RECIPROCITY

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The third assumption of [the reciprocal system of physics] is that space and time exist in discrete units. This, too, is an extrapolation from known facts into the region that is unknown. In the early days of science it was generally believed that all of the primary physical phenomena were continuous and infinitely divisible, but as knowledge has grown during the succeeding centuries one after another of these phenomena has been found to exist only in units. The atomic structure of matter was the first to be demonstrated. Later the unit of electricity was isolated and still more recently the work of Planck made it clear that radiant energy follows the pattern.....
... Since experience shows that as our knowledge widens more and more physical phenomena are proved to exist only in discrete units, it is merely a reasonable extrapolation to assume that if all the facts were known, this would also be found to be true with respect to the basic entities, space and time.

Dewey B. Larson, 1

I am tending to the belief that it is impossible to continue further with this continuum theory.

Albert Einstein, 1

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THE LIQUID STATE IN THE RECIPROCAL SYSTEM: THE VOLUME/TEMPERATURE RELATION, A CONTEMPORARY MATHEMATICAL TREATMENT

by
Ronald W. Satz, Ph.D.

This paper provides a step-by-step procedure for the calculation of liquid specific volume as a function of composition and temperature, based on the Reciprocal System of D. B. Larson[1]. In this theory, each individual molecule may be in the solid, liquid, or gaseous (or vapor) state, regardless of the state of the majority of molecules of the substance.

First let's define some terms:

V_L = overall specific volume of liquid (cm^3/g) (total volume/total mass)

V_1 = specific volume increment at 0 °K and that due to the solid molecules in solution of the liquid (solid volume/total mass)

V_2 = specific volume increment due to the liquid molecules of the substance, temperature above 0 °K (liquid volume/total mass)

V_3 = specific volume increment due to the critical (gaseous or vapor) molecules in solution of the liquid (gaseous volume/total mass)

Then,

$$V_L = V_1 + V_2 + V_3 \qquad (1)$$

The initial values of these three components are designated V_{01}, V_{02}, V_{03}. These differ only by a geometric factor (designated k_{s1}, k_{s2}, k_{s3}) applied to a base initial value, V_{00}, determined as follows.

Just as the volume of a gas is determined by the number of molecules, so the volume of a liquid is determined by the number of volumetric groups which it contains. In an organic compound, for instance, each of the common interior groups, such as CH_2, CH, or CO, constitutes one volumetric group. The CH_3 groups in the end positions of the aliphatic chains occupy two units each. So hexane, represented as $CH_3CH_2CH_2CH_2CH_2CH_3$, has 8 volumetric groups. Let n_v be the number of volumetric groups and recall that the factor .707 expresses the geometric reduction obtained by the close-packed arrangement of the liquid groups because of their flexibility of movement. Then, in natural units, the base initial volume is directly proportional to the number of volumetric units, reduced by close-packing:

$$V_{00} = .707 n_v \qquad (2)$$

Let m be the molecular weight (non-dimensional) of the molecule of the substance, m_u be the value of the natural unit of atomic mass in g, and V_{lnu} be the value of the natural unit of liquid volume expressed in cm^3. Then, in conventional units, the basic initial value is

$$V_{00} = \frac{.707 n_v V_{lnu}}{m m_u} \ cm^3/g \qquad (3)$$

V_{lnu} is *not* the cube of the natural unit of space in the time-space region, which is applicable only to the gaseous state. Rather, V_{lnu} is the cube of the natural unit of space in the time region, which is 1/156.45 (the inter-regional ratio) of that in time-space region, or 2.9139×10^{-8} cm. Cubing this we get

$$V_{lnu} = 2.47417 \times 10^{-23} \ cm^3$$

The natural unit of mass is 1 atomic mass unit, so m_u is 1.65979×10^{-24} g. Putting these values in eq. 3, we get

$$V_{00} = \frac{10.5389 n_v}{m} \ cm^3/g \qquad (4)$$

For hexane, n_v is 8 and the molecular weight is 86.18. Therefore,

$$V_{00} = .9783 \ cm^3/g$$

For the critical (gaseous or vapor) specific volume increment, the geometric factor k_{s3} is always 1.00. For the solid specific volume increment, the geometric factor k_{s1} is .891 (the cube root of .707) where close-packing in the solid state can be achieved. Where such packing cannot be achieved, the geometric factor k_{s1} is 1.000. The same applies to the geometric factor for the liquid specific volume increment, k_{s2}. Therefore, the initial values of the three volume components may be expressed as

$$V_{01} = V_{00} k_{s1} \qquad (6)$$

$$V_{02} = V_{00} k_{s2} \qquad (7)$$

$$V_{03} = V_{00} k_{s3} = V_{00} \qquad (8)$$

In a multi-group molecule, the value of the geometric factors K_{s1} and K_{s2} represent *averages*, since some groups may be at .891 while others at 1.000. Let n_{s1} = the number of close-packed groups per molecule in the solid state, and let n_{s2} = the number of close-packed groups per molecule in the liquid state. Then

$$k_{s1} = (n_{s1} \times .891 + (n_v - n_{s1}) \times 1.000) / n_v \qquad (9)$$

$$k_{s2} = (n_{s2} \times .891 + (n_v - n_{s2}) \times 1.000) / n_v \qquad (10)$$

