



Analysis of isothermal EOS for NaCl under extreme compression

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ABSTRACT

Different isothermal EOS, which expresses volume ratio as a function of pressure for materials at given temperature has been discussed. During our computational investigation it is observed that Holzapfel EOS does not satisfy the agreement of $K_T K_T''$ as calculated by using Brennan Stacey EOS, Shanker EOS, and Vinet EOS. The critical test of EOS for solids under extreme compressions has been discussed by evaluating the pressure and volume derivative properties viz. isothermal bulk modulus and its pressure derivative, according to the data calculated for NaCl up to extremely high pressure. Among the four EOS viz Holzapfel EOS, Brennan Stacey EOS, Shanker EOS, and Vinet EOS, it is found that, Holzapfel EOS is not suitable for calculating higher pressure derivative of isothermal bulk modulus under extreme compression

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Introduction

The exploration of matter at extreme conditions is a central theme in a broad range of scientific disciplines (e.g. material science, chemistry, physics and Earth and planetary science). The application of pressure can induces both continuous and discontinuous changes in atomic and electronic structure of a material. Learning how atomic and electronic arrangements change under extreme conditions, provide insight into the nature of phase transformations, chemical reaction, and also evolution in micro- and nanostructural components, such as crystallite size, dislocations, voids, and grain boundaries. Once these processes are understood, it will be possible to predict responses of materials under thermo-mechanical extremes using advanced computational tools. Further, this fundamental knowledge will open new avenues for designing and synthesizing materials with unique properties. These thermo-mechanical extremes will allow the tuning of atomic structure and the varying nature of chemical bonds to produce revolutionary new materials.

The properties of solids at high pressure and temperature are very important for their application point of view. NaCl is an important alkali halide that is used as a pressure gauge in laboratory measurements of compression data. It is one of the most widely used internal pressure standards in high-pressure diffraction experiments owing to the availability of a large body of experimental data. For instance, the equation of state for B1-type NaCl has been investigated in several studies up to the limit of its stability [1–8]. It is also known that the B1-type NaCl is only stable up to a pressure of about 30 GPa, where the occurrence of a pressure-induced phase transition from B1 type (rocksalt) to B2-type (cesium chloride) as it has been reported by different group of researchers. [9–15] Although it is experimentally possible to study the B2-type NaCl at elevated pressures, its equation of state has not been investigated well yet, especially at high temperatures. This, therefore, limits the use of NaCl as a pressure standard to relatively low pressures and temperatures. Therefore, the P - V - T equation of state

reported in this article will be fundamentally important for extending its scientific and engineering applications including its usefulness as a pressure calibrant.

The main objective of present paper is to reduce the gap between theoretical and practical approach of investigations for the solids at high pressure in context to NaCl crystal with only moderate computations.

In present paper an attempt has been made to find suitable EOS for calculating pressure P , bulk modulus K_T and its higher order pressure derivatives K_T' and K_T'' for NaCl crystal by using four empirical isothermal EOS viz. Holzapfel EOS [16], Brennan Stacey EOS[17], Shanker EOS [17] and Vinet EOS[17] between the temperature range 300K-1050K.

Theory

The EOS have fundamental basis. Shock wave reduced isotherms (SWRI) are commonly considered as most reliable EOS data for the realization of a practical pressure scale. Holzapfel considered a comparison of SWRI for different metals and also the calibration of the ruby luminescence line shift stresses as secondary pressure scale and discussed corrections for the deviatoric stresses, effects from uncertainties in the theoretically derived *Grüneisen* parameter, to derive an EOS [16] as given below:

$$P = 3K_0 x^{-5} (1-x) \exp[f(1-x)] \quad (1)$$

$$\text{Where } x = \left(\frac{V}{V_0}\right)^{\frac{1}{3}} \text{ and } f = \frac{3}{2}(K_0' - 3)$$

Brennan Stacey EOS derived, using the thermodynamic formulation for the *Grüneisen* parameter [18-19] is as follows:

$$P = \frac{3K_0 \left(\frac{V}{V_0}\right)^{\frac{4}{3}}}{(3K_0' - 5)} \left[\exp \left\{ \left(\frac{3K_0' - 5}{3} \right) \times \left(1 - \frac{V}{V_0} \right) \right\} - 1 \right] \quad (2)$$

The Shanker EOS derived using a modified exponential dependence for the short range constant on volume [20] is as follows:

$$P = \frac{3K_0 \left(\frac{V}{V_0}\right)^{-\frac{4}{3}}}{(3K_0' - 8)} \left[\left(1 - \frac{1}{t} + \frac{1}{t^2}\right)(\exp ty - 1) + y \left(1 + y - \frac{2}{t}\right) \exp ty \right] \quad (3)$$

$$\text{Where } y = \left(1 - \frac{V}{V_0}\right) \text{ and } t = \left(K_0' - \frac{8}{3}\right)$$

Vinet EOS based on universal relationship between binding energy and interatomic separation for solids [21, 22] is as follows:

$$P = 3K_0 x^{-2} (1-x) \exp[\eta(1-x)] \quad (4)$$

$$\text{Where } \eta = \frac{3}{2} (K_0' - 1)$$

Expression for isothermal bulk modulus corresponding to equations (1), (2) and (3) obtained by using the

relationship $K_T = -V \left(\frac{dP}{dV}\right)_T$ given as

$$K_T = \frac{1}{3} fPx - K_0 x^{-5} (4x - 5) \exp[f(1-x)] \quad (5)$$

$$K_T = K_0 \left(\frac{V}{V_0}\right)^{-\frac{4}{3}} \exp \left\{ \left(K_0' - \frac{5}{3}\right) \left(1 - \frac{V}{V_0}\right) \right\} + \frac{4}{3} P \quad (6)$$

$$K_T = \frac{4}{3} P + K_0 \left(\frac{V}{V_0}\right)^{-\frac{4}{3}} \exp \left\{ \left(K_0' - \frac{8}{3}\right) \left(1 - \frac{V}{V_0}\right) \right\} \quad (7)$$

and

$$K_T = K_0 x^{-2} [1 + (\eta x + 1)(1-x)] \exp\{\eta(1-x)\} \quad (8)$$

The expression for first pressure derivative of isothermal bulk modulus can be given as

$$K_T' = \frac{\partial K_T}{\partial P} = \frac{\partial K_T}{\partial V} \frac{\partial V}{\partial P} \quad (9)$$

