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A New Formulation of Generalized Equation of State (GEOS) based on Finite Strain Theory and Comparison with other Equations of State (EOSs)

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Abstract

Objective: To formulate the equation of state as well as their isothermal bulk modulus using the basic laws of thermodynamics and Identities. **Method:** This study has considered a relation of Eulerian finite strain having two arbitrary parameters $a_\in$ and $b_\in$ $(a_\in, b_\in \leq 1)$. The salient feature of this equation of state is that by substituting the values of parameters, the expressions for the prominent equations of state and their bulk modulus can be obtained. **Findings :** Four prototype solids viz. MgO, CaO, NaCl, and Al_2O_3 have been applied to the equation of state to test its validity and applicability. The results were compared with experimental data and other equations of state. Consequently, the proposed equation of state exhibits the same trend as prominent equations of state and provides better results. It corresponds well with the experimental curve at high pressure. **Novelty:** The GEOS can be used in the future for planning high-pressure experiments on the compression behavior of several materials, minerals, and solids.

Keywords: The Eularian Finite Stain Theory; Equation of State; Prototype Solids; High Pressure

1 Introduction

Generally, equations of state (EOS) at constant temperature are referred to as isothermal EOS, whereas those at constant pressure and volume are referred to as isochoric EOS and isobaric EOS, respectively. The EOS of materials has been the subject of a number of empirical and phenomenological attempts in the past. Basic EOSs can be categorized into three categories: (a) Based on the solid mechanics' definition of finite strain, such as Birch-Murnaghan, Thomsen and Ullman-Pan'kov[1](b) assumption-based relationships among the variables in EOS, such as Murnaghan, Keane, Brennam-Stacey and Barton-Stacey[2](c) based on interatomic potentials, such as Bardeen, Libby-

Libby, Born-Mie and Born-Mayer [1,3]. In the past decades, a number of researchers have studied various forms of the equation of state at high pressures and temperatures [1,3–8]. It is a subject of interest in basic and applied sciences to derive equations of state (EOS) from both of theoretical and experimental aspects. It provides insight into the nature of solid-state theories and determines the thermodynamic parameters which are of crucial importance in high-pressure research.

A number of theoretical, empirical, and quantum simulation methods are widely used to explain a wide variety of equations of state [9–11]. At different pressures and temperatures, these models are used to study the thermodynamic properties, elastic properties, structural phase transitions, and stability of the earth-forming minerals. Recently, Dehant et al. [12] interpreted the structure and materials processes in the mantle and core of the earth using a high-pressure and high-temperature experimental technique. In addition, Katsura and Tange [13] reformulated the Birch-Murnaghan (BM) and other EOS using finite strain theory and also applied it to standard materials. In the present study, we constructed the generalized form of the equation of state (GEOS) and also derived the expression for its isothermal bulk modulus. In addition, we also reconstructed the prominent equations of state (EOSes) and their bulk modulus from GEOS. We tested the validity and applicability of the GEOS on four prototype solids viz. MgO, CaO, NaCl, and Al_2O_3. The results from GEOS have been compared to existing experimental data along with other theoretical models.

2 Methodology

Let us assume that generalized form of the Eulerian finite strain in terms of the volume ratio $\left(\frac{V_0}{V}\right)$ as

$$f = a_\in \left[\left(\frac{V_0}{V} \right)^{b_\in} - 1 \right] \tag{1}$$

Where $V_0$is the volume at$P = 0$. $a_\in$ and $b_\in (a_\in, b_\in \leq 1)$ are the new arbitrary parameters.

The partial derivative of Eulerian finite Strain$f$ with respect to volume is given as follows:

$$\frac{\partial f}{\partial V} = -\frac{a_\in b_\in}{V_0} \left(1 + \frac{f}{a_\in} \right)^{\frac{1}{b_\in} + 1} \tag{2}$$