For hexane, for instance, K_{s1} is .9864 (with 1 group at .891 and 7 groups at 1.0000, the average is 7.891/8 or .9864) and K_{s2} is .9728 (with 2 groups at .891 and 6 groups at 1.0000). Therefore, for hexane, the initial values of the specific volume increments are

$$V_{01} = .9783 \times .9864 = .9650 \ \text{cm}^3/\text{g}$$

$$V_{02} = .9783 \times .9728 = .9517 \ \text{cm}^3/\text{g}$$

$$V_{03} = .9783 \times 1.0000 = .9783 \ \text{cm}^3/\text{g}$$

From eq. 10 it's clear that ordinarily $n_v \geq n_{s1}, n_v \geq n_{s2}$. However, for lower group elements, hyrdrogen through fluorine, closer packing than normal can be achieved because of inactive dimensions of the gravitational repulsion force. This means that, in effect, for lower group elements the geometric factors can be less than .891. We can still use eq. 10, though, if we allow the value of the number of solid groups to exceed the number of volumetric units.

Now that we have the initial values as a function of composition, we can determine the values of the three components as a function of temperature. The solid specific volume increment not only includes the initial volume at 0 ^{o}K but also a factor proportional to the number of solid molecules in the substance at any temperature, Δs, which can be determined by probability considerations.

$$V_1 = V_{01} + \Delta s \qquad (11)$$

To use the normal probability function or table we need to know the value of the normal random variable, z_s, applicable. It should be proportional to the difference between the liquid temperature T and the melting point T_M, in degrees K, divided by the melting point. The coefficient and the intercept have unfortunately not been worked out theoretically, but are given empirically by Larson (Ref. 1) as follows:

$$z_s = \frac{4(T - T_M)}{T_M} + .40 \qquad (12)$$

We want the right tail of the distribution, so we subtract the value of the normal function, denoted by erf(z_S), from 1 and then multiply by the average difference in specific volume between solid and liquid molecules, denoted by Δv:

$$\Delta s = (1 - erf(z_s))\Delta v \tag{13}$$

Larson uses an average value of Δv of .080 for paraffin hydrocarbons (C_{14} and below) and .084 for paraffins above C_{14} (rather than computing the individual values). For hexane, T_M = 178 K (-95 °C). At T = -50 °C, z_S=1.41 and from the normal probability table, erf(z_S) ≈ .9207. Subtracting this from 1.0000, we get .0793, which means that 7.93 % of the molecules in the liquid hexane aggregate at -50 °C are in the solid state. Multiplying this figure by the approximate difference in specific volume between solid and liquid molecules, .080, we get .0063 cm^3/g for the value of Δs.

The thermal motion beyond the initial point of the liquid (considered as starting at 0 °K) is the one-dimensional equivalent of the thermal motion of a gas, and thus the volume generated is directly proportional to the temperature, T. Let T_{Inu} be the natural unit of temperature in the time region (for the condensed states of matter) and n_t be the temperature factor. Then

$$V_2 = \frac{T}{n_t T_{Inu}} V_{02} \tag{14}$$

In Ref. 2, Larson derived the value of T_{Inu} to be 510.8 K. For simple substances, n_t is 1. More complex or more electropositive substances have values of n_t of 2 up to 16. Hexane has a value of 1; water, 2; silver, 16. Compounds of electropositive and electronegative elements have intermediate values (some with half-integral values, which are averages), as would be expected.

The gaseous or vapor increment of specific volume depends on the proportion of critical molecules existing in the aggregate at each temperature, which can be computed from probability considerations. Larson uses two random variables for this computation, both a function of the critical temperature, T_c:

$$z_{c1} = \frac{9(T_c - T)}{T_c + T_{Inu}/2} \tag{15}$$

$$z_{c2} = \frac{27(T_c - T)}{T_c + T_{Inu}/2} \tag{16}$$

Then the specific volume increment due to critical molecules in the substance is

$$V_3 = (2 - (erf(z_{c1}) + erf(z_{c2})))V_{03} \qquad (17)$$

For hexane, T_c = 508 K. At T = 210 °C, z_{c1} = .2947 and z_{c2} =.8106. The corresponding values of the normal probability function are .6144 and .8109. Then, from eq. 17,

$$V_3 = (2 - (.6144 + .8109))(.9783) = (.5747)(.9783) = .5622 \ \ cm^3/g$$

The .5747 factor means that 57.47% of the molecules at this temperature are in the critical state.

