

Model for Calculating the Density of Aqueous Electrolyte Solutions

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A new model for calculating the density of aqueous solutions of electrolytes has been developed. Parameters for 59 electrolytes were established on the basis of an extensive critical review of the published literature for solutions of one electrolyte in water, with over 10 700 points included. The average difference between the calculated and experimental density of solutions of water and one electrolyte is 0.10 kg m^{-3} with a standard deviation of 1.44 kg m^{-3} . The model was validated by predicting the density of systems of two or more electrolytes in water. The average difference between experimental and calculated values for over 1600 points is 0.003 kg m^{-3} with a standard deviation of 1.39 kg m^{-3} . The electrolytes studied are AlCl_3 , $\text{Al}_2(\text{SO}_4)_3$, BaCl_2 , CaCl_2 , CdCl_2 , CdSO_4 , CoCl_2 , CoSO_4 , CrCl_3 , $\text{Cr}_2(\text{SO}_4)_3$, CuCl_2 , CuSO_4 , FeCl_2 , FeSO_4 , FeCl_3 , $\text{Fe}_2(\text{SO}_4)_3$, HCl , HCN , HNO_3 , H_3PO_4 , H_2SO_4 , KCl , K_2CO_3 , KNO_3 , KOH , K_2SO_4 , LiCl , Li_2SO_4 , MgCl_2 , MgSO_4 , MnCl_2 , MnSO_4 , NaBr , NaCl , NaClO_3 , Na_2CO_3 , NaF , NaHCO_3 , NaH_2PO_4 , Na_2HPO_4 , NaHSO_3 , NaI , Na_2MoO_4 , NaNO_2 , NaNO_3 , NaOH , Na_3PO_4 , Na_2SO_3 , $\text{Na}_2\text{S}_2\text{O}_3$, Na_2SO_4 , NH_3 , NH_4Cl , NH_4NO_3 , $(\text{NH}_4)_2\text{SO}_4$, NiCl_2 , NiSO_4 , SrCl_2 , ZnCl_2 , and ZnSO_4 .

Introduction

The density of aqueous electrolyte solutions is useful in the design and control of chemical processes. It is used in pipe sizing, pump calculations, heat transfer calculations, and other common problems.

Despite the importance of density data in engineering calculations, finding the relevant data can be frustrating. Perry's Chemical Engineers' Handbook⁹⁰ has a short section on density with good data for commercially important chemicals (H_2SO_4 , HCl , HNO_3 , NaOH , NH_3 , etc.) and with fragmentary and often dated information for about 70 other electrolytes. There is no other practical reference available to engineers. This is surprising because chemists have been studying the density of electrolyte solutions for over a century and have measured the density of all common electrolyte solutions over a range of concentration and temperature.

One of the reasons for this discrepancy may be confusion regarding units. Chemists often use mole-based units for concentration (molality and molarity), but mass-based units are more practical for engineers (mass fraction and mass per volume are most common). Furthermore, published data are often reported as apparent molal volume instead of density.

The units of concentration used in this paper are mass based instead of mole based as is more traditional. This should help make the model more immediately useful for engineering calculations. More importantly, mole-based units, especially molality, are not very well suited for calculating the density of solutions containing a large number of electrolytes in water, the molality being by definition the number of moles of a solute in a kilogram of solvent excluding any other solute present in this solution. As will be demonstrated later in looking at data for multielectrolyte solutions, the other solutes, if present, will have an effect on the density of the solution, and ignoring this effect significantly decreases the accuracy of the model prediction.

Review of Available Data

The first step of the study was to assemble published data from the literature. Density data are readily available going back to the late 1800s. Measurements using modern tube vibration techniques are now common and are considered quite accurate and consistent.³⁴ The measurement of concentration is also more accurate because of the use of modern analytical techniques. Data from as far back as the early 1900s were reviewed: data from before 1970 might be less reliable, but some of the early literature data are still of excellent quality.

One secondary source that was used extensively is a compilation of data from 1900 to about 1985 by Lobo.⁶⁴ Additional searches were performed for electrolytes that are not well covered in Lobo, as well as for more recent data.

Fifty nine electrolytes were selected for this review. The electrolytes selected consist of the chloride and sulfate salts of most common metals plus a selection of common acids and bases and other electrolytes such as carbonates, nitrates, and bromides of alkali metals. The model proposed here works well for all selected electrolytes, and there is no reason to believe that it would not work for any other electrolyte.

Density Model

The first step in developing a density model was to develop a simple mixing rule that could be used for a solution containing an arbitrary number of components. We based our mixing rule on the well-known fact that the volume of a mixture of ideal liquids can be calculated with the following equation:

$$v_m = v_{\text{H}_2\text{O}} + \sum_i v_i \quad (1)$$

where $v_{\text{H}_2\text{O}}$, v_m , and v_i are the volumes of the water, the mixture, and ideal component i , respectively.

Equation 1 can be transformed to calculate density. For all ideal mixtures,

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$$\frac{1}{\rho_m} = \frac{w_{\text{H}_2\text{O}}}{\rho_{\text{H}_2\text{O}}} + \sum_i \frac{w_i}{\rho_i} \quad (2)$$

where $w_{\text{H}_2\text{O}}$ and $\rho_{\text{H}_2\text{O}}$ are the mass fraction and the density of water, w_i is the mass fraction of component i , ρ_i is its density, and ρ_m is the density of the mixture. All densities are expressed in kg m^{-3} .

In the model presented here, it is assumed that the density (or the volume) of water is not a function of concentration but only of temperature. The density (or volume) of the electrolyte has been assumed to vary with both temperature and composition and is called "apparent" density or volume. (The pressure dependency of the density and volume of water and electrolytes is small and was not considered in this model. The limited data at high pressure in the literature were not used to calculate the model's coefficients.)

Equation 1 then becomes

$$V_m = V_{\text{H}_2\text{O}} + \sum_i V_{\text{app},i} \quad (3)$$

where $V_{\text{H}_2\text{O}}$ is the volume of water in m^3 and $V_{\text{app},i}$ is the apparent volume of electrolyte i , also in m^3 .

Equation 3 can be rewritten using the specific volume, the volume occupied per unit of mass

$$V_m = w_{\text{H}_2\text{O}} V_{\text{H}_2\text{O}} + \sum_i w_i \bar{V}_{\text{app},i} \quad (4)$$

where $\bar{V}_{\text{app},i}$ indicates the electrolyte i specific volume in $\text{m}^3 \text{kg}^{-1}$. This can be rewritten in terms of density

$$\rho_m = \frac{1}{\frac{w_{\text{H}_2\text{O}}}{\rho_{\text{H}_2\text{O}}} + \sum_i \frac{w_i}{\rho_{\text{app},i}}} \quad (5)$$

or, alternatively,

$$\rho_m = \frac{1}{w_{\text{H}_2\text{O}} \bar{V}_{\text{H}_2\text{O}} + \sum_i w_i \bar{V}_{\text{app},i}} \quad (6)$$

where $\rho_{\text{app},i}$ is the apparent density of electrolyte i .

