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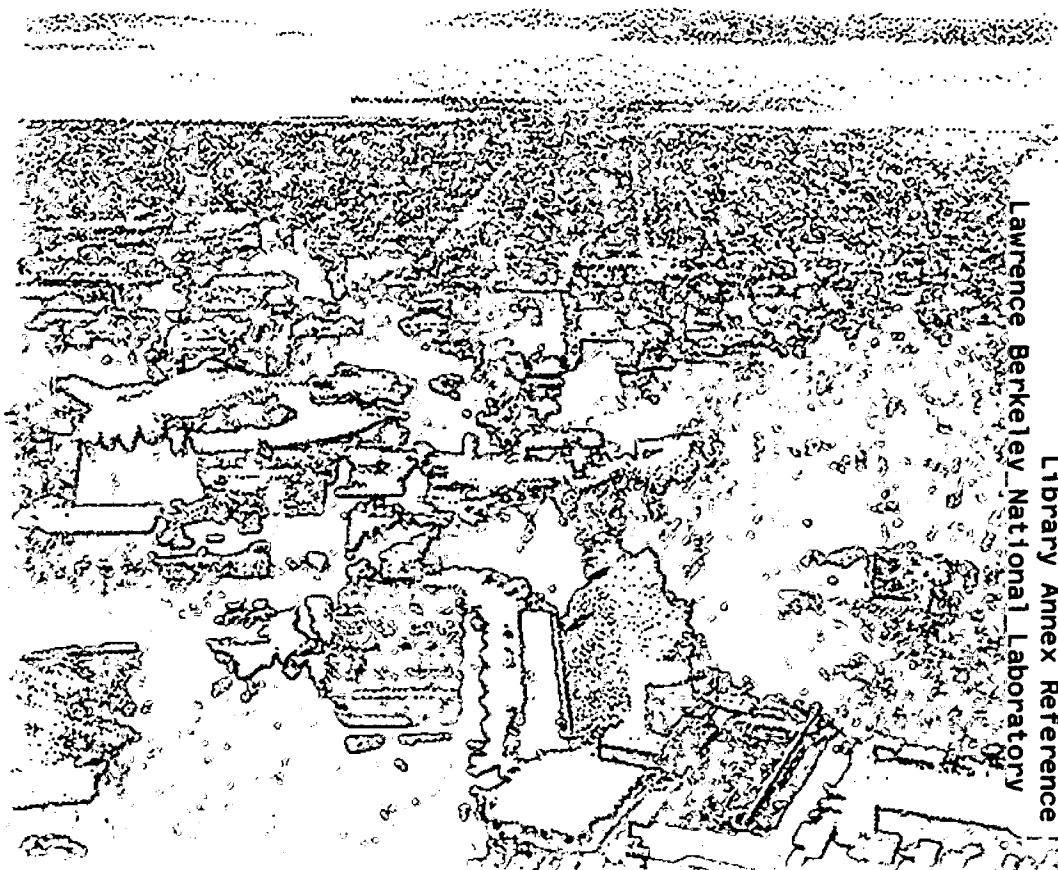
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Julio E. García

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October 2001

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Density of Aqueous Solutions of CO$_2$

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October 2001

Density of Aqueous Solutions of CO_2 *

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October 11, 2001

Abstract

In this report, we present a numerical representation for the partial molar volume of CO_2 in water and the calculation of the corresponding aqueous solution density. The motivation behind this work is related to the importance of having accurate representations for aqueous phase properties in the numerical simulation of carbon dioxide disposal into aquifers as well as in geothermal applications. According to reported experimental data the density of aqueous solutions of CO_2 can be as much as 2-3 % higher than pure water density. This density variation might produce an influence on the groundwater flow regime. For instance, in geologic sequestration of CO_2, convective transport mixing might occur when, several years after injection of carbon dioxide has stopped, the CO_2-rich gas phase is concentrated at the top of the formation, just below an overlaying caprock. In this particular case the heavier CO_2 saturated water will flow downward and will be replaced by water with a lesser CO_2 content.

1 Introduction

Disposal of CO_2 into geological formations requires, among other conditions, the presence of a regional caprock for confinement. In order to avoid two-phase conditions in the injection line, geological disposal of CO_2 would be made at supercritical conditions. Under such conditions, CO_2 is less dense than water and would have a tendency to migrate to the top of the formation (Pruess and García, 2001). After a relatively long time (decades after ending injection) almost all gas would be stored at the top, underlying

the caprock. Because the density of CO_2 saturated water is slightly higher than the density of pure water, density driven flow will occur enhancing the dissolution process by convective mixing. In such flow problems, numerical simulation capabilities that take into account variable density brines are crucial (Oldenburg and Pruess, 1995).