The ratio of compression volume to the reference volume is also expressed in the terms of generalized Eulerian Finite Strain $f$given as

$$\frac{V_0}{V} = \left(1 + \frac{f}{a_\in} \right)^{\frac{1}{b_\in}} \tag{3}$$

However, on the compression, the Helmholtz free energy of the matter can be expressed in the form of the Taylor series expansion of the Eulerian finite strain

$$F = a_0 + a_1 f + a_2 f^2 + a_3 f^3 + a_4 f^4 + \ldots \tag{4}$$

2.1 Second-Order Generalized Equation of State

For the second-order equation of state (SO-EOS) the Eq.(4) is truncated up to the second terms. Therefore, Eq. (4) reduces to

$$F = a_0 + a_1 f + a_2 f^2 \tag{5}$$

The coefficient of the first term in Eq. (5) can be $a_0 = 0$ because pressure should be zero in an uncompressed condition i.e. $V = V_0$ and$F = 0$, we have

$$F \cong a_1 f + a_2 f^2 \tag{6}$$

In isothermal EOS, the pressure P is expressed as a function of the volume V. From the thermodynamics identity, the pressure is the volume derivative of Helmholtz energy F as

$$P = -\left(\frac{\partial F}{\partial V} \right)_T \tag{7}$$

By substituting Eq. (1) and (6) in (7), we obtained the pressure and volume relation in terms of assumed fitting parameters $a_\in$ and$b_\in$. Thus

$$P = (a_1 + 2a_2 f)\,\frac{a_\in b_\in}{V_0}\left(1+\frac{f}{a_\in}\right)^{\frac{1}{b_\in}+1} \tag{8}$$

The coefficient $a_1 = 0$ under the uncompressed condition and $V = V_0$ at $P = 0$then Eq. (8) may be written as follow

$$P = 2a_2 f\frac{a_\in b_\in}{V_0}\left(1+\frac{f}{a_\in}\right)^{\frac{1}{b_\in}+1} \tag{9}$$

Therefore, the second coefficient $a_2$of Eq. (8) can easily be evaluated using the definition of the isothermal bulk modulus.

$$K_T = -V\left(\frac{\partial P}{\partial V}\right)_T \tag{10}$$

The partial derivative of pressure with respect to the volume in the uncompressed condition of matter$P = 0$ and f vanishes at$V = V_0$is, therefore

$$\left(\frac{\partial P}{\partial V}\right)_{T,\ P=0} = -\frac{K_{T0}}{V_0} \tag{11}$$

Where $K_{To}$is the isothermal bulk modulus at standard temperature.

Using Eqs.(9)-(11) under the uncompressed condition we can be gets the coefficient a_2. Therefore,

$$a_2 = \frac{V_0 K_{T0}}{2a_\in^2 b_\in^2} \tag{12}$$

Substituting the coefficient a_2 from Eq. (12) in P-V Relation Eq. (9) can be written as follow

$$P = \frac{K_{T0}}{a_\in b_\in} f\left(1+\frac{f}{a_\in}\right)^{\frac{1}{b_\in}+1} \tag{13}$$

This Eq.(13) is the second-order generalized equation of state (SO-GEOS) in terms of Eulerian Finite Strain f and arbitrary parameters.

The isothermal bulk modulus can be evaluated using the definition Eq. (10). Therefore

$$K_T = K_{T0}\left(1+\frac{f}{a_\in}\right)^{\frac{1}{b_\in}+1}\left\{1+\left(2+\frac{1}{b_\in}\right)\frac{f}{a_\in}\right\} \tag{14}$$

This Eq. (14) is the required expression for isothermal bulk modulus in terms of f and arbitrary parameters.

2.2 Third Order Generalized Equation of State

For the third-order equation of state (TO-EOS), the Eq. (4) is truncated up to the third terms as and Eq. (4) may be written as follow:

$$F \cong a_2 f^2 + a_3 f^3 \tag{15}$$

Thus the P-V relation may write as follow:

$$P = \left(2a_2 f + 3a_3 f^2\right)\frac{a_\in b_\in}{V_0}\left(1+\frac{f}{a_\in}\right)^{\frac{1}{b_\in}+1} \tag{16}$$

Where $a_2 = \frac{V_0 K_{T0}}{2a_{\in}^2 b_{\in}^2}$. The undetermined third coefficient $a_3$can be easily evaluated in the identical manner as fora_2.

