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Subject: Density-Weight Percent Molarity Conversion Equations for Uranyl Sulfate-Water Solutions at 25.0°C and Between 100-300°C

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DISCLAIMER

DENSITY-WEIGHT PERCENT-MOLARITY CONVERSION EQUATIONS FOR URANYL SULFATE-WATER SOLUTIONS AT 25.0°C AND BETWEEN 100-300°C

A. Equations Applicable at 25°C.

The equations given are evaluated from density-molarity data for uranyl sulfate-water solutions at 25.0 ± 0.2°C as determined by Lietzke, Wright, and Marshall[1]. The initial equation is derived from the linear relationship of density to molarity. Experimental average deviation of the slope constant so calculated is 0.57 percent. The probable error of ± 0.45 percent for this constant is used to determine the accuracy of the specific equations for the dependent variable if the independent variable is not in error.

I. Density-Volume Concentrations.

(1) $d = 0.9970 + 0.316_5\ M$

(2) $d = 0.9970 + 0.001329\ g_u$

(3) $d = 0.9970 + 0.000864_5\ g_s$

Accuracy: d to ± 0.45 (1 - 1/d) percent

M, g_u, g_s to ± 0.45 percent

where

d = density in grams per cc

M = molarity UO_2SO_4

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[1] J. A. Swartout, et al. Homogeneous Reactor Quarterly Report for period ending August 15, 1951, ORNL 1121, P. 124 (December 27, 1951).

g_u = grams uranium per liter

g_s = grams UO_2SO_4 per liter

II. Density-Weight Concentrations.

(4) $$d = \frac{0.9970}{1 - 0.01329\ U}$$

(5) $$d = \frac{0.9970}{1 - 0.00864_5\ S}$$

(6) $$U = 75.2_2 - \frac{75.0_0}{d}$$

(7) $$S = 115.7 - \frac{115.3}{d}$$

Accuracy: d to ± 0.45 (d - 1) percent

U, S to ± 0.45 percent

where

d = density in grams per cc

U = weight percent uranium

S = weight percent UO_2SO_4

III. Molarity-Weight Concentrations.

(8) $$1/M = \frac{23.88}{U} - 0.317_4$$

(9) $$1/M = \frac{36.7_2}{S} - 0.317_4$$

(10) $$1/U = \frac{0.0418_8}{M} + 0.01329$$

(11) $$1/S = \frac{0.02723}{M} + 0.00864_5$$

Accuracy: M to ± 0.45 $(\frac{24M}{U} - 1)$ percent

or to ± 0.45 $(\frac{37M}{S} - 1)$ percent

U to ± 0.45 $(\frac{U}{24M} - 1)$ percent

S to ± 0.45 $(\frac{S}{37M} - 1)$ percent

where

M = molarity UO_2SO_4

U = weight percent uranium

S = weight percent UO_2SO_4

B. Equations Applicable Between 100-300°C.

Sources of data from which the final equations were derived are given as follows, together with some of the density values and brief explanations if deemed necessary.

1. Reference 1 above. Density data at 25.0 ± 0.2°C.
2. I. Helmholz and G. Friedlander. Physical Properties of Uranyl Sulfate Solutions, LAMS 30 (December 15, 1943). Density Data from 30 to 100°.
3. W. H. Davenport and R. H. Powell. Private Communication.

The following density data were obtained by the method described in Reference 1, page 75:

t°C	Molarity UO_2SO_4 at 25°C	Density at t°C
50	.08732	1.0159
50	.125	1.0278
50	.1622	1.0397
184	.1299	.9248 ± .0005
203	.1299	.9015 ± .0005
232	.1299	.8630 ± .0005

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4. J. A. Swartout, et al. Chemistry Division Quarterly
Progress Report for Period Ending February , 1949.
ORNL 336, pp. 24-27 (May 4, 1949).

Density Data of C. H. Secoy: The density data for an initial 34.9 percent uranyl sulfate solution were corrected for loss of water to the vapor phase by using the densities of saturated water vapor (Reference 6). The vapor pressures of this system are not more than 10 psi different from that of pure water (Experimental Data, H. O. Day of this laboratory).

