064	1.0040
3.96	79.67	0.066	1.0034	950	3.17	79.66	0.066	1.0043
4.17	84.80	0.068	1.0036	1000	3.34	84.79	0.068	1.0045

TABLE 4. Solute properties at infinite dilution — Continued

<i>p</i> = 3.0 MPa					<i>p</i> = 4.0 MPa				
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	
0.044	39.57	0.063	274.7	400	0.044	39.59	0.062	208.8	
0.047	44.96	0.063	205.3	450	0.047	44.97	0.061	155.9	
0.054	51.86	0.090	153.2	500	0.054	51.81	0.086	116.4	
0.056	53.07	0.097	146.6	507.04					
1.603	43.02	-0.064	1.0799	507.04					
				523.54	0.060	56.16	0.121	100.2	
				523.54	1.294	45.51	-0.113	1.0989	
1.591	43.25	-0.033	1.0615	520					
1.598	44.05	-0.002	1.0425	540	1.264	45.44	-0.056	1.0704	
1.624	45.16	0.014	1.0303	560	1.259	46.05	-0.016	1.0487	
1.660	46.46	0.025	1.0223	580	1.273	47.06	0.005	1.0349	
1.703	47.89	0.033	1.0168	600	1.297	48.31	0.019	1.0258	
1.749	49.41	0.038	1.0131	620	1.327	49.71	0.029	1.0197	
1.799	51.00	0.043	1.0104	640	1.360	51.21	0.035	1.0155	
1.850	52.63	0.046	1.0086	660	1.396	52.79	0.040	1.0126	
1.902	54.31	0.048	1.0073	680	1.434	54.43	0.044	1.0106	
1.955	56.03	0.051	1.0063	700	1.473	56.11	0.047	1.0091	
2.09	60.46	0.055	1.0051	750	1.573	60.49	0.052	1.0072	
2.23	65.05	0.058	1.0047	800	1.676	65.06	0.057	1.0066	
2.37	69.78	0.061	1.0047	850	1.780	69.78	0.059	1.0065	
2.51	74.66	0.064	1.0049	900	1.885	74.65	0.063	1.0068	
2.65	79.66	0.065	1.0052	950	1.990	79.65	0.065	1.0071	
2.79	84.78	0.067	1.0055	1000	2.100	84.77	0.067	1.0075	

<i>p</i> = 5.0 MPa					<i>p</i> = 6.0 MPa				
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	
0.044	39.62	0.065	169.2	400	0.044	39.65	0.060	142.9	
0.047	44.98	0.061	126.3	450	0.047	44.99	0.063	106.6	
0.054	51.77	0.086	94.3	500	0.053	51.73	0.083	79.6	
0.064	59.12	0.151	74.1	537.13					
1.109	47.92	-0.174	1.1182	537.13					
				548.77	0.069	62.07	0.183	57.5	
				548.77	0.991	50.35	-0.250	1.1385	
1.099	47.74	-0.155	1.1109	540					
1.058	47.37	-0.065	1.0735	560	0.947	49.39	-0.152	1.1076	
1.051	47.90	-0.024	1.0512	580	0.913	49.07	-0.067	1.0724	
1.059	48.87	-0.001	1.0372	600	0.907	49.61	-0.024	1.0513	
1.077	50.10	0.015	1.0279	620	0.914	50.59	-0.001	1.0378	
1.100	51.49	0.026	1.0217	640	0.929	51.83	0.014	1.0290	
1.126	52.99	0.034	1.0174	660	0.947	53.23	0.025	1.0230	
1.154	54.57	0.038	1.0144	680	0.969	54.75	0.032	1.0189	
1.184	56.22	0.042	1.0124	700	0.993	56.35	0.037	1.0160	
1.263	60.54	0.050	1.0096	750	1.056	60.60	0.047	1.0122	
1.344	65.08	0.055	1.0086	800	1.124	65.11	0.053	1.0109	
1.428	69.79	0.058	1.0085	850	1.193	69.80	0.057	1.0106	
1.512	74.65	0.061	1.0087	900	1.263	74.64	0.060	1.0108	
1.596	79.64	0.064	1.0091	950	1.333	79.63	0.063	1.0112	
1.680	84.76	0.066	1.0096	1000	1.404	84.75	0.065	1.0117	

TABLE 4. Solute properties at infinite dilution — Continued

<i>p</i> = 7 MPa					<i>p</i> = 8 MPa				
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	
0.044	39.68	0.062	124.1	400	0.044	39.70	0.062	110.0	
0.047	44.99	0.060	92.5	450	0.047	45.00	0.060	82.0	
0.053	51.68	0.087	69.1	500	0.053	51.64	0.085	61.2	
0.069	62.20	0.187	49.6	550	0.068	61.98	0.178	44.0	
0.075	65.09	0.235	46.2	559.01					
0.911	52.90	-0.339	1.160	559.01					
				568.19	0.081	68.27	0.297	38.0	
				568.19	0.857	55.64	-0.459	1.183	
0.830	50.75	-0.137	1.100	580	0.789	53.28	-0.260	1.137	
0.806	50.61	-0.062	1.069	600	0.739	51.96	-0.116	1.091	
0.802	51.23	-0.024	1.050	620	0.723	52.05	-0.053	1.064	
0.809	52.26	-0.001	1.038	640	0.722	52.80	-0.019	1.048	
0.822	53.53	0.014	1.029	660	0.729	53.90	0.001	1.037	
0.838	54.96	0.024	1.024	680	0.741	55.22	0.015	1.030	
0.857	56.50	0.032	1.020	700	0.756	56.69	0.024	1.025	
0.910	60.67	0.043	1.015	750	0.800	60.76	0.040	1.018	
0.967	65.14	0.051	1.013	800	0.849	65.18	0.048	1.016	
1.026	69.81	0.055	1.013	850	0.900	69.83	0.054	1.015	
1.086	74.64	0.059	1.013	900	0.953	74.65	0.058	1.015	
1.146	79.63	0.062	1.013	950	1.005	79.62	0.061	1.016	
1.206	84.74	0.065	1.014	1000	1.059	84.74	0.064	1.016	

<i>p</i> = 9 MPa					<i>p</i> = 10 MPa				
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	
0.044	39.73	0.064	99.1	400	0.044	39.76	0.065	90.4	
0.047	45.01	0.060	73.8	450	0.046	45.02	0.060	67.2	
0.053	51.61	0.079	55.1	500	0.053	51.57	0.081	50.3	
0.068	61.77	0.173	39.7	550	0.067	61.57	0.162	36.3	
0.088	71.65	0.373	31.9	576.53					
0.823	58.66	-0.617	1.208	576.53					
				584.18	0.097	75.32	0.484	27.1	
				584.18	0.804	62.08	-0.834	1.236	
0.792	57.39	-0.504	1.190	580					
0.700	53.85	-0.196	1.120	600	0.685	56.60	-0.344	1.157	
0.667	53.12	-0.092	1.082	620	0.630	54.53	-0.151	1.104	
0.658	53.47	-0.042	1.060	640	0.610	54.30	-0.072	1.074	
0.660	54.35	-0.014	1.046	660	0.606	54.88	-0.032	1.056	
0.667	55.53	0.004	1.036	680	0.609	55.90	-0.008	1.044	
0.679	56.91	0.018	1.030	700	0.618	57.16	0.008	1.036	
0.715	60.86	0.036	1.022	750	0.648	60.97	0.032	1.026	
0.758	65.22	0.045	1.019	800	0.685	65.28	0.043	1.022	
0.803	69.85	0.052	1.018	850	0.726	69.87	0.050	1.020	
0.849	74.66	0.057	1.018	900	0.767	74.67	0.055	1.020	
0.896	79.62	0.060	1.018	950	0.809	79.63	0.059	1.020	
0.944	84.73	0.063	1.019	1000	0.852	84.73	0.063	1.021	

TABLE 4. Solute properties at infinite dilution — Continued

<i>p</i> = 12 MPa					<i>p</i> = 14 MPa			
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>
0.043	39.82	0.065	77.30	400	0.043	39.88	0.061	68.01
0.046	45.04	0.058	57.42	450	0.046	45.07	0.059	50.45
0.052	51.50	0.079	42.95	500	0.052	51.44	0.076	37.74
0.066	61.19	0.155	31.13	550	0.065	60.84	0.146	27.46
				600	0.115	83.15	0.746	17.68
0.119	84.04	0.831	20.19	597.86				
0.805	70.67	-1.518	1.300	597.86				
				609.85	0.152	95.82	1.594	15.47
				609.85	0.861	83.29	-2.898	1.3824
				600				
0.767	68.43	-1.254	1.280	620	0.660	69.03	-1.075	1.271
0.605	59.02	-0.373	1.166	640	0.533	60.74	-0.366	1.167
0.551	56.70	-0.167	1.112	660	0.491	58.52	-0.166	1.116
0.532	56.34	-0.084	1.081	680	0.474	58.18	-0.088	1.086
0.527	56.85	-0.040	1.062	700	0.469	58.70	-0.041	1.068
0.529	57.82	-0.014	1.050	720	0.471	59.68	-0.015	1.056
0.535	59.06	0.004	1.042	740	0.476	60.93	0.002	1.048
0.543	60.49	0.016	1.036	760	0.483	62.37	0.015	1.042
0.554	62.05	0.025	1.033	780	0.491	63.94	0.023	1.038
0.565	63.70	0.032	1.030	800	0.501	65.60	0.030	1.036
0.577	65.42	0.037	1.028	850	0.528	70.03	0.042	1.032
0.610	69.94	0.046	1.026	900	0.556	74.75	0.050	1.031
0.644	74.70	0.053	1.026	950	0.586	79.66	0.055	1.031
0.679	79.64	0.057	1.026	1000	0.616	84.75	0.060	1.032
0.714	84.73	0.061	1.026					