Having determined V_1, V_2, and V_3 we can now calculate V_L from eq. 1.

To automate the task of comparing the theoretical values with those observed, I've prepared a computer program and run it on most of the same liquids Larson used in the original series of papers: hexane, hexadecane, benzene, acetic acid, ethyl acetate, ethyl chloride, ethanethiol, fluorine, hydrochloric acid, sulfur dioxide, carbon tetrachloride, and water. Printouts from the program for all of these liquids follow. The observed values come from the same sources Larson used: Timmermans' *Physico-chemical Constants of Pure Organic Compounds*, the American Petroleum Institute, and the *International Critical Tables*.

Most of the computer results are in harmony with Larson's manual calculations. The two seeming exceptions are for acetic acid and water. For acetic acid, Larson used a value of initial liquid specific volume of .5469, which is .7795 that of his base initial volume, .7016; but .891 is supposedly the smallest allowed fraction. For water, Larson used a value of .7640 for both the initial solid and liquid specific volumes, but this is only .8713 that of his base initial volume, .8769, not .891. Actually. these differences are due to "hydrogen bonding", which can allow closer packing than normal. In a second calculation for water, I input 1.78 for Π_{s1} and Π_{s2} so as to get the initial volumes to be .7640. The theoretical results computed came out to be much closer to the experimental ones than the previous run.

To compute the specific volume for any liquid of your choice, follow these steps:

1. Determine the formula of the compound and its molecular weight.

2. From the formula, determine the number of volumetric units and number of temperature units.

3. Use equation 4 to obtain the base initial volume.

4. Use equations 9 and 10 to compute the geometric factors; some iteration here may be required to the get the right values.

5. Compute the initial volumes with equations 6, 7, and 8.

6. Using equations 12 and 13, compute the solid specific volume increment, equation 11.

7. Use equation 14 to compute the liquid specific volume increment.

8. Using equations 15 and 16, compute the critical specific volume increment, equation 17.

9. Sum the results to get the final value, from equation 1.

References:

1. D. Larson, *The Liquid State* , privately circulated series of papers on the liquid state, circa. 1960-1964. Note: I made use of the papers numbered I, II, II-supplement, and III. I've reorganized all of the equations and changed some of the symbols for the sake of clarity. I've also used the latest values of the conversion constants. The computer program is entirely original.

2. D. Larson, *Basic Properties of Matter* (Salt Lake City, UT: International Society of Unified Science, 1959-1988), pp. 59-60.

Appendix: The Computer Program

The following pages show the input screens of the program. The data base language is *filePro Plus* and the computation language is *TrueBasic*. This is the first of what will be a comprehensive series of programs for the calculation of all properties of matter based on the Reciprocal System of theory. Eventually the programs will be made available for purchase.

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Hexane
Representation: CH3CH2CH2CH2CH2CH3 Mol. Wt.: 86.17848
Melting Temperature: -95.00 Critical Temperature: 234.84 deg. C

Volumetric Units :	NV: 8.0	NS1: 1.0	NS2: 2.0		
Geometric Factors:		KS1: .9864	KS2: .9728	KS3: 1.0000	
INITIAL VOLUMES :	V00: .9783	V01: .9650	V02: .9517	V03: .9783	
Delta Vol.: .0800	Temperature Factor: 1.0		Corr. Coef.: 1.0000		

Temp.-deg. C	V1	V2	V3	VL	VO	Diff. cm3/g
-100.00	.9959	.3226	.0000	1.3185	1.3130	.0055
-90.00	.9893	.3413	.0001	1.3307	1.3270	.0037
-80.00	.9835	.3599	.0001	1.3435	1.3420	.0015
-70.00	.9785	.3785	.0002	1.3572	1.3570	.0002
-60.00	.9744	.3972	.0002	1.3718	1.3730	-.0012
-50.00	.9713	.4158	.0004	1.3875	1.3890	-.0015
-40.00	.9691	.4344	.0006	1.4041	1.4050	-.0009
-30.00	.9675	.4530	.0009	1.4214	1.4220	-.0006
-20.00	.9665	.4717	.0013	1.4395	1.4400	-.0005
-10.00	.9658	.4903	.0019	1.4580	1.4580	.0000
.00	.9655	.5089	.0028	1.4772	1.4770	.0002
10.00	.9652	.5276	.0039	1.4967	1.4960	.0007
20.00	.9651	.5462	.0055	1.5168	1.5160	.0008
30.00	.9651	.5648	.0077	1.5376	1.5370	.0006
40.00	.9650	.5835	.0106	1.5591	1.5600	-.0009
50.00	.9650	.6021	.0143	1.5814	1.5830	-.0016
60.00	.9650	.6207	.0192	1.6049	1.6070	-.0021
70.00	.9650	.6394	.0254	1.6298	1.6330	-.0032
80.00	.9650	.6580	.0332	1.6562	1.6610	-.0048
90.00	.9650	.6766	.0429	1.6845	1.6900	-.0055
100.00	.9650	.6953	.0547	1.7150	1.7200	-.0050
110.00	.9650	.7139	.0690	1.7479	1.7530	-.0051
120.00	.9650	.7325	.0860	1.7835	1.7900	-.0065
130.00	.9650	.7511	.1060	1.8221	1.8290	-.0069
140.00	.9650	.7698	.1293	1.8641	1.8720	-.0079
150.00	.9650	.7884	.1565	1.9099	1.9200	-.0101
160.00	.9650	.8070	.1887	1.9607	1.9750	-.0143
170.00	.9650	.8257	.2282	2.0189	2.0350	-.0161
180.00	.9650	.8443	.2790	2.0883	2.1050	-.0167
190.00	.9650	.8629	.3472	2.1751	2.1880	-.0129
200.00	.9650	.8816	.4398	2.2864	2.2910	-.0046
210.00	.9650	.9002	.5622	2.4274	2.4250	.0024