Equations 4–6 are mathematically equivalent, and any of them can be used. Because in some cases the apparent specific volume of an electrolyte tends to 0 and its apparent density tends to infinity, eq 5 can cause some numerical problems. Equation 6 was used hereafter, but this is mostly a matter of preference.

Solving eq 6 for $\bar{V}_{\text{app},i}$ yields the following equation for calculating the apparent specific volume of one electrolyte in solution with water:

$$\bar{V}_{\text{app},i} = \frac{1 - \frac{\rho_m(1 - w_i)}{\rho_{\text{H}_2\text{O}}}}{\rho_m w_i} \quad (7)$$

The density of water instead of its apparent volume was used for convenience only. Either can be used. The density

of water was calculated using a correlation from Kell (eq 8):⁵¹ where t is the temperature in $^{\circ}\text{C}$.

At high concentration, the numerical value used for the density of water has little impact on the value of the apparent specific volume. At low concentration ($w_i < 0.01$), this is not the case.

The numerical values for the density of water predicted by eq 8 were compared to those in the Revised Supplementary Release on Saturation Properties of Ordinary Water Substance edited by the International Association for the Properties of Water and Steam⁴³ (IAPWS) and to those in Recommended Reference Materials for the Realization of Physicochemical Properties edited by Marsh.⁶⁸ Equation 8 was found to be in very close agreement with the values in Marsh (average deviation 0.003, maximum 0.005 kg m^{-3}), but those found by eq 8 are systematically higher than those in IAPWS at temperatures below about 110 $^{\circ}\text{C}$ by about 0.05 kg m^{-3} at 25 $^{\circ}\text{C}$. This may be explained by the fact that the densities in Lobo and Marsh are at atmospheric pressure below 100 $^{\circ}\text{C}$ whereas those from the IAPWS are at saturation pressure. Because of the agreement between the values in Lobo and Marsh, the fact that most engineering calculations will be done for processes at atmospheric pressure, and that most experimental measurements of density were taken at that same pressure, eq 8 was used hereafter.

Figure 1 shows how the apparent specific volume, in this case, MgSO_4 , can be either positive or negative. Apparent specific volume typically has a low value at low concentration and then increases toward a linear relationship with mass fraction at higher concentration. The inflection point where this relationship becomes linear, the slope of that linear relationship, and the influence of temperature on both of these factors, however, are difficult to predict.

Finding a mathematical model to represent the apparent specific volume suitably was a challenge. The following was found to adequately represent all electrolytes studied and is suitable for interpolation as well as extrapolation, as will be demonstrated later:

$$\bar{V}_{\text{app},i} = \frac{w_i + c_2 + c_3 t}{(c_0 w_i + c_1) e^{(0.000001(t+c_4)^2)}} \quad (9)$$

where c_0 to c_4 are empirical constants. c_0 and c_1 are in kg m^{-3} , c_2 is dimensionless, c_3 is in $^{\circ}\text{C}^{-1}$ and c_4 is in $^{\circ}\text{C}$, and t is the temperature in $^{\circ}\text{C}$. The fractional term of this equation was formulated by examining many sets of experimental data using residual plots of $\rho_{\text{app},i}$. The original form of the equation included only terms c_0 to c_2 . The exponential term with the c_4 constant was added for the temperature dependence and is based on the findings of Sangwal.¹¹⁶ The term $c_3 t$ was added after looking at residual plots and noting that the point where the apparent specific volume switched from negative to positive changed slowly with temperature even with the exponential term included.

Calculation of Terms c_0 to c_4

To calculate terms c_0 to c_4 , we calculated the apparent specific volume using eq 7 for all 10 700 data points studied. A nonlinear least-squares method was then used to estimate terms c_0 to c_4 from eq 9:

Initial values were entered for c_0 to c_4 (1, 1, 1, 0.0025, and 1500 are typical values).

$$\rho_{\text{H}_2\text{O}} = \frac{(((((-2.8054253 \times 10^{-10} t + 1.0556302 \times 10^{-7}) t - 4.6170461 \times 10^{-5}) t - 0.0079870401) t + 16.945176) t + 999.83952)}{1 + 0.01687985 t} \quad (8)$$

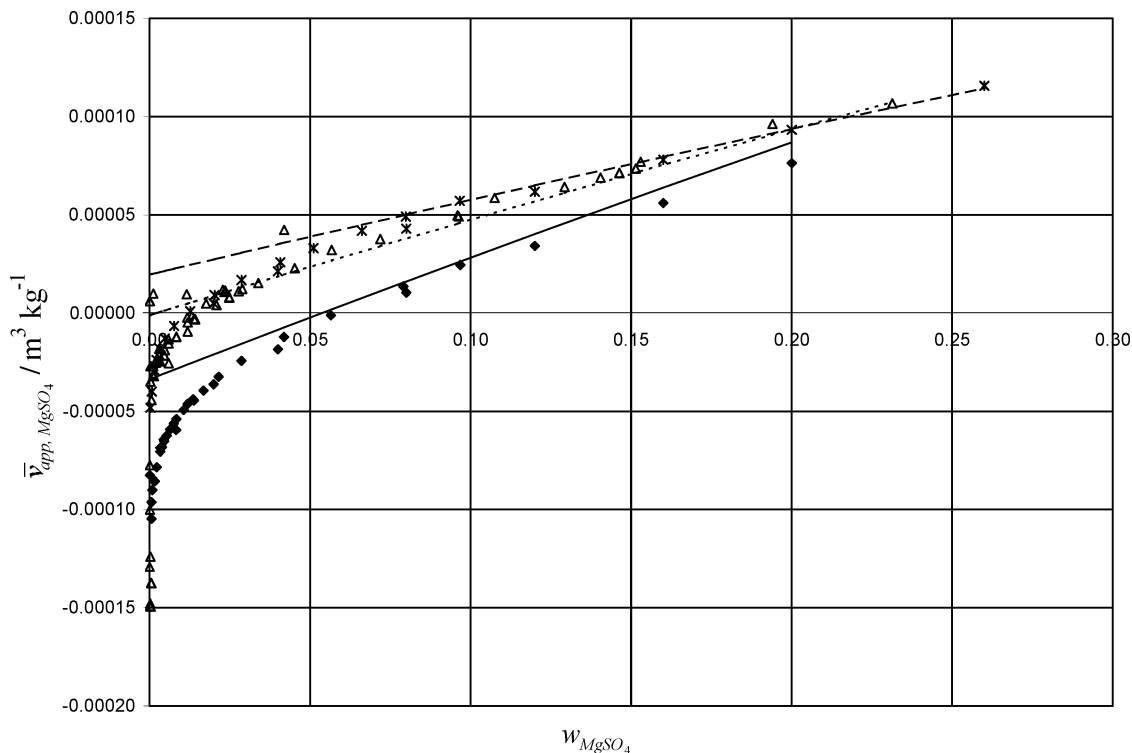


Figure 1. Specific volume of MgSO_4 in solution with water: \blacklozenge , exptl data at $0\text{ }^\circ\text{C}$; $-$, calcd data at $0\text{ }^\circ\text{C}$; Δ , exptl data at $25\text{ }^\circ\text{C}$; $- - -$, calcd data at $25\text{ }^\circ\text{C}$; $*$, exptl data at $50\text{ }^\circ\text{C}$; $- \cdot - \cdot -$, calcd data at $50\text{ }^\circ\text{C}$.