In this report we present a new correlation for the partial molar volume of CO_2 in water and the calculation of the corresponding aqueous solution density. This aqueous phase density correlation is then incorporated into the TOUGH2 Equation-of-State (EOS) module for carbon dioxide ECO2 (under development) (Pruess and García, 2001; Pruess et al., 1999). Currently, the brine density correlation considers only salinity effects with no CO_2 dependency (Battistelli et al., 1997). Figure 1 shows the computed brine density from 10 to 110 °C at various salt mass fractions (XNaCl=0.00, 0.05, 0.10 and 0.25) as implemented inside EWASG. The density increase due to salinity is up to almost 20%.

Experimental data for the system H_2O-CO_2 show that the carbon dioxide content produce an increase in aqueous phase density on the order of 2 to 3 %. Because the salinity effect is considerable higher, the dependency on CO_2 content is often ignored. This assumption is perfectly acceptable in geothermal applications. Nevertheless, as discussed before, it can conceal key processes in fluid flow dynamics of carbon dioxide sequestration.

Based on thermodynamic theory (Söhnel and Novotný, 1985; Anderson and Crerar, 1993), the density of aqueous solutions of CO_2 may be expressed as:

$$\rho_{aq} = \rho_1 + M_2 \cdot c - c \cdot \rho_1 \cdot V_\phi \qquad (1)$$

where V_ϕ is the apparent molar volume of dissolved CO_2; M_2 is the molecular weight of CO_2; ρ_1 is the density of pure water and c is the CO_2 concentration

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*Research Advisors: Dr. Karsten Pruess, Earth Sciences Division, Lawrence Berkeley National Laboratory and Prof. Nicholas Sitar, Department of Civil and Environmental Engineering, University of California at Berkeley
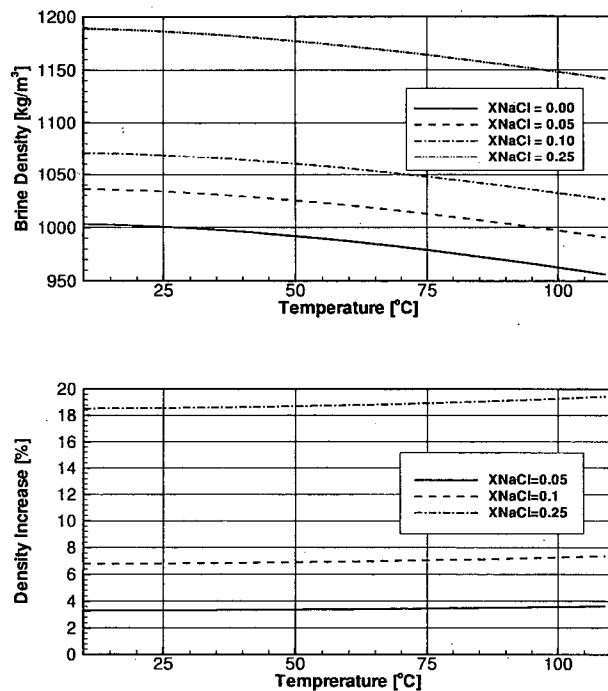
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Figure 1: Computed density and density increase of NaCl solutions for salt mass fraction (XNaCl) from 0 to 0.25 using the EWASG correlation.

expressed by the number of moles of solute in 1 m^3 of solution (for details see Appendix A).

2 Experimental Data and Preliminary Correlations

A large number of data exist on the solubility of CO_2 in water (Scharlin (1996) and Drummond (1981)). In spite of their significance, there is limited experimental data on densities of the aqueous system H_2O-CO_2-NaCl. Usually, there is two sets of data, one for the system H_2O-NaCl and another for the system H_2O-CO_2. Because the effect of salinity on density is considerably higher than the effect of carbon dioxide, the latter is often ignored. The most significant investigations of partial molar volume of CO_2 and density of aqueous solutions of CO_2 along with experimental conditions are listed in Table 1.

The data collected indicate that CO_2 saturated water is heavier than pure water below 300 °C and down to at least 5 °C. Some measurements were done at CO_2 saturation, while others were for very low mole fraction. Apparent molar volumes for data sets re-

Table 1: Experimental data for partial molar volume and density of aqueous solutions for the system CO_2-H_2O.

NP *	T [^oC]	P [MPa]	Reference
24	5-20	6.4-29.5	Teng et al. (1997)
14	25-300	20-35	Hnědkovský et al. (1996)
5	274-297	19.6-29.4	Malinin (1974)
8	25-100	1.96	Ellis and McFadden (1972)
1	5-40	NR **	Parkinson and Nevers (1969)
1	25	NR **	Moore et al. (1982)

* Number of points used in this study
** Not reported

porting only densities and solubilities were calculated using the theory presented in Appendix A.

Experimental results show that the partial molar volume (approximated here as the apparent molar volume) is weakly dependent on CO_2 mole fraction (Parkinson and Nevers, 1969) and, for temperatures below 300°C is independent of pressure (Malinin, 1974). Salinity effects on partial molar volume of CO_2 in water are not considered in this study. There are limited data that consider salinity. Malinin (1974) presented several data points for solutions of 1 M NaCl at high temperatures and pressures. His findings showed that the salinity effects are weak and within experimental uncertainty.