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Fluorine
Representation: F Mol. Wt.: 18.99840
Melting Temperature: -219.62 Critical Temperature: -155.00 deg. C

Volumetric Units :	NV:	1.00	NS1:	.50	NS2:	1.00	
Geometric Factors:			KS1:	.9455	KS2:	.8910	KS3: 1.0000
INITIAL VOLUMES :	V00:	.5547	V01:	.5245	V02:	.4942	V03: .5547
Delta Vol.:	.0000	Temperature Factor:		1.0	Corr. Coef.:		.9958

Temp.-deg. C	V1	V2	V3	VL	VO	Diff.	cm3/g
-208.00	.5245	.0630	.0560	.6435	.6100	.0335	
-203.00	.5245	.0679	.0688	.6612	.6210	.0402	
-198.00	.5245	.0727	.0838	.6810	.6340	.0470	
-193.00	.5245	.0776	.1015	.7036	.6460	.0576	
-188.00	.5245	.0824	.1230	.7299	.6620	.0679	

Using the standard critical temperature--poor results.

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Fluorine
Representation: F Mol. Wt.: 18.99840
Melting Temperature: -219.62 Critical Temperature: -131.00 deg. C

Volumetric Units :	NV:	1.00	NS1:	.50	NS2:	1.00		
Geometric Factors:			KS1:	.9455	KS2:	.8910	KS3:	1.0000
INITIAL VOLUMES :	V00:	.5547	V01:	.5245	V02:	.4942	V03:	.5547
Delta Vol.:	.0000	Temperature Factor:		1.0	Corr. Coef.:		1.0000	

Temp.-deg. C	V1	V2	V3	VL	VO	Diff.	cm3/g
-208.00	.5245	.0630	.0226	.6101	.6100	.0001	
-203.00	.5245	.0679	.0286	.6210	.6210	.0000	
-198.00	.5245	.0727	.0359	.6331	.6340	-.0009	
-193.00	.5245	.0776	.0445	.6466	.6460	.0006	
-188.00	.5245	.0824	.0546	.6615	.6620	-.0005	

Critical temperature is given in handbooks as -155 C, but -131 C works better!

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Carbon Tetrachloride
Representation: CCl4
Melting Temperature: -23.00 Critical Temperature: 283.10 deg. C Mol. Wt.: 153.81000

Volumetric Units : NV: 6.0 | NS1: .0 | NS2: 4.5 |
Geometric Factors: | KS1: 1.0000 | KS2: .9183 | KS3: 1.0000
INITIAL VOLUMES : V00: .4111 | V01: .4111 | V02: .3775 | V03: .4111
Delta Vol.: .0000 Temperature Factor: 1.0 Corr. Coef.: .9999