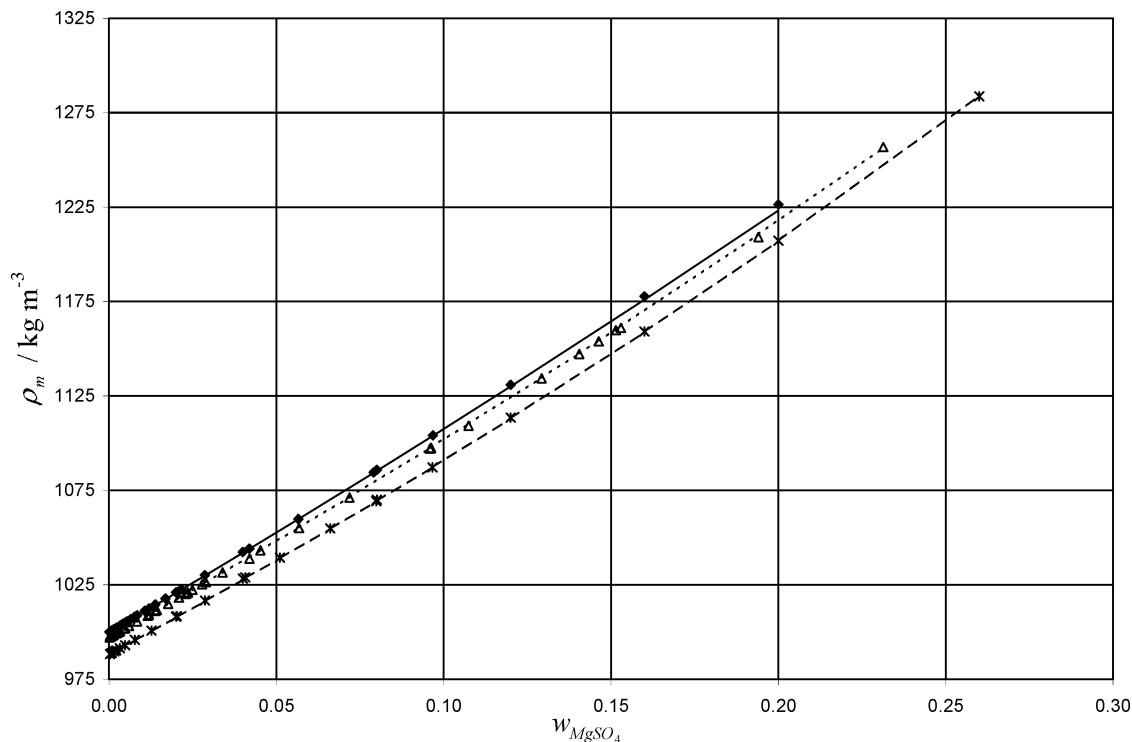


Figure 2. Density of solutions of MgSO_4 and water: \blacklozenge , exptl data at $0\text{ }^\circ\text{C}$; $-$, calcd data at $0\text{ }^\circ\text{C}$; Δ , exptl data at $25\text{ }^\circ\text{C}$; $- - -$, calcd data at $25\text{ }^\circ\text{C}$; $*$, exptl data at $50\text{ }^\circ\text{C}$; $- \cdot - \cdot -$, calcd data at $50\text{ }^\circ\text{C}$.

A residual was calculated by subtracting the calculated solution density from its experimental value.

The sum of the square of the residuals was calculated, and this value was minimized by varying c_0 to c_4 . It was found that alternating between the conjugate gradient and the Newton methods of seeking the minimum value significantly increased the quality of the fit.

The data were checked for consistency (see below). If an inconsistent datum was found, then it was removed and steps 2 and 3 were repeated. This was repeated until there were no more inconsistent data.

Because the constant c_4 can sometimes be negative and the solver program does not always converge to the absolute minimum square of the residuals, especially if c_4