2.1 Previous Work

There are correlations available for the partial molar volume as a function of temperature. Most of these representations consider a polynomial fit as follows:

$$V_\phi = a + bT + cT^2 + dT^3 + eT^4 \qquad (2)$$

Table 2 summarizes the different fits for Equation 2 found in the literature as well as other types of correlations.

2.2 Novel Correlation

The fit to Equation 2 proposed in this study considers 53 data points (See Figure 2). The following equation adequately represents the data with an $R^2 = 0.98$.

$$V_\phi = 37.51 - 9.585 * 10^{-2}T \\ + 8.740 * 10^{-4}T^2 - 5.044 * 10^{-7}T^3 \qquad (3)$$

Equation 3 and 1 were used to compute densities of aqueous solutions of CO_2 at a pressure of 100 bar

Table 2: Correlations used by other authors for partial molar volume of CO_2 in water.

a	b	c	d	e	Reference
37.36	$-7.109*10^{-2}$	$-3.812*10^{-5}$	$+3.296*10^{-6}$	$-3.702*10^{-9}$	Andersen et al. (1992) *
1799.36	-17.8218	0.0659297	$-1.0579*10^{-4}$	$+6.200*10^{-8}$	Enick and Klara (1990) **
35.663	$-5.960*10^{-2}$	$+6.308*10^{-4}$			Jonathan Ennis-King[1] *
37.51	$-9.585*10^{-2}$	$+8.740*10^{-4}$	$-5.044*10^{-7}$		This work *
$V_\phi = e^{154.7881 - \frac{3582.452}{T} - 26.7757773 log(T) + 0.045234908T}$					Iglesias and Moya (1992) ***

* Equation 2 V_ϕ is in $cm^3/mole$ and T is in degrees Celsius
** Equation 2 V_ϕ is in $cm^3/mole$ and T is in degrees Kelvin
*** V_ϕ is in $cm^3/mole$ and T is in degrees Kelvin
[1] Personal Communication
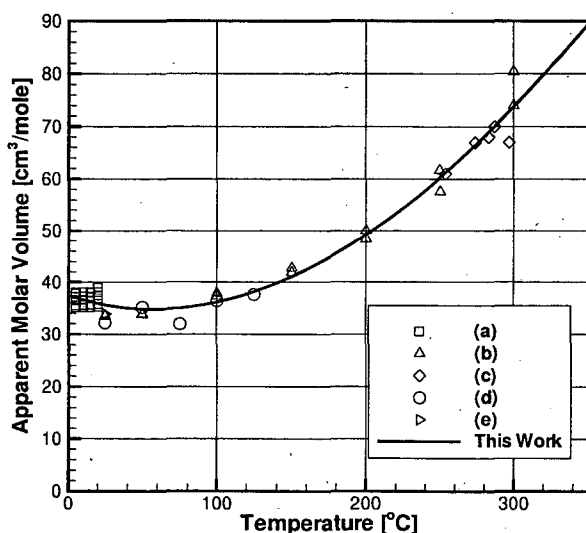
Figure 2: Fit of Partial Molar Volume Vs. Temperature. (a) Teng et al Teng et al. (1997), (b) Hnedkosky et al Hnědkovský et al. (1996), (c)Malinin Malinin (1974), (d) Ellis and McFadden Ellis and 'McFadden (1972), (e)Moore et al Moore et al. (1982)

Figure 3: Computed density of aqueous solutions of CO_2 (P=100 bar)

for mole fractions (Xmole) of 0.02 and 0.05 (Figure 3). A maximum density increase of 2.5 % is obtained for a solution with a CO_2 mole fraction of 0.05.