Using expression (9) in equations (5), (6), (7) and (8), the first derivative of isothermal bulk modulus K_T' becomes

$$K_T' = \frac{fx}{3} \left[\left(1 - \frac{P}{3K_T}\right) - \frac{1}{K_T} \left(\frac{fPx}{3} - K_T\right) \right] - \frac{K_0 x^{-5}}{3K_T} (16x - 25) \exp[f(1-x)] \quad (10)$$

$$K_T' = \frac{16}{9} \frac{P}{K_T} + \left(1 - \frac{4P}{3K_T}\right) \left\{ \frac{V}{V_0} \left(K_0' - \frac{5}{3}\right) + \frac{5}{3} \right\} \quad (11)$$

$$K_T' = \frac{16}{9} \frac{P}{K_T} + \left(1 - \frac{4P}{3K_T}\right) \left\{ \frac{V}{V_0} \left(K_0' - \frac{8}{3}\right) + \frac{8}{3} \right\} \quad (12)$$

and

$$K_T' = \frac{1}{3} \left[\frac{x(1-\eta) + 2\eta x^2}{1 + (\eta x + 1)(1-x)} + \eta x + 2 \right] \quad (13)$$

The corresponding expression for second order pressure derivative of isothermal bulk modulus

$$K_T'' = \frac{\partial K_T'}{\partial P}, \text{ obtained from further derivation of (10), (11),}$$

(12) and (13) are written as follows:

$$K_T K_T'' = -\frac{fx}{9} \left[2 \left(1 - \frac{fPx}{3K_T}\right) - \frac{P}{3K_T} + \left(1 - \frac{PK_T'}{K_T}\right) (1 + fx) \right] + \frac{K_0}{3K_T} \times \left[\left\{ (16x^{-4} - 25x^{-5}) \left(K_T' - \frac{fx}{3}\right) \right\} - \frac{1}{3} \{64x^{-4} - 125x^{-5}\} \right] \exp[f(1-x)] \quad (14)$$

$$K_T K_T'' = \frac{16}{9} - \frac{16K_T'}{9K_T} - \frac{V}{V_0} \left(K_0' - \frac{5}{3}\right) \left(1 - \frac{4P}{3K_T}\right) - \frac{4}{3} \left(1 - \frac{PK_T'}{K_T}\right) \left\{ \frac{V}{V_0} \left(K_0' - \frac{5}{3}\right) + \frac{5}{3} \right\} \quad (15)$$

$$K_T K_T'' = \frac{4}{3} \left[1 - \frac{PK_T'}{K_T} \right] \left[\frac{4}{3} - \left\{ \frac{V}{V_0} \left(K_0' - \frac{8}{3}\right) + \frac{8}{3} \right\} \right] - \frac{V}{V_0} \left(K_0' - \frac{8}{3}\right) \left(1 - \frac{4P}{3K_T}\right) \quad (16)$$

and

$$K_T K_T'' = \frac{x}{9} \left[\frac{\{x(1-\eta) + 2\eta x^2\} \{\eta(1-2x) - 1\}}{\{1 + (\eta x + 1)(1-x)\}^2} - 1 - 4\eta x \right] \quad (17)$$

Results and Discussion

In the present work we have described four different forms of EOS, equations (1), (5), (10) and (14) corresponds for Holzapfel EOS, equation (2), (6), (11) and (15) corresponds for Brennan Stacey EOS, equations (3), (7), (12) and (16) corresponds for Shanker EOS and equations (4), (8), (13) and (17) corresponds for Vinet EOS. All the four EOS contains only two parameters K_0 and K_0' both at zero pressure at different temperature. These values of K_0 and K_0' have been recommended by Anderson [23]. The value of input parameters K_0 (GPa) and K_0' given in the Table-1 are obtained from the literature [24-26]. The values of pressure P (GPa) for NaCl were computed for given increments of V/V_0 by using equation (1), (2), (3) and (4) at different temperature ranges from 300K - 1050K.

Using the value of pressure P computed as above, the value of isothermal bulk modulus K_T has been calculated by using equation (5), (6), (7) and (8). Substituting these values of P and K_T in equation (10), (11), (12) and (13), the values of first pressure derivative of K_T i.e. K_T' have been obtained. Further substituting the values of P, K_T , K_T' in equation (14), (15), (16)

and (17), second pressure derivative of K_T i.e. K_T'' has been calculated in terms of $K_T K_T''$.

These calculated values of P , K_T , K_T' and $K_T K_T''$ for NaCl at different temperature shown in Table (2 – 7). The graphs plotted between V/V_0 vs P , P vs K_T , P vs K_T' , P vs $-K_T K_T''$ shown in fig. (1 – 24).

By presenting a comprehensive analysis for EOS in the limit of extreme compression, Stacey [27-28] has given some basic criteria which must be satisfied by an EOS for its validity and applicability. We list these criteria as

(i) In the limit $\frac{V}{V_0} \rightarrow 0$, the pressure should not remain finite

but it must approach infinity.

(ii) The isothermal bulk modulus must increase regularly and continuously with the increase in pressure such that $K_T \rightarrow \infty$ in the limit of infinitely large pressure.

(iii) The pressure derivative of isothermal bulk modulus K_T' must decreases progressively with the increase in pressure such that K_T' remains greater than 5/3 in the limit of infinitely large pressure i.e. $P \rightarrow \infty$ and $\frac{V}{V_0} \rightarrow 0$.

(iv) $K_0 K_0''$ must be negative and will decreases with increase in temperature and $-K_T K_T'' \rightarrow 0$ as $P \rightarrow \infty$.

From the fig. (1 – 6), showing the graph P vs V/V_0 , it is observed that the values of pressure calculated by using equations (1 – 4) are in good agreement with each other in the entire temperature ranges having a slight deviation at higher temperature above 600K. Also from fig. (1 – 6) it is clear that in

the limit $\frac{V}{V_0} \rightarrow 0$, the pressure should not remain finite but it

approaches to infinity. It is also observed that the amount of pressure required for producing the same change in V/V_0 decreases continuously with increase in temperature. This is related to the fact that the bulk modulus becomes less and the material becomes more compressible at higher temperature. It is also clear from fig. (7-12) that bulk modulus increases with the increase in pressure such that $K_T \rightarrow \infty$ in the limit of infinitely large pressure, whereas it decreases with increase in temperature but at higher compressions the rate of decrement in bulk modulus with temperature becomes slow.

Bulk modulus is thus found to depend strongly on pressure as well as temperature. From fig. (13-18) it is also clear that the pressure derivative of isothermal bulk modulus decreases with increase in pressure and when $P \rightarrow \infty$, K_T' remains greater than 5/3.

From fig. (7 – 24) it is observed that for K_T , K_T' and $-K_T K_T''$, Holzapfel is distinguished from other three EOS i.e. Brennan Stacey, Shanker, and Vinet as these are in good agreement with each other among all the graphs while Holzapfel curve is differ from them. The basic foundation of Holzapfel EOS depends on single parameter. This one parameter EOS

[29 – 34], based on the assumption that under very strong compression all solids approaches to the Thomas- Fermi state has a certain degree of predictive capability. Thomas-Fermi state is given by [34]

$$P = 1003.6 \left(\frac{Z}{V} \right)^{\frac{5}{3}} \quad (18)$$

Where Z and V are atomic number and molar volume (cm^3/mole) respectively. Stacey has emphases in a very convincing way that analytical EOS describing the phase transition from zero pressure to infinite pressure. The Thomas-Fermi state is not valid mainly because parameters appearing in such equations cannot remain unchanged through phase transition.

