Measurement and Prediction of Physicochemical Properties of Liquors Relevant to the Sulfate Process for Titania Production. 1. Densities in the $TiOSO_4 + FeSO_4 + H_2SO_4 + H_2O$ System[†]

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No reliable model for the prediction of densities has been reported for the title system. Since this is partly due to conflicting experimental data available in the literature, densities in the title system have been measured by high-precision vibrating-tube densimetry over wide concentration ranges. Measurements comprise binary (single electrolyte) and mixed (ternary) acidic solutions of titanyl sulfate at (25 and 50) °C as well as binary, ternary, and quaternary mixtures containing iron(II) sulfate at 25 °C. We have found that a pro-rata additivity rule for densities applies to a series of aqueous metal sulfate + sulfuric acid mixtures at constant total sulfate concentration, based on hypothetical densities in the supersaturated concentration ranges of the binary metal sulfate subsystems. These hypothetical densities can be readily obtained by extrapolation of the properties of mixed solutions. When included in Masson-type density correlations for the binary metal sulfate systems, the resulting model resolves the reported inconsistencies in density predictions for the $FeSO_4 + H_2SO_4 + H_2O$ system. This is the first density model that includes $TiOSO_4$ as a component.

Introduction

The sulfate process for titania (TiO_2) production[1] involves leaching of ilmenite (ideal composition $FeTiO_3$) in sulfuric acid, followed by reduction of Fe(III) (arising from appreciable Fe_2O_3 contents of some ores[2]) and precipitation of $FeSO_4 \cdot 7H_2O$ ("copperas"). Finally, the purified, acidic solution of titanyl sulfate ($TiOSO_4$) is decomposed hydrolytically to form titania.

The densities of such plant liquors are important parameters for process control and engineering design purposes related to sizing and various heat and mass transfer operations. In particular, density is needed for the conversion of concentration units, e.g., from the frequently reported mass-based units to the industry-preferred unit, $g \cdot L^{-1}$. Also, volumetric properties of solutions are required to calculate the variation of other thermodynamic quantities as a function of pressure.

In the industrial context, physicochemical property models are often parametrized by regression of data which have in general been measured on multicomponent solutions, the industrial plant liquors themselves in most cases. Such purely empirical models are highly susceptible to parameter correlation, leading to propagation in the uncertainties and consequent failures when attempts are made to extrapolate to smaller subsystems or beyond the ranges of parametrization.

More fundamental models thus start from accurate, semi-empirical descriptions of the solvent and the constituent binary systems (in the present case, one electrolyte plus water). Properties of the multicomponent system are then frequently predicted by simple, linear chemical "mixing rules". Such rules, which have been well established experimentally, include those of Harned, Lietzke & Stoughton, and others for activity coefficients,[3−5] Robinson and Stokes for vapor pressure,[3] Zdanovskii for isopiestic molalities and solubilities,[6] Young's pro-rata additivity rule for densities and heat capacities,[7−9] and Young's "cross-square" rule for enthalpies.[10] It should be noted that these linear rules operate at constant total concentration, ionic strength, or water activity.

Laliberté and Cooper[11] have presented a model for the calculation of densities of mixed electrolyte solutions which employs a linear mixing rule for apparent specific volumes. The model is based on data for 59 binary electrolytes, including $FeSO_4$, $Fe_2(SO_4)_3$, and H_2SO_4. $TiOSO_4$ was, however, not considered. Laliberté and Cooper concluded that densities reported for some ternary (two electrolytes plus water) and quaternary (three electrolytes plus water) systems, including $FeSO_4 + H_2SO_4 + H_2O$ and $FeSO_4 + Fe_2(SO_4)_3 + H_2SO_4 + H_2O$, were inconsistent with model predictions based on data for the constituent binary systems.

Acidic leach liquors may reach high acid concentrations in certain stages of the refinement process. The prediction of properties of mixed solutions by the mixing rules mentioned above would then require the knowledge of these properties for the binary (salt) solutions at high supersaturation. In this paper, we focus especially on this aspect which has often been overlooked in the literature.