Table 1. Values of Constants c_0 to c_4 from Equation 9

	$c_0/\text{kg/m}^3$	$c_1/\text{kg/m}^3$	$c_2/\text{dimensionless}$	$c_3/1/^\circ\text{C}$	$c_4/^\circ\text{C}$	$\bar{V}_{\text{app},t}$ at $w = 0.01$ and $t = 25^\circ\text{C}/\text{m}^3/\text{kg}$	references
AlCl ₃	221.68	160.90	0.15125	0.002500	1500.0	0.0001340	23, 70
Al ₂ (SO ₄) ₃	-0.0017202	0.0018967	-0.030904	0.004087	3804.2	0.0000185	18, 90, 121
BaCl ₂	-0.0030518	0.00526670	4.1785	0.068274	3971.9	0.0001299	45, 67, 87, 90, 129
CaCl ₂	-0.63254	0.93995	4.2785	0.048319	3180.9	0.0002025	28, 45, 57, 87, 90, 113, 123, 133, 136
CdCl ₂	-0.090879	0.29116	7.3827	-0.031855	-3477.5	0.0001513	9, 23, 37, 104, 107
CdSO ₄	-1.0440 × 10 ⁻⁷	6.1070 × 10 ⁻⁸	-0.003761	0.004108	5007.7	0.0000182	6, 7, 117
CoCl ₂	-8.0924 × 10 ⁻⁸	8.0261 × 10 ⁻⁸	410.24	9.1808	5619.8	0.0001169	37, 93, 99, 123
CoSO ₄	-118.36	1368.1	0.01304	-0.000145	-294.02	0.0000132	7, 117
CrCl ₃	3.1469	232.160	0.20191	0.002500	1500.0	0.0001155	90
Cr ₂ (SO ₄) ₃	1.0045	1.7697	-0.085017	0.002500	1500.0	-0.0006873	6
CuCl ₂	1868.5	1137.20	0.07185	0.002565	575.7	0.0000880	23, 26, 90, 97
CuSO ₄	-1.9827 × 10 ⁻⁷	1.0883 × 10 ⁻⁷	-0.12506	0.003831	4936.8	-0.0000037	84, 80, 95, 101, 125
FeCl ₂	98.654	199.51	0.33639	0.0038444	1650.1	0.0001334	48, 99
FeSO ₄	-3.6737 × 10 ⁻⁶	1.2465 × 10 ⁻⁴	-0.062861	0.0015696	3943.0	-0.0000159	7, 21, 90
FeCl ₃	-1333.8	4369.2	1.5298	0.007099	829.21	0.0001901	90
Fe ₂ (SO ₄) ₃	0.47444	-0.64624	-713.10	-25.569	4023.2	0.0001610	14, 75, 90
HCl	-80.061	255.42	118.42	1.0164	2619.5	0.0005186	3, 30, 39, 90, 98, 128
HCN	255.82	283.11	0.66888	0.0062057	891.0	0.0012616	53, 90
HNO ₃	12.993	-23.579	-3.6070	0.0079416	-2427.1	0.0004521	35, 82, 90
H ₃ PO ₄	1358.3	-4327.7	-4.5950	0.0043831	-912.45	0.0004720	17, 25, 90
H ₂ SO ₄	89.891	224.48	0.82285	0.0068422	1571.5	0.0003482	35, 90, 103
KCl	-0.46782	4.30800	2.3780	0.022044	2714.0	0.0003769	20, 28, 31, 32, 44, 49, 52, 62, 65, 73, 79-81, 90, 114, 135
K ₂ CO ₃	-1.4313	2.49170	1.1028	0.013116	2836.0	0.0001621	29, 41, 73, 90
KNO ₃	7.5436	26.38800	1.2396	0.011656	2214.0	0.0003872	7, 22, 45, 73, 79, 82, 90, 110
KOH	194.85	407.31	0.14542	0.002040	1180.9	0.0001178	4, 41, 69, 81, 90, 109, 127
K ₂ SO ₄	-2.6681 × 10 ⁻⁵	3.0412 × 10 ⁻⁵	0.97118	0.019816	4366.1	0.0002071	20, 49, 72, 78, 88, 90, 114
LiCl	17.807	32.011	1.3951	-0.006234	-2131.6	0.0004588	28, 45, 62, 73, 80, 130, 133
Li ₂ SO ₄	0.0014730	0.0026934	0.17699	0.0041319	3640.7	0.0001565	12, 48, 85, 134
MgCl ₂	-0.00051500	0.0013444	0.58358	0.0085832	3843.6	0.0001910	5, 13, 28, 45, 49, 72, 87, 90, 113, 129
MgSO ₄	3.9412 × 10 ⁻⁷	1.4425 × 10 ⁻⁶	-0.05372	0.002062	4563.3	0.0000039	6, 13, 27, 45, 49, 52, 72, 74, 88, 90
MnCl ₂	0.000001869	0.00004545	1.5758	-0.010776	-4369.9	0.0001832	37, 40, 92, 97, 104, 128
MnSO ₄	0.0032447	0.057246	0.05136	0.002146	3287.8	0.0000344	6, 7, 19, 40, 75, 103, 117
NaBr	109.770	513.04	1.54540	0.011019	1618.1	0.0002394	24, 28, 32, 45, 73, 90, 118, 119, 130
NaCl	-0.00433	0.06471	1.01660	0.014624	3315.6	0.0003065	13, 20, 27, 28, 31, 32, 44, 48, 52, 62, 67, 73, 74, 79, 80, 90, 135
NaClO ₃	0.014763	0.024913	1.2924	-0.0076175	-3454.3	0.0003465	11, 90, 108
Na ₂ CO ₃	0.012755	0.014217	-0.091456	0.0021342	3342.4	-0.0000233	38, 41, 73, 88
NaF	2.8191 × 10 ⁻⁶	2.1777 × 10 ⁻⁷	-0.041483	0.00021765	4586.9	-0.0000613	55, 72, 73, 86, 114
NaHCO ₃	-9.4794 × 10 ⁻⁸	1.5657 × 10 ⁻⁷	0.9912	0.022644	4900.2	0.0002939	38, 73, 88, 106
NaH ₂ PO ₄	208.77	641.05	0.78893	0.0045520	1198.4	0.0003177	71, 122
Na ₂ HPO ₄	1096.7	937.57	0.01424	-0.0005595	-860.20	0.0000054	122
NaHSO ₃	6.1384 × 10 ⁻⁶	1.3029 × 10 ⁻⁶	0.13635	-0.0014624	-4472.5	0.0002066	16
NaI	626.15	1858.2	1.7387	0.010500	1203.3	0.0002386	62, 65, 73, 112, 118, 119, 130
Na ₂ MoO ₄	-2.0813	4.8446	4.4342	-0.020815	-2942.3	0.0001638	78, 122
NaNO ₂	78.365	298.00	0.96246	0.0021999	1500.0	0.0003360	33, 90
NaNO ₃	49.209	94.737	0.77927	0.0075451	1819.2	0.0003423	8, 22, 45, 50, 73, 82, 90, 102, 110
NaOH	385.55	753.47	-0.10938	0.0006953	542.88	-0.0000784	3, 39, 41, 54, 66, 73, 81, 88, 90, 109
Na ₃ PO ₄	1015.6	1533.7	-0.15180	0.00013660	173.71	-0.0000862	122
Na ₂ SO ₃	1.5197 × 10 ⁻⁵	4.3766 × 10 ⁻⁷	0.10296	-0.0015271	-4500.9	0.0002528	90, 122, 131
Na ₂ S ₂ O ₃	0.84462	-1.5142	-42.949	0.19335	-3425.9	0.0002400	78, 90, 122
Na ₂ SO ₄	-1.2095 × 10 ⁻⁷	4.3474 × 10 ⁻⁷	0.15364	0.0072514	4731.5	0.0001189	13, 20, 27, 45, 47, 52, 72, 88, 90, 114, 134
NH ₃	0.12693	0.10470	1.0302	-0.0050803	-2973.7	0.0014430	90, 106
NH ₄ Cl	6.56150	89.772	4.9024	-0.016574	-2089.3	0.0007061	40, 45, 47, 73, 74, 84, 90, 106
NH ₄ NO ₃	1379.3	1124.4	0.65598	0.0014106	176.41	0.0005916	1, 10, 90, 108, 110, 120
(NH ₄) ₂ SO ₄	-123.22	452.59	3.2898	0.016292	1692.4	0.0004301	30, 46, 90
NiCl ₂	-1.3900 × 10 ⁻⁶	4.1879 × 10 ⁻⁶	0.77734	-0.0066936	-4638.1	0.0000851	23, 37, 83, 90, 91, 97, 105, 117, 123, 124
NiSO ₄	-0.03894	0.22109	-0.14443	0.0009867	3073.8	-0.0000336	44, 90, 94, 117
SrCl ₂	1.3534 × 10 ⁻⁶	-7.4877 × 10 ⁻⁷	-1.9356	0.010704	-4882.1	0.0001281	40, 45, 73, 87, 96, 113
ZnCl ₂	1943.6	304.34	-0.013753	0.0011543	573.79	0.0000542	37, 90, 100, 104, 132
ZnSO ₄	18.378	35.927	-0.089193	0.0010773	2066.3	-0.0000182	5, 7, 44, 90, 101, 126
median	0.00324470	0.9400	0.33639	0.0025646	1500.0		

crosses 0, results from step 4 were saved, and steps 1 to 4 were repeated with new initial values, this time using -1500 as an initial guess for c_4 .

If the solver found different values for constants c_0 to c_4 after step 5, then the ones with the lowest sum of the square of residuals was used.

As mentioned above, the value minimized was the square of the solution density residual. The square of the electrolyte apparent specific volume residual could have been used instead. This would have given a better fit for the apparent specific volume at low mass fraction at the expense of the fit at high mass fraction. However, the accuracy of the

calculated solution density would not have been significantly improved at low electrolyte concentration because the water density is the most important term in eq 6 in this situation. At high electrolyte concentration, however, the additional error in determining the electrolyte apparent specific volume would have caused a significantly worse estimation of the solution density.