<i>p</i> = 16 MPa					<i>p</i> = 18 MPa			
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>
0.043	39.94	0.060	61.08	400	0.043	40.00	0.061	55.72
0.046	45.09	0.059	45.24	450	0.046	45.12	0.055	41.21
0.051	51.38	0.075	33.86	500	0.051	51.33	0.071	30.84
0.064	60.53	0.138	24.72	550	0.063	60.24	0.135	22.59
0.108	80.66	0.587	16.17	600	0.102	78.65	0.496	15.00
0.210	114.02	3.505	12.02	620.54				
0.997	104.13	-6.446	1.493	620.54				
				630.19	0.330	147.95	10.234	9.34
				630.19	1.298	145.22	-18.181	1.652
				640	0.701	86.79	-2.651	1.402
0.564	68.37	-0.832	1.252	660	0.488	67.52	-0.625	1.230
0.475	61.93	-0.322	1.163	680	0.433	62.67	-0.269	1.157
0.442	60.09	-0.154	1.117	700	0.403	61.51	-0.140	1.117
0.429	59.89	-0.084	1.090	720	0.394	61.52	-0.078	1.093
0.426	60.48	-0.041	1.072	740	0.391	62.21	-0.040	1.077
0.427	61.49	-0.016	1.061	760	0.392	63.28	-0.015	1.066
0.431	62.77	0.001	1.053	780	0.396	64.61	0.003	1.059
0.437	64.24	0.013	1.048	800	0.402	66.10	0.014	1.054
0.445	65.82	0.021	1.044	850	0.420	70.30	0.032	1.047
0.467	70.15	0.038	1.039	900	0.441	74.90	0.043	1.044
0.491	74.81	0.047	1.038	950	0.463	79.75	0.050	1.043
0.517	79.70	0.053	1.037	1000	0.486	84.80	0.055	1.043
0.543	84.77	0.057	1.037					

TABLE 4. Solute properties at infinite dilution — Continued

$p = 20$ MPa					$p = 22$ MPa				
$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$	$T$ K	$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$	
0.043	40.06	0.059	51.46	400	0.043	40.12	0.058	48.01	
0.045	45.14	0.057	38.00	450	0.045	45.17	0.054	35.40	
0.051	51.28	0.074	28.45	500	0.050	51.24	0.069	26.50	
0.062	59.97	0.119	20.89	550	0.061	59.72	0.118	19.51	
0.097	76.99	0.418	14.06	600	0.093	75.59	0.366	13.27	
0.148	94.89	1.25	11.10	620	0.133	90.39	0.918	10.66	
0.710	243.1	58.2	7.090	638.95					
2.150	260.5	-90.1	1.917	638.95					
1.636	200.5	-42.0	1.819	640	0.349	151.4	9.02	7.393	
0.543	77.88	-1.35	1.333	660	0.694	101.5	-3.90	1.510	
0.429	66.94	-0.464	1.211	680	0.451	73.36	-0.816	1.285	
0.389	63.71	-0.223	1.151	700	0.385	66.75	-0.347	1.195	
0.371	62.87	-0.122	1.117	720	0.357	64.63	-0.181	1.146	
0.364	63.11	-0.067	1.095	740	0.345	64.24	-0.103	1.117	
0.363	63.92	-0.035	1.081	760	0.340	64.69	-0.057	1.098	
0.365	65.07	-0.012	1.071	780	0.340	65.62	-0.028	1.086	
0.368	66.45	0.004	1.065	800	0.342	66.86	-0.008	1.077	
0.383	70.48	0.027	1.055	850	0.353	70.69	0.021	1.064	
0.401	75.00	0.039	1.052	900	0.368	75.12	0.035	1.059	
0.421	79.81	0.048	1.051	950	0.386	79.89	0.046	1.057	
0.441	84.84	0.054	1.050	1000	0.404	84.89	0.052	1.056	

$p = 24$ MPa					$p = 26$ MPa				
$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$	$T$ K	$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$	
0.043	40.18	0.060	45.16	400	0.043	40.24	0.059	42.77	
0.045	45.20	0.054	33.24	450	0.045	45.23	0.053	31.43	
0.050	51.20	0.064	24.88	500	0.050	51.17	0.067	23.52	
0.053	54.13	0.080	22.12	520	0.053	54.04	0.081	20.93	
0.058	57.53	0.103	19.58	540	0.057	57.38	0.100	18.54	
0.064	61.66	0.135	17.19	560	0.063	61.37	0.122	16.30	
0.073	66.94	0.193	14.89	580	0.072	66.42	0.176	14.16	
0.090	74.38	0.314	12.61	600	0.086	73.33	0.280	12.06	
0.123	87.02	0.697	10.26	620	0.115	84.39	0.576	9.921	
0.243	122.86	3.50	7.548	640	0.196	109.75	1.94	7.559	
1.258	191.84	-24.9	1.924	660	1.739	401.46	39.1	3.669	
0.501	84.11	-1.56	1.392	680	0.599	103.90	-3.34	1.557	
0.391	71.01	-0.545	1.251	700	0.409	77.12	-0.866	1.324	
0.350	66.91	-0.262	1.182	720	0.349	69.90	-0.381	1.226	
0.332	65.65	-0.146	1.143	740	0.323	67.40	-0.206	1.173	
0.323	65.63	-0.084	1.118	760	0.311	66.78	-0.121	1.141	
0.320	66.29	-0.048	1.102	780	0.305	67.08	-0.069	1.120	
0.321	67.35	-0.023	1.090	800	0.303	67.92	-0.038	1.105	
0.329	70.95	0.013	1.074	850	0.308	71.24	0.006	1.085	
0.342	75.27	0.031	1.067	900	0.319	75.44	0.027	1.076	
0.357	79.98	0.042	1.064	950	0.333	80.09	0.040	1.072	
0.374	84.95	0.050	1.063	1000	0.348	85.02	0.048	1.070	

TABLE 4. Solute properties at infinite dilution — Continued

<i>p</i> = 30 MPa					<i>p</i> = 40 MPa			
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>
0.043	40.36	0.057	39.00	400	0.042	40.68	0.057	33.21
0.043	42.28	0.054	34.30	420	0.043	42.55	0.054	29.08
0.044	44.26	0.053	30.33	440	0.043	44.49	0.053	25.63
0.045	46.36	0.055	26.93	460	0.044	46.51	0.054	22.71
0.047	48.63	0.057	23.98	480	0.046	48.68	0.055	20.20
0.049	51.11	0.064	21.37	500	0.048	51.03	0.059	18.00
0.052	53.90	0.076	19.03	520	0.050	53.62	0.066	16.06
0.056	57.09	0.091	16.89	540	0.053	56.53	0.075	14.30
0.061	60.86	0.113	14.90	560	0.058	59.87	0.095	12.69
0.069	65.51	0.151	13.01	580	0.064	63.80	0.116	11.19
0.081	71.59	0.233	11.17	600	0.072	68.57	0.157	9.77
0.103	80.49	0.401	9.35	620	0.085	74.69	0.219	8.40
0.150	96.48	0.943	7.44	640	0.106	83.13	0.356	7.05
0.335	143.67	4.266	5.20	660	0.147	96.15	0.609	5.69
0.947	201.28	-11.003	2.34	680	0.238	118.51	1.088	4.28
0.489	99.18	-2.270	1.556	700	0.406	142.32	-0.291	2.90
0.305	70.71	-0.280	1.220	750	0.316	87.94	-0.869	1.498
0.278	69.37	-0.077	1.140	800	0.248	75.11	-0.222	1.264
0.277	71.97	-0.012	1.109	850	0.232	74.68	-0.074	1.188
0.284	75.86	0.017	1.095	900	0.231	77.39	-0.014	1.154
0.295	80.35	0.033	1.089	950	0.235	81.32	0.014	1.137
0.307	85.20	0.043	1.085	1000	0.242	85.85	0.030	1.128

<i>p</i> = 50 MPa					<i>p</i> = 60 MPa			
<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>	<i>T</i> K	<i>V</i> <sub>2</sub> dm <sup>3</sup> ·mol <sup>-1</sup>	<i>H</i> <sub>2</sub> kJ·mol <sup>-1</sup>	<i>C</i> <sub><i>p</i>2</sub> kJ mol <sup>-1</sup> K <sup>-1</sup>	φ <sub>2</sub>
0.042	41.01	0.055	30.13	400	0.041	41.35	0.055	28.42
0.042	42.85	0.051	26.26	420	0.042	43.15	0.051	24.67
0.043	44.73	0.050	23.07	440	0.042	44.99	0.046	21.59
0.044	46.69	0.051	20.38	460	0.043	46.90	0.050	19.02
0.045	48.77	0.052	18.10	480	0.044	48.91	0.047	16.86
0.046	51.01	0.057	16.13	500	0.045	51.05	0.050	15.01
0.049	53.45	0.061	14.40	520	0.047	53.37	0.052	13.40
0.051	56.15	0.070	12.85	540	0.049	55.90	0.061	11.98
0.055	59.18	0.081	11.45	560	0.052	58.69	0.070	10.70
0.059	62.63	0.095	10.16	580	0.056	61.80	0.077	9.55
0.066	66.64	0.113	8.97	600	0.061	65.31	0.093	8.48
0.075	71.43	0.155	7.83	620	0.068	69.34	0.105	7.49
0.088	77.34	0.198	6.75	640	0.077	74.01	0.132	6.57
0.108	84.93	0.270	5.71	660	0.090	79.52	0.162	5.69
0.141	94.95	0.365	4.70	680	0.108	86.05	0.195	4.86
0.194	107.34	0.354	3.72	700	0.133	93.55	0.208	4.08
0.294	106.40	-0.988	1.978	750	0.216	105.56	-0.345	2.48
0.237	83.78	-0.414	1.456	800	0.219	92.14	-0.491	1.712
0.210	78.73	-0.151	1.296	850	0.195	83.65	-0.231	1.438
0.201	79.64	-0.056	1.230	900	0.183	82.50	-0.095	1.324
0.201	82.73	-0.009	1.197	950	0.180	84.54	-0.035	1.268
0.205	86.82	0.015	1.178	1000	0.180	88.06	0.001	1.236