Experimental

Density Measurements. Densities were measured at (25.00 and 50.00) °C (± 0.02 °C) using an Anton Paar (Austria) vibrating tube density meter (model DMA 602), calibrated with high-purity water and nitrogen. Since the densities of aqueous solutions are higher than those of the reference substances, this demands that the calibration constant be applicable at densities outside the calibration range, i.e., that the vibrating tube acts as a strictly harmonic oscillator under all conditions. This assumption appears to be reasonable under near-ambient conditions.[12]

Samples were injected into the dry vibrating tube using syringes equipped with 0.45 μm membrane filters. The sample was allowed to reach thermal equilibrium for several minutes,

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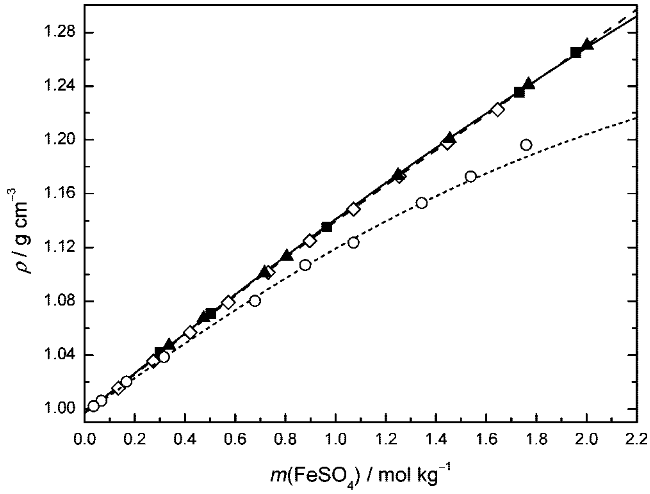

Figure 1. Densities of $FeSO_4$(aq) at 25 °C. ▲, this work, set 1; ■, this work, set 2; ○, ref 14; ◇, ref 15. The two sets of data measured in this work were obtained with independently prepared stock solutions. For a discussion of the various correlations, see text.

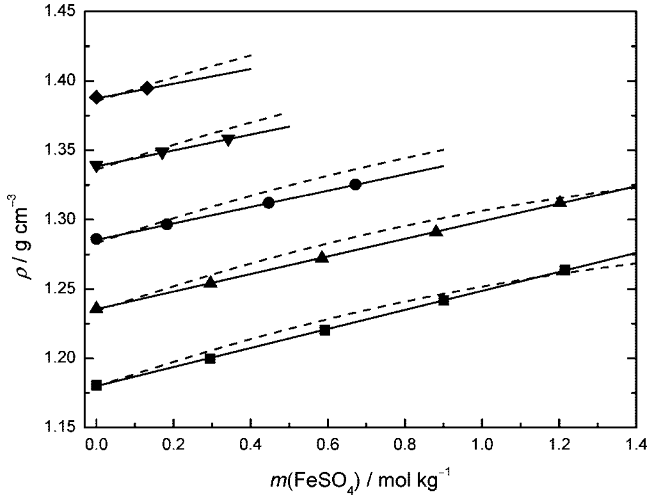

Figure 2. Densities of $FeSO_4 + H_2SO_4$ solutions at 25 °C and constant total sulfate concentrations of ■, 300 $g\cdot L^{-1}$; ▲, 400 $g\cdot L^{-1}$; ●, 500 $g\cdot L^{-1}$; ▼, 600 $g\cdot L^{-1}$; ◆, 700 $g\cdot L^{-1}$. At higher total sulfate concentration, the experimentally accessible range is limited by the solubility of iron sulfate monohydrate. Solid lines, linear mixing rule; dashed lines, model of Laliberté and Cooper[11] for ternary $FeSO_4 + H_2SO_4$ solutions.

and the periods of vibration were measured. Two such readings were taken for each of the solutions and only recorded when the periods obtained were stable within a random variation in the last (sixth) digit. The uncertainty in the measured density was therefore less than $1\cdot10^{-5}$ $g\cdot cm^{-3}$. After each reading, the tube was washed with dilute acid solution and water, then emptied, rinsed with analytical-grade acetone, and dried using compressed nitrogen. The period readings of water and nitrogen were checked frequently to ensure that the performance of the glass vibrating tube had not been compromised by chemical attack or deposition of solids.