Temp.-deg. C	V1	V2	V3	VL	VO	Diff.	cm3/g
.00	.4111	.2019	.0003	.6133	.6120	.0013	
10.00	.4111	.2093	.0005	.6209	.6200	.0009	
20.00	.4111	.2167	.0007	.6285	.6270	.0015	
30.00	.4111	.2240	.0010	.6361	.6350	.0011	
40.00	.4111	.2314	.0014	.6439	.6430	.0009	
50.00	.4111	.2388	.0020	.6519	.6510	.0009	
60.00	.4111	.2462	.0027	.6600	.6600	.0000	
70.00	.4111	.2536	.0037	.6684	.6680	.0004	
80.00	.4111	.2610	.0050	.6771	.6770	.0001	
90.00	.4111	.2684	.0066	.6861	.6870	-.0009	
100.00	.4111	.2758	.0087	.6956	.6970	-.0014	
110.00	.4111	.2832	.0113	.7056	.7080	-.0024	
120.00	.4111	.2906	.0145	.7162	.7190	-.0028	
130.00	.4111	.2980	.0184	.7275	.7310	-.0035	
140.00	.4111	.3053	.0231	.7395	.7440	-.0045	
150.00	.4111	.3127	.0288	.7526	.7570	-.0044	
160.00	.4111	.3201	.0354	.7666	.7700	-.0034	
170.00	.4111	.3275	.0432	.7818	.7850	-.0032	
180.00	.4111	.3349	.0521	.7981	.8020	-.0039	
190.00	.4111	.3423	.0625	.8159	.8200	-.0041	
200.00	.4111	.3497	.0745	.8353	.8410	-.0057	
210.00	.4111	.3571	.0889	.8571	.8640	-.0069	
220.00	.4111	.3645	.1069	.8825	.8910	-.0085	
230.00	.4111	.3719	.1302	.9132	.9210	-.0078	
240.00	.4111	.3792	.1612	.9515	.9580	-.0065	
250.00	.4111	.3866	.2024	1.0001	1.0020	-.0019	
260.00	.4111	.3940	.2549	1.0600	1.0630	-.0030	

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Hexadecane
Representation: CH3(CH2)14CH3 Mol. Wt.: 226.45000
Melting Temperature: 18.20 Critical Temperature: 454.84 deg. C

Volumetric Units : NV: 18.0	NS1: 3.5	NS2: 12.0	
Geometric Factors:	KS1: .9788	KS2: .9273	KS3: 1.0000
INITIAL VOLUMES : V00: .8377	V01: .8199	V02: .7768	V03: .8377

Delta Vol.: .0840 Temperature Factor: 1.0 Corr. Coef.: .9996

Temp.-deg. C	V1	V2	V3	VL	VO	Diff. cm3/g
20.00	.8481	.4458	.0000	1.2939	1.2930	.0009
30.00	.8440	.4610	.0000	1.3050	1.3050	.0000
40.00	.8402	.4762	.0001	1.3165	1.3160	.0005
50.00	.8368	.4914	.0001	1.3283	1.3280	.0003
60.00	.8338	.5067	.0001	1.3406	1.3410	-.0004
70.00	.8311	.5219	.0002	1.3532	1.3530	.0002
80.00	.8288	.5371	.0003	1.3662	1.3660	.0002
90.00	.8269	.5523	.0004	1.3796	1.3790	.0006
100.00	.8253	.5675	.0005	1.3933	1.3920	.0013
110.00	.8240	.5827	.0007	1.4074	1.4070	.0004
120.00	.8229	.5979	.0009	1.4217	1.4210	.0007
130.00	.8221	.6131	.0012	1.4364	1.4360	.0004
140.00	.8215	.6283	.0017	1.4515	1.4510	.0005
150.00	.8210	.6435	.0022	1.4667	1.4660	.0007
160.00	.8207	.6587	.0029	1.4823	1.4830	-.0007
170.00	.8204	.6739	.0038	1.4981	1.4990	-.0009
180.00	.8203	.6891	.0050	1.5144	1.5160	-.0016
190.00	.8201	.7044	.0064	1.5309	1.5330	-.0021
200.00	.8201	.7196	.0082	1.5479	1.5510	-.0031
210.00	.8200	.7348	.0105	1.5653	1.5700	-.0047
220.00	.8200	.7500	.0132	1.5832	1.5900	-.0068
230.00	.8199	.7652	.0166	1.6017	1.6020	-.0003
240.00	.8199	.7804	.0206	1.6209	1.6330	-.0121
250.00	.8199	.7956	.0255	1.6410	1.6550	-.0140
260.00	.8199	.8108	.0312	1.6619	1.6790	-.0171
270.00	.8199	.8260	.0380	1.6839	1.7040	-.0201
280.00	.8199	.8412	.0459	1.7070	1.7300	-.0230
290.00	.8199	.8564	.0550	1.7313	1.7590	-.0277

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Ethanethiol
Representation: C2H5SH
Mol. Wt.: 62.13000
Melting Temperature: -144.40 Critical Temperature: 224.84 deg. C

Volumetric Units : NV: 4.5	NS1: .5	NS2: .5		
Geometric Factors:	KS1: .9879	KS2: .9879	KS3: 1.0000	
INITIAL VOLUMES : V00: .7633	V01: .7541	V02: .7541	V03: .7633	
Delta Vol.: .0000 Temperature Factor: 1.0		Corr. Coef.: .9999		