The validity of equation (1-4) can also be checked by using two well accepted constraints [27, 28]. The first constraint reveals that $K_0 K_0''$ must be negative i.e. less than zero where as the second constraint reveals that the first pressure derivative of isothermal bulk modulus at extreme compression must be greater than or equal to 5/3 i.e. $K_\infty' \geq 5/3$.

The first set of constraints is based on the fact that K_T' decreases with increase in the pressure, this has been supported theoretically as shown in fig. (13-18).

For second set of constraints, Keane [35-37] and Stacey EOS yields an identical relationship given as

$$K_0 K_0' = -K_0' (K_0' - K_\infty') \quad (19)$$

Using the value of K_0'' and K_0' from Table (2-7), it is observed that the value of K_∞' / K_0' yields a result ≈ 0.9 which is greater than 3/5 upto 600K for all the four EOS whereas beyond 600K Holzapfel equation fails hopelessly to satisfy the constraint $K_\infty' \geq 5/3$.

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Table1: Values of Input parameters of Isothermal bulk modulus (K_0) and its first pressure derivative (K'_0) at zero pressure for NaCl at different temperature [24, 25, 26].

S. No.	Temperature (K)	K_0 (GPa)	K'_0
1.	300	24.0	5.35
2.	450	21.6	5.51
3.	600	19.0	5.73
4.	750	16.5	6.03
5.	900	14.1	6.40
6.	1050	11.7	6.85

Table 2: Values of P(GPa), K_T (GPa), K'_T and $K_T K''_T$ calculated by using (A)Holzapfel EOS, (B) Brennan Stacey EOS, (C) Shanker EOS and (D) Vinet EOS for NaCl at 300K.

V/V ₀	P(A)	P(B)	P(C)	P(D)	K_T (A)	K_T (B)	K_T (C)	K_T (D)	K'_T (A)	K'_T (B)	K'_T (C)	K'_T (D)	$K_T K''_T$ (A)	$K_T K''_T$ (B)	$K_T K''_T$ (C)	$K_T K''_T$ (D)
1	0	0	0	0	24	24	24	24	5.35	5.35	5.35	5.35	-8.30	-9.04	-9.04	-9.30
0.95	1.41	1.41	1.41	1.41	31.26	31.2	31.27	31.23	4.98	4.93	4.98	4.93	-6.41	-7.26	-7.25	-7.42
0.9	3.34	3.34	3.34	3.34	40.56	40.38	40.58	40.37	4.67	4.58	4.67	4.54	-5.07	-5.97	-5.94	-6.11
0.85	5.99	5.97	5.99	5.97	52.56	51.98	52.57	52.02	4.41	4.27	4.4	4.29	-4.07	-5.00	-4.96	-5.04
0.8	9.64	9.55	9.62	9.56	68.18	66.74	68.09	66.95	4.19	3.99	4.16	4.04	-3.32	-4.26	-4.20	-3.96
0.75	14.7	14.45	14.6	14.5	88.75	85.6	88.35	86.25	3.99	3.73	3.94	3.82	-2.74	-3.66	-3.59	-3.46
0.7	21.7	21.17	21.5	21.3	116.2	109.83	115	111.44	3.82	3.5	3.75	3.62	-2.29	-3.18	-3.10	-3.36
0.65	31.6	30.43	31	30.7	153.2	141.14	150.4	144.68	3.66	3.28	3.56	3.43	-1.92	-2.77	-2.70	-3.05

Table3: Values of of P(GPa), K_T (GPa), K'_T and $K_T K''_T$ calculated by using (A)Holzapfel EOS, (B) Brennan Stacey EOS, (C) Shanker EOS and (D) Vinet EOS for NaCl at 450K.

V/V ₀	P(A)	P(B)	P(C)	P(D)	K_T (A)	K_T (B)	K_T (C)	K_T (D)	K'_T (A)	K'_T (B)	K'_T (C)	K'_T (D)	$K_T K''_T$ (A)	$K_T K''_T$ (B)	$K_T K''_T$ (C)	$K_T K''_T$ (D)
1	0	0	0	0	21.6	21.6	21.6	21.6	5.51	5.51	5.51	5.51	-8.82	-9.41	-9.41	-9.82
0.95	1.28	1.28	1.28	1.27	28.35	28.33	28.36	28.32	5.11	5.08	5.13	5.07	-6.76	-7.53	-7.52	-7.79
0.9	3.04	3.03	3.04	3.03	37.04	36.9	37.08	36.87	4.79	4.71	4.8	4.71	-5.31	-6.18	-6.15	-6.39
0.85	5.46	5.44	5.46	5.44	48.32	47.84	48.38	47.82	4.52	4.39	4.52	4.4	-4.25	-5.17	-5.13	-5.37
0.8	8.82	8.75	8.81	8.75	63.09	61.86	63.11	61.95	4.29	4.1	4.27	4.14	-3.46	-4.40	-4.34	-4.60
0.75	13.5	13.31	13.4	13.3	82.63	79.89	82.45	80.31	4.08	3.83	4.1	3.91	-2.85	-3.79	-3.72	-4.01
0.7	20.1	19.6	19.9	19.7	108.8	103.19	108.1	104.42	3.9	3.6	3.8	3.7	-2.37	-3.29	-3.21	-3.54
0.65	29.4	28.34	28.9	28.6	144.5	133.5	142.3	136.44	3.74	3.36	3.6	3.52	-1.99	-2.87	-2.80	-3.16

Table4: Values of P(GPa), K_T (GPa), K'_T and $K_T K''_T$ calculated by using (A)Holzapfel EOS, (B) Brennan Stacey EOS, (C) Shanker EOS and (D) Vinet EOS for NaCl at 600K.

V/V ₀	P(A)	P(B)	P(C)	P(D)	K_T (A)	K_T (B)	K_T (C)	K_T (D)	K'_T (A)	K'_T (B)	K'_T (C)	K'_T (D)	$K_T K''_T$ (A)	$K_T K''_T$ (B)	$K_T K''_T$ (C)	$K_T K''_T$ (D)
1	0	0	0	0	19	19	19	19	5.73	5.73	5.73	5.73	-9.55	-9.93	-9.93	-10.50
0.95	1.13	1.13	1.13	1.13	25.2	25.19	25.22	25.17	5.3	5.28	5.32	5.26	-7.25	-7.89	-7.89	-8.30
0.9	2.69	2.7	2.7	2.7	33.24	33.14	33.31	33.09	4.96	4.89	4.98	4.88	-5.65	-6.46	-6.43	-6.76
0.85	4.89	4.88	4.89	4.87	43.76	43.4	43.89	43.31	4.67	4.55	4.69	4.56	-4.50	-5.40	-5.35	-5.65
0.8	7.95	7.89	7.95	7.88	57.63	56.66	57.81	56.6	4.42	4.25	4.42	4.28	-3.64	-4.59	-4.53	-4.83
0.75	12.2	12.1	12.2	12.1	76.13	73.87	76.25	74.82	4.21	3.98	4.19	4.04	-2.99	-3.96	-3.88	-4.20
0.7	18.3	17.93	18.2	18	101.1	96.31	100.9	97.07	4.02	3.72	3.97	3.83	-2.48	-3.44	-3.36	-3.71
0.65	27	26.13	26.6	26.2	135.4	125.78	134.1	127.93	3.85	3.48	3.78	3.63	-2.08	-3.00	-2.93	-3.30

Table 5: Values of P(GPa), K_T (GPa), K'_T and $K_T K''_T$ calculated by using (A)Holzapfel EOS, (B) Brennan Stacey EOS, (C) Shanker EOS and (D) Vinet EOS for NaCl at 750K.