As expected according Equation 1, the density variation of the aqueous solutions of CO_2 is nearly linear with respect to CO_2 mole fraction (See Figure 4). Figure 5 and 6 show a comparison between the measured and predicted values of the partial molar volume of CO_2 in water and the density of aqueous solutions of CO_2, respectively. Predicted values using Equation 3 agree very well with the measured data.
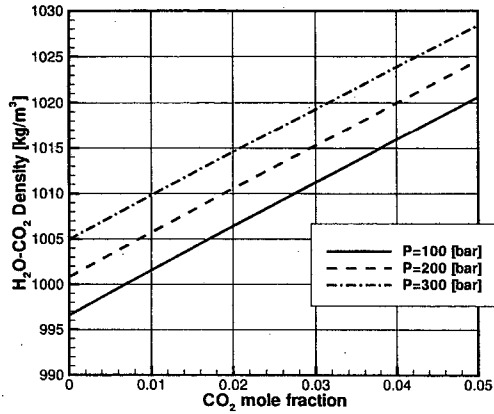
Figure 4: Computed density of aqueous solutions of CO_2 (P=100 bar)
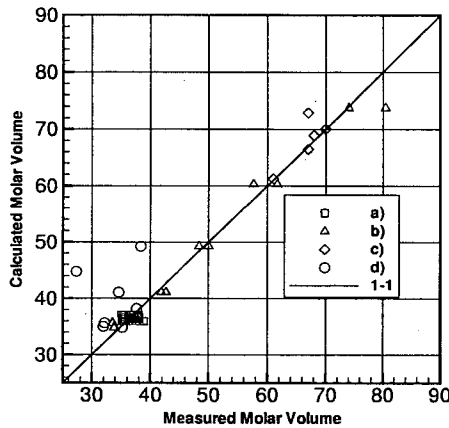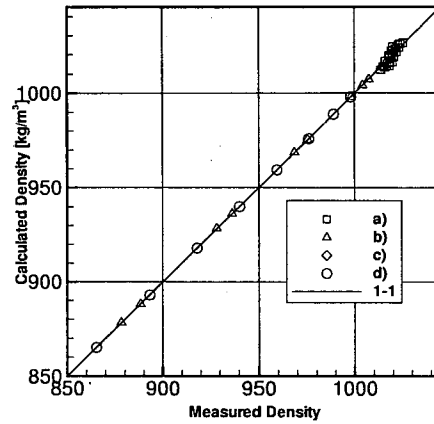
Figure 5: Comparison between measured and predicted partial molar volume of CO_2 in water
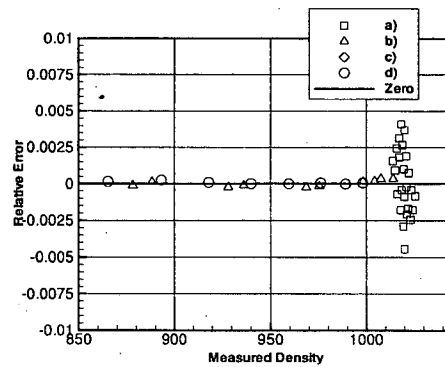
Figure 6: Comparison between measured and predicted density of aqueous solution of CO_2
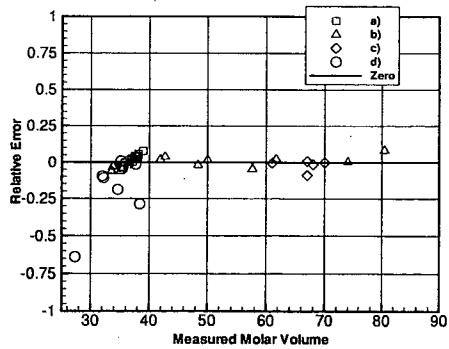
3 TOUGH2-ECO2 Implementation

The proposed new formulation for the partial molar volume of CO_2 in water and the corresponding aqueous solution density is incorporated into the TOUGH2 Equation-of-State module ECO2 through the new subroutine COCO2. Only few changes are required in the rest of the module. Calls to subroutine COCO2 require the following arguments: aqueous phase temperature and pressure, CO_2 and Salt mass fractions, and brine density:

CALL COCO2(TX,PL,XG,XSA,DB)

The CO_2 dependency on brine density can be turned on through parameter specification in data block SELEC. A description of additional SELECtion options is provided in Pruess et al. (1999).

4

IE(9) Allows to select brine density as a function of CO$_2$ content
      0: Brine density independent of CO$_2$ content
      1: Full dependence

The beta version of subroutine COCO2 is presented in Appendix B.

4 Nomenclature

c	molarity of solution (moles/m^3)
M	molecular weight (kg/mol)
m	molality of the solution expressed in moles of solute in 1 kg of solvent (mol/kg)
n_i	number of moles of the i-th component in the mixture (mol)
P	pressure (Pa)
T	temperature (°C)
V	volume (m^3)
$\overline{V}_i$	partial molar volume of the i-th component (m^3/mol)
V_m	molar volume (m^3/mol)
V_ϕ	apparent molar volume of dissolved CO$_2$ (m^3/mol)
x_i	molar fraction
ρ	density of the solution (kg/m^3)
ρ_1	density of water (kg/m^3)

Subscripts

aq	aqueous phase
s	mixture
1	solvent (H$_2$O)
2	solute (CO$_2$)

Superscripts

o	at infinite dilution

Acknowledgement

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A Density of Binary Aqueous Solutions

The partial molar volume is an important thermodynamic quantity since: (1) its value may be used to correct Henry's constant when the gas pressure is large (Prausnitz et al., 1986) and; (2) the knowledge of its value can be used to estimate the density of the solution. In this appendix we present an overview of theory related to partial molar volumes and estimation of the corresponding binary aqueous solutions density. For additional details the reader is referred to Prausnitz et al. (1986) and Anderson and Crerar (1993).