Temp.-deg. C	V1	V2	V3	VL	VO	Diff. cm3/g
.00	.7541	.4033	.0028	1.1602	1.1600	.0002
10.00	.7541	.4180	.0039	1.1760	1.1830	-.0070
20.00	.7541	.4328	.0055	1.1924	1.1960	-.0036
30.00	.7541	.4476	.0076	1.2093	1.2115	-.0022
40.00	.7541	.4623	.0104	1.2268	1.2270	-.0002
50.00	.7541	.4771	.0140	1.2452	1.2450	.0002
60.00	.7541	.4918	.0187	1.2646	1.2660	-.0014
70.00	.7541	.5066	.0246	1.2853	1.2870	-.0017
80.00	.7541	.5214	.0319	1.3074	1.3120	-.0046
90.00	.7541	.5361	.0409	1.3311	1.3350	-.0039
100.00	.7541	.5509	.0519	1.3569	1.3610	-.0041
110.00	.7541	.5657	.0649	1.3847	1.3870	-.0023
120.00	.7541	.5804	.0804	1.4149	1.4160	-.0011
130.00	.7541	.5952	.0984	1.4477	1.4510	-.0033
140.00	.7541	.6100	.1195	1.4836	1.4880	-.0044
150.00	.7541	.6247	.1445	1.5233	1.5310	-.0077
160.00	.7541	.6395	.1751	1.5687	1.5770	-.0083
170.00	.7541	.6542	.2144	1.6227	1.6310	-.0083
180.00	.7541	.6690	.2673	1.6904	1.6950	-.0046
190.00	.7541	.6838	.3393	1.7772	1.7730	.0042
200.00	.7541	.6985	.4351	1.8877	1.8730	.0147

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Ethyl Chloride
Representation: CH3CH2Cl
Melting Temperature: -136.40 Critical Temperature: 187.20 deg. C Mol. Wt.: 64.52000

Volumetric Units : NV: 4.5 | NS1: .0 | NS2: 4.5
Geometric Factors: | KS1: 1.0000 | KS2: .8910 | KS3: 1.0000
INITIAL VOLUMES : V00: .7350 | V01: .7350 | V02: .6549 | V03: .7350
Delta Vol.: .0000 Temperature Factor: 1.0 Corr. Coef.: .9998

Temp.-deg. C	V1	V2	V3	VL	VO	Diff.	cm3/g
20.00	.7350	.3759	.0131	1.1240	1.1190	.0050	
30.00	.7350	.3887	.0177	1.1414	1.1380	.0034	
40.00	.7350	.4015	.0236	1.1601	1.1590	.0011	
50.00	.7350	.4143	.0311	1.1804	1.1810	-.0006	
60.00	.7350	.4271	.0403	1.2024	1.2040	-.0016	
70.00	.7350	.4400	.0517	1.2267	1.2290	-.0023	
80.00	.7350	.4528	.0653	1.2531	1.2560	-.0029	
90.00	.7350	.4656	.0815	1.2821	1.2870	-.0049	
100.00	.7350	.4784	.1007	1.3141	1.3200	-.0059	
110.00	.7350	.4913	.1232	1.3495	1.3570	-.0075	
120.00	.7350	.5041	.1504	1.3895	1.3990	-.0095	
130.00	.7350	.5169	.1848	1.4367	1.4470	-.0103	
140.00	.7350	.5297	.2307	1.4954	1.5040	-.0086	
150.00	.7350	.5425	.2942	1.5717	1.5720	-.0003	
160.00	.7350	.5554	.3812	1.6716	1.6610	.0106	
170.00	.7350	.5682	.4944	1.7976	1.7890	.0086	

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Ethyl Acetate
Representation: CH3COOC2H5 Mol. Wt.: 88.10000
Melting Temperature: -83.60 Critical Temperature: 250.10 deg. C

Volumetric Units : NV: 6.0	NS1: 1.0	NS2: 1.0	
Geometric Factors:	KS1: .9818	KS2: .9818	KS3: 1.0000
INITIAL VOLUMES : V00: .7177	V01: .7046	V02: .7046	V03: .7177
Delta Vol.: .0000 Temperature Factor: 1.0		Corr. Coef.:	.9998

Temp.-deg. C	V1	V2	V3	VL	VO	Diff. cm3/g
.00	.7046	.3768	.0014	1.0828	1.0820	.0008
10.00	.7046	.3906	.0020	1.0972	1.0960	.0012
20.00	.7046	.4044	.0028	1.1118	1.1100	.0018
30.00	.7046	.4182	.0039	1.1267	1.1250	.0017
40.00	.7046	.4320	.0054	1.1420	1.1410	.0010
50.00	.7046	.4458	.0074	1.1578	1.1580	-.0002
60.00	.7046	.4596	.0100	1.1742	1.1750	-.0008
70.00	.7046	.4734	.0134	1.1914	1.1940	-.0026
80.00	.7046	.4872	.0177	1.2095	1.2130	-.0035
90.00	.7046	.5009	.0231	1.2286	1.2330	-.0044
100.00	.7046	.5147	.0297	1.2490	1.2540	-.0050
110.00	.7046	.5285	.0378	1.2709	1.2770	-.0061
120.00	.7046	.5423	.0476	1.2945	1.3020	-.0075
130.00	.7046	.5561	.0593	1.3200	1.3270	-.0070
140.00	.7046	.5699	.0730	1.3475	1.3550	-.0075
150.00	.7046	.5837	.0889	1.3772	1.3870	-.0098
160.00	.7046	.5975	.1075	1.4096	1.4220	-.0124
170.00	.7046	.6113	.1292	1.4451	1.4600	-.0149
180.00	.7046	.6251	.1553	1.4850	1.5030	-.0180
190.00	.7046	.6389	.1882	1.5317	1.5530	-.0213
200.00	.7046	.6527	.2314	1.5887	1.6100	-.0213
210.00	.7046	.6665	.2897	1.6608	1.6820	-.0212
220.00	.7046	.6803	.3677	1.7526	1.7710	-.0184