Figure 2 shows the experimental and calculated density of MgSO₄ solutions at the same temperatures as in Figure 1. The fit is excellent, even at low concentration where there is a significant difference between the experimental and calculated apparent specific volumes.

Table 2. Statistical Results for Fit of Constants c_0 to c_4 from Equation 9

	t min/°C	t max/°C	w min	w max	average solution density residual/kg/m ³	standard deviation of solution density residual/kg/m ³	average electrolyte specific volume residual/l/kg	standard deviation of electrolyte specific volume residual/l/kg	number of points used in the correlation	number of inconsistent point
AlCl ₃	25	25	0.00230	0.19356	0.08084	0.27545	-0.01943	0.04774	21	2
Al ₂ (SO ₄) ₃	15	95	0.00972	0.39800	0.06667	0.65002	-0.00255	0.00586	64	4
BaCl ₂	0	140	0.00081	0.26000	0.03801	0.49239	-0.00186	0.00482	140	1
CaCl ₂	0	100	0.00139	0.51320	0.20714	1.03856	-0.00841	0.01250	357	2
CdCl ₂	25	75	0.00190	0.53833	0.10512	0.41154	-0.00280	0.01455	88	90
CdSO ₄	25	75	0.00001	0.29671	0.08388	0.54655	-0.01114	0.02463	45	24
CoCl ₂	15	75	0.00131	0.34452	0.11563	0.69019	-0.00610	0.00861	171	1
CoSO ₄	25	75	0.00008	0.33050	-0.03259	1.68202	-0.01342	0.11682	34	7
CrCl ₃	18	18	0.01000	0.12000	-0.06859	0.13855	0.00313	0.00281	5	0
Cr ₂ (SO ₄) ₃	25	25	0.00001	0.00149	0.00515	0.01167	-0.10673	0.19405	16	0
CuCl ₂	0	55	0.00135	0.42036	0.00418	0.62217	-0.00092	0.01241	116	3
CuSO ₄	0	60	0.00161	0.28440	0.03240	0.98107	-0.00382	0.01693	232	3
FeCl ₂	15	45	0.00012	0.20968	0.01412	0.13982	-0.00864	0.01622	93	0
FeSO ₄	15	75	0.00200	0.27401	-0.34048	4.95152	0.01509	0.03989	72	5
FeCl ₃	0	30	0.01000	0.50000	0.21341	1.24076	-0.00832	0.01396	47	0
Fe ₂ (SO ₄) ₃	15	25	0.01000	0.60000	0.08538	9.26838	-0.00123	0.03505	67	0
HCl	-5	100	0.00037	0.40000	0.08895	0.84965	-0.00566	0.01024	331	0
HCN	0	15	0.01000	1.00000	0.15182	2.12717	-0.00933	0.02463	18	0
HNO ₃	-10	100	0.00104	0.80110	-0.04043	2.29532	0.00331	0.00963	476	2
H ₃ PO ₄	15.85	81.4	0.00100	0.85000	0.10601	0.37553	-0.00518	0.00971	196	0
H ₂ SO ₄	0	100	0.00005	0.77060	0.08914	1.14088	-0.01912	0.06636	332	6
KCl	0	125	0.00007	0.28000	0.06154	0.22885	-0.00971	0.02848	688	5
K ₂ CO ₃	0	100	0.01000	0.58240	0.50966	2.75832	-0.00978	0.01984	170	1
KNO ₃	0	100	0.00105	0.24000	0.03281	0.21962	-0.00279	0.00458	206	27
KOH	0	100	0.00084	0.59460	0.15383	1.51866	-0.00991	0.01879	421	9
K ₂ SO ₄	0	98.67	0.00035	0.10970	0.03750	0.15534	-0.00915	0.01927	230	7
LiCl	5	95	0.00212	0.45390	0.34210	0.92901	-0.01654	0.01959	332	0
Li ₂ SO ₄	0	65	0.00009	0.26021	0.04565	0.35769	-0.01014	0.01923	145	1
MgCl ₂	0	100	0.00024	0.32748	0.23446	0.85186	-0.02122	0.02081	400	6
MgSO ₄	0	125	0.00006	0.26000	0.16889	0.75475	-0.02575	0.05259	331	17
MnCl ₂	15	75	0.00122	0.43468	0.08571	0.61832	-0.00496	0.00867	186	0
MnSO ₄	0	45	0.00001	0.36398	0.01826	0.94715	-0.01108	0.02885	114	36
NaBr	15	91.95	0.00512	0.54816	0.03090	0.32130	-0.00182	0.00386	139	20
NaCl	0	140	0.00006	0.26031	0.07133	0.33349	-0.00568	0.01129	630	7
NaClO ₃	18	35	0.00053	0.50097	0.06097	0.79294	-0.01679	0.06039	79	1
Na ₂ CO ₃	0	45	0.00042	0.30824	0.06081	0.84564	-0.00819	0.01590	147	0
NaF	0	98.67	0.00041	0.03744	0.02489	0.29430	-0.01375	0.07657	85	6
NaHCO ₃	0	45	0.00025	0.07810	0.01642	0.12809	-0.00381	0.00745	91	176
NaH ₂ PO ₄	5	80	0.00012	0.60000	0.47090	2.35507	-0.07216	0.09928	38	3
Na ₂ HPO ₄	40	80	0.05000	0.30000	-0.00875	0.62112	0.00038	0.00355	12	0
NaHSO ₃	10	40	0.00103	0.24298	-0.00850	1.14795	-0.01228	0.05942	91	1
NaI	0	99.96	0.00656	0.75037	0.05082	0.80436	-0.00171	0.00400	92	3
Na ₂ MoO ₄	25	80	0.00611	0.35000	0.09456	0.28754	-0.00540	0.00753	30	0
NaNO ₂	15	20	0.01000	0.20000	0.00892	0.17519	-0.00086	0.00259	11	0
NaNO ₃	0	100	0.00128	0.68820	0.04938	0.60805	-0.00306	0.00716	252	29
NaOH	0	120	0.00050	0.70000	0.17220	2.71593	-0.01094	0.02659	623	12
Na ₃ PO ₄	40	80	0.05000	0.30000	-0.02280	0.83275	0.00075	0.00388	14	0
Na ₂ SO ₃	19	80	0.01000	0.20000	-0.02610	3.08175	-0.00230	0.06546	43	0
Na ₂ S ₂ O ₃	20	80	0.00399	0.60000	0.84240	1.83868	-0.02573	0.02516	50	0
Na ₂ SO ₄	0	125	0.00032	0.24000	0.16611	0.51522	-0.01924	0.04224	340	9
NH ₃	0	100	0.01000	0.30000	0.05431	0.73499	-0.00363	0.01578	172	4
NH ₄ Cl	0	100	0.00005	0.40000	0.10373	0.59267	-0.00599	0.01778	387	2
NH ₄ NO ₃	0	95	0.00448	0.78740	-0.00268	1.35067	0.00037	0.00426	162	26
(NH ₄) ₂ SO ₄	0	100	0.00656	0.50000	0.27713	1.03004	-0.01061	0.01354	174	0
NiCl ₂	15	75	0.00045	0.39244	0.12238	0.56366	-0.00722	0.01108	224	6
NiSO ₄	15	60	0.00005	0.35329	0.04764	0.35323	-0.00456	0.01012	107	8
SrCl ₂	15	98.81	0.00059	0.28382	-0.00564	1.25027	-0.00131	0.00738	98	6
ZnCl ₂	0	100	0.00138	0.70000	-0.02405	0.85636	0.00357	0.01414	240	7
ZnSO ₄	15	60	0.00165	0.36772	0.03498	0.96533	-0.00401	0.00990	227	33
average					0.10438		-0.00866			