The definition of a partial molar property is applicable only to extensive properties differentiated at constant temperature and pressure. The total volume of a system with j-components can be expressed by the relation:

$$V = \sum_{i=1}^{j} n_i \overline{V_i} \qquad (4)$$

where

$$\overline{V_i} = \left(\frac{\partial V}{\partial n_i}\right)_{T,P,n_{j \neq i}} \qquad (5)$$

is the partial molar volume of the i-th component.

In practice, the apparent molar quantities are more easy to be determined, and the partial molar quantities are calculated from these. For binary solutions the apparent molar volume, V_ϕ, is defined as:

$$V_\phi = \frac{V - n_1 V_{m,1}}{n_2} \qquad (6)$$

As illustrated in Figure 7, the apparent molar volume is the volume that should be attributed to the solute in the solution if one assumes that the solvent contributes the same volume it has in its pure state. Alternatively,

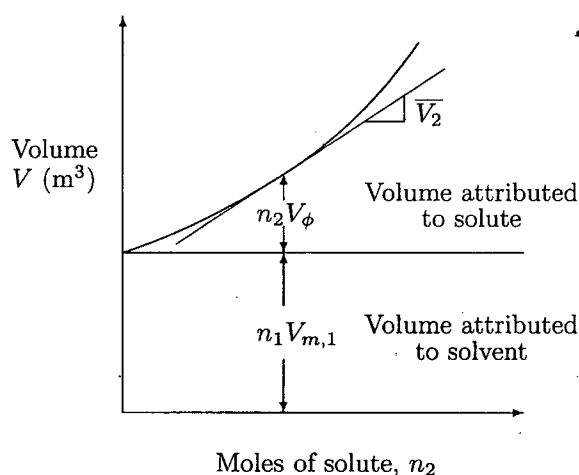$$V = n_1 V_{m,1} + n_2 V_\phi \qquad (7)$$

Figure 7: Total volume of a solution as a function of solute concentration showing the difference between partial molar volume and apparent molar volume. Adapted from Anderson and Crerar (1993).

Dividing Equation 7 by $(n_1 + n_2)$ we obtain:

$$V_m = x_1 V_{m,1} + x_2 V_\phi \qquad (8)$$

The apparent molar volume V_ϕ can be seen (Figure 8) to be the intercept on the solute axis.
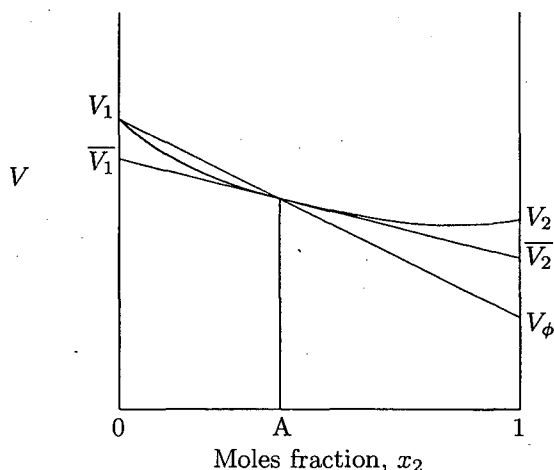
Figure 8: Molar volume of a binary solution versus mole fraction showing the difference between partial molar volume and apparent molar volume for solution at composition A. Adapted from Anderson and Crerar (1993)

The partial molar volume of solute and solvent in a binary solution can be obtained from V_ϕ as:

$$\overline{V}_2 = \left(\frac{\partial V}{\partial n_2}\right)_{T,P,n_1} = V_\phi + n_2 \left(\frac{\partial V_\phi}{\partial n_2}\right)_{T,P,n_1} \qquad (9)$$

at infinite dilution (i.e. $n_2 \rightarrow 0$) the following relation holds

$$\overline{V}_2^o = V_\phi^o \qquad (10)$$

i.e. the partial molar volume of a solute at infinite dilution is equal to its apparent molar volume at infinite dilution.

The apparent partial molar volume can be expressed in terms of densities and molecular weights (Teng et al., 1997).

$$V_\phi = \frac{1}{n_2}\left(\frac{n_1 M_1 + n_2 M_2}{\rho} - n_1 \frac{M_1}{\rho_1}\right) \qquad (11)$$