Preparation and Analysis of $FeSO_4 + H_2SO_4$ Solutions. Two stock solutions of $FeSO_4$ were prepared by dissolving iron(II) sulfate heptahydrate (BDH, AnalaR) in high purity, CO_2-free water (Millipore MilliQ system). The densities of (0.25 to 1.75) $mol\cdot kg^{-1}$ $FeSO_4$ solutions were measured in duplicate at 25 °C. Using concentrated sulfuric acid and Millipore MilliQ water, solutions of H_2SO_4 concentrations from (300 to 700) $g\cdot L^{-1}$ were made in 250 mL volumetric flasks, and their densities were determined at 25 °C using the procedure mentioned above. Ternary $FeSO_4 + H_2SO_4 + H_2O$ mixtures were prepared by dissolving high-purity metallic iron (Merck, p. a.) in these sulfuric acid solutions.

The determination of the Fe(II) content was carried out in acidic solution with a 0.001667 $mol\cdot L^{-1}$ potassium dichromate standard solution prepared from Volucon (France) ampoules and sodium diphenylamine sulfonate indicator. Determination of Fe(III) was performed by iodometric titration, using a 500 $g\cdot L^{-1}$ KI solution (which was stored in the dark) and a 0.1 $mol\cdot L^{-1}$ $Na_2S_2O_3$ solution standardized with KIO_3. The concentration of sulfuric acid was determined by titration with standard, carbonate-free NaOH solution with methyl orange as the indicator. Sulfuric acid in acidic iron(II) sulfate solutions was determined after addition of potassium oxalate as a complexing agent. Using bromothymol blue indicator, the solution was titrated against standard, carbonate-free NaOH solution.[13]

The concentrations of Fe(II) and Fe(III) in acidic ferrous sulfate solutions were determined as described above. The uncertainty in the Fe(II) molality was 0.1 %. Fe(III) was generally found to be negligible.

Preparation and Analysis of $TiOSO_4 + H_2SO_4$ Solutions. The preparation of sulfuric acid solutions is described above. Titanyl sulfate solutions were prepared using a solid "$TiOSO_4\cdot 2H_2O + H_2SO_4$ complex" (Aldrich) that had been purified of sulfuric acid by thorough washing with ethanol. Gravimetric and X-ray diffraction analyses showed that the purified material corresponded to $TiOSO_4\cdot 2H_2O$. The exact Ti content was determined UV−vis spectrophotometrically via the Ti(IV) complex with hydrogen peroxide.[13] Standard solutions were made from high-purity Ti metal (Aldrich, 99.98 %) dissolved in H_2SO_4 solutions of appropriate concentration. Some of these solutions were used for density measurements after oxidizing Ti(III) with pure oxygen supplied from a cylinder. The uncertainty in the resulting $TiOSO_4$ concentration was estimated as 0.1 %.

Results and Discussion

$FeSO_4 + H_2SO_4 + H_2O$ System. Densities measured at 25 °C for binary $FeSO_4$(aq) solutions were correlated using the Masson equation (eq 1) for which the constants a to d were adjusted with respect to experimental density data.

$$\rho = \rho o + a(m/m°) + b(m/m°)^{3/2} + c(m/m°)^2 + d(m/m°)^{5/2} \qquad (1)$$

where ρ is the density of the binary solution; $\rho°$ is the density of water (0.997047 $g\cdot cm^{-3}$ at 25 °C); m is the $FeSO_4$ molality in moles per kilogram of water; and $m° \equiv 1$ $mol\cdot kg^{-1}$. For H_2SO_4(aq), the temperature-dependent correlation of Laliberté and Cooper[11] was employed as it agreed very well with the present measurements.

Figure 1 is a graphical representation of the present densities of $FeSO_4$ at 25 °C. There are conflicting data sets in the literature.[14,15] The values of Bakeev et al.[14] have been used by Laliberté and Cooper[11] for parametrization of their model (dotted line in Figure 1). However, the densities measured in the present work agree much better with the data compiled by Aseyev and Zaytsev[15] and were used to obtain the constants a to d of the Masson equation (eq 1). Our recommended set of constants, given in Table 1 and corresponding to the solid line in Figure 1, includes the density data for the hypothetical, supersaturated solutions that were obtained by extrapolation (see below). Another set of constants, obtained by excluding these hypotheti-

Table 1. Masson Parameters for $FeSO_4(aq)$ and $TiOSO_4(aq)$ at 25 °C

	$FeSO_4(aq)$	$TiOSO_4(aq)$
a	0.14219422	0.13065842
b	0.02261627	−0.0076366091
c	−0.024811662	−0.0016696575
d	0.003945851	−