TABLE 4. Solute properties at infinite dilution — Continued

$p = 70 \text{ MPa}$					$p = 80 \text{ MPa}$				
$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$	$T$ K	$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$	
0.041	41.70	0.049	27.56	400	0.040	42.06	0.048	27.24	
0.041	43.47	0.047	23.80	420	0.041	43.79	0.046	23.41	
0.042	45.27	0.046	20.74	440	0.041	45.56	0.045	20.32	
0.042	47.12	0.047	18.23	460	0.042	47.37	0.046	17.80	
0.043	49.07	0.048	16.12	480	0.042	49.26	0.047	15.70	
0.044	51.14	0.049	14.33	500	0.044	51.26	0.048	13.94	
0.046	53.35	0.050	12.79	520	0.045	53.38	0.049	12.43	
0.048	55.74	0.052	11.44	540	0.047	55.66	0.051	11.12	
0.050	58.35	0.055	10.25	560	0.049	58.12	0.054	9.97	
0.054	61.21	0.060	9.17	580	0.051	60.78	0.058	8.94	
0.058	64.37	0.067	8.19	600	0.055	63.69	0.064	8.02	
0.063	67.89	0.078	7.29	620	0.059	66.86	0.073	7.18	
0.070	71.84	0.096	6.46	640	0.064	70.33	0.084	6.41	
0.079	76.28	0.117	5.68	660	0.071	74.12	0.094	5.69	
0.090	81.26	0.131	4.96	680	0.080	78.24	0.098	5.04	
0.106	86.71	0.130	4.28	700	0.090	82.63	0.096	4.43	
0.160	98.66	-0.076	2.86	750	0.126	93.06	-0.004	3.15	
0.189	96.05	-0.382	1.996	800	0.158	95.93	-0.234	2.27	
0.180	88.25	-0.272	1.607	850	0.163	91.45	-0.254	1.792	
0.169	85.61	-0.130	1.436	900	0.157	88.51	-0.155	1.562	
0.164	86.62	-0.055	1.350	950	0.152	88.77	-0.076	1.443	
0.163	89.52	-0.017	1.302	1000	0.150	91.10	-0.030	1.376	

$p = 90 \text{ MPa}$					$p = 100 \text{ MPa}$				
$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$	$T$ K	$V_2$ $\text{dm}^3\text{-mol}^{-1}$	$H_2$ $\text{kJ}\cdot\text{mol}^{-1}$	$C_{p2}$ $\text{kJ mol}^{-1} \text{K}^{-1}$	$\varphi_2$	
0.040	42.42	0.051	27.32	400	0.040	42.79	0.050	27.71	
0.040	44.13	0.047	23.34	420	0.040	44.47	0.046	23.58	
0.041	45.86	0.045	20.19	440	0.040	46.17	0.044	20.29	
0.041	47.64	0.044	17.63	460	0.041	47.91	0.041	17.65	
0.042	49.38	0.043	15.51	480	0.041	49.71	0.043	15.49	
0.043	51.21	0.044	13.74	500	0.042	51.59	0.042	13.70	
0.044	53.36	0.045	12.24	520	0.043	53.57	0.044	12.18	
0.045	55.64	0.048	10.95	540	0.044	55.67	0.048	10.89	
0.047	57.68	0.051	9.82	560	0.046	57.91	0.052	9.77	
0.050	60.489	0.056	8.83	580	0.048	60.29	0.051	8.79	
0.052	63.19	0.061	7.94	600	0.050	62.83	0.055	7.91	
0.056	66.10	0.067	7.13	620	0.053	65.55	0.062	7.13	
0.060	69.594	0.073	6.40	640	0.057	68.43	0.064	6.43	
0.066	72.30	0.076	5.73	660	0.061	71.49	0.064	5.79	
0.072	76.68	0.079	5.12	680	0.066	74.71	0.068	5.20	
0.080	79.94	0.078	4.56	700	0.073	78.03	0.065	4.67	
0.106	89.09	0.017	3.37	750	0.092	86.25	0.031	3.55	
0.133	94.14	-0.132	2.51	800	0.114	92.06	-0.069	2.71	
0.145	93.00	-0.205	1.981	850	0.129	93.33	-0.150	2.16	
0.144	90.84	-0.156	1.698	900	0.132	92.45	-0.141	1.838	
0.141	90.79	-0.087	1.544	950	0.131	92.52	-0.091	1.652	
0.140	92.69	-0.041	1.456	1000	0.134	96.48	-0.050	1.541	



## Appendix B. The FORTRAN Programs

A listing is presented of the FORTRAN source code for the calculation of thermodynamic properties of mixtures of CO<sub>2</sub> and H<sub>2</sub>O. The purpose of each of the subroutines is explained in its preface in the form of a comment statement. The listing is given in order to enable the user to incorporate property calculations into existing or emerging programs. The program has only limited "user-friendliness", as explained further on.

The main program MIXPROP, together with the subroutines called by it, produces a collection of thermodynamic properties of the homogeneous mixture, such as Helmholtz and Gibbs free energies, enthalpy, entropy, heat capacities, fugacities and fugacity coefficients. This program, which can be used as an example for the use of the routines, calculates the properties along an isobar at constant composition for a range of temperatures specified by the user. The user may also specify the system of units to be used (note that the composition is always taken to be mole fractions). This will enable the user to check correct operation by comparing with the tables presented in this paper.

The rather simplified program should not be used blindly since no information is available as to the location

of phase boundaries, which must be determined from another program, such as COEX shown in the following example. The phase for which calculation will be made is determined by the initial guess for the densities, and in this example a vapor-like guess is used.

The next example is the main program COEX, using the same subroutines, which demonstrates a method for the prediction of coexisting phases. This uses a non-linear equation solver SNSQ which is commonly available in math packages, but other convenient packages may also be used. The formulation for the saturated liquid and vapor densities, DLEQ and DVEQ, for pure water developed by Saul and Wagner<sup>41</sup> are used to supply initial guesses for the densities in the iteration.

Another main program, APPMOLP, is also included, illustrating the method by which the apparent molar properties may be calculated. This example calculates the apparent molar volume, the apparent molar heat capacity, and also  $V_2$  and  $C_{p,2}$ , along an isobar at constant composition for a range of temperatures, as in the first program.

## PROGRAM MIXPROP

C

C PROGRAM FOR CALCULATING THERMODYNAMIC PROPERTIES OF CO2-H2O MIXTURES  
C THIS IS A PROGRAM DESIGNED TO CALCULATE TABLES OF PROPERTIES SUCH AS  
C THE TABLES IN THIS PAPER, AND IS INTENDED TO SERVE AS AN EXAMPLE FOR  
C THE USE OF THE VARIOUS SUBROUTINES WHICH FOLLOW.

C

```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /PROPS/ P,A,G,H,U,S,CV,CP,DPDD,DPDT,W
COMMON /CRITC / PC0,PC1,DC0,DC1,TC0,TC1,PI0,PI1,DIO,DI1,TI0,TI1
COMMON /THPH/ PH0,PHT,PHD,THT,THD,PHC,THC
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VX,TX
COMMON /DERIVS/ DADT,CVR,DPDTR,D2P
COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK
CHARACTER*8 ND,NH,NT,NP
COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH,/UNITC/NT,ND,NP,NH,IFL
COMMON /FUGETC/ TT,PIN,FUG1,FUG2,PHI1,PHI2
CHARACTER*1 IFL
CALL FACTOR(0.,1.,1.)
CALL UNIT
71  FORMAT('1PH=',F6.3,' FFT=',F6.4,' FFV=',F6.3,6F6.3)
188  FORMAT(' INPUT PRESSURE, X(CO2), INIT, FINAL AND INCR OF T')
189  FORMAT(4X,'X',7X,'T',5X,'Pressure Volume Enthalpy fug1  phi1'
1,6X,'fug2  phi2'/12X,A3,5X,A4,3X,A7,2X,A8,2X,A4,14X,A4/)
WRITE(*,71) PH0,FFT,FFV,PHD,PHT,THD,THT,PHC,THC
1  WRITE(*,188)
READ(*,*,END=9) PIN,X,TT1,TT2,TTI
WRITE(*,189) NT,NP,ND,NH,NP,NP
TT = TT1-TTI
3  TT = TT + TTI
IF(TT.GT.TT2) GO TO 1
CALL FACTOR(0.,1.,1.)

