International Journal of Advance Research in Science and Engineering
Vol. No.4, Issue 09, September 2015
www.ijarse.com
IJARSE
ISSN 2319 - 8354

NEW RELATION BETWEEN VOLUME THERMAL EXPANSION AND THERMAL PRESSURE FOR SOLIDS

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ABSTRACT

A new relation between volume thermal expansion and thermal pressure for NaCl, KCl, MgO, CaO, Al_2O_3, and Mg_2SiO_4 has been derived. The results from this relation have been compared with experimental data and the results obtained by Kushwah *et.al.*. It has been observed that the new relation is in close agreement with experimental data.

Keywords: Equation of State; Bulk Modulus; Thermal Pressure; Thermal Expansion.

I INTRODUCTION

Volume expansion of solids due to rise in temperature is directly related to thermal pressure [1, 2]. Anderson[3] gave a relation for thermal pressure as

$$P(V,T) = P(V,T_0) + \Delta P_{th} \qquad \ldots (1)$$

where V is the volume, T the temperature and T_0 is initial value of temperature taken here is equal to 300 K. The last term in Equation (1) represents the difference in values of thermal pressure at two temperatures T and T_0 . i.e.

$$\Delta P_{th} = P_{th}(T) - P_{th}(T_0) \qquad \ldots (2)$$

In Equation (1) and (2), it has been assumed that the thermal pressure is a function of temperature only. At atmospheric pressure, i.e. at P (V, T) = 0, we have:

$$P(V,T_0) = -\Delta P_{th} \qquad \ldots (3)$$

II. METHOD OF ANALYSIS

The generalized Kushwah logarithmic EOS can be written as[4]

$$P(1-x)^{K_\infty'} = A_1 \ln(1+x) + A_2[\ln(1+x)]^2 + A_3[\ln(1+x)]^3 \qquad \dots (4)$$

where x = (1 – V/V_0), V_0 is the volume at atmospheric pressure, the constants A_1, A_2, and A_3 are defined by Kushwah *et al*[5]. as

$$A_1 = K_0 \qquad \dots (5)$$

$$A_2 = K_0\left(-\frac{K_0'}{10} + 1\right) \qquad \dots (6)$$

$$A_3 = K_0\left(-\frac{K_0'^2}{50} - \frac{K_0'}{5} + 1\right) \qquad \dots (7)$$

where K_0 and K_0' are isothermal bulk modulus and its first derivative at zero atmospheric pressure. Values of K_0 and K_0' for NaCl, KCl, MgO, CaO, Al_2O_3, and Mg_2SiO_4 are given in Table 1.

Table 1- Values of input data used in calculations, isothermal bulk modulus K_0 (GPa) and pressure derivative of isothermal bulk modulus K_0' are at T = 300 K and atmospheric pressure[5].

Solids	K_0	K_0'	K_∞'
NaCl	24.0	5.38	3.23
KCl	17.0	5.46	3.28
MgO	162	4.15	2.49
CaO	111	4.85	2.91
Al_2O_3	252	3.99	2.39
Mg_2SiO_4	127	5.40	3.24

From Equation (3) and (4) ΔP_{th} i.e. difference in thermal pressure can be obtained as

$$-\Delta P_{th}(1-x)^{K_\infty'} = A_1 \ln(1+x) + A_2[\ln(1+x)]^2 + A_3[\ln(1+x)]^3 \qquad \dots (8)$$

Here V/V_0 is the volume expansion with increase in temperature for solids at atmospheric pressure (P = 0)

We suggest a new relation for ΔP_{th} for solids as

$$\Delta P_{th} = B_0 - B_1 Exp\left(-\frac{V/V_0}{B_2}\right) \qquad \dots (9)$$

where B_0, B_1, and B_2 are constants and values of these constants are given in table 2 and obtained values of thermal pressure ΔP_{th} and volume thermal expansion V/V_0 for NaCl, KCl, MgO, CaO, Al_2O_3, and Mg_2SiO_4 as a function of temperature as given in Table 3.

Table 2----Values of constants B_0, B_1, and B_2 for NaCl, KCl, MgO, CaO, Al_2O_3, and Mg_2SiO_4 obtained from mat lab.

Solids	B_0	B_1	B_2
NaCl	3.7026	2471.01644	0.15377
KCl	2.59103	1866.23596	0.15197
MgO	28.65951	7937.78069	0.17782
CaO	18.42856	7675.73465	0.16579
Al_2O_3	50.878	7143.459	0.20226
Mg_2SiO_4	14.14074	15549.06156	0.14926

Table 3 --- values of thermal pressure ΔP_{th} and volume thermal expansion V/V_0 for NaCl, KCl, MgO, CaO, Al_2O_3, and Mg_2SiO_4 as a function of temperature.