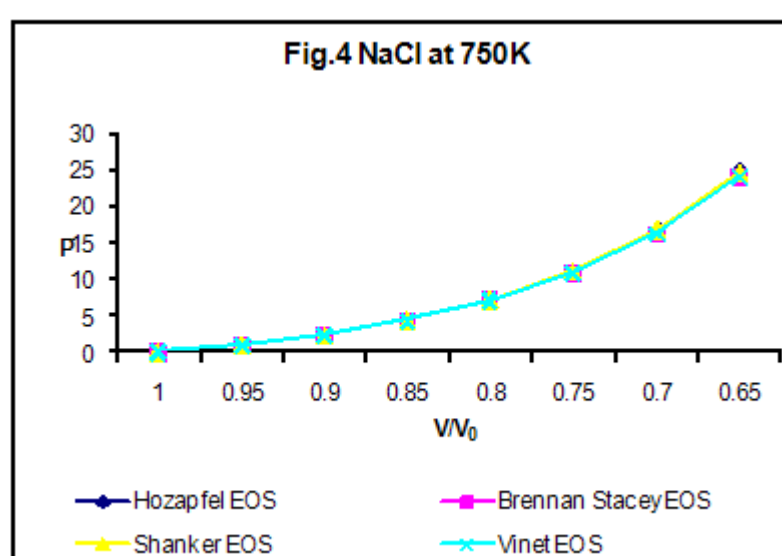
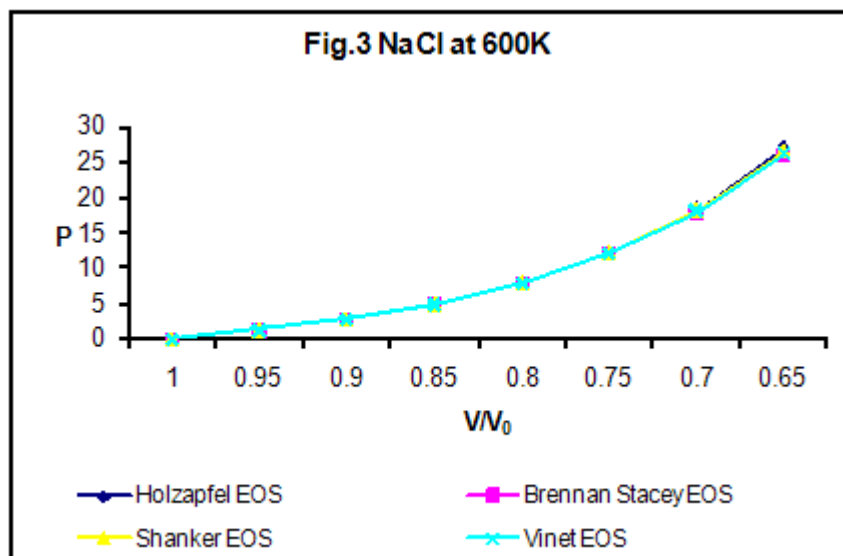
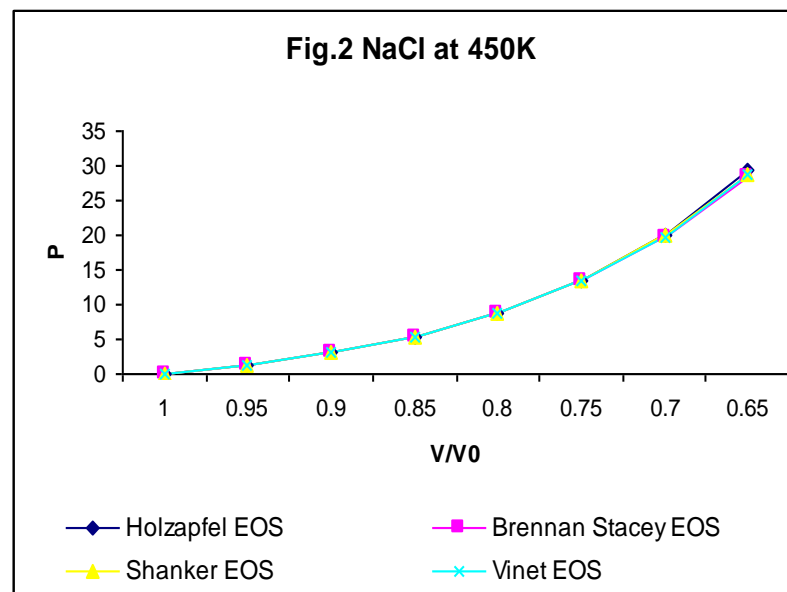
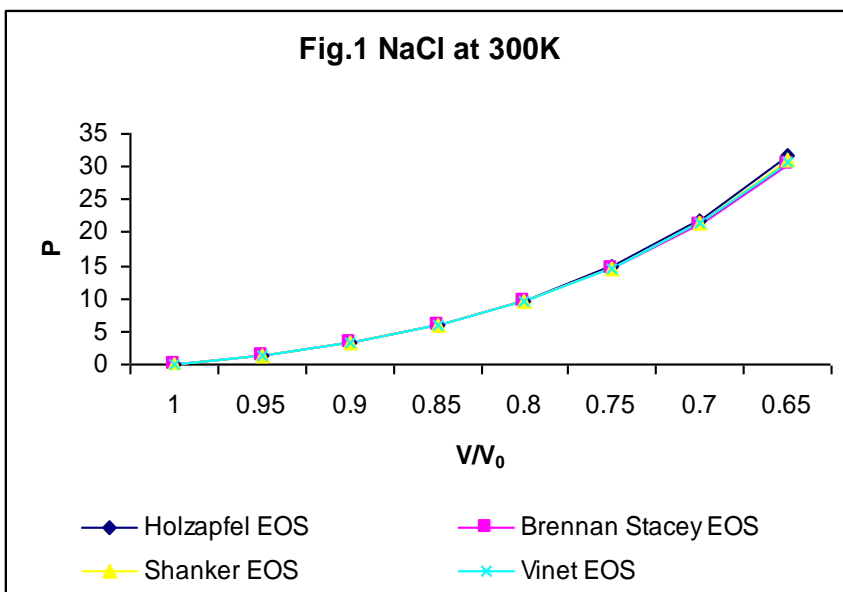
V/V ₀	P(A)	P(B)	P(C)	P(D)	K_T (A)	K_T (B)	K_T (C)	K_T (D)	K'_T (A)	K'_T (B)	K'_T (C)	K'_T (D)	$K_T K''_T$ (A)	$K_T K''_T$ (B)	$K_T K''_T$ (C)	$K_T K''_T$ (D)
1	0	0	0	0	16.5	16.5	16.5	16.5	6.03	6.03	6.03	6.03	-10.60	-10.63	-10.60	-11.60
0.95	0.99	0.99	0.99	0.99	22.2	22.19	22.22	22.17	5.56	5.55	5.59	5.52	-7.93	-8.40	-8.39	-9.00
0.9	2.38	2.38	2.38	2.38	29.67	29.61	29.76	29.53	5.18	5.14	5.23	5.1	-6.12	-6.80	-6.81	-7.30
0.85	4.35	4.34	4.36	4.33	39.53	39.2	39.75	39.13	4.87	4.78	4.91	4.76	-4.84	-5.70	-5.65	-6.04
0.8	7.13	7.09	7.14	7.07	52.68	51.99	53.06	51.75	4.61	4.46	4.64	4.47	-3.89	-4.80	-4.78	-5.15
0.75	11.1	10.97	11.1	10.9	70.4	68.69	70.91	68.47	4.38	4.17	4.39	4.21	-3.18	-4.20	-4.10	-4.46
0.7	16.7	16.4	16.7	16.4	94.59	90.73	95.06	90.84	4.18	3.9	4.16	3.99	-2.63	-3.60	-3.56	-3.93
0.65	24.9	24.21	24.7	24.2	128.1	120	128	121.14	4.01	3.65	3.95	3.78	-2.20	-3.20	-3.12	-3.49