```

```

T = TTT(TT)
FDD = FD
IF(ID.NE.3) FDD = FD/WM0
FHH = FH
IF(ID.NE.3) FHH = FH*WM0
D = .001
IF(X.LT..02 .AND. PIN*FP/PR.GT.PV(T)) D = 3.
CALL SHAPIT(X,TT,PIN,T,D,PP)
CALL THERM(D,T,X)
DOUT = D*DR/FDD/HX
DPDT = DPDT*FT/FP *PR/TR
DPDD = DPDD*FDD/FP *PR/DR
CVOUT = CV*FT/FHH *SR
CPOUT = CP*FT/FHH *SR
SOUT = S*FT/FHH *SR
HOUT = H/FHH *AR *.001
UOUT = U/FHH *AR
AOUT = A/FHH *AR
GOUT = G/FHH *AR
VOUT = 1./DOUT
CALL MU(XMU1,XMU2,D2ADX2,D,T,X)
WRITE(*,33) X,TT,PIN,VOUT,HOUT,FUG1,PHI1,FUG2,PHI2
WRITE(7,33) X,TT,PIN,VOUT,HOUT,FUG1,PHI1,FUG2,PHI2
33 FORMAT(F8.5,F8.2,F8.3,F9.4,F9.3,F9.5,F9.4,F9.5,F9.4)
GO TO 3
9 STOP
END
C
BLOCK DATA
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK
COMMON /CRITC / PC0,PC1,DC0,DC1,TC0,TC1,PI0,PI1,DI0,DI1,TI0,TI1
COMMON /IDEAL5/ TBT(16),A5BT(16),S5BT(16),CV5BT(16),TCT(16)
1,G5CT(16),S5CT(16),CP5CT(16)
COMMON /CONVRT/ FFP(6),FFD(6),FFT(6),FFH(6)
COMMON /THPH/ PH0,PHT,PHD,THT,THD,PHC,THC
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FTT,FVV,V45,T45,VX,TX
COMMON/COEFS/A0(18),A1(5),A20,Y(4),A3(36),RR(4),TEE(4),A4(4)
1,K(36),L(36),M(4),N(4),ALPHA(4),BETA(4),Z0
C THE CONVERSION FACTORS FOR DIFFERENT SYSTEMS OF UNITS ARE AS
C RECOMMENDED BY THE ASTM IN THEIR 'STANDARD FOR METRIC PRACTICE'
C (STANDARD E380-79).
DATA PH0,FTT,FVV,PHC,THC/1.196D0,0.9044D0,1.078D0,-.66D0,.08D0/
DATA PHD,PHT,THD,THT/-0.22D0,-0.15D0,-.01D0,-.048D0/
DATA FFP/1.D0,.1D0,.101325D0,.006894757D0,2*1.D0/
DATA FFD/1.D0,1.D3,1.D0,16.01846D0,2*1.D0/
DATA FFH/2*1.D0,4.1868D0,2.326D0,2*1.D0/
C THE ABOVE CONVERSION FACTORS FOR THE CAL AND BTU ARE THE
C 'INTERNATIONAL' CAL AND BTU.
DATA TI0,PI0,DI0/647.27D0,22.115D0,317.763D0/
DATA TI1,PI1,DI1/304.04D0,7.38D0,460.D0/
*, WM0,WM1,R/18.0152D0,44
C THE VALUES USED FOR WM0, WM1 AND R ARE THOSE RECOMMENDED BY COHEN AND
C TAYLOR IN 'THE 1973 LEAST-SQUARES ADJUSTMENT OF THE FUNDAMENTAL
C CONSTANTS', JPCRD VOL 2 P 663 (1973).
C THE A0 THROUGH A4 ARE THE PARAMETERS FOR THE IAPS-84 FORMULATION FOR H2O
DATA A3/-7.6221190138079D0, 32.661493707555D0, 11.305763156821D0,
*-1.0015404767712D0, .12830064355028D3, -.28371416789846D3,
*.24256279839182D3, -.99357645626725D2, -.12275453013171D4,

```

```

* .23077622506234D4, -.16352219929859D4, .58436648297764D3,
* .42365441415641D4, -.78027526961828D4, .38855645739589D4,
*-.91225112529381D3, -.90143895703666D4, .15196214817734D5,
*-.39616651358508D4, -.72027511617558D3, .11147126705990D5,
*-.17412065252210D5, .99918281207782D3, .33504807153854D4,
*-.64752644922631D4, .98323730907847D4, .83877854108422D3,
*-.27919349903103D4, .11112410081192D4, -.17287587261807D4,
*-.36233262795423D3, .61139429010144D3, .32968064728562D2,
* .10411239605066D3, -.38225874712590D2, -.20307478607599D3/
DATA K/4*1,4*2,4*3,4*4,4*5,4*6,4*7,4*9,3,3,1,5/
DATA L/ 1, 2, 4, 6, 1, 2, 4, 6, 1, 2, 4, 6, 1, 2, 4, 6, 1, 2,
* 4, 6, 1, 2, 4, 6, 1, 2, 4, 6, 1, 2, 4, 6, 0, 3, 3, 3/
DATA A0/- .130840393653E2,-.857020420940E2, .765192919131D-2,
1-.620600116069D0,-.106924329402D2,-2.80671377296D0,
2 .119843634845D3,-.823907389256D2, .555864146443D2,
3-31.0698122980D0, 13.6200239305D0,-4.57116129409D0,
4 1.15382128188D0,-.214242224683D0, .0282800597384D0,
5-.250384152737D-2, .132952679669D-3, -.319277411208D-5/
DATA A1/ 1.53830530000D0, -.810483670000D0, -6.83057480000D0,
1 0., .86756271D0/, A20/ 4.2923415D0/,Z0/0.317763D0/
DATA Y/ .59402227D-1, -.28128238E-1, .56826674E-3,-.27987451E-3/
DATA RR/ 3*1.0038928D0,4.8778492/
DATA TEE/ 2*.98876821D0,.99124013D0,.41713659D0/
DATA A4/- .32329494D-2,-.024139355D0,.79027651D-3,-1.3362857D0/
DATA M,N/2,2,2,4,0,2,0,0/
DATA ALPHA/34.D0,40.D0,30.D0,1050.D0/,BETA/2*2.D4,4.D4,25.D0/
END

```

C

## SUBROUTINE UNIT

C THIS SUBROUTINE ALLOWS THE USER TO CHOOSE THE SYSTEM OF UNITS TO BE  
C USED AND ESTABLISHES THE PROPER CONVERSION FACTORS.

```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH,/UNITC/NT,ND,NP,NH,IFL
COMMON /CRITC / PC0,PC1,DC0,DC1,TC0,TC1,PI0,PI1,DI0,DI1,TI0,TI1
COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK
COMMON /CONVRT/ FFP(6),FFD(6),FFT(6),FFH(6)
CHARACTER*8 NNT(4),NNP(4),NND(4),NNH(4),NNHM(4),NT,ND,NP,NH
CHARACTER*1 IFL
DATA NNT/'K','C','R','F'/
DATA NND/'m3/kg ','cm3/g ','dm3/mol','ft3/lb'/
DATA NNP/'MPa','bar','atm','psia'/
DATA NNH/'kJ/kg',' J/g ','cal/g','BTU/lb'/
DATA NNHM/'kJ/kmol','J/mol','cal/mol',' '/
WRITE(*,12)
READ *,IT
IF(IT-3) 102,105,105
102 PRINT 13
READ *,ID
PRINT 14
READ *,IP
IF(ID.EQ.3) THEN
PRINT 151
ELSE
PRINT 15
ENDIF
READ *,IH
GO TO 109
105 ID=4
IP=4

```

```

      IH = 4
109 NP = NNP(IP)
      FP = FFP(IP)
      NT = NNT(IT)
      ND = NND(ID)
      NH = NNH(IH)
      IF(ID.EQ.3) NH = NNHM(IH)
      FD = FFD(ID)
      FH = FFH(IH)
140 DRK = DIO
      PR = PIO
      TR = TIO
      DR = DRK/WMO
      AR = 1000.*PR/DR
      SR = AR/TR
      WR = (AR)**(.5)
      RSS = R/SR
      PC0 = PIO/PR
      DC0 = DIO/WMO /DR
      TC0 = TIO/TR
      PC1 = PI1/PR
      DC1 = DC0 * TIO/TI1 * PI1/PIO
      TC1 = TI1/TR
      RETURN
12  FORMAT(' CHOOSE FROM 1 = K, 2 = Deg C, 3 = Deg R, 4 = Deg F')
13  FORMAT(' CHOOSE FROM 1 = m3/kg, 2 = cm3/g, 3 = dm3/mol, 4 = ft3/lb')
14  FORMAT(' CHOOSE FROM 1 = MPa, 2 = bar, 3 = atm, 4 = psia')
15  FORMAT(' CHOOSE FROM 1 = kJ/kg, 2 = J/g, 3 = cal/g, 4 = BTU/lb')
151 FORMAT(' CHOOSE FROM 1 = kJ/mol, 2 = J/mol, 3 = cal/mol')
      END

```

C

```

      FUNCTION TTT(T)
C THIS FUNCTION CONVERTS THE EXTERNAL T TO THE INTERNAL REDUCED TTT
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WMO,WM1,WMX,DRK
      CHARACTER*8 NT,ND,NP,NH
      COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH
      GO TO (1,2,3,4),IT
1  TTT = T/TR
      FT = 1.
      RETURN
2  TTT = T + 273.15
      FT = 1.
      TTT = TTT/TR
      RETURN
3  TTT = T/1.8
      FT = 5./9.
      TTT = TTT/TR
4  TTT = (T + 459.67)/1.8
      FT = 5./9.
      TTT = TTT/TR
      RETURN
      END

```

C

```

      FUNCTION TTI(T)
C THIS FUNCTION CONVERTS THE INTERNAL REDUCED T TO THE EXTERNAL TTI
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WMO,WM1,WMX,DRK
      COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH

```

```

GO TO (5,6,7,8),IT
5 TTI = T*TR
RETURN
6 TTI = T*TR-273.15
RETURN
7 TTI = T*TR*1.8
RETURN
8 TTI = T*TR*1.8 - 459.67
RETURN
END