Table 2. Densities in the $FeSO_4 + H_2SO_4 + H_2O$ System at 25 °C

$c(H_2SO_4)$ $g\cdot L^{-1}$	$m(H_2SO_4)$ $mol\cdot kg^{-1}$	$m(FeSO_4)$ $mol\cdot kg^{-1}$	ρ $g\cdot cm^{-3}$
	0	2.002	1.27016
	0	1.769	1.24105
	0	1.454	1.20059
	0	1.248	1.17352
	0	0.805	1.11332
	0	0.717	1.10109
	0	0.474	1.06739
	0	0.336	1.04699
	0	1.957	1.26518
	0	1.957	1.26468
	0	1.732	1.23526
	0	1.732	1.23557
	0	0.965	1.13521
	0	0.503	1.07099
	0	0.301	1.04175
300	3.498	0	1.18069
	3.204	0.295	1.19994
	2.905	0.593	1.22046
	2.598	0.901	1.24170
	2.283	1.215	1.26383
400	4.863	0	1.23579
	4.568	0.296	1.25419
	4.278	0.585	1.27229
	3.982	0.881	1.29090
	3.661	1.202	1.31207
500	6.265	0	1.28607
	6.082	0.183	1.29660
	5.818	0.447	1.31210
	5.593	0.672	1.32539
600	8.016	0	1.33933
	7.846	0.171	1.34890
	7.674	0.342	1.35832
700	9.900	0	1.38824
	9.767	0.132	1.39496

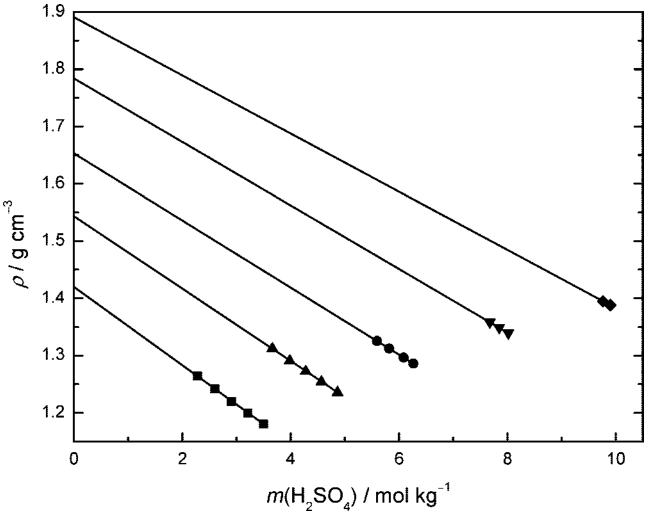

Figure 3. Densities of $FeSO_4 + H_2SO_4$ solutions at 25 °C and constant total sulfate concentrations of ■, 300 $g\cdot L^{-1}$; ▲, 400 $g\cdot L^{-1}$; ●, 500 $g\cdot L^{-1}$; ▼, 600 $g\cdot L^{-1}$; ◆, 700 $g\cdot L^{-1}$. The extrapolation to zero sulfuric acid concentration corresponds to binary, hypothetical (supersaturated) $FeSO_4$ solutions.

cal data, results in an almost identical (dashed) curve for the concentration range shown in Figure 1.

The present experimental data are collected in Table 2. Figure 2 represents the measured densities of mixed electrolyte solutions of iron sulfate plus sulfuric acid in water at constant sulfate concentrations of (300, 400, 500, 600, and 700) $g\cdot L^{-1}$. In contrast to the nonlinear density predictions of Laliberté and Cooper's model,[11] a linear relationship between the density and the molality of iron(II) sulfate in the mixed solutions was found experimentally. To derive a linear pro-rata additivity rule for mixed solutions at high sulfuric acid molalities, hypothetical values for "pure", supersaturated $FeSO_4$ solutions are required. These values were obtained by linear extrapolation as illustrated in Figure 3, in which the densities are plotted vs the sulfuric acid concentration in the mixtures so that the densities of the hypothetical $FeSO_4$ solutions correspond to the intercepts. Then, Young's pro-rata additivity rule can be applied

$$\rho_{mix} = (1 + x)\rho_1 + x\rho_2 \qquad (2)$$

where ρ_{mix} is the density of the mixture; x is the mole fraction of the solute component 2; and ρ_1 and ρ_2 are the densities of the constituent binary solutions at the total sulfate molalities. In the present case, ρ_1 and ρ_2 are calculated from the model of Laliberté and Cooper[11] for $H_2SO_4(aq)$ and the present Masson correlation for $FeSO_4(aq)$ (including the "hypothetical" values at high molalities). This model results in average relative deviations between experimental and calculated densities, $|\rho_{exp} - \rho_{calc}|/\rho_{calc}$, of better than 0.1 % (all data) and 0.062 % (binary system).