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Acetic Acid
Representation: CH3COOH Mol. Wt.: 60.05000
Melting Temperature: 16.70 Critical Temperature: 321.60 deg. C

Volumetric Units :	NV: 4.00	NS1: 4.00	NS2: 4.00		
Geometric Factors:		KS1: .8910	KS2: .8910	KS3: 1.0000	
INITIAL VOLUMES :	V00: .7020	V01: .6255	V02: .6255	V03: .7020	
Delta Vol.:	.0000	Temperature Factor: 1.0		Corr. Coef.: .9998	

Temp.-deg. C	V1	V2	V3	VL	VO	Diff. cm3/g
20.00	.6255	.3590	.0005	.9850	.9530	.0320
30.00	.6255	.3712	.0007	.9974	.9620	.0354
40.00	.6255	.3835	.0010	1.0100	.9720	.0380
50.00	.6255	.3957	.0014	1.0226	.9830	.0396
60.00	.6255	.4080	.0020	1.0355	.9940	.0415
70.00	.6255	.4202	.0027	1.0484	1.0050	.0434
80.00	.6255	.4325	.0037	1.0617	1.0170	.0447
90.00	.6255	.4447	.0050	1.0752	1.0290	.0462
100.00	.6255	.4570	.0067	1.0892	1.0420	.0472
110.00	.6255	.4692	.0088	1.1035	1.0550	.0485
120.00	.6255	.4814	.0115	1.1184	1.0680	.0504
130.00	.6255	.4937	.0149	1.1341	1.0830	.0511
140.00	.6255	.5059	.0191	1.1505	1.1000	.0505
150.00	.6255	.5182	.0243	1.1680	1.1160	.0520
160.00	.6255	.5304	.0306	1.1865	1.1330	.0535
170.00	.6255	.5427	.0381	1.2063	1.1500	.0563
180.00	.6255	.5549	.0470	1.2274	1.1690	.0584
190.00	.6255	.5672	.0574	1.2501	1.1890	.0611
200.00	.6255	.5794	.0695	1.2744	1.2100	.0644
210.00	.6255	.5917	.0835	1.3007	1.2330	.0677
220.00	.6255	.6039	.0995	1.3289	1.2590	.0699
230.00	.6255	.6161	.1179	1.3595	1.2880	.0715
240.00	.6255	.6284	.1394	1.3933	1.3210	.0723
250.00	.6255	.6406	.1655	1.4316	1.3580	.0736
260.00	.6255	.6529	.1982	1.4766	1.4010	.0756
270.00	.6255	.6651	.2408	1.5314	1.4490	.0824
280.00	.6255	.6774	.2970	1.5999	1.5090	.0909
290.00	.6255	.6896	.3698	1.6849	1.5790	.1059
300.00	.6255	.7019	.4605	1.7879	1.6810	.1069

Poor results using usual values of NS1 and NS2.

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Acetic Acid
Representation: CH3COOH Mol. Wt.: 60.05000
Melting Temperature: 16.70 Critical Temperature: 321.60 deg. C

Volumetric Units :	NV:	4.00	NS1:	3.50	NS2:	8.00		
Geometric Factors:			KS1:	.9046	KS2:	.7820	KS3:	1.0000
INITIAL VOLUMES :	V00:	.7020	V01:	.6350	V02:	.5490	V03:	.7020
Delta Vol.:	.0000	Temperature Factor:		1.0	Corr. Coef.:			.9998