```

CC

SUBROUTINE IDEALF(TT,X)

```

C IDEALF CALCULATES THE IDEAL GAS PROPERTIES OF THE MIXTURE OF
C COMPOSITION X, STORING THE RESULTS IN COMMON /IDEAL/
  IMPLICIT DOUBLE PRECISION(A-H,O-Z)
  COMMON /IDEAL/ AZ,SZ,CVZ
  COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK
  COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VCX,TCX
  T = TT*FX
  CALL FZ0(T,AZ0,SZ0,CVZ0)
  CALL FZ1(T,AZ1,SZ1,CVZ1)
  TERM = 0.
  IF(X.GT.0.D0 .AND. X.LT.1.D0) TERM = X*DLOG(X) + (1.-X)*DLOG(1.-X)
  AZ = (X*AZ1 + (1.-X)*AZ0) + RSS*T*TERM
  SZ = (X*SZ1 + (1.-X)*SZ0) - RSS*TERM
  CVZ = (X*CVZ1 + (1.-X)*CVZ0)
  RETURN
END

```

C

SUBROUTINE FZ0(T,F0,S0,C0)

IMPLICIT DOUBLE PRECISION(A-H,O-Z)

```

C FZ0 CALCULATES THE IDEAL GAS PROPERTIES OF H2O
COMMON/COEFS/A0(18),A1(5),A20,Y(4),A3(36),RHO(4),TEE(4),A4(4)
1,K(36),L(36),M(4),N(4),ALPHA(4),BETA(4),Z0
TI=1./T
TLN=DLOG(T)
F0=(A0(1)+A0(2)*T)*TLN
S0=-A0(1)*TI-A0(2)*TLN-A0(2)
C0=-A0(2)+A0(1)*TI
DO 10 I=3,18
TERM=A0(I)*T**(I-6)
F0=F0+TERM*T
S0=S0-TERM*(I-5)
10 C0=C0-TERM*(I-5)*(I-6)
RETURN
END

```

C

SUBROUTINE FZ1(T,AZ,SZ,CVZ)

```

C FZ1 CALCULATES AN APPROXIMATION TO THE IDEAL GAS PROPERTIES
C OF CO2 (ESTIMATED FROM SUPERTRAPP)
  IMPLICIT DOUBLE PRECISION(A-H,O-Z)
  DIMENSION A0(3)
  DATA A0/-1.967246D0,-26.95374D0,-7.657489D0/
  TI=1./T
  TLN=DLOG(T)
  AZ=(A0(1)+A0(2)*T)*TLN + A0(3)*T*T
  SZ=-A0(1)*TI-A0(2)*TLN-A0(2) - 2.*A0(3)*T
  CVZ=-A0(2)+A0(1)*TI - 2.*A0(3)*T

```

```

RETURN
END
C
SUBROUTINE FACTOR(X,D,T)
C THE MIXING RULES AND SHAPE FACTOR ARE APPLIED, PRODUCING FX, HX AND QX
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
CALL MIXRUL(X)
CALL SHAPE(X,D,T)
RETURN
END
C
SUBROUTINE SHAPE(X,D,T)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VCX,TCX
COMMON /CRITC / PC0,PC1,DC0,DC1,TC0,TC1,PI0,PI1,DI0,DI1,TI0,TI1
COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK
COMMON /THPH/ PH0,PHT,PHD,THT,THD,PHC,THC
WMX = (1.-X)*WM0 + X*WM1
TT=T-1.
DD=D-1.
TH = 1. + THD*DD + THT*TT + THC*TT*DD
PH = PH0 + PHD*DD + PHT*TT + PHC*DD*TT
IF(X.LT.1.E-5) THEN
FX=1.
HX=1.
GO TO 6
ENDIF
IF(X.GT..99999) THEN
FX=TH*TC1/TC0
HX=PH*DC0/DC1
GO TO 6
ENDIF
FX = TCX/TC0 *((1.-X)**2 + 2.*X*(1.-X)*(TH)**(.5) + X*X*TH)
HX = VCX*DC0 *((1.-X) + X*PH)
6 QX = FX/HX
RETURN
END
C
SUBROUTINE MIXRUL(X)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VCX,TCX
COMMON /CRITC / PC0,PC1,DC0,DC1,TC0,TC1,PI0,PI1,DI0,DI1,TI0,TI1
T45 = FFT*(TC0*TC1)**(.5)
V45 = FFV*(.5*DC0**(-.3333) + .5*DC1**(-.3333))**3
VCX = (1.-X)**2/DC0 + 2.*X*(1.-X)*V45 + X*X/DC1
TCX = (1.-X)**2*TC0 + 2.*X*(1.-X)*T45 + X*X*TC1
RETURN
END
C
SUBROUTINE THERM(D,T,X)
C THIS SUBROUTINE CALLS THE IDEAL GAS FUNCTION, THE HELMHOLTZ ENERGY
C FUNCTION AND ALL THE NECESSARY DERIVATIVES OF THE HELMHOLTZ
C ENERGY AND FROM THESE ASSEMBLES THE LIST OF THERMODYNAMIC FCTS.
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VX,TX
COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH,/UNITC/NT,ND,NP,NH,IFL
COMMON /IDEAL / AZ,SZ,CVZ
COMMON/COEFS/A0(18),A1(5),A20,Y(4),A3(36),RHO(4),TEE(4),A4(4)

```

```

1,K(36),L(36),M(4),N(4),ALPHA(4),BETA(4),Z0
COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK
COMMON /PROPS/ P,A,G,H,U,S,CV,CP,DPDD,DPDT,W
COMMON /FUGETC/ TT,PIN,FUG1,FUG2,PHI1,PHI2
COMMON /RESPROP/ ARES,PRES,GRES
CHARACTER*1 IFL
CHARACTER*8 NT,ND,NP,NH
CALL IDEALF(T,X)
CALL HELM(D,T,X,ACF)
CALL PDP(D,T,X,PCF,DPDDCF)
GRES = ARES + (PRES*FX)/D
CALL DADTF(D,T,X,DADT,D2ADT2)
CALL DPDTF(D,T,X,DPT)
P = PCF * QX
DPDD = DPDDCF * QX
A=AZ+ACF
S = SZ - DADT
CV = CVZ - T*FX*D2ADT2
DPDT = DPT*QX
DVDT = DPDT/DPDD/D/D/DR/DR
G = A + PCF/D *FX
U = A + T*S*FX
H = G + T*S*FX
CP = CV + FX*HX*HX*T*DPDT**2/DPDD/D/D
W = SQRT(DABS(1.E6*CP*DPDD/CV))
RETURN
END

```

C

SUBROUTINE HELM(D,T,X,ACF)

C THIS SUBROUTINE CALCULATES THE HELMHOLTZ FUNCTION FROM D, T AND X  
C FROM THE PARAMETERS FOUND IN THE BLOCK DATA ROUTINE

```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VX,TX
COMMON/COEFS/A0(18),A1(5),A20,Y(4),A3(36),RHO(4),TEE(4),A4(4)
1,K(36),L(36),M(4),N(4),ALPHA(4),BETA(4),Z0
COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK
COMMON /RESPROP/ ARES,PRES,GRES
TI = 1./T
TLN = DLOG(T)
F1 = 0.
DO 11 I = 1,5
TERM = D*A1(I)*TI**(I-2)
11 F1 = F1 + TERM
YY = D*(Y(1) + Y(2)*TLN + Y(3)*TI**3 + Y(4)*TI**5)
Y1 = 1.-YY
Y2 = 130./(3.*Y1)
Y3 = 169./(6.*Y1*Y1)
F2 = A20*T*(DLOG(D/Y1)-Y2 + Y3-14.*YY)
Z = 1.-DEXP(-Z0*D)
F3 = 0.
DO 13 I = 1,36
TERM = A3(I)*TI**L(I)*Z**(K(I)-1)
13 F3 = F3 + TERM*Z
F4 = 0.
DO 14 I = 1,4
DEL = (D-RHO(I))/RHO(I)
TAU = (T-TEE(I))/TEE(I)
DELN = DEL**N(I)

```

```

TERM=A4(I)*DEXP(-ALPHA(I)*DEL**M(I)-BETA(I)*TAU**2)
14 F4=F4+TERM*DELN
RLH=-RSS*DLOG(HX)
ACF=(F1+F2+F3+F4)*FX+RLH*T*FX
ARES=(F1+F2+F3+F4+RSS*T*(91./6.-DLOG(D)))*FX
RETURN
END

```

C

```

SUBROUTINE PDP(D,T,X,P,DPD)
C THE PRESSURE AND ITS DERIV W.R.T. D ARE CALCULATED BY NUMERICAL
C DIFFERENTIATION OF THE HELMHOLTZ FUNCTION.