If the composition is expressed by the number of moles of solute in 1 kg of solvent (i.e. $n_2 = m\, n_1 = 1/M_1$), we obtain:

$$V_\phi = \frac{\rho_1 - \rho}{m\rho\rho_1} + \frac{M_2}{\rho} \qquad (12)$$

Or, if the composition is expressed by the number of moles of solute in 1 m^3 of solution (i.e. $n_2 = c\, n_1 = (\rho - cM_2)/M_1$):

$$V_\phi = \frac{\rho_1 - \rho}{c\rho_1} + \frac{M_2}{\rho_1} \qquad (13)$$

Either Equation 12 or 13 can be used to obtain an expression for aqueous density. From equation 13

$$\rho_{aq} = \rho_1 + M_2 \cdot c - c \cdot \rho_1 \cdot V_\phi \qquad (14)$$

Or from equation 12:

$$\rho = \frac{1 + mM_2}{mV_\phi + \frac{1}{\rho_1}} \qquad (15)$$

where m can be expressed in terms of mol fractions (x_1, x_2) as:

$$m = \frac{1}{M_1\left(\frac{1}{x_2} - 1\right)} = \frac{x_2}{M_1 x_1} \qquad (16)$$

$$x_2 = \frac{mM_1}{1 + mM_1} \qquad (17)$$

Replacing equation 16 into equation 15

$$\rho = \frac{1 + \frac{x_2 M_2}{M_1 x_1}}{\frac{x_2 V_\phi}{M_1 x_1} + \frac{1}{\rho_1}} \qquad (18)$$

After further simplification we obtain an alternative equation for the aqueous phase density

$$\frac{1}{\rho} = \frac{x_2 V_\phi}{M_T} + \frac{M_1 x_1}{\rho_1 M_T} \qquad (19)$$

where $M_T = M_1 x_1 + M_2 x_2$

A.1 Ideal Solutions

For an *ideal solution*, the partial molar volumes of the species in solution are equal to the molar volumes of pure species at the same temperature and pressure. In this event, the total volume becomes:

$$V = n_1 V_{m,1} + n_2 V_{m,2} \qquad (20)$$

Expressing the molar volumes in terms of densities $(V_{m,i} = \frac{M_i}{\rho_i})$:

$$V = n_1 \frac{M_1}{\rho_1} + n_2 \frac{M_2}{\rho_2} \qquad (21)$$

$$\frac{n_1 M_1 + n_2 M_2}{\rho} = n_1 \frac{M_1}{\rho_1} + n_2 \frac{M_2}{\rho_2} \qquad (22)$$

7

Dividing Equation 22 by the total mass:

$$\frac{1}{\rho} = \frac{X_1}{\rho_1} + \frac{X_2}{\rho_2} \qquad (23)$$

Where $X_i = \frac{n_1 M_i}{n_1 M_1 + n_2 M_2}$ is the mass fraction of specie i.

B   Subroutine COCO2

```
01715          — C
01716        [[SUBROUTINE COCO2(TX,PX,XG,XSA,DBJ)]]
01717          — C        IMPLICIT DOUBLE PRECISION (A-H,O-Z)
01718          — COMMON/GASLAW/R,AMS,AMA,CVNCG
01719          — COMMON/EOSG/ZA,AMSALT,GAST
01720          — COMMON/EOSEL/IE(16),FE(512)
01721          — COMMON/VISWAT/DW0
01722          — COMMON/KONIT/KON,DELT,IGOOD
01723          — SAVE ICALL
01724          — DATA ICALL/0/
01725          — ICALL=ICALL+1
01726          —[IF(ICALL.EQ.1) WRITE(11,899)]
01727    899  — FORMAT(6X,'COCO2     0.9        19 September 2001',6X,
01728             X'DENSITY OF AQUEOUS PHASE AS FUNCTION OF T, P',
01729             X' AND CO2 MOLE FRACTION')
01730          — C
01731          — C-----WHEN IE(9)>1 INCLUDE CO2 MOLE FRACTION DEPENDENCY.
01732          — C
01733          — DBC=DBJ
01734          — C        Compute effective molecular weight
01735          — EMW=(1.0-XG)/((1.0-XG-XSA)/AMS+XSA/AMSALT)
01736          — C        Compute mole fraction.
01737          — XMG=XG/(XG+AMA*(1.-XG)/EMW)
01738          — C        Correlation for partial molar volume JULIO GARCIA (2001)
01739          —[IF(IE(9).EQ.1) THEN]
01740             — VPH=37.51-9.585E-2*TX+8.740E-4*TX*TX-5.044E-7*TX*TX*TX
01741          [END IF]
01742          — C        Unit Conversion
01743          — VPHI=VPH/1000000.
01744          — TOTM=(1.0-XMG)*EMW+XMG*AMA
01745          — DBINV=(XMG*VPHI/TOTM)+(EMW*(1.0-XMG))/(DBC*TOTM)
01746          — DBJ=1./DBINV
01747          — C-----IDEAL SOLUTIONS
01748          — C        Partial molar volumes of species in solution are
01749          — c        equal to molar volumes of pure species.
01750          — c        To be included only for testing purposes...
01751          — C        Get pure CO2 density at saturated conditions
01752          — c        Calculate TOT1 and TOT2 and evaluate density of aqueous solution.
01753          — C        DBINV1=TOT1/DBC+TOT2/DCO2
01754          — C        DB2=1./DBINV1
01755          —[IF (IGOOD.NE.0) RETURN]
01756          — C-----Viscosity OF CO2 SATURATED AQUEOUS PHASE
01757          — C        There are few data points for this. To be included in a
01758          — C        next version if COCO2.
01759          — RETURN
01760          — END
```