The volume second-order derivative of pressure can be evaluated using definitions of the isothermal bulk modulusand its pressure derivative. Therefore

$$\left(\frac{\partial^2 P}{\partial V^2}\right)_T = \frac{K_T}{V^2}\left(K'_T + 1\right) \tag{17}$$

Where $K'_T$is first order derivative of bulk modulus. Under the condition of the uncompressed state of matter i.e. $P = 0$ and f vanishesat$V = V_0$, is, therefore, the Eq. (17) expressed as follow

$$\left(\frac{\partial^2 P}{\partial V^2}\right)_{T,0} = \frac{K_{T0}}{{V_0}^2}\left(K'_{T0} + 1\right) \tag{18}$$

Where $K'_{T0}$is the pressure derivative of isothermal bulk modulus at $P = 0$ and standard temperature. Now using the Eqs. (16)-(18) and the second coefficient$a_2 = \frac{V_0 K_{T0}}{2a_{\in}^2 b_{\in}^2}$, the value of third coefficient $a_3$can be determined as follow

$$a_3 = \frac{K_{T0} V_0}{6a_{\in}^3 b_{\in}^3}\left\{K'_{To} - (3b_{\in} + 2)\right\} \tag{19}$$

Substituting the values of coefficient $a_2$and $a_3$in Eq. (16), the TO-GEOS can be written as follows:

$$P = \frac{K_{T0}}{a_{\in} b_{\in}} f\left(1 + \frac{f}{a_{\in}}\right)^{\frac{1}{b_{\in}} + 1}\left[1 + \frac{f}{2a_{\in} b_{\in}}\left(K'_{T0} - (3b_{\in} + 2)\right\}\right] \tag{20}$$

The second term appears in curly brackets shows up due to the truncation of the Helmholtz free energy to the third-order term. The type of curly bracket can be attributed to the considered generalized Eulerian finite strain Eq. (1). The TO-EOS (20) becomes indistinguishable from the SO-GEOS (16) when $K'_{T0} = (3b_{\in} + 2)$. In other words, if $K'_{T0} = 0$, the TO-GEOS (20) differs from SO-GEOS (16).

In order to evaluate the expression for isothermal bulk modulus for third-order, the approach isidentical as in Eq. (14) when the definition (10) is used. Therefore, one gets

$$K_T = K_{T0}\left(1 + \frac{f}{a_{\in}}\right)^{\frac{1}{b_{\in}} + 1}\left[1 + \frac{2f}{a_{\in}} + \frac{f}{a_{\in} b_{\in}} + \frac{1}{2a_{\in} b_{\in}}\left\{K'_{T0} - (3b_{\in} + 2)\right\}\left\{2f + \frac{3f^2}{a_{\in}} + \frac{f^2}{a_{\in} b_{\in}}\right\}\right] \tag{21}$$

This Eq. (21) represents the expression for isothermal bulk modulus of third-order in terms of arbitrary parameters and f. Note that Eq. (21) is identical to isothermal bulk modulus (14) for SO-GEOS if $K'_{T0} = (3b_{\in} + 2)$. In other words, if $K'_{T0} = 0$, Eq. (21) should differs from the Eq. (14).

2.3 Identifying the other prominent EOSs from the GEOSs

In this section, we would test newly formulated GEOS for the following four cases by substituting arbitrary parameters,$a_{\in}$ and$b_{\in}$.

3.3.1 Case I if $a_{\varepsilon} = 1/2$ and $b_{\varepsilon} = 2/3$ then

$$f = \frac{1}{2}\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right] \tag{22}$$

$$\frac{\partial f}{\partial V} = -\frac{1}{3V_0}(1 + 2f)^{5/2} \tag{23}$$

$$a_2 = \frac{9}{2} K_{T0} V_0 \tag{24}$$

$$a_3 = \frac{9}{2} K_{T0} V_0 \left(K'_{To} - 4\right\} \tag{25}$$

Therefore Eq. (13) and (14) can be rewritten as follows

$$P = 3K_{T0} f(1+2f)^{5/2} \tag{26}$$

$$K_T = K_{T0}(1+2f)^{5/2} (1+7f\} \tag{27}$$

In a similar way the Eq. (20) and (21) can be written as follow:

$$P = 3K_{T0} f\,(1+2f)^{5/2} \left\{1 + \frac{3}{2} f(K'_{T0} - 4)\right\} \tag{28}$$

$$K_T = K_{T0}\,(1+2f)^{5/2} \left\{1 + 7f + \frac{3}{2}\left(K'_{T0} - 4\right)(2f + 9f^2)\right\} \tag{29}$$

It is evident from Eq. (26) and (28), the result has obtained the PV-relation identical to the BM-EOS of second and third-order. Eq. (27) and (29) represent expression for the bulk modulus corresponding to second and third order BM-EOS.