```

```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VX,TX
COMMON /RESPROP/ ARES,PRES,GRES
D0=D
V0=1./D
DV=.0005*D0
D1=D0-DV
D2=D0+DV
V1=1./D1
V2=1./D2
CALL FACTOR(X,D0,T)
FX0=FX
HX0=HX
QX0=QX
CALL FACTOR(X,D1,T)
T1=T*FX0/FX
CALL FACTOR(X,D1,T1)
HX1=HX
T1=T*FX0/FX
CALL HELM(D1,T1,X,A1)
ARES1=ARES
FX=FX0
HX=HX0
QX=QX0
CALL FACTOR(X,D2,T)
T2=T*FX0/FX
CALL FACTOR(X,D2,T2)
T2=T*FX0/FX
HX2=HX
CALL HELM(D2,T2,X,A2)
ARES2=ARES
FX=FX0
HX=HX0
QX=QX0
CALL HELM(D0,T,X,A0)
P=-(A1-A2)/(V1*HX1-V2*HX2)/QX
PRES=-(ARES1-ARES2)/(V1*HX1-V2*HX2)/QX
P1=-(A1-A0)/(V1*HX1-V0*HX0)/QX
P2=-(A2-A0)/(V2*HX2-V0*HX0)/QX
DPD=2.*(P1-P2)/(D1/HX1-D2/HX2)
RETURN
END

```

C

```

SUBROUTINE DADTF(D,T,X,DADT,D2ADT2)
C IN THIS SUBROUTINE, THE FIRST AND SECOND DERIVATIVES OF THE
C HELMHOLTZ FCT W.R.T. TEMPERATURE ARE CALCULATED BY NUMERICAL
C DIFFERENTIATION

```



```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VX,TX
D0=D
T0=T
DT=.0002
T1=T0-DT
T2=T0+DT
CALL FACTOR(X,D0,T0)
CALL HELM(D0,T0,X,A0)
FX0=FX
HX0=HX
QX0=QX
CALL SHAXIT(X,D0,T1,D1,T1)
FX1=FX
CALL HELM(D1,T1,X,A1)
FX=FX0
HX=HX0
QX=QX0
CALL SHAXIT(X,D0,T2,D2,T2)
FX2=FX
CALL HELM(D2,T2,X,A2)
FX=FX0
HX=HX0
QX=QX0
DADT=(A1-A2)/(T1*FX1-T2*FX2)
DADT1=(A1-A0)/(T1*FX1-T0*FX0)
DADT2=(A2-A0)/(T2*FX2-T0*FX0)
D2ADT2=2.*(DADT1-DADT2)/(T1*FX1-T2*FX2)
RETURN
END

```

C

```

SUBROUTINE DPDTF(D,T,X,DPT)

```

C HERE THE DERIVATIVE OF THE PRESSURE W.R.T. TEMPERATURE IS CALCULATED

C AGAIN BY NUMERICAL DIFFERENTIATION

```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VX,TX
COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK
D0=D
T0=T
DT=.0002
T1=T0-DT
T2=T0+DT
CALL FACTOR(X,D0,T0)
FX0=FX
HX0=HX
QX0=QX
CALL SHAXIT(X,D0,T1,D1,T1)
FX1=FX
CALL PDP(D1,T1,X,P1,DPD1)
PP1=P1*QX
FX=FX0
HX=HX0
QX=QX0
CALL SHAXIT(X,D0,T2,D2,T2)
FX2=FX
CALL PDP(D2,T2,X,P2,DPD2)
PP2=P2*QX
FX=FX0

```

```

HX = HX0
QX = QX0
DPT = (PP1-PP2)/(T1*FX1-T2*FX2)
RETURN
END

```

C

```

SUBROUTINE SHAPIT(X,TT,PP,T,D,P)

```

C THIS SUBROUTINE ITERATES TO FIND THE SHAPE FACTORS CONSISTANT WITH

C THE EXTERNAL TT AND PP (AND ALSO RETURNS THE REDUCED T, D AND P)

```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)

```

```

COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH

```

```

COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VX,TX

```

```

COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK

```

```

T = 1.

```

```

DD = D

```

```

2 CALL FACTOR(X,D,T)

```

```

T = TTT(TT)/FX

```

```

P = PP*FP/PR/QX

```

```

CALL DFIND(D,X,P,DD,T,DQ)

```

```

IF(DABS(DD/D - 1.).LT.1.E-6) RETURN

```

```

DD = D

```

```

GO TO 2

```

```

END

```

C

```

SUBROUTINE SHAXIT(X,D,T,D1,T1)

```

C THIS IS A RESTRICTED ITERATION FOR THE SHAPE FACTORS USED IN THE

C FUNCTIONS FOR DERIVATIVES W.R.T. T

```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)

```

```

COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VCX,TCX

```

```

DD = D

```

```

D1 = D

```

```

T1 = T

```

```

HX0 = HX

```

```

FX0 = FX

```

```

QX0 = QX

```

```

2 CALL FACTOR(X,D1,T1)

```

```

D1 = D*HX/HX0

```

```

IF(DABS(D1/DD-1.).LT.1.E-10) RETURN

```

```

DD = D1

```

```

GO TO 2

```

```

END

```

C

```

SUBROUTINE SHAPDT(X,DIN,TT,D,T)

```

C ANOTHER SHAPE FACTOR ITERATION ROUTINE WHICH FINDS THE SHAPE FACTORS

C AND REDUCED DENSITY AND TEMPERATURE CORRESPONDING TO THE EXTERNAL

C DENSITY AND TEMPERATURE 'DIN' AND 'TT'.

```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)

```

```

COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VX,TX

```

```

COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK

```

```

D = DIN*HX/DR

```

```

T = TTT(TT)/FX

```

```

1 CALL FACTOR(X,D,T)

```

```

D1 = DIN*HX/DR

```

```

T1 = TTT(TT)/FX

```

```

IF(DABS(D1/D-1.).LT.1.E-8) RETURN

```

```

D = D1

```

```

T = T1

```

```

GO TO 1

```

END

C

SUBROUTINE MU(XMU1,XMU2,D2ADX2,D,T,X)

C IN THIS SUBROUTINE, THE RELATED QUANTITIES OF THE CHAMICAL POTENTIAL

C FUGACITIES, AND FUGACITY COEFFICIENTS ARE CALCULATED FOR EACH

C COMPONENT. THE CHEMICAL POTENTIALS ARE RETURNED IN THE CALLING

C LIST AND THE OTHER PREOPERTIES IN THE COMMON BLOCK /FUGETC/

IMPLICIT DOUBLE PRECISION(A-H,O-Z)

COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VCX,TCX

COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH

COMMON /IDEAL / AZ,SZ,CVZ

COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM0,WM1,WMX,DRK

COMMON /PROPS / P,A,G,H,U,S,CV,CP,DPDD,DPDT,W

COMMON /FUGETC/ TT,PIN,FUG1,FUG2,PHI1,PHI2

COMMON /RESPROP/ ARES,PRES,GRES

D0 = D

FDD = FD

IF(ID.NE.3) FDD = FD/WMX

T0 = T

HX0 = HX

FX0 = FX

QX0 = QX

CALL THERM(D,T,X)

A0 = A

ARES0 = ARES

G0 = (A + P/D \*HX)\*AR

GRES0 = GRES

776 FORMAT(2F10.3,F10.5,2F15.9)

P0 = P

Z0 = P/D/T/RSS

DOUT = D\*DR/HX

TOUT = TT1(T\*fx)

DELX = 2.E-5

IF(X.GT..99998) DELX = 1.-X

IF(X.LT.2.E-5) DELX = X

X2 = X-DELX

IF(X.EQ.1.) X2 = .999999

CALL SHAPDT(X2,DOUT,TOUT,D2,T2)

CALL THERM(D2,T2,X2)

P2 = P

A2 = A

ARES2 = ARES

FX = FX0

HX = HX0

QX = QX0

X1 = X + DELX

IF(X.EQ.0.) X1 = 1.E-6

CALL SHAPDT(X1,DOUT,TOUT,D1,T1)

CALL THERM(D1,T1,X1)

P1 = P

A1 = A

ARES1 = ARES

IF(DELX.EQ.0.) DELX = 5.E-7

DADX = (A1-A2)/(X1-X2) \*AR

DARESDX = (ARES1-ARES2)/(X1-X2)

D2ADX2 = (A1 + A2 - 2.\*A0)/DELX/DELX

DPDX = (P1-P2)/(X1-X2)

XMU1 = G0 - X\*DADX

```

XMU2 = G0 + (1.-X)*DADX
RESMU1 = (GRES0 - X*DARESDX)/RSS/T /FX
RESMU2 = (GRES0 + (1.-X)*DARESDX)/RSS/T /FX
PHI1 = DEXP(RESMU1) *D*RSS*T/P *FX/HX
PHI2 = DEXP(RESMU2) *D*RSS*T/P *FX/HX
FUG1 = PHI1*PIN*(1.-X)
FUG2 = PHI2*PIN*X
FX = FX0
HX = HX0
QX = QX0
RETURN
END

```

C

```

SUBROUTINE DFIND(DOUT,X,P,D,T,DPD)
C THIS IS THE SUBROUTINE WHICH ITERATES TO FIND THE DENSITY AS A
C FUNCTION OF TEMPERATURE AND PRESSURE. THE 'D' INPUT IN THE CALLING
C LIST IS AN INITIAL GUESS FOR THE DENSITY, AND DOUT (AND ALSO
C DPD=DP/DD) ARE OUTPUT. ALL QUANTITIES ARE IN REDUCED FORM.
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
TOL = 1.0E-8
IF(T.LT..7) TOL = 1.0E-7
IF(T.LT..6) TOL = 1.0E-6
DD = D
L = 0
9 L = L + 1
IF(DD.LE.1.E-8) DD = 1.E-8
IF(DD.GT.5.5) DD = 5.5
CALL PDP(DD,T,X,PP,DPD)
IF(DPD.GT.0.) GOTO 13
IF(D.GE..9337) DD = DD*1.02
IF(D.LT..9337) DD = DD*.98
IF(L.LE.10) GOTO 9
13 DPDX = DPD*1.1
IF(DPDX.LT..0005) DPDX = .0005
IF(DABS(1.-PP/P).LT.TOL) GO TO 20
DX = (P-PP)/DPDX
IF(DABS(DX).GT..3) DX = DX*.3/DABS(DX)
15 DD = DD + DX
IF(DD.LE.1.E-8) DD = 1.E-8
IF(L.LE.30) GO TO 9
DD = DD - DX
IF(DABS(1.-PP/P).GT.1.E-3) PRINT 1000,P,PP,D,DD,DPD
20 CONTINUE
DOUT = DD
1000 FORMAT(' 30 ITER IN DFIND: PIN PCALC DIN DCALC DPD'
1/10X,5E12.5)
RETURN
END