Solids	Temperature T (K)	Thermal pressure ΔP_{th} (GPa) Kushwah EOS Eq. (8)	Experimental Ref. [3]	Volume thermal expansion V/V_0 Ref [3]	Thermal pressure ΔP_{th} (GPa) Eq. (9)
NaCl	300	0.00	0.00	1.0000	0.00
	350	0.14	0.14	1.0060	0.14
	400	0.28	0.28	1.0123	0.28
	450	0.43	0.43	1.0188	0.43
	500	0.57	0.57	1.0256	0.57
	550	0.71	0.71	1.0328	0.71
	600	0.85	0.85	1.0402	0.85
	650	0.99	0.99	1.0480	0.99
	700	1.13	1.13	1.0561	1.13
	750	1.26	1.27	1.0645	1.27
KCl	300	0.00	0.00	1.0000	0.00
	350	0.09	0.09	1.0054	0.09
	400	0.18	0.19	1.0112	0.19
	450	0.28	0.28	1.0172	0.28
	500	0.37	0.37	1.0235	0.37
	550	0.46	0.47	1.0301	0.47
	600	0.56	0.56	1.0370	0.56
	650	0.65	0.65	1.0442	0.65
	700	0.75	0.75	1.0517	0.75
	750	0.84	0.84	1.0594	0.84

	800	0.93	0.93	1.0675	0.93
	850	1.01	1.02	1.0759	1.02

Table 3 --- - values of thermal pressure ΔP_{th} and volume thermal expansion V/V_0 for NaCl, KCl, MgO, CaO, Al_2O_3, and Mg_2SiO_4 as a function of temperature

Solids	Temperature T (K)	Thermal pressure ΔP_{th} (GPa) Kushwah EOS Eq. (8)	Thermal pressure ΔP_{th} (GPa) Experimental Ref. [3]	Volume thermal expansion V/V_0 Ref [3]	Thermal pressure ΔP_{th} (GPa) Eq. (9)
MgO	300	0.00	0.00	1.0000	0.00
	400	0.53	0.54	1.0033	0.54
	500	1.16	1.12	1.0073	1.12
	600	1.76	1.73	1.0112	1.73
	700	2.38	2.35	1.0153	2.35
	800	3.02	2.98	1.0196	2.98
	900	3.66	3.61	1.0240	3.61
	1000	4.28	4.24	1.0284	4.24
	1100	4.93	4.87	1.0331	4.87
	1200	5.58	5.50	1.0379	5.50
	1300	6.21	6.12	1.0427	6.12
	1400	6.83	6.74	1.0476	6.74
	1500	7.48	7.36	1.0528	7.36
	1600	8.12	7.97	1.0581	7.97
	1700	8.76	8.58	1.0635	8.58
	1800	9.37	9.20	1.0688	9.20
CaO	300	0.00	0.00	1.0000	0.00
	400	0.36	0.36	1.0033	0.36
	500	0.74	0.74	1.0066	0.74
	600	1.14	1.13	1.0106	1.13
	700	1.54	1.53	1.0145	1.53
	800	1.96	1.94	1.0186	1.94
	900	2.35	2.34	1.0226	2.34
	1000	2.74	2.74	1.0267	2.74
	1100	3.15	3.13	1.0311	3.13
	1200	3.56	3.53	1.0356	3.53
Al_2O_3	300	0.00	0.00	1.0000	0.00
	400	0.45	0.45	1.0018	0.45
	500	1.00	0.98	1.0040	0.98
	600	1.56	1.55	1.0063	1.55
	700	2.17	2.15	1.0088	2.15
	800	2.79	2.76	1.0114	2.76
	900	3.45	3.43	1.0142	3.43
	1000	4.06	4.01	1.0168	4.01
	1100	4.68	4.64	1.0195	4.64
	1200	5.32	5.27	1.0223	5.27

	1300	5.97	5.90	1.0252	5.90
	1400	6.56	6.53	1.0279	6.53
	1500	7.19	7.16	1.0308	7.16
	1600	7.81	7.79	1.0337	7.79
	1700	8.38	8.42	1.0364	8.42
	1800	9.01	9.05	1.0394	9.05

Table 3 --- - values of thermal pressure ΔP_{th} and volume thermal expansion V/V_0 for NaCl, KCl, MgO, CaO, Al_2O_3, and Mg_2SiO_4 as a function of temperature

Solids	Temperature T (K)	Thermal pressure ΔP_{th} (GPa) Kushwah EOS Eq. (8)	Experimental Ref. [3]	Volume thermal expansion V/V_0 Ref [3]	Thermal pressure ΔP_{th} (GPa) Eq. (9)
Mg_2SiO_4	300	0.00	0.00	1.0000	0.00
	400	0.35	0.36	1.0028	0.36
	500	0.74	0.75	1.0059	0.75
	600	1.16	1.16	1.0094	1.16
	700	1.57	1.57	1.0129	1.57
	800	1.98	1.98	1.0164	1.98
	900	2.37	2.40	1.0199	2.40
	1000	2.80	2.83	1.0238	2.83
	1100	3.22	3.25	1.0277	3.25
	1200	3.67	3.69	1.0320	3.69
	1300	4.11	4.13	1.0363	4.13
	1400	4.54	4.56	1.0407	4.56
	1500	4.97	5.00	1.0451	5.00
	1600	5.40	5.43	1.0498	5.43
	1700	5.84	5.87	1.0547	5.87

III. CONCLUSION

Comparison of difference in thermal pressure with respect to volume expansion for NaCl, KCl, MgO, CaO, Al_2O_3, and Mg_2SiO_4 is given in Table 3. Which show that values of ΔP_{th} predicted from Equation (9) is accurate and close to experimental data as compared to Equation (8) proposed by Kushwah *et al.*

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