2.3.2 Case II if $a_\varepsilon = 1$ and $b_\varepsilon = 1/3$ then

$$f = \left[\left(\frac{V_0}{V}\right)^{1/3} - 1\right] \tag{30}$$

$$\frac{\partial f}{\partial V} = -\frac{1}{3V_0}(1+f)^4 \tag{31}$$

$$a_2 = \frac{9}{2} K_{T0} V_0 \tag{32}$$

$$a_3 = \frac{9}{2} K_{T0} V_0 \left(K'_{To} - 3\right\} \tag{33}$$

Eqs. (13), (14), (20) and (21) become the form as follow

$$P = 3K_{T0} f(1+f)^4 \tag{34}$$

$$K_T = K_{T0}\,(1+f)^4 \{1+5f\} \tag{35}$$

$$P = 3K_{T0} f\,(1+f)^4 \left\{1 + \frac{3}{2} f(K'_{T0} - 3)\right\} \tag{36}$$

$$K_T = K_{T0}\,(1+f)^4 \left\{1 + 5f + 3\left(K'_{T0} - 3\right)(f + 3f^2)\right\} \tag{37}$$

In a similar way, the Eq. (34) and(36) provides the PV-relation parallel to the Bardeen EOS of second and third-order. Eq. (35) and (37) represents the expression for the bulk modulus corresponding to second and third-order Bardeen EOS.

2.3.3 Case III if $a_\varepsilon = 1/3$ and $b_\varepsilon = 1$ then

$$f = \frac{1}{3}\left[\frac{V_0}{V} - 1\right] \tag{38}$$

$$\frac{\partial f}{\partial V} = -\frac{1}{3V_0}(1+f)^2 \tag{39}$$

$$a_2 = \frac{9}{2}K_{T0}V_0 \tag{40}$$

$$a_3 = \frac{9}{2}K_{T0}V_0\left(K'_{To} - 5\right\} \tag{41}$$

Eq. (13), (14), (20) and (21) take the form as follow

$$P = 3K_{T0}f(1+3f)^2 \tag{42}$$

$$K_T = K_{T0}(1+3f)^2\{1+9f\} \tag{43}$$

$$P = 3K_{T0}f(1+3f)^2\left\{1+\frac{3}{2}f(K'_{T0}-5)\right\} \tag{44}$$

$$K_T = K_{T0}(1+3f)^2\left\{1+9f+3\left(K'_{T0}-5\right)(f+6f^2)\right\} \tag{45}$$

It is interesting to note that Eq. (42) and (44) indicate the PV-relation for SO and TO. This is identical to the Third-power Eulerian equation of state (TPE-EOS) for second and third-order recently reported by Katsura and Tange[13]. Eq. (43) and (45) are the expression for the bulk modulus corresponding to second and third-order TPE-EOS.

2.3.4 Case IV if $a_\varepsilon = 2/3$ and $b_\varepsilon = 1/2$ then

$$f = \frac{2}{3}\left[\left(\frac{V_0}{V}\right)^{1/2} - 1\right] \tag{46}$$

$$\frac{\partial f}{\partial V} = -\frac{1}{3V_0}\left(1+\frac{3}{2}f\right)^3 \tag{47}$$

$$a_2 = \frac{9}{2}K_{T0}V_0 \tag{48}$$

$$a_3 = \frac{9}{2}K_{T0}V_0\left\{K'_{To} - \frac{7}{2}\right\} \tag{49}$$

Eqs. (13), (14), (20) and (21) becomes the form as follow

$$P = 3K_{T0}f\left(1+\frac{3}{2}f\right)^3 \tag{50}$$

$$K_T = K_{T0}\left(1+\frac{3}{2}f\right)^3\{1+6f\} \tag{51}$$

$$P = 3K_{T0}f\left(1+\frac{3}{2}f\right)^3\left\{1+\frac{3}{2}f(K'_{T0}-\frac{7}{2})\right\} \tag{52}$$

$$K_T = K_{T0}\left(1+\frac{3}{2}f\right)^3\left\{1+6f+\frac{3}{4}\left(K'_{T0}-\frac{7}{2}\right)(4f+15f^2)\right\} \tag{53}$$

The Eq. (50) and (52) represent the PV-relation for SO and TO. This indicates other form of GEOS for second and third-order. Eq. (51) and (53) represent the expression for the bulk modulus corresponding to the special form of GEOS of second and third-order.