```

C

```

SUBROUTINE GUESS(T,P,X,Y)
C THIS SUBROUTINE PROVIDES AN INITIAL GUESS FOR THE LIQUID AND VAPOR
C COMPOSITIONS (X,Y) AT T AND P, AND MAY BE USED AS A STARTING POINT
C FOR ITERATIONS WHICH NEED A GUESS. IT USES PV WHICH FOLLOWS.
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /CRITC / PC0,PC1,DC0,DC1,TC0,TC1,PI0,PI1,DI0,DI1,TI0,TI1
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VCX,TCX
P4S = PV(T)
TX = T*TI0/TI1

```

```

P5S = PV(TX)*PI1/PI0
IF(P4S.EQ.0.) GO TO 10
X = (P-P4S)/(P5S-P4S)
Y = 1.-(1.-X)*P4S/P
RETURN

```

```

10 IF(P5S.EQ.0.) GO TO 20
XS = (T-TC0)/(TC1-TC0)
CALL FACTOR(XS,1.,1.)
PXS = QX
X = XS + (1.-XS)*(P-PXS)/(P5S-PXS)
Y = 1.-(1.-X)*(1.-XS)*PXS/P
IF(X.LT..001) X = .001
IF(X.GT..999) X = .999
IF(Y.GT.X) Y = .9*X
IF (Y.LT..001) Y = .001
RETURN
20 X = -1.
Y = -1.
RETURN
END

```

C

FUNCTION PV(T)

```

C THIS FUNCTION CALCULATES AN APPROXIMATE VAPOR PRESSURE, PV, FOR PURE
C H2O AS A FUNCTION OF THE INPUT TEMPERATURE. THE VAPOR PRESSURE
C CALCULATED AGREES WITH THE VAPOR PRESSURE PREDICTED BY THE SURFACE
C TO WITHIN .02% TO WITHIN A DEGREE OR SO OF THE CRITICAL TEMPERATURE,
C AND CAN SERVE AS AN INITIAL GUESS FOR FURTHER REFINEMENT BY
C IMPOSING THE CONDITION THAT GL = GV.

```

```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
DIMENSION A(8)
DATA A/-7.8889166D0,2.5514255D0,-6.716169D0,33.239495D0,
1-105.38479D0,174.35319D0,-148.39348D0,48.631602D0/
PV = 0.
IF(T.GT..9997775D0) RETURN
W = DABS(1.-T*.9997)
B = 0.
DO 4 I = 1,8
Z = I
4 B = B + A(I)*W**((Z + 1.)/2.)
Q = B/T
PV = 1.001*DEXP(Q)
RETURN
END

```

C

FUNCTION TSAT(P)

```

C THIS FUNCTION CALCULATES THE SATURATION TEMPERATURE FOR A GIVEN
C PRESSURE. BY AN ITERATIVE PROCESS USING PSAT AND TDPSDT.

```

```

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
TSAT = 0.
IF(P.GT.1.) RETURN
K = 0
PL = 7.1226152D0 + 2.302585D0*DLOG(P)
TG = .57602D0 + PL*(.042887D0 + PL*(.00368D0 + PL*(3.837D-4 + PL*3.D-5)))
1 IF(TG.LT..422D0) TG = .422D0
IF(TG.GT..9996D0) TG = .9996D0
IF(K.LT.8) GO TO 2
GO TO 8
2 K = K + 1

```

```

PP = PV(TG)
DP = TDPSDT(TG)
IF(DABS(1.-PP/P).LT.1.D-5) GO TO 8
TG = TG*(1. + (P-PP)/DP)
GO TO 1
8 TSAT = TG
RETURN
END

```

C

```

FUNCTION TDPSDT(T)
C THIS FUNCTION CALCULATES T*(DPS/DT), AND IS USED BY THE FUNCTION TSAT.
  IMPLICIT DOUBLE PRECISION(A-H,O-Z)
  DIMENSION A(8)
  DATA A/-7.8889166D0,2.5514255D0,-6.716169D0
  1,33.239495D0,-105.38479D0,174.35319D0,-148.39348D0
  2,48.631602D0/
  IF(T.GE.1.D0) T = .99999D0
  W = 1.-T
  B = 0.
  C = 0.
  DO 4 I = 1,8
  Z = I
  Y = A(I)*W**((Z+1.)/2.)
  C = C + Y/W*(.5-.5*Z-1./T)
4 B = B + Y
  Q = B/T
  TDPSDT = DEXP(Q)*C
RETURN
END

```

C

```

C *****
C *****

```

C

## PROGRAM COEX

```

C THIS PROGRAM CALCULATES THE PREDICTED COMPOSITIONS AND DENSITIES OF
C COEXISTING PHASES OF H2O-CO2 MIXTURES AT A SPECIFIED TEMPERATURE
C AND PRESSURE. THE FUGACITIES OF EACH COMPONENT ARE CALCULATED IN
C THE SUBROUTINE FCN, AND THE NON-LINEAR EQUATION SOLVER ADJUSTS THE
C COMPOSITIONS SUCH AS TO REDUCE THE DIFFERENCE IN THE FUGACITIES
C FOR EACH COMPONENT ACROSS THE PHASE BOUNDARY TO ZERO. THIS USES
C A WIDELY AVAILABLE ROUTINE SNSQ FOR THE SOLUTION.
C IN THIS VERSION, AN INITIAL GUESS FOR THE COMPOSITIONS IS SUPPLIED
C BY THE USER.
C THIS PROGRAM USES THE BLOCKDATA ROUTINE AND SUBROUTINES FROM THE
C FIRST PROGRAM (MIXPROP)
  IMPLICIT DOUBLE PRECISION(A-H,O-Z)
  CHARACTER*8 NT,ND,NP,NH
  DIMENSION X(2),FVEC(2),DIAG(2),FJAC(2,2),R(3),QTF(2),WA1(2),WA2(2)
  COMMON /FUGETC/ TIN,PIN,FUG1,FUG2,PHI1,PHI2
  COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH,/UNITC/NT,ND,NP,NH,IFLAG
  COMMON /RCONST/ TR,PR,DR,AR,SR,WR,RR,RSS,WM4,WM5,WMX
  COMMON /THPH/ PH0,PHT,PHD,THT,THD,PHC,THC
  COMMON /CRITC / PC4,PC5,DC4,DC5,TC4,TC5,PI4,PI5,DI4,DI5,TI4,TI5
  COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VCX,TCX
1, WA3(2),WA4(2)
  COMMON /DPARMS/ TT,PP,DGL,DGV,DLL,DVW,Q,XIN
  COMMON /PROPS / P,A,G,H,U,S,CV,CP,DPDD,DPDT,W
  COMMON /START/ XSTART.YSTART

```

```

CHARACTER*1 IFLAG
EXTERNAL FCN
OPEN(5,FILE = 'INPUT')
OPEN(6,FILE = 'OUTPUT')
IOPT = 2
N = 2
XTOL = 2.E-5
LDFJAC = 2
LR = 3
MAXFEV = 300
ML = 1
MU = 1
EPSFCN = 2.E-6
MODE = 1
FACT = 10.
NPRINT = 1
CALL FACTOR(0.D0,1.D0,1.D0)
CALL UNIT
WRITE(*,71) PH0,FFT,FFV,PHD,PHT,THD,THT,PHC,THC
71 FORMAT('1PH = ',F6.3,' FFT = ',F6.3,' FFV = ',F6.3,6F7.3/)
1 READ(*,*,END = 99) TT,PP,XIN,YIN
C TT, PP ARE THE TEMPERATURE AND PRESSURE, AND XIN, YIN THE INTIAL
C GUESSES FOR THE LIQ AND VAP COMPOSITIONS.
CALL INIT(XIN,YIN)
WRITE(*,*) XIN,YIN,DGL,DGV
XV = YIN
XL = XIN
X(1) = XL
X(2) = XV
TIN = TT
PIN = PP
C CALL SNSQ(FCN,JAC,IOPT,N,X,FVEC,FJAC,LDFJAC,XTOL,MAXFEV,ML,MU,
C * EPSFCN,DIAG,MODE,FACT,NPRINT,INFO,NFEV,NJEV,
C * R,LR,QTF,WA1,WA2,WA3,WA4)
FNORM = ENORM(N,FVEC)
WRITE (6,1000) FNORM,(X(J),J = 1,N)
WRITE(6,1001) TT,PP,X(1),X(2),DLL,DVV
1001 FORMAT(1X,F8.3,F10.6,F9.6,F8.5,2F10.5,F10.5,F10.5)
1011 FORMAT(F9.3,F9.4,2F9.6,2F9.4,F9.4,F8.4)
GO TO 1
1000 FORMAT (5X,31H FINAL L2 NORM OF THE RESIDUALS,E15.7 //
* 5X,27H FINAL APPROXIMATE SOLUTION // (5X,3E15.7))
99 STOP
END
C
SUBROUTINE INIT(XL,XV)
C THIS ROUTINE GENERATES INITIAL GUESSES FOR THE LIQUID AND VAPOR
C DENSITIES FROM THE DENSITIES OF PURE H2O AT T.
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
COMMON /DPARMS/ TT,PP,DGL,DGV,DLL,DVV,Q,XIN
COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH
COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM4,WM5,WMX
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VCX,TCX
T = TTT(TT)
CALL DLEQ(T,DL)
CALL DVEQ(T,DV)
DGL = DL*1.04
DGV = DV*.9