Experimental data points with significant error were removed from the calculation of the constants but are included for reference. Significant error here is defined as a point where the residual is greater than the average residual plus or minus 4 times the standard deviation of the residuals. This was tested for both the density residual and the apparent specific volume residual. This rule was not blindly followed, however. If the residual could be

seen as being part of a pattern of residuals going steadily worse, typically as the electrolyte mass fraction was going toward a minimum or a maximum, then the point was kept. However, if the residual was found to be significantly different from similar data points, then it was removed. This is usually a sign of a measurement or a transcription error. All inconsistent data points have been kept in the Supporting Information for further study and

Table 3. Interpolating and Extrapolating Density Data for NH₄NO₃ over Mass Fraction

range	all data: constants c_0 to c_4 fitted over the entire data/kg m ⁻³		interpolation: constants c_0 to c_4 fitted only where $w_i \leq 0.25$ or $w_i \geq 0.55$ /kg m ⁻³		extrapolation: constants c_0 to c_4 fitted only where $w_i \leq 0.4$ /kg m ⁻³	
	residual	standard deviation	residual	standard deviation	residual	standard deviation
$w_i \leq 0.1$	-0.0126	0.3134	-0.0800	0.3219	0.0545	0.2168
$0.1 < w_i \leq 0.2$	-0.0247	0.9325	-0.1546	0.9315	-0.0107	0.8179
$0.2 < w_i \leq 0.3$	-0.0053	1.1657	-0.0839	1.1982	0.0443	0.5680
$0.3 < w_i \leq 0.4$	-0.1505	1.0908	-0.1394	1.1334	-0.2966	0.6659
$0.4 < w_i \leq 0.5$	-0.0845	1.2968	-0.0007	1.3734	0.3383	0.3960
$0.5 < w_i \leq 0.6$	0.7051	1.7808	0.7975	1.8365	3.9139	2.8375
$0.6 < w_i \leq 0.7$	-0.6898	2.0528	-0.6531	1.9793	5.4216	4.0500
$0.7 < w_i \leq 0.8$	0.1778	1.3411	0.1352	1.3466	9.3939	2.4608

Table 4. Interpolating and Extrapolating Density Data for NH₄NO₃ over Temperature

range	all data: constants c_0 to c_4 fitted over the entire data/kg m ⁻³		interpolation: constants c_0 to c_4 fitted only where $t \leq 30$ °C or 70 °C/ t /kg m ⁻³		extrapolation: constants c_0 to c_4 fitted only where $t \leq 55$ °C/kg m ⁻³	
	residual	standard deviation	residual	standard deviation	residual	standard deviation
$t < 10$ °C	1.3701	0.7059	1.1927	0.5773	0.5837	0.3488
10 °C $\leq t < 20$ °C	0.1487	0.1458	0.0025	0.1237	-0.1210	0.3108
20 °C $\leq t < 30$ °C	-0.7216	0.9689	-0.6451	0.9487	-0.4019	0.8846
30 °C $\leq t < 40$ °C	0.1736	1.1701	1.3485	0.7956	0.7904	1.1278
40 °C $\leq t < 50$ °C	-0.3461	1.1309	0.2488	1.6369	0.1297	1.0129
50 °C $\leq t < 60$ °C	0.3468	1.3913	1.6458	1.4481	-0.1526	1.5924
60 °C $\leq t < 70$ °C	0.0034	1.1681	0.5982	1.5558	-0.4191	1.6686
70 °C $\leq t < 80$ °C	0.3847	1.8403	1.4270	1.7511	-1.9591	2.5133
80 °C $\leq t < 90$ °C	0.4964	0.5605	0.2839	0.4698	1.3804	1.1177
90 °C $\leq t < 100$ °C	-0.1185	2.7742	-0.2839	2.5867	-0.8945	4.5935

are identified by an exclamation point “!” to the right of the residuals.

Although the occasional single experimental point had to be removed, sometimes an entire data set was inconsistent with several others. If the data set was from an older publication, then it was usually ignored and is not necessarily presented in the Supporting Information, especially if the electrolyte has been well studied and many other data are available. However, if the inconsistent data set was from a more recent publication, then it was not used in the estimation of constants c_0 to c_4 but was kept in the Supporting Information for reference.

A good example is CdCl₂, where the set of data from Call⁹ and the three sets from Herrington,³⁷ Rard,¹⁰⁴ and Reilly¹⁰⁷ are mutually inconsistent. The densities measured by Call are systematically higher than those measured by Herrington, Rard, and Reilly. (The densities from Dolian²³ could be interpreted as being consistent with any of these sets.) In this case, we have used the densities from Herrington, Rard, and Reilly, reasoning that three sets of data were less likely to be wrong than one. We have also kept Dolian's set. It is perhaps significant that Call did not check the purity of the CdCl₂ he used in his experiments but trusted the certificate of analysis provided by his supplier. In the same paper, Call reported measurements on MgCl₂ that are consistent with other data sets for this electrolyte.

Results and Discussion

The values of constants c_0 to c_4 from eq 9 are given in Table 1. Also included in Table 1 is the calculated specific volume $\bar{v}_{app,i}$ of the electrolyte at $w_i = 0.01$ and $t = 25$ °C. This value can be used to determine whether the constants were properly entered when recalculating specific volume. Statistical results, including the average residual and standard deviation for both the solution density and the

electrolyte apparent specific volume, are given in Table 2. The apparent specific volume residual is on average -0.0087 l kg⁻¹ with a standard deviation of 0.028 l kg⁻¹. When using these apparent specific volumes in eq 6, the average solution density residual is 0.10 kg m⁻³ with a standard deviation of 1.44 kg m⁻³. These values are calculated over all consistent points and are not an average of the average value for each electrolyte.

Equations 6 and 9 were tested for their usefulness in predicting density outside the range used in estimating their coefficients, both for extrapolation and interpolation. NH₄NO₃ was chosen as the test case because its density residual standard deviation is 1.35 kg m⁻³, close to the average value for all data sets, and because data are available for it over a wide range of concentration and temperature.

Equations 6 and 9 were first tested for extrapolation and interpolation over the mass fraction. The data were split by slices of 0.1 mass fraction, and the model predictions were compared for the full data set, fitting the data only where the mass fraction is below 0.25 or above 0.55 (interpolation) or fitting the data only where the mass fraction is below 0.4 (extrapolation). Results are found in Table 3.