Water - Carbon Dioxide Data

Temperature Range 0-300 °C
Julio Garcia

Summary

Ref	NP	T [°C]	P [Mpa]	Authors	Comments
1	24	5.0-20.0	6.44-29.49	Teng et al. 1997	
2	14	25.0-300.0	20.0-35.0	Hnedkosky et al 1996	
3	5	274-297	19.6-29.41	Malinin 1972	High T
4	8	25.0-100.0	1.96	Ellis and McFadden	Low P
5	1	5.0-40.0	?	Parkinson and De Nevers 1969	
6	1	25.00	0.1	Moore et al. 1982	

Total   53

Reference	Point #	Temperature	Pressure	reported mol fraction	calculated molality	reported density	TOUGH2	calculated part. m. vol.		Correlation Estimated	Correlation Calculated
Ref	PN	T [°C]	P [Mpa]	x_{co2}	m [mol/kg]	ρ_e [kg/m³]	ρ_{H2O} [kg/m³]	V [cm³/mol]	$\Delta\rho/\rho$	V [cm³/mol]	ρ_e [kg/m³]
1	1	5.00	6.44	2.93E-02	1.677	1018.10	1003.10	35.10518	0.0150	37.0425	1013.93
1	2	5.00	9.87	3.08E-02	1.765	1019.77	1004.70	35.46292	0.0150	37.0425	1015.99
1	3	5.00	14.77	3.20E-02	1.837	1020.63	1007.10	36.52252	0.0134	37.0425	1018.69
1	4	5.00	19.68	3.31E-02	1.902	1022.01	1009.40	37.16304	0.0125	37.0425	1021.25
1	5	5.00	24.58	3.41E-02	1.961	1023.33	1011.70	37.76369	0.0115	37.0425	1023.76
1	6	5.00	29.49	3.49E-02	2.009	1025.33	1014.00	37.96816	0.0112	37.0425	1026.20
1	7	10.00	6.44	2.79E-02	1.594	1016.97	1002.80	35.16296	0.0141	36.6284	1013.78
1	8	10.00	9.87	2.94E-02	1.683	1018.60	1004.40	35.55935	0.0141	36.6284	1015.88
1	9	10.00	14.77	3.05E-02	1.748	1019.40	1006.60	36.57429	0.0127	36.6284	1018.38
1	10	10.00	19.68	3.16E-02	1.813	1020.75	1008.90	37.26453	0.0117	36.6284	1020.98
1	11	10.00	24.58	3.26E-02	1.872	1021.70	1011.10	38.03609	0.0105	36.6284	1023.43
1	12	10.00	29.49	3.34E-02	1.920	1023.98	1013.30	38.06063	0.0105	36.6284	1025.80
1	13	15.00	6.44	2.69E-02	1.536	1015.75	1002.10	35.17582	0.0136	36.2572	1013.28
1	14	15.00	9.87	2.80E-02	1.600	1017.10	1003.70	35.63583	0.0134	36.2572	1015.25
1	15	15.00	14.77	2.96E-02	1.695	1018.22	1006.60	37.02130	0.0115	36.2572	1018.65
1	16	15.00	19.68	3.09E-02	1.771	1019.68	1008.10	37.28695	0.0115	36.2572	1020.59
1	17	15.00	24.58	3.19E-02	1.831	1020.96	1010.30	37.90595	0.0106	36.2572	1023.07
1	18	15.00	29.49	3.27E-02	1.878	1022.87	1012.40	38.07764	0.0103	36.2572	1025.37
1	19	20.00	6.44	2.50E-02	1.425	1013.68	1001.20	35.31489	0.0125	35.9286	1012.09
1	20	20.00	9.87	2.58E-02	1.471	1014.80	1002.70	35.79922	0.0121	35.9286	1013.87
1	21	20.00	14.77	2.75E-02	1.571	1015.97	1004.90	36.88348	0.0110	35.9286	1016.70
1	22	20.00	19.68	2.93E-02	1.677	1017.72	1007.10	37.51087	0.0105	35.9286	1019.55
1	23	20.00	24.58	3.04E-02	1.742	1019.05	1009.20	38.10025	0.0098	35.9286	1022.00
1	24	20.00	29.49	3.12E-02	1.789	1019.79	1011.30	38.90718	0.0084	35.9286	1024.32