```

RETURN  
END

```
C*****
SUBROUTINE DLEQ(T,DL)
DOUBLE PRECISION T,DL
DIMENSION G(6),TPOT(6)
DATA N/6,TPOT/.33333333,.66666667,1.6666667,5.3333333,14.333333,
*36.666667/, G/1.99206,1.10123,-.512506,-1.75263,-45.4485,-675615./
TAU = 1.-T
DL = 1.
DO 10 I = 1,N
10 DL = DL + G(I)*TAU**TPOT(I)
RETURN
END
```

```
C*****
SUBROUTINE DVEQ(T,DV)
DOUBLE PRECISION T,DV
DIMENSION G(6),TPOT(6)
DATA N/6, TPOT/.3333333333,.6666666667,1.33333333,3.,
*.616666666666667E1, .118333333333333E2/,
* G / - 2.02957,-2.68781,-5.38107,-17.3151,-44.6384,-64.3486/
TAU = 1.-T
DV = 0.
DO 10 I = 1,N
10 DV = DV + G(I)*TAU**TPOT(I)
DV = EXP(DV)
RETURN
END
```

```
C
SUBROUTINE FCN(N,XX,FVEC,JFLAG)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
DIMENSION XX(2),FVEC(2)
COMMON /DPARMS/ TT,PP,DGL,DGV,DDL,DDV,Q,XIN
COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM4,WM5,WMX
COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VCX,TCX
COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH,/UNITC/NT,ND,NP,NH,IFLAG
COMMON /FUGETC/ TIN,PIN,FUG1,FUG2,PHI1,PHI2
CHARACTER*8 NT,ND,NP,NH
CHARACTER*1 IFLAG
IF(XX(1).GT.1.D0) XX(1) = .999995D0
IF(XX(1).LT.0.D0) XX(1) = .000005D0
IF(XX(2).GT.1.D0) XX(2) = .999995D0
IF(XX(2).LT.0.D0) XX(2) = .000005D0
TIN = TT
FDD = FD
X = XX(1)
Y = XX(2)
YP1 = XIN/(WM5*XIN + WM4*(1.D0-XIN))
3 CALL FACTOR(X,1.D0,1.D0)
T = TTT(TT)/FX
CALL FACTOR(X,DGL,T)
DL = DGL
CALL SHAPIT(X,TT,PP,T,DL,P)
FDD = FD
IF(ID.NE.3) FDD = FD/WMX
YY = XIN
IF(ID.NE.3) YY = YP1
YL = X
```



```

IF(ID.NE.3) YL=X/WMX
CALL MU(XMU1,XMU2,D2ADX2,DL,T,X)
FUGX1=FUG1
FUGX2=FUG2
DDL=DL*DR/HX/FDD
CALL FACTOR(Y,DGV,1.D0)
T=TTT(TT)/FX
CALL FACTOR(Y,DGV,T)
T=TTT(TT)/FX
DV=DGV
CALL SHAPIT(Y,TT,PP,T,DV,P)
YV=Y
DGV=DV
Q=(YL-YV)/(YL-YV)
CALL MU(YMU1,YMU2,D2ADX2,DV,T,Y)
FUGY1=FUG1
FUGY2=FUG2
DDV=DV*DR/HX/FDD
FVEC(1)=(FUGY1-FUGX1)/FUGY1
FVEC(2)=(FUGY2-FUGX2)/FUGY2
IF(JFLAG.EQ.0) WRITE(6,6) X,Y,Q,DDL,DDV,FVEC
6 FORMAT(1X,3F7.4,2F10.5,2F8.3)
RETURN
END

```

```

C
C *****
C *****
C

```

## PROGRAM APPMOLP

```

C PROGRAM FOR CALCULATING APPARENT MOLAR V AND CP (ALSO V2, CP2)
C THIS PROGRAM ALSO USED THE BLOCKDATA AND SUBROUTINES FROM MIXPROP
  IMPLICIT DOUBLE PRECISION(A-H,O-Z)
  COMMON /PROPS/ P,A,G,H,U,S,CV,CP,DPDD,DPDT,W
  COMMON /CRITC / PC4,PC5,DC4,DC5,TC4,TC5,PI4,PI5,DI4,DI5,TI4,TI5
  COMMON /MIXFAC/ FX,HX,QX,TH,PH,FFT,FFV,V45,T45,VX,TX
  COMMON /DERIVS/ DADT,CVR,DPDTR,D2P
  COMMON /QQQQ/ Q,ARES,QAB,Q10,Q20,Q11,QUB,QSB,CVB,DPDTB,DPDDB
  COMMON /RCONST/ TR,PR,DR,AR,SR,WR,R,RSS,WM4,WM5,WMX,DRK
  COMMON /THPH/ PH0,PHT,PHD,THT,THD,PHC,THC
  CHARACTER*8 ND,NH,NT,NP
  COMMON /UNITS/ IT,ID,IP,IH,FT,FD,FP,FH,/UNITC/NT,ND,NP,NH,IFL
  CHARACTER*1 IFL
71 FORMAT('1PH=',F6.3,' FFT=',F6.3,' FFV=',F6.3,6F6.3/)
  WRITE(7,71) PH0,FFT,FFV,PHD,PHT,THD,THT,PHC,THC
  CALL FACTOR(0.D0,1.D0,1.D0)
  CALL UNIT
  WRITE(*,71) PH0,FFT,FFV,PHD,PHT,THD,THT,PHC,THC
1 WRITE(*,63)
63 FORMAT(' input mole frac, p, t1,t2,delt')
  READ(*,*,END=9) X,PIN,TT1,TT2,TTI
  TT=TT1-TTI
C IF YOU WISH TO INPUT COMPOSITIONS AS MOLALITY (XM), THE FOLLOWING
C LINES MAY BE USED TO CONVERT TO MOLE FRACTIONS
C X = XM*WM4/1000.
C X = X/(1.+X)
IF(X.EQ.0.) GO TO 2
C The following starting point for the density iteration is appropriate
C for higher temperature liquids or supercritical liquid-like states.

```

```

DDD = 2.
C The following two lines indicate a possible way to furnish a vapor-
C like starting density should one be necessary.
C   PSAT = PV(T)
C   IF(DDD.GT.1. .AND. PP.LT.PSAT) DDD = PP/RSS/T
3 TT = TT + TTI
  IF(TT.GT.TT2) GO TO 1
  CALL FACTOR(0.,1.,1.)
  IF(TT.GT.TS) DDD = PIN/R/TT/DR
  T = TTT(TT)
  FDD = FD
  IF(ID.NE.3) FDD = FD/WM4
  FHH = FH
  IF(ID.NE.3) FHH = FH*WM4
  PP = PIN*FP/PR
  CALL DFIND(D,X,PP,DDD,T,DQ)
C PROPERTIES FOR PURE H2O AT T AND P ARE NOW CALCULATED
  CALL THERM(D,T,0.)
  P0 = P*PR/FP
  D0 = D*DR/FDD
  DPDT0 = DPDT*FT/FP *PR/TR
  DPDD0 = DPDD*FDD/FP *PR/DR
  CV0 = CV*FT/FHH *SR
  CP0 = CP*FT/FHH *SR
  S0 = S*FT/FHH *SR
  H0 = H/FHH *AR
  U0 = U/FHH *AR
  A0 = A/FHH *AR
  G0 = G/FHH *AR
C NOW THE PROPERTIES AT COMPOSITION X ARE CALCULATED
  CALL FACTOR(X,D,T)
  FDD = FD
  IF(ID.NE.3) FDD = FD/WMX
  FHH = FH
  IF(ID.NE.3) FHH = FH*WMX
  PP = PIN*FP/PR/QX
  T = TTT(TT)/FX
  CALL DFIND(D,X,PP,DDD,T,DQ)
  DDD = D
  CALL FACTOR(X,D,T)
  T = TTT(TT)/FX
  PP = PIN*FP/PR/QX
  CALL DFIND(D,X,PP,DDD,T,DQ)
  DDD = D
  CALL FACTOR(X,D,T)
  T = TTT(TT)/FX
  PP = PIN*FP/PR/QX
  CALL DFIND(D,X,PP,DDD,T,DQ)
  DDD = D
  FDD = FD
  IF(ID.NE.3) FDD = FD/WMX
  FHH = FH
  IF(ID.NE.3) FHH = FH*WMX
  CALL THERM(D,T,X)
  PPP = P/FP *PR
  DD = D*DR/FDD/HX
  DPDT = DPDT*FT/FP *PR/TR
  DPDD = DPDD*FDD/FP *PR/DR

```

```
CV = CV*FT/FHH *SR
CP01 = CP*FT/FHH *SR
S = S*FT/FHH *SR
H = H/FHH *AR
U = U/FHH *AR
A=A/FHH *AR
G=G/FHH *AR
V=1./DD
V0=1./D0
XX = (1.-X)/X
VA = ( V/X - XX*V0)*1000.
CPA = CP01/X - XX*CP0
VV=1000.*V
X1=X+.00001
CALL FACTOR(X1,D,T)
FDD=FD
IF(ID.NE.3) FDD=FD/WMX
FHH= FH
IF(ID.NE.3) FHH= FH*WMX
PP = PIN*FP/PR/QX
T= TTT(TT)/FX
CALL DFIND(D,X,PP,DDD,T,DQ)
CALL THERM(D,T,X1)
CP1 = CP*FT/FHH *SR
D1 = D*DR/FDD/HX
V1=1./D1
DVDX=(V1-V)*100000.
DCPDX=(CP1-CP01)*100000.
CP2=CP01+(1.-X)*DCPDX
V2=V+(1.-X)*DVDX
V2=V2*1000.
WRITE(*,33) X,TT,PIN,VV,V2,VA,CP2,CPA
33 FORMAT(F9.5,F9.3,F9.3,F9.2,4F10.1)
GO TO 3
9 STOP
END
```