Temp.-deg. C	V1	V2	V3	VL	VO	Diff. cm3/g
20.00	.6350	.3151	.0005	.9506	.9530	-.0024
30.00	.6350	.3258	.0007	.9615	.9620	-.0005
40.00	.6350	.3366	.0010	.9726	.9720	.0006
50.00	.6350	.3473	.0014	.9837	.9830	.0007
60.00	.6350	.3581	.0020	.9951	.9940	.0011
70.00	.6350	.3688	.0027	1.0065	1.0050	.0015
80.00	.6350	.3796	.0037	1.0183	1.0170	.0013
90.00	.6350	.3903	.0050	1.0303	1.0290	.0013
100.00	.6350	.4011	.0067	1.0428	1.0420	.0008
110.00	.6350	.4118	.0088	1.0556	1.0550	.0006
120.00	.6350	.4226	.0115	1.0691	1.0680	.0011
130.00	.6350	.4333	.0149	1.0832	1.0830	.0002
140.00	.6350	.4441	.0191	1.0982	1.1000	-.0018
150.00	.6350	.4548	.0243	1.1141	1.1160	-.0019
160.00	.6350	.4656	.0306	1.1312	1.1330	-.0018
170.00	.6350	.4763	.0381	1.1494	1.1500	-.0006
180.00	.6350	.4870	.0470	1.1690	1.1690	.0000
190.00	.6350	.4978	.0574	1.1902	1.1890	.0012
200.00	.6350	.5085	.0695	1.2130	1.2100	.0030
210.00	.6350	.5193	.0835	1.2378	1.2330	.0048
220.00	.6350	.5300	.0995	1.2645	1.2590	.0055
230.00	.6350	.5408	.1179	1.2937	1.2880	.0057
240.00	.6350	.5515	.1394	1.3259	1.3210	.0049
250.00	.6350	.5623	.1655	1.3628	1.3580	.0048
260.00	.6350	.5730	.1982	1.4062	1.4010	.0052
270.00	.6350	.5838	.2408	1.4596	1.4490	.0106
280.00	.6350	.5945	.2970	1.5265	1.5090	.0175
290.00	.6350	.6053	.3698	1.6101	1.5790	.0311
300.00	.6350	.6160	.4605	1.7115	1.6810	.0305

Much better results using NS2=8.00; must be because of hydrogen bonding.

*** L I Q U I D SPECIFIC VOLUME AS A FUNCTION OF TEMPERATURE ***

CHEMICAL NAME : Water
Representation: H2O Mol. Wt.: 18.01530
Melting Temperature: .00 Critical Temperature: 374.15 deg. C

Volumetric Units : NV: 1.50	NS1: 1.50	NS2: 1.50	
Geometric Factors:	KS1: .8910	KS2: .8910	KS3: 1.0000
INITIAL VOLUMES : V00: .8775	V01: .7819	V02: .7819	V03: .8775

Delta Vol.: .0275 Temperature Factor: 2.0 Corr. Coef.: .9987

Temp.-deg. C	V1	V2	V3	VL	VO	Diff. cm3/g
.00	.7914	.2091	.0001	1.0006	1.0002	.0004
10.00	.7899	.2167	.0001	1.0067	1.0004	.0063
20.00	.7886	.2244	.0002	1.0132	1.0018	.0114
30.00	.7874	.2320	.0003	1.0197	1.0044	.0153
40.00	.7864	.2397	.0004	1.0265	1.0079	.0186
50.00	.7854	.2473	.0005	1.0332	1.0121	.0211
60.00	.7847	.2550	.0008	1.0405	1.0171	.0234
70.00	.7840	.2626	.0011	1.0477	1.0228	.0249
80.00	.7835	.2703	.0015	1.0553	1.0290	.0263
90.00	.7831	.2780	.0020	1.0631	1.0359	.0272
100.00	.7828	.2856	.0028	1.0712	1.0435	.0277
110.00	.7825	.2933	.0037	1.0795	1.0515	.0280
120.00	.7823	.3009	.0049	1.0881	1.0603	.0278
130.00	.7822	.3086	.0065	1.0973	1.0697	.0276
140.00	.7821	.3162	.0086	1.1069	1.0798	.0271
150.00	.7820	.3239	.0112	1.1171	1.0906	.0265
160.00	.7820	.3315	.0144	1.1279	1.1021	.0258
170.00	.7820	.3392	.0183	1.1395	1.1144	.0251
180.00	.7819	.3468	.0232	1.1519	1.1275	.0244
190.00	.7819	.3545	.0291	1.1655	1.1415	.0240
200.00	.7819	.3621	.0362	1.1802	1.1565	.0237
210.00	.7819	.3698	.0446	1.1963	1.1726	.0237
220.00	.7819	.3774	.0545	1.2138	1.1900	.0238
230.00	.7819	.3851	.0661	1.2331	1.2087	.0244
240.00	.7819	.3928	.0795	1.2542	1.2291	.0251
250.00	.7819	.4004	.0948	1.2771	1.2512	.0259
260.00	.7819	.4081	.1122	1.3022	1.2755	.0267
270.00	.7819	.4157	.1320	1.3296	1.3023	.0273
280.00	.7819	.4234	.1548	1.3601	1.3321	.0280
290.00	.7819	.4310	.1813	1.3942	1.3655	.0287
300.00	.7819	.4387	.2134	1.4340	1.4036	.0304

Rather poor results using usual NS1 and NS2 values.