Reference	Point #	Temperature	Pressure	calculated mol fraction	reported molality	reported density	TOUGH2	reported part. m. vol.		Correlation Estimated	Correlation Calculated
Ref	PN	T [°C]	P [Mpa]	x_{co2}	m [mol/kg]	ρ_e [kg/m³]	ρ_{H2O} [kg/m³]	V [cm³/mol]	$\Delta\rho/\rho$	V [cm³/mol]	ρ_e [kg/m³]
2	25	25.00	20.00	2.80E-03	0.155	1007.51	1005.90	33.49272	0.0016	35.64212	1007.16
2	26	50.00	20.01	2.80E-03	0.155	998.17	996.59	33.90330	0.0016	34.82945	998.02
2	27	100.00	20.00	2.80E-03	0.155	968.53	967.42	37.83881	0.0011	36.15060	968.77
2	28	150.00	20.00	2.80E-03	0.155	928.36	927.73	42.70850	0.0007	41.08515	928.57
2	29	200.00	19.99	2.80E-03	0.155	878.20	878.19	50.01913	0.0000	49.25480	878.30
2	30	250.00	19.99	3.34E-03	0.185	815.53	816.49	61.68213	-0.0012	60.28125	815.71
2	31	300.00	20.00	3.34E-03	0.185	732.90	734.95	80.44028	-0.0028	73.78620	733.57
2	32	25.00	35.00	2.80E-03	0.155	1013.87	1012.30	33.59630	0.0016	35.64212	1013.54
2	33	50.00	35.00	2.80E-03	0.155	1004.28	1002.70	33.75875	0.0016	34.82945	1004.10
2	34	100.00	34.99	2.80E-03	0.155	975.21	974.05	37.29369	0.0012	36.15060	975.37
2	35	150.00	35.00	2.80E-03	0.155	936.25	935.55	41.87511	0.0007	41.08515	936.35
2	36	200.00	34.99	2.80E-03	0.155	888.27	888.13	48.39760	0.0002	49.25480	888.16
2	37	250.00	35.00	3.34E-03	0.185	829.82	830.41	57.61381	-0.0007	60.28125	829.49
2	38	300.00	35.00	2.80E-03	0.155	756.66	758.08	74.01220	-0.0019	73.78620	756.69

Reference	Point #	Temperature	Pressure	calculated mol fraction	reported molality	reported density	TOUGH2	reported part. m. vol.		Correlation Estimated	Correlation Calculated
Ref	PN	T [°C]	P [Mpa]	x_{co2}	m [mol/kg]	ρ_e [kg/m³]	ρ_{H2O} [kg/m³]	V [cm³/mol]	$\Delta\rho/\rho$	V [cm³/mol]	ρ_e [kg/m³]
3	39	287.00	19.61	1.09E-02	0.597	783.69	758.39	70.00000	0.0334	70.0576	754.38
3	40	274.00	19.61	2.19E-02	1.190	833.30	780.24	67.00000	0.0680	66.4776	773.36
3	41	297.00	29.41	1.09E-02	0.597	756.41	755.30	67.00000	0.0015	72.9129	750.46
3	42	283.00	29.41	2.19E-02	1.190	778.80	778.17	68.00000	0.0008	68.9399	769.77
3	43	254.00	29.41	4.48E-02	2.380	820.13	820.12	61.00000	0.0000	61.2754	809.22

Reference	Point #	Temperature	Pressure	calculated mol fraction	reported molality	reported density	TOUGH2	reported part. m. vol.		Correlation Estimated	Correlation Calculated
Ref	PN	T [°C]	P [Mpa]	x_{co2}	m [mol/kg]	ρ_e [kg/m³]	ρ_{H2O} [kg/m³]	V [cm³/mol]	$\Delta\rho/\rho$	V [cm³/mol]	ρ_e [kg/m³]
4	44	25.00	1.96	2.88E-04	0.016	998.10	997.91	32.16963	0.0002	35.6421	998.04
4	45	50.00	1.96	2.88E-04	0.016	989.03	988.88	35.15829	0.0001	34.8295	989.04
4	46	75.00	1.96	2.88E-04	0.016	975.88	975.68	31.96852	0.0002	35.0147	975.83
4	47	100.00	1.96	2.88E-04	0.016	959.40	959.26	36.36107	0.0001	36.1506	959.40
4	48	125.00	1.96	2.88E-04	0.016	940.06	939.93	37.61656	0.0001	38.1898	940.05
4	49	150.00	1.96	2.88E-04	0.016	918.08	917.90	34.58565	0.0002	41.0852	917.99
4	50	175.00	1.96	2.88E-04	0.016	893.18	892.90	27.33462	0.0003	44.7892	892.96
4	51	200.00	1.96	2.88E-04	0.016	865.25	865.10	38.33659	0.0002	49.2548	865.12

Reference	Point #	Temperature	Pressure	not reported	not reported	not reported		reported part. m. vol.		Correlation Estimated	Correlation Calculated
Ref	PN	T [°C]	P [Mpa]	x_{co2}	m [mol/kg]	ρ_e [kg/m³]	ρ_{H2O} [kg/m³]	V [cm³/mol]	$\Delta\rho/\rho$	V [cm³/mol]	ρ_e [kg/m³]
6	52	25.00	0.10	-	-	-	-	33.90000	-	35.64211875	

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