Table 6: Values of P(GPa), K_T (GPa), K'_T and $K_T K''_T$ calculated by using (A)Holzapfel EOS, (B) Brennan Stacey EOS, (C) Shanker EOS and (D) Vinet EOS for NaCl at 900K.

V/V ₀	P(A)	P(B)	P(C)	P(D)	K_T (A)	K_T (B)	K_T (C)	K_T (D)	K'_T (A)	K'_T (B)	K'_T (C)	K'_T (D)	$K_T K''_T$ (A)	$K_T K''_T$ (B)	$K_T K''_T$ (C)	$K_T K''_T$ (D)
1	0	0	0	0	14.1	14.1	14.1	14.1	6.4	6.4	6.4	6.4	-11.90	-11.50	-11.50	-12.90
0.95	0.85	0.85	0.85	0.85	19.3	19.31	19.33	19.28	5.88	5.88	5.93	5.83	-8.79	-9.00	-8.99	-9.90
0.9	2.07	2.08	2.08	2.07	26.21	26.21	26.34	26.09	5.46	5.44	5.53	5.38	-6.71	-7.30	-7.26	-7.90
0.85	3.83	3.82	3.84	3.81	35.46	35.38	35.78	35.1	5.12	5.06	5.2	5.01	-5.25	-6.10	-6.02	-6.53
0.8	6.34	6.33	6.37	6.29	47.94	47.58	48.55	47.1	4.84	4.72	4.9	4.7	-4.19	-5.20	-5.09	-5.53
0.75	9.96	9.9	10	9.83	64.97	63.88	65.96	63.1	4.59	4.41	4.63	4.43	-3.41	-4.50	-4.37	-4.78
0.7	15.2	15.04	15.3	14.9	88.52	85.75	89.87	85.06	4.38	4.12	4.39	4.19	-2.81	-3.90	-3.80	-4.20
0.65	22.9	22.44	22.9	22.3	121.6	115.24	123	115.06	4.19	3.85	4.16	3.97	-2.34	-3.40	-3.34	-3.73

Table7: Values of P(GPa), K_T (GPa), K'_T and $K_T K''_T$ calculated by using (A)Holzapfel EOS, (B) Brennan Stacey EOS, (C) Shanker EOS and (D) Vinet EOS for NaCl at 1050K

V/V ₀	P(A)	P(B)	P(C)	P(D)	K_T (A)	K_T (B)	K_T (C)	K_T (D)	K'_T (A)	K'_T (B)	K'_T (C)	K'_T (D)	$K_T K''_T$ (A)	$K_T K''_T$ (B)	$K_T K''_T$ (C)	$K_T K''_T$ (D)
1	0	0	0	0	11.7	11.7	11.7	11.7	6.85	6.85	6.85	6.85	-13.60	-12.54	-12.50	-14.60
0.95	0.71	0.72	0.72	0.71	16.36	16.38	16.4	16.34	6.26	6.28	6.33	6.21	-9.80	-9.72	-9.71	-11.00
0.9	1.76	1.76	1.77	1.76	22.65	22.7	22.82	22.54	5.79	5.81	5.91	5.71	-7.42	-7.83	-7.80	-8.70
0.85	3.29	3.3	3.31	3.28	31.19	31.27	31.63	30.88	5.42	5.41	5.54	5.31	-5.75	-6.50	-6.45	-7.12
0.8	5.52	5.53	5.57	5.48	42.9	42.91	43.8	42.16	5.11	5.04	5.22	4.97	-4.55	-5.52	-5.45	-5.99
0.75	8.79	8.79	8.81	8.67	59.14	58.78	60.71	57.56	4.85	4.71	4.93	4.68	-3.68	-4.77	-4.69	-5.17
0.7	13.6	13.56	13.8	13.3	81.95	80.48	84.39	78.8	4.62	4.4	4.67	4.43	-3.02	-4.57	-4.10	-4.50
0.65	20.8	20.29	21	20.2	114.5	110.33	117.9	108.44	4.41	4.11	4.42	4.2	-2.51	-3.68	-3.61	-4.02

Fig.(1-6) :Plots of compressions V/V_0 vs P for NaCl by using equations (1-4) at different temperature.