There is no significant difference when comparing the results over the entire data set and when interpolating over the mass fraction. Results when extrapolating over the mass fraction are different. When extrapolating by less than a mass fraction of 0.1, the fit is still quite good. With an extrapolation of 0.2 mass fraction, there is some degradation in the fit quality, and above this value the degradation becomes significant both in terms of the average residual and in terms of the standard deviation. The density of solutions of NH₄NO₃ of a mass fraction of 0.7 is on the order of 1350 kg m⁻³, however, and an average residual of 9 kg m⁻³ with a standard deviation of 2.5 kg m⁻³ might still be acceptable for many calculations.

Table 5. Statistical Results for Solutions of More than One Electrolyte in Water (Part 1)

electrolyte 1	electrolyte 2	electrolyte 3	electrolyte 4	average density residual kg/m ³ (eqs 6 and 9)	std dev of density residual kg/m ³ (eqs 6 and 9)	average density residual kg/m ³ (eqs 6 and 10)	std dev of density residual kg/m ³ (eqs 6 and 10)	number of points used	number of inconsistent points
BaCl ₂	NaCl			-1.03	1.80	0.27	0.69	288	0
CaCl ₂	KCl			-1.76	2.83	0.26	0.67	162	0
CaCl ₂	KCl	MgCl ₂	NaCl	-14.41	0.96	-3.64	0.97	75	0
CaCl ₂	MgCl ₂			-0.42	1.85	0.88	1.48	72	0
CaCl ₂	NaCl			-2.75	3.29	-0.11	1.38	222	0
CdCl ₂	HCl			-9.68	8.19	-3.91	3.86	19	0
CuCl ₂	HCl			-8.07	7.26	-1.30	1.82	20	0
CuSO ₄	H ₂ SO ₄			-6.90	5.37	-2.10	1.33	36	0
Fe ₂ (SO ₄) ₃	Na ₂ SO ₄			-2.81	3.39	0.87	2.47	9	3
Fe ₂ (SO ₄) ₃	NaBr			1.21	0.99	3.03	1.43	16	0
Fe ₂ (SO ₄) ₃	NaCl			0.84	2.28	4.20	1.81	12	0
Fe ₂ (SO ₄) ₃	NaNO ₃			1.82	0.93	3.84	1.75	16	0
HCl	MnCl ₂			-5.85	4.05	3.94	3.71	76	0
KCl	K ₂ SO ₄			-1.61	0.62	-0.26	0.28	30	0
KCl	MgCl ₂			-1.97	2.37	-0.61	0.80	36	0
KCl	NaBr			-1.73	1.65	0.23	0.25	31	0
KCl	NaCl			-2.50	2.48	-0.16	0.70	145	0
KCl	Na ₂ SO ₄			-1.44	0.80	-0.28	0.41	30	0
KCl	(NH ₄) ₂ SO ₄			-2.10	1.30	-0.27	0.48	6	0
K ₂ SO ₄	NaCl			-1.66	0.68	-0.45	0.36	32	0
K ₂ SO ₄	Na ₂ SO ₄			-1.99	3.95	-0.80	3.80	28	0
MgCl ₂	NaCl			-1.35	1.72	0.72	0.98	72	0
MgSO ₄	NaCl			0.34	1.36	1.10	1.15	66	0
MgSO ₄	Na ₂ SO ₄			0.71	0.97	0.80	0.95	54	61
NaCl	Na ₂ SO ₄			-0.38	1.01	0.12	0.78	81	0
NaCl	NH ₄ NO ₃			-6.12	6.64	-0.44	0.83	17	0
Na ₂ SO ₄	(NH ₄) ₂ SO ₄			-10.87	5.79	-0.91	1.67	6	0
average std dev number				-0.050		0.003			
					2.750		1.393	1657	64
inconsistent data sets									
FeSO ₄	H ₂ SO ₄			-8.07	11.74	16.65	13.89	0	26
Fe ₂ (SO ₄) ₃	FeSO ₄	H ₂ SO ₄		-32.64	40.53	-14.58	40.31	0	112
H ₂ SO ₄	MnSO ₄			-32.17	34.45	-16.57	34.61	0	38
MnSO ₄	Na ₂ SO ₄			-40.59	16.79	-26.75	13.64	0	13
number									189

The same method was used to evaluate the usefulness of eqs 6 and 9 when interpolating or extrapolating over temperature. Refer to Table 4.

Once again this proves that there is no significant degradation of the fit quality when interpolating data. When extrapolating, there is a significant increase in the standard deviation as the temperature difference increases to 40 °C or more, but this increase is less pronounced than when extrapolating over mass fraction. It should also be noted that restricting the range of mass fraction or temperature used in calculating constants c_0 to c_4 does slightly increase the accuracy of the fit over that range, as indicated by the decrease in the standard deviation.

Prediction of the Density of Solutions of More Than One Electrolyte in Water

Equations 6 and 9 were tested to determine if they could accurately predict data for solutions of more than one electrolyte in water. Data for these solutions are limited, but measurements for 29 different systems of 2 electrolytes in water, 1 system of 3 electrolytes in water, and 1 system of 5 electrolytes in water were found, close to 2000 data points. Not all of these data points were consistent, however; see below.

During the course of this validation, it was found that eqs 6 and 9 were adequate for multielectrolyte solutions at low concentrations. However, at higher concentrations, the error in the calculated density was higher than desired.

It was found that a subtle modification of eq 9 decreased this error significantly. By using the total electrolyte concentration ($1 - w_{\text{H}_2\text{O}}$) instead of the concentration of just the electrolyte in question (w_i) to calculate the electrolyte apparent specific volume, the model was found to be significantly more accurate. The modified form of eq 9 is

$$\bar{V}_{\text{app},i} = \frac{(1 - w_{\text{H}_2\text{O}}) + c_2 + c_3 t}{(c_0(1 - w_{\text{H}_2\text{O}}) + c_1)e^{(0.000001(t+c_4)^2)}} \quad (10)$$

This equation reduces to eq 9 for a solution of just one electrolyte in water. Using eq 10 to calculate the apparent specific volume and eq 6 to calculate the solution density yielded excellent results. Tables 5 and 6 show the results; with eqs 6 and 9, the average solution density residual is -0.05 kg m^{-3} with a standard deviation of 2.75 kg m^{-3} . Using eq 6 and 10 gives an average solution density residual of 0.003 kg m^{-3} with a standard deviation of 1.39 kg m^{-3} . This standard deviation compares favorably with the standard deviation of 1.44 kg m^{-3} for systems of one electrolyte in water.