A similar extrapolation procedure[8,9] has been applied to aqueous $NaOH(aq) + NaAl(OH)_4(aq)$ mixtures, since $NaAl(OH)_4(aq)$ does not exist in the pure binary solution because it is unstable with respect to precipitation of $Al(OH)_3(s)$. This problem has been circumvented by measuring appropriate (stable) ternary mixtures of $NaOH(aq) + NaAl(OH)_4(aq)$. The properties of the hypothetical binary solutions of "$NaAl(OH)_4(aq)$" were then obtained by linear extrapolation.[8,9] Similar approaches to isopiestic measurements involving hydrolysing salts that are only stable in acidic solution have been described in the literature.[16]

Figure 4 shows the densities of $H_2SO_4(aq)$ and $FeSO_4(aq)$ in water at 25 °C. The solid dots are for the density of $H_2SO_4(aq)$, and the solid squares denote the densities of $FeSO_4(aq)$. The open squares are the hypothetical values (*y*-axis) read from Figure 3. The density of any mixed solution falls between the curves and can be obtained by Young's rule. The dashed line corresponds to a Masson model excluding hypothetical data, whereas the dotted line shows the model of Laliberté and Cooper.[11] These results confirm that purely empirical models for the correlation of physicochemical properties are highly susceptible to parameter correlation and consequent error propagation. Extrapolations beyond the range of data used in their parametrization must accordingly be made with considerable caution.

Figure 5 is a graphical representation of the difference between the calculated and experimental densities of saturated iron(II) sulfate in sulfuric acid solutions. The squares represent values obtained in our laboratory. The triangles correspond to the literature data[17] that were found by Laliberté and Cooper[11] not to be well represented by their model. It is evident that the present model (solid symbols) predicts densities of mixed $FeSO_4 + H_2SO_4 + H_2O$ solutions in better agreement with the experimental data than the model of Laliberté and Cooper[11] (open symbols).

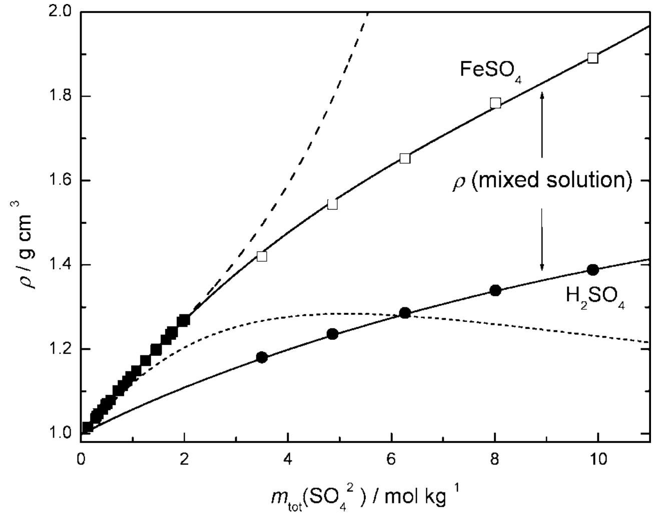

Figure 4. Densities of $FeSO_4 + H_2SO_4$ solutions at 25 °C measured in this work. ■, $FeSO_4$(aq); □, hypothetical (supersaturated) $FeSO_4$ solutions; ●, H_2SO_4 solutions. Upper solid line, present model including data for hypothetical $FeSO_4$ solutions. Dashed line, Masson equation excluding hypothetical data. Dotted line, model of Laliberté and Cooper[11] for $FeSO_4$(aq). Lower solid line, model of Laliberté and Cooper[11] for H_2SO_4 solutions. The densities of ternary $FeSO_4 + H_2SO_4 + H_2O$ mixtures are located between the two solid lines and are calculated according to the pro-rata additivity rule at constant total sulfate molality, eq 2.