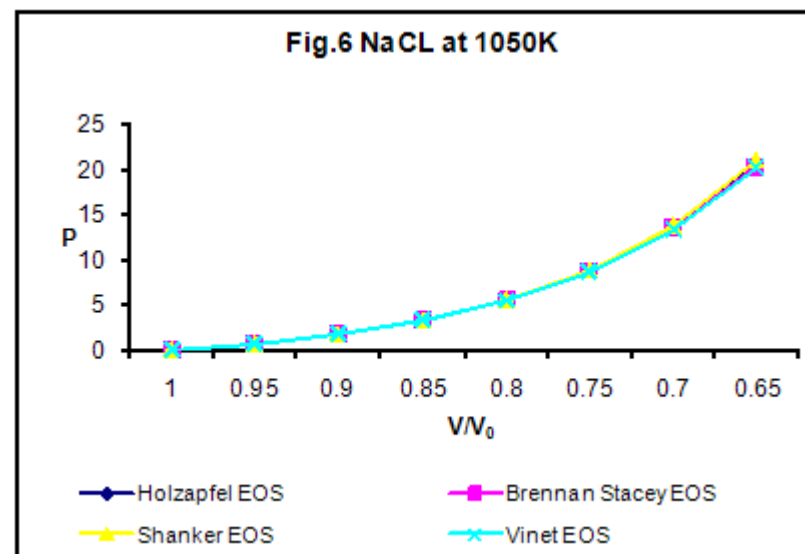
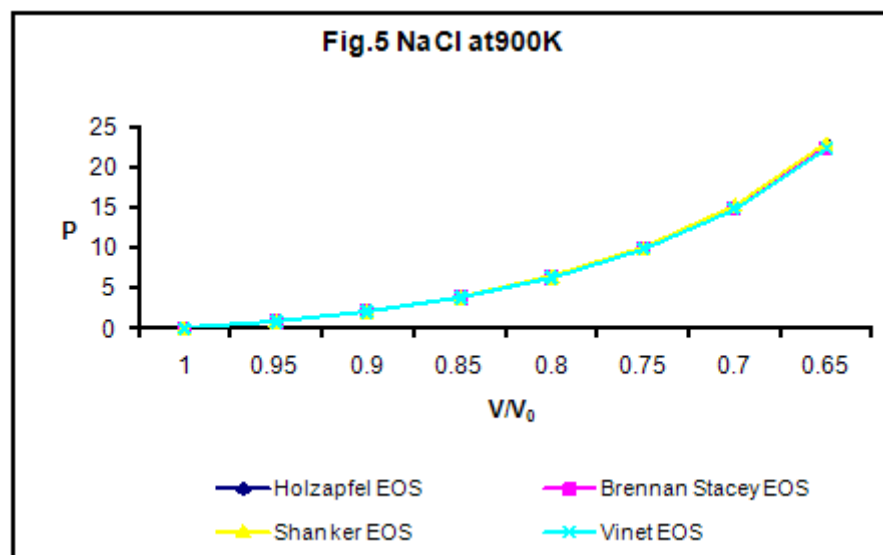
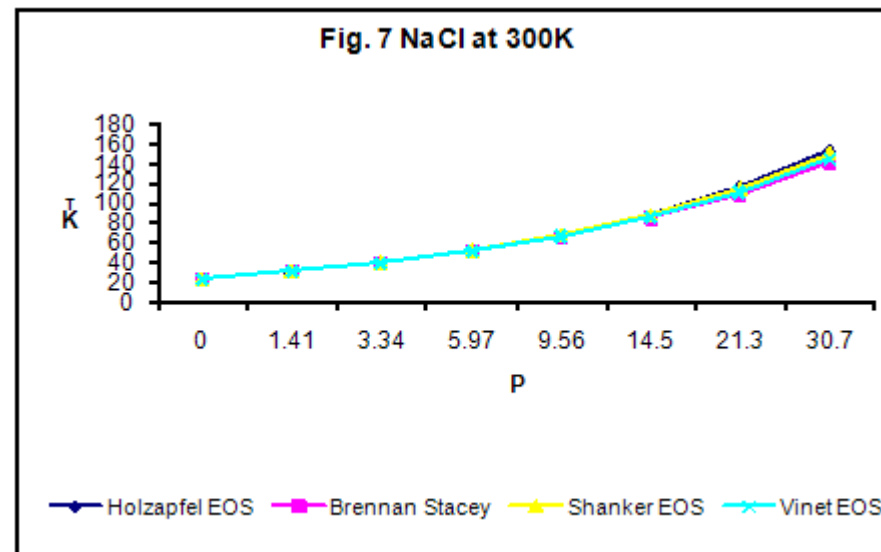
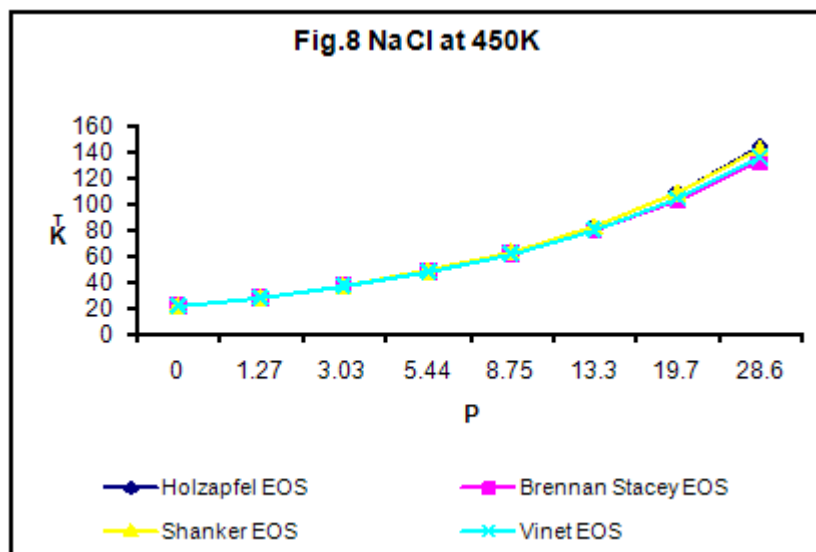


Fig. (7-12): Plots of pressure P vs K_T for NaCl by using equations (5-8) at different temperature.