Thus, it is evident from the above derivations the proposed GEOS plays a crucial role and is capable of producing prominent equations of states. This indicates justification and the validity of the proposed work and may be useful in the field of research and geophysical applications.

3 Results and Discussion

To test the validity of the proposed work, we have applied it on four prototype solids viz. MgO, CaO, NaCl, and Al_2O_3. The used input parameters[14–17] for these prototype materials bulk moduli and their pressure derivative at room temperature and zero pressure have shown in Table 1. The finite strain as a function of compression $(V/V0)$hasbeen calculated using the Eqs. (22), (30), (38) and (46). As shown in Figure 1, the finite strain increases nearly in the same manner up to the compression $V/V0 = 0.8$ for all cases. The finite strains rapidly increases and then diverge to infinity as $V/V_0 \to 0$. Consequently, the Helmholtz free energy and pressure also increase infinity with $V/V_0 \to 0$. There is an interesting correlation between the curves for Case I and Case IV lies between Case II and Case III i.e. a finite strain is steeper for Case III (TPE-EOS) than it is for Case I, II, and IV. The behavior of Case IV (GEOS) and Case I (BM-EOS) are very close to Case II (Bardeen EOS). It is also noticeable that the rate of pressure increase is very similar in BM-EOS and special form of GEOS under low compression. Thus the special form of GEOS shows the validation because of the closeness of BM-EOS, this is widely, used in geophysical studies.

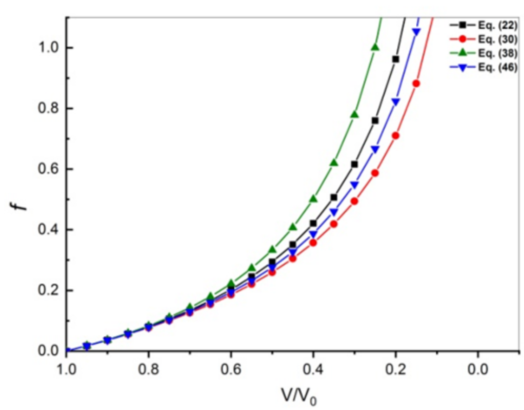

Fig 1. Comparison the finite strains $f$as a function of compression $\left(\frac{V_0}{V}\right)$

We have made an attempt to examine the validity of SO and TO-EOS with the available experimental data considering four cases. The pressure has been calculated at different isothermal compression ranging from 1 to 0.6 at room temperature for prototype solids viz. MgO, CaO, NaCl, and Al_2O_3 using the SO and TO-EOS for all cases (i) Eq. (26) and (28) (second and third-order BM-EOS; (ii) Eq. (34) and (36) (second and third order Bardeen EOS); (iii) Eq. (42) and (44) (second and third-order TPE-EOS; (iv) Eq.(50) and (52) i.e. second and third order GEOS (Special form). The graphs have been plotted with the help of Origin Lab ProV2019.

As shown in Figure 2 , the pressure obtained for four cases of EOSs for MgO, CaO, NaCl, and Al_2O_3. Out of these prototype solids, MgO and NaCl are frequently used in high pressure experiments. The input parameters K_{T0}, K'_{T0} at zero pressure, and room temperature have been used to calculate the pressure and are shown in Table 1. We can see that the pressure increases continually with the decrease of compression. It is evident that the PV-curves have been diverged according the value of pressure derivative of bulk moduli. As the value $K'_{T0} = 5.15$ for NaCl, the PV-curve is more diverse in compare with the value $K'_{T0} = 3.9$ for Al_2O_3.

From Figure 2 a, we have found that the PV-curve for SO-EOS has more deviated in comparison to TO-EOS with the experimental data by Marsh[18]. The SO-TPE