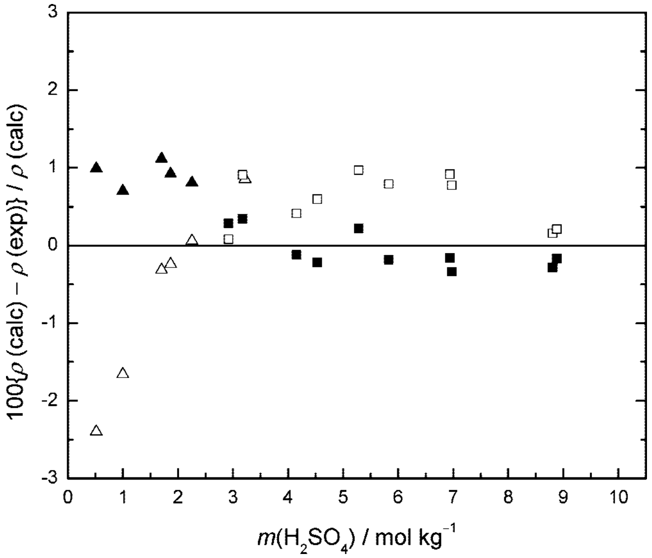

Figure 5. Differences between calculated and experimental densities of saturated $FeSO_4$ in H_2SO_4 solutions. Squares, data from this laboratory; triangles, ref 17. Solid symbols, present model; open symbols, model of Laliberté and Cooper[11] for mixed $FeSO_4 + H_2SO_4$ solutions.

Table 3. Densities in the $TiOSO_4 + H_2SO_4 + H_2O$ System

$c(H_2SO_4)$ / $g \cdot L^{-1}$	$m(H_2SO_4)$ / $mol \cdot kg^{-1}$	$m(TiOSO_4)$ / $mol \cdot kg^{-1}$	ρ / $g \cdot cm^{-3}$	ρ / $g \cdot cm^{-3}$
			25 °C	50 °C
	0	0.979	1.11775	1.10674
	0	2.953	1.33369	–
	0	4.917	1.51432	1.49743
	0	5.895	1.58995	1.57456
	0	0.980	1.11597	–
	0	1.047	1.11895	–
	0	1.994	1.23002	–
	0	3.873	1.41898	–
	0	3.998	1.42908	–
	0	4.985	1.51392	–
	0	5.916	1.58796	–
	1.997	0	1.11044	1.09625
	1.624	0.369	1.13364	1.11948
	1.242	0.746	1.15672	1.14263
	0.844	1.139	1.18085	1.16649
	0.431	1.547	1.20569	1.19040
	0	1.973	1.23098	1.21497
	3.999	0	1.20185	1.18490
	3.295	0.693	1.24196	1.22545
	2.549	1.427	1.28343	1.26710
	1.705	2.258	1.33120	1.31458
	0.905	3.045	1.37663	1.35984
	0	3.935	1.42828	1.40955
500	6.258	0	1.28290	1.26458
	6.230	0.0273	1.28448	1.26619
	6.203	0.0548	1.28601	1.26781
	6.175	0.0822	1.28751	1.26925
	6.148	0.1093	1.28898	1.27072
	6.120	0.1372	1.29048	1.27227
600	7.953	0	1.33417	1.31538
	7.943	0.0101	1.33468	1.31594
	7.934	0.0196	1.33515	1.31641
	7.924	0.0292	1.33564	1.31691
	7.915	0.0385	1.33609	1.31735
	7.904	0.0489	1.33659	1.31788
700	10.117	0	1.39019	1.37091
	10.111	0.0062	1.39050	1.37123
	10.105	0.0122	1.39080	1.37156
	10.099	0.0183	1.39112	1.37182
	10.092	0.0245	1.39140	1.37216
	10.086	0.0306	1.39182	1.37256

$TiOSO_4 + H_2SO_4 + H_2O$ System. Densities for this system were measured at (25 and 50) °C (Table 3). The purity of ethanol-washed $TiOSO_4 \cdot 2H_2O$ was found to be 99.15 %. Binary $TiOSO_4$(aq) solutions of higher concentrations contained small amounts of insoluble matter, probably some hydrolysis products. We therefore estimated their concentrations to be uncertain by 0.5 % and consequently assigned lower weights to these data points in the derivation of the present density model. Density data measured at 25 °C are shown in Figure 6. As for the $FeSO_4 + H_2SO_4 + H_2O$ system, the densities of ternary $TiOSO_4 + H_2SO_4 + H_2O$ solutions are calculated according to the pro-rata additivity rule given by eq 2, combined with the model of Laliberté and Cooper[11] for H_2SO_4(aq).