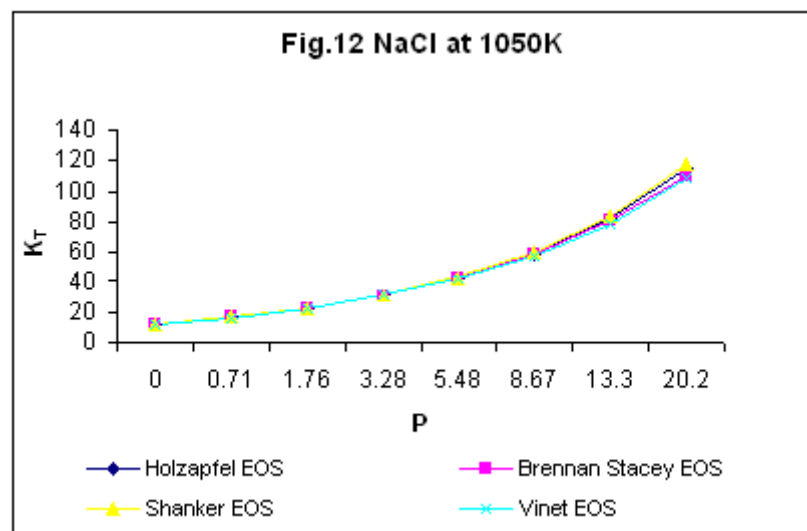
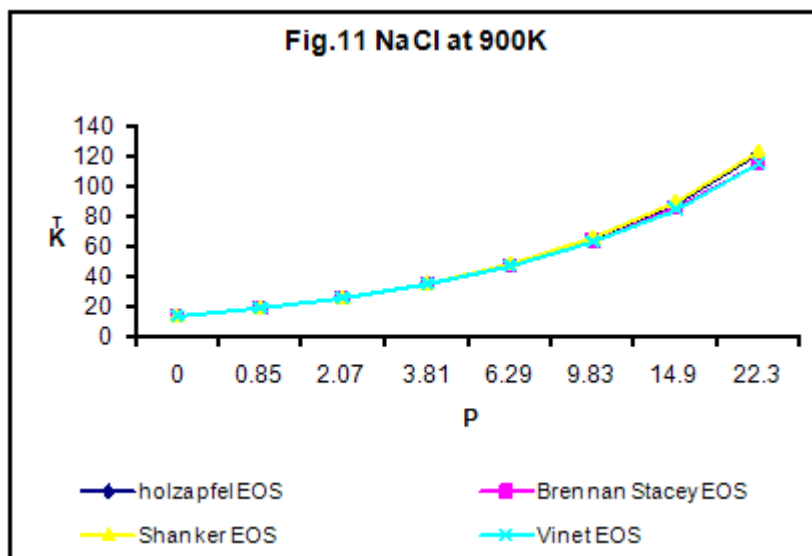
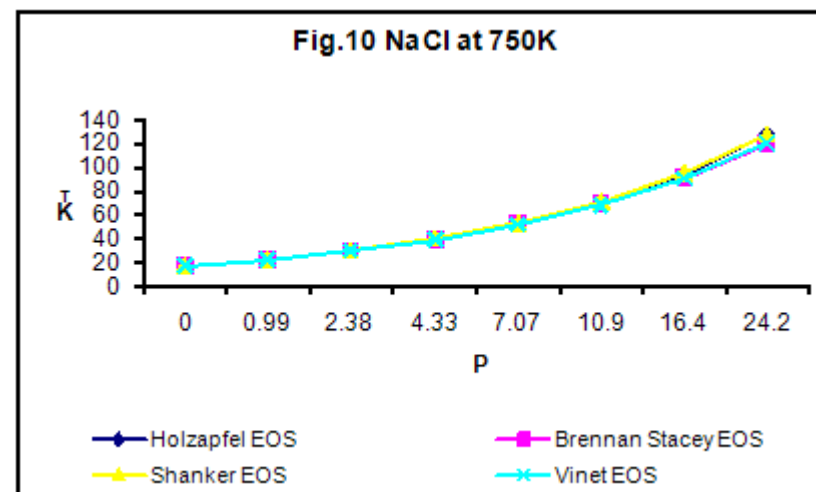
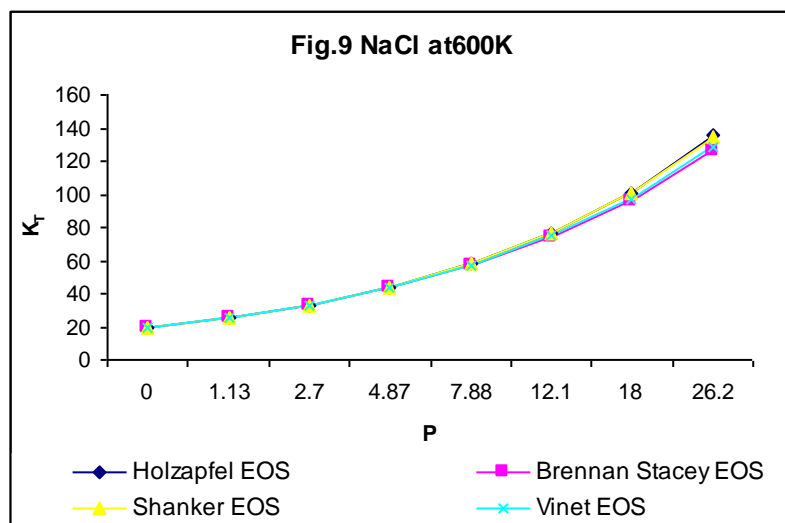
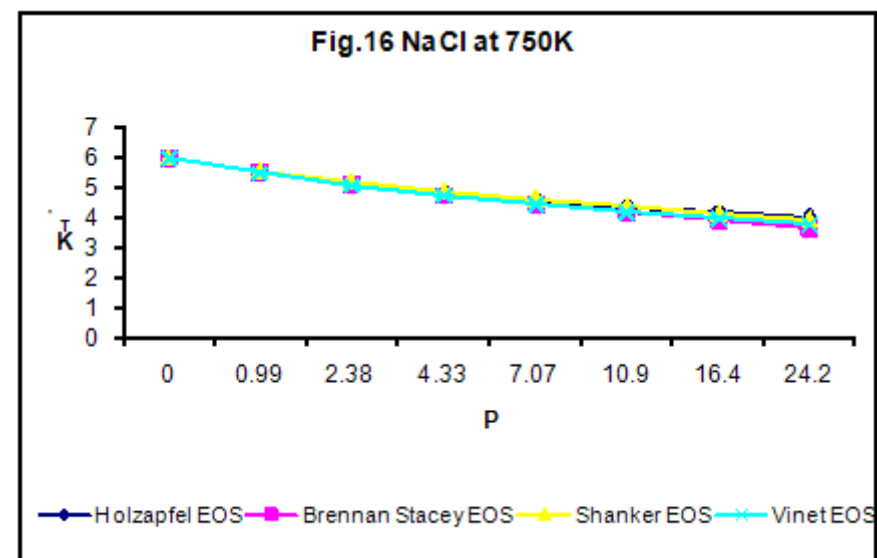
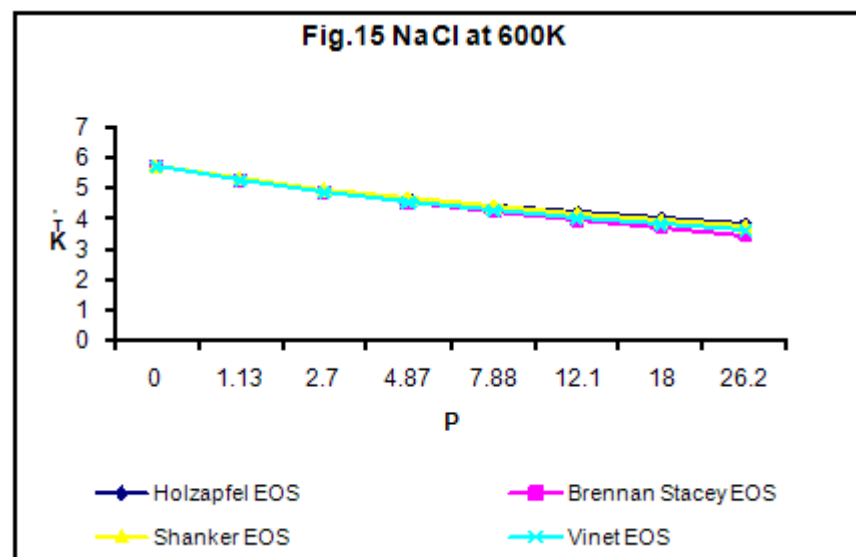
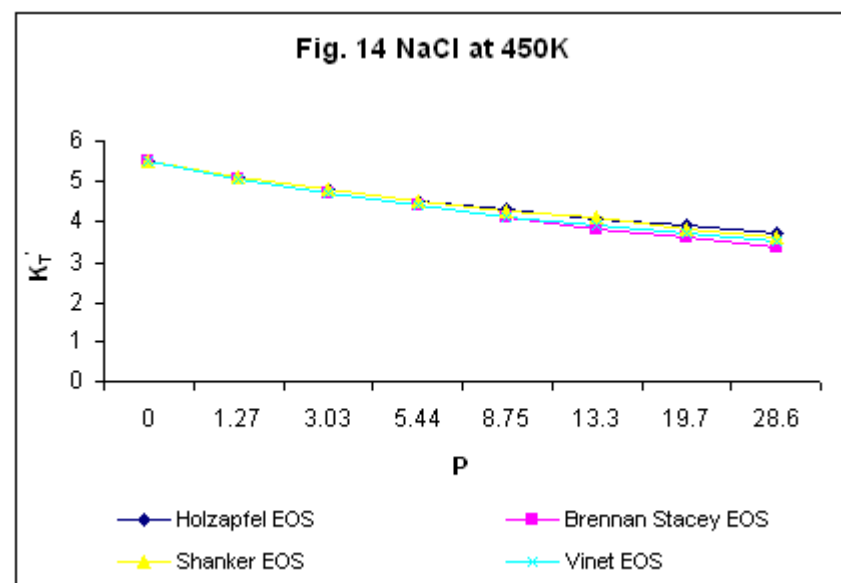
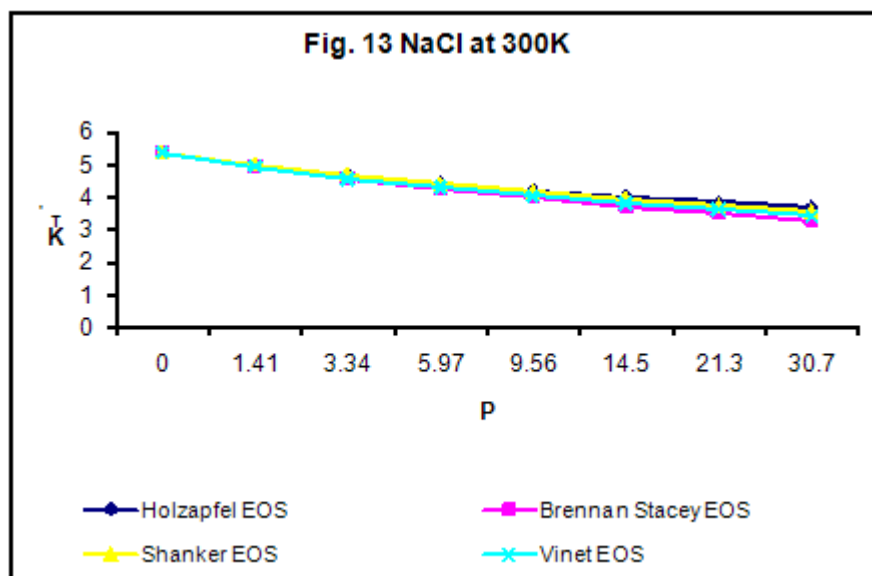