Concentration changes were corrected to the original value, 34.9 percent, by subtracting an equivalent number of density units as would be required for correction at 25°. No corrections were made on densities or concentrations below 108.8°. The following are the corrected values for C. H. Secoy's data:

t°C	Density
22.3	1.432*
48.8	1.410*
70.0	1.393*
88.0	1.380*
108.8	1.360
129.2	1.340
152.6	1.317
175.7	1.294
187.0	1.282
231.7	1.227
249.4	1.199
274.0	1.153
303.8	1.081
325.8	1.004
345.8	.911
356.3	.861
366.5	.787
371.5	.753

*No correction necessary.

5. J. D. Roarty, Oak Ridge National Laboratory, Density Data Between 25-100° to be published soon. (Private Communication).

6. N. E. Dorsey, Properties of Ordinary Water Substances. Reinhold Publishing Corporation; p. 577 (1940). Density Data for Water at Saturated Vapor Pressures.

Evaluation of Data. At the suggestion of E. L. Compere, an empirical temperature versus a linear density scale was constructed on a graph to show a straight line relationship of water density values (densities at saturated vapor pressure). All solution densities were plotted on this scale. The density lines were found to be parallel to the water curve between 120° and 280° for the 34.9 percent uranyl sulfate solution and from 25° to at least 232° for the 4.58 percent solution. Below 120° there was a definite upswing which appeared proportional to the molarity. From these data and the density equations at 25°, the following equations are derived to express the solution density of water-uranyl sulfate solutions between 120° and 280° for concentrations up to 51 percent salt.

$$d_{\text{solution}_t} = \frac{1}{\frac{78.65}{U} - 1.046} + d_{H_2O_t} \tag{12}$$

$$d_{\text{solution}_t} = \frac{1}{\frac{120.9}{S} - 1.046} + d_{H_2O_t} \tag{13}$$

where

$d_{H_2O_t}$ = density of water at t°C (at saturated vapor pressure)

U = weight percent uranium

S = weight percent UO_2SO_4

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These equations are believed to be accurate to ±0.5 percent from 25° to approximately 300° for uranyl sulfate solutions not over about 10 weight percent. For higher concentrations they appear accurate to better than ± 1.0 percent between 120° and 250°, the limitation at the lower and higher temperatures being due to deviations in the linearity relationships. If these deviations are ignored then the equations are accurate to ± 2% in the temperature ranges 25-120° and 250-280° for concentrations above approximately 10 percent.

The above empirical equations for upper temperatures were derived and checked with experimental data at hand. R. Van Winkle of the Experimental Engineering Division, Oak Ridge National Laboratory, has accomplished the same purpose with an equation derived purely on a theoretical basis. His equation is not quite as accurate as the above expressions, but fits the data well if its theoretical origin is considered.

C. <u>Addendum</u>:

I. The following equations for D_2O-UO_2SO_4 solutions are derived by substitution of D_2O density for H_2O density in the previous relationships. There are no experimental data to justify the correctness of these equations.

1. At 25.0 ± 0.2°C

$$d_{solution} = 1.1044 + .316_5 M$$

$$d_{solution} = \frac{1.1044}{1 - 0.01329 U}$$

$$\frac{1}{M} = \frac{21.55}{U} - 0.286_6$$

2. Between 120°-280°C:

$$d_{\text{solution}_t} = \frac{1}{\frac{71.0_0}{U} - .943_9} + d_{D_2O}^{t}$$

where

d = density of D_2O-UO_2SO_4 solution

U = weight percent uranium

M = molarity UO_2SO_4

$d_{D_2O}^{t}$ = density of D_2O at t

II. Equations Derived Before Final Substitutions for Densities.

(a) $$d_{\text{solution}_{25^\circ}} = d_{H_2O}^{25^\circ} + .31651\,M$$

(b) $$d_{\text{solution}}^{25^\circ} = \frac{d_{H_2O}^{25^\circ}}{1 - .013295\,U}$$

(c) $$\frac{1}{M^{25^\circ}} = \frac{23.806}{d_{H_2O}^{25^\circ}\;U} - \frac{.31651}{d_{H_2O}^{25^\circ}}$$

(d) $$d_{\text{solution}_t} = \frac{1}{\frac{78.410}{d_{H_2O}^{25^\circ}\;U} - \frac{1.0425}{d_{H_2O}^{25^\circ}}} + d_{H_2O}^{t}$$

where $d_{H_2O}^{25^\circ} = 0.99704$

or

$d_{D_2O}^{25^\circ} = 1.1044$