Ternary mixtures with H_2SO_4 included two series over the complete compositional range at (2 and 4) $mol \cdot kg^{-1}$ total sulfate molalities. An analysis of these data showed that deviations of mixture densities from linearity (Young's rule) were less than 0.18 %. This is limited by the analytical uncertainties described above. However, it confirms that eq 2 can be applied for most practical purposes (Figure 7).

In addition, mixtures were prepared at higher total sulfate molalities and the measured densities extrapolated to pure hypothetical, supersaturated $TiOSO_4$ solutions. For the densities of these ternary mixtures, a linear dependence was found as well so that eq 2 could be applied. The 25 °C data, including the hypothetical values, were correlated using the Masson equation (eq 1). The results are reported in Table 1. The uncertainties in $TiOSO_4$(aq) concentration and the small departures from linearity discussed above are reflected in somewhat larger average relative deviations between experimental and calculated densities of < 0.14 % (all data) and < 0.30 % (binary system).

The Masson parameters in Table 1 also predict the 50 °C density data reasonably well, provided that the density of water at 50 °C (0.988047 $g \cdot cm^{-3}$) is substituted for $\rho°$ in eq 1. This is in accordance with our recent findings for the densities of $NiCl_2$(aq).[18] However, a very slight temperature dependence of

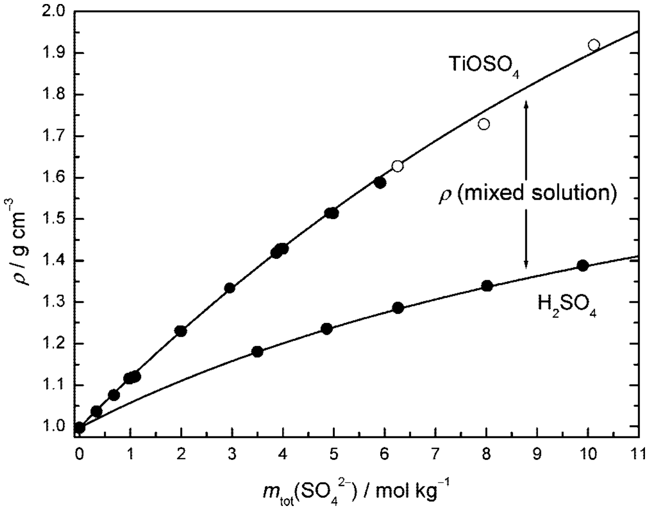

Figure 6. Densities of binary $TiOSO_4$ solutions at 25 °C. ●, this work; ○, densities of mixed $H_2SO_4 + TiOSO_4$ solutions extrapolated to $m(H_2SO_4) = 0$, this work. Solid lines, present correlation for $TiOSO_4$(aq) (Table 1) and model of Laliberté and Cooper[11] for H_2SO_4(aq). The densities of ternary $TiOSO_4 + H_2SO_4 + H_2O$ mixtures are located between the two solid lines corresponding to the binary systems and are calculated according to the pro-rata additivity rule at constant total sulfate molality, eq 2.

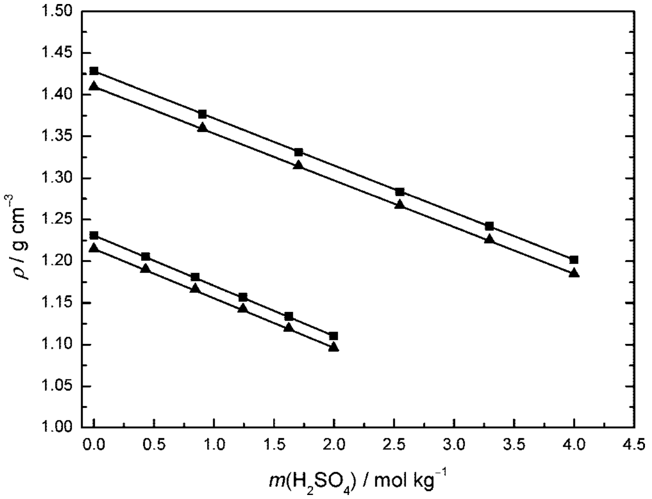

Figure 7. Densities of mixed $H_2SO_4 + TiOSO_4$ solutions at 25 °C (squares) and 50 °C (triangles) at (2 and 4) mol·kg^{-1} total sulfate concentrations. The lines indicate a linear change of density on mixing.

the *a* parameter (a decrease by 0.0001 per Kelvin) for $TiOSO_4$(aq) gives a better agreement. It should be noted that, judging from the density data compiled by Aseyev and Zaytsev[15] (which are, however, the results of a correlation rather than primary experimental data), the temperature dependence of *a* is larger (a decrease by 0.0002 to 0.0003 per Kelvin) for $FeSO_4$(aq).