Fig. (13-18): Plots of pressure P vs K_T' for NaCl by using equations (10-13) at different temperature.



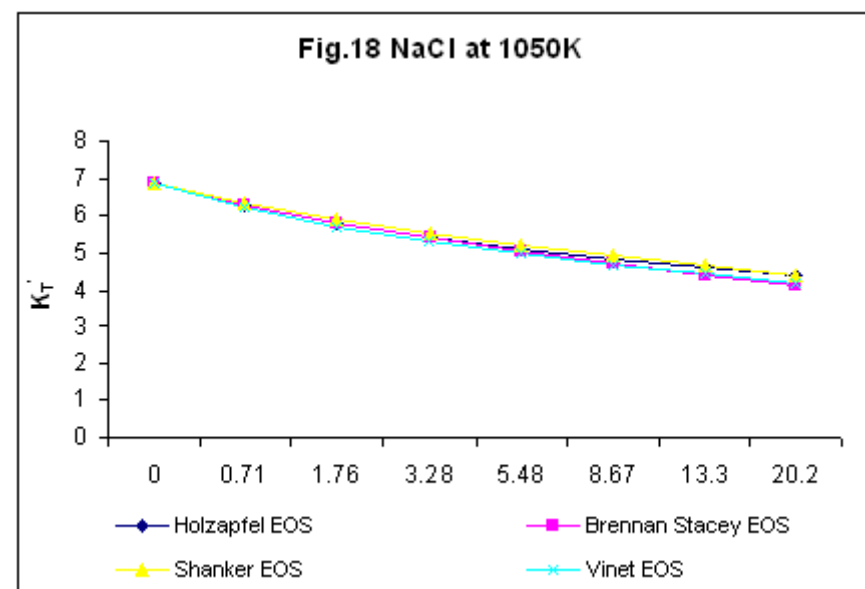
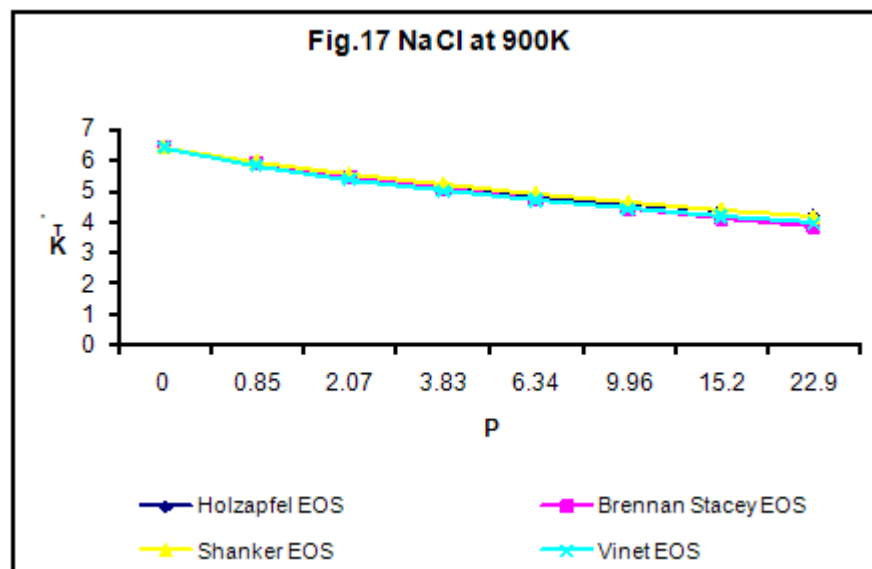


Fig. (19-24): Plots of pressure P vs $-K_T K_T''$ for NaCl by using equations (14-17) at different temperature.