Four data sets have a much higher standard deviation: solutions of FeSO₄ and H₂SO₄, of FeSO₄, Fe₂(SO₄)₃, and H₂SO₄, of H₂SO₄ and MnSO₄, and finally of MnSO₄ and Na₂SO₄. For all of these data sets, no recent references were found (except data from Przepiera,¹⁰³ which date from 2000). For these four systems, the standard deviation is

Table 6. Statistical Results for Solutions of More than One Electrolyte in Water (Part 2)

electrolyte 1	electrolyte 2	electrolyte 3	electrolyte 4	<i>t</i> min °C	<i>t</i> max °C	w min electro- lyte 1	w max electro- lyte 1	w min electro- lyte 2	w max electro- lyte 2	w min electro- lyte 3	w max electro- lyte 3	w min electro- lyte 4	w max electro- lyte 4	refs
BaCl ₂	NaCl			25	140	0.003	0.215	0.003	0.187	0.000	0.000	0.000	0.000	67
CaCl ₂	KCl			25	25	0.000	0.267	0.000	0.251	0.000	0.000	0.000	0.000	59, 136
CaCl ₂	KCl	MgCl ₂	NaCl	20	40	0.036	0.040	0.010	0.012	0.117	0.141	0.079	0.083	56
CaCl ₂	MgCl ₂			22.87	98.67	0.009	0.136	0.008	0.109	0.000	0.000	0.000	0.000	115
CaCl ₂	NaCl			5	98.67	0.001	0.259	0.000	0.203	0.000	0.000	0.000	0.000	58, 77, 115, 136
CdCl ₂	HCl			25	25	0.000	0.379	0.000	0.267	0.000	0.000	0.000	0.000	128
CuCl ₂	HCl			25	25	0.000	0.309	0.000	0.267	0.000	0.000	0.000	0.000	128
CuSO ₄	H ₂ SO ₄			25	40	0.032	0.128	0.000	0.200	0.000	0.000	0.000	0.000	42
Fe ₂ (SO ₄) ₃	Na ₂ SO ₄			25	25	0.043	0.168	0.030	0.123	0.000	0.000	0.000	0.000	14
Fe ₂ (SO ₄) ₃	NaBr			25	25	0.045	0.169	0.022	0.093	0.000	0.000	0.000	0.000	15
Fe ₂ (SO ₄) ₃	NaCl			25	25	0.045	0.169	0.025	0.105	0.000	0.000	0.000	0.000	14
Fe ₂ (SO ₄) ₃	NaNO ₃			25	25	0.046	0.170	0.018	0.078	0.000	0.000	0.000	0.000	15
HCl	MnCl ₂			25	25	0.001	0.335	0.005	0.412	0.000	0.000	0.000	0.000	128
KCl	K ₂ SO ₄			5	95	0.012	0.115	0.010	0.092	0.000	0.000	0.000	0.000	20
KCl	MgCl ₂			25	25	0.004	0.220	0.003	0.113	0.000	0.000	0.000	0.000	60
KCl	NaBr			25	25	0.007	0.200	0.008	0.263	0.000	0.000	0.000	0.000	61
KCl	NaCl			5	95	0.001	0.210	0.001	0.184	0.000	0.000	0.000	0.000	20, 30, 77, 135
KCl	Na ₂ SO ₄			5	95	0.012	0.115	0.008	0.076	0.000	0.000	0.000	0.000	20
KCl	(NH ₄) ₂ SO ₄			25	25	0.032	0.062	0.059	0.113	0.000	0.000	0.000	0.000	30
K ₂ SO ₄	NaCl			5	95	0.011	0.092	0.010	0.092	0.000	0.000	0.000	0.000	20
K ₂ SO ₄	Na ₂ SO ₄			5	95	0.002	0.092	0.008	0.083	0.000	0.000	0.000	0.000	20
MgCl ₂	NaCl			22.87	98.67	0.009	0.107	0.015	0.203	0.000	0.000	0.000	0.000	115
MgSO ₄	NaCl			25	125	0.001	0.152	0.006	0.127	0.000	0.000	0.000	0.000	27, 77
MgSO ₄	Na ₂ SO ₄			25	125	0.001	0.035	0.001	0.021	0.000	0.000	0.000	0.000	27, 63
NaCl	Na ₂ SO ₄			5	125	0.006	0.127	0.001	0.076	0.000	0.000	0.000	0.000	20, 27
NaCl	NH ₄ NO ₃			25	25	0.007	0.218	0.010	0.386	0.000	0.000	0.000	0.000	77
Na ₂ SO ₄	(NH ₄) ₂ SO ₄			25	25	0.051	0.101	0.058	0.236	0.000	0.000	0.000	0.000	30
average														
std dev														
number														
inconsistent	data sets													
FeSO ₄	H ₂ SO ₄			-10	25	0.024	0.207	0.014	0.250	0.000	0.000	0.000	0.000	63
Fe ₂ (SO ₄) ₃	FeSO ₄	H ₂ SO ₄		25	80	0.000	0.220	0.000	0.152	0.001	0.067	0.000	0.000	76
H ₂ SO ₄	MnSO ₄			12.6	45	0.058	0.991	0.001	0.297	0.000	0.000	0.000	0.000	63, 103
MnSO ₄	Na ₂ SO ₄			97	97	0.007	0.265	0.022	0.295	0.000	0.000	0.000	0.000	63
number														

more than 6 times the standard deviation of all of the other data. This makes the data for these systems highly suspect, and the data sets have been excluded from the calculation of the average and standard deviation. They have been included for reference in the supplementary data.

Conclusions

An empirical model has been developed that can predict the density of aqueous solutions of one or more electrolytes. Experimental data from 59 electrolytes have been fit to the model over a wide range of temperature and concentration. The model has been tested by calculating the difference between the experimental and predicted density of solutions of more than one electrolyte in water. The average difference was found to be 0.10 with a standard deviation of 1.42 kg m⁻³ over a wide range of temperature and concentration.

Further Work

As explained above, one of the main sources of inaccuracy in the model presented here is the lack of consistency between different data sets. This is particularly the case for many metal sulfates, where there is very little published information and what has been published is often of poor quality. The data for CoSO₄, FeSO₄, and Fe₂(SO₄)₃ are especially poor. Additional experimental data for these electrolytes, perhaps also as mixtures with H₂SO₄, over a wide range of concentration and temperature would definitely be helpful.

For some electrolytes such as NaOH and HNO₃, there is a lot of consistent information available, but eqs 6 and 9 do not represent the data perfectly. In addition to the

expected apparent volume residual at low concentration, the model tends to over or underestimate the density at various mass fractions, and this over or underestimation varies with temperature. We are reasonably confident that this effect is real and is not caused by inconsistent data, but there is no obvious modification to eq 9 that could represent this behavior easily.

List of Symbols

- c_0 , empirical constant in eqs 9 and 10, kg m⁻³
- c_1 , empirical constant in eqs 9 and 10, kg m⁻³
- c_2 , empirical constant in eqs 9 and 10, dimensionless
- c_3 , empirical constant in eqs 9 and 10, °C⁻¹
- c_4 , empirical constant in eqs 9 and 10, °C
- t , temperature, °C
- $V_{app,i}$, apparent volume of component i , m³
- $\bar{V}_{app,i}$, specific volume of component i , m³ kg⁻¹
- V_i , volume of ideal component i , m³
- V_{H_2O} , volume of water, m³
- V_m , volume of the mixture, m³
- w_{H_2O} , mass fraction of water
- w_i , mass fraction of component i
- $\rho_{app,i}$, apparent density of component i , kg m⁻³
- ρ_{H_2O} , density of water, kg m⁻³
- ρ_i , density of ideal component i , kg m⁻³
- ρ_m , density of the mixture, kg m⁻³

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Supporting Information Available:

Calculation spreadsheets for all of the electrolyte solutions presented in Tables 1, 2, and 5. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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