Literature data for various molar total acid/titania ratios[19] are reproduced reasonably well by the present density model for mixed $TiOSO_4 + H_2SO_4$ solutions (Figure 8). The literature data[19] for $TiOSO_4$(aq) appear to be systematically (albeit slightly) higher than the values measured in this study.

$FeSO_4 + TiOSO_4 + H_2SO_4 + H_2O$ System. Densities in the quaternary system were measured at 25 °C for two series of solutions at constant total sulfate and sulfuric acid concentrations. Titanyl and iron(II) ions were replacing each other to form complete series of mixtures (Table 4). The present model predicts densities for the quaternary system very well. The average relative deviation between these experimental densities and values calculated from the present model is 0.068 %.

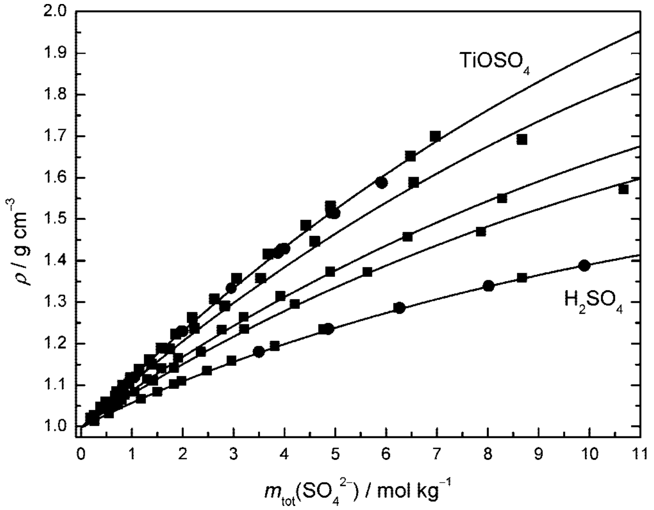

Figure 8. Densities of $TiOSO_4 + H_2SO_4$ solutions at 25 °C. ●, This work; lines, calculation based on present correlation for $TiOSO_4$ (Table 1) and model of Laliberté and Cooper[11] for H_2SO_4(aq), combined with a linear mixing rule (eq 2). ■, Data of Hixson and Stetkewicz[19] for various molar ratios of total sulfuric acid to titania (A/T) in solution. From top to bottom, A/T = 1.00, 1.26, 2.06, 2.93, ∞.

Table 4. Densities in the $TiOSO_4 + FeSO_4 + H_2SO_4 + H_2O$ System at 25 °C

$m(H_2SO_4)$ / mol·kg^{-1}	$m(TiOSO_4)$ / mol·kg^{-1}	$m(FeSO_4)$ / mol·kg^{-1}	ρ / g·cm^{-3}
4.891	0	0.4982	1.28439
4.891	0.0992	0.398	1.28411
4.891	0.199	0.299	1.28357
4.891	0.298	0.199	1.28296
4.892	0.393	0.103	1.28230
4.892	0.497	0	1.28170
3.533	0	0.794	1.26617
3.532	0.159	0.636	1.26508
3.531	0.319	0.477	1.26319
3.530	0.475	0.322	1.26142
3.530	0.633	0.165	1.25914
3.529	0.799	0	1.25716

Conclusions

A consistent model for the prediction of densities over wide concentration ranges in the industrially important $TiOSO_4 + FeSO_4 + H_2SO_4 + H_2O$ system is presented. This work demonstrates the importance of binary property data for supersaturated concentration ranges when mixing rules are applied to predict the properties of ternary solutions. The problem with property model extrapolations can be circumvented by properly exploiting mixture properties to predict properties of the binary subsystems. The extrapolated properties can then be included in the model for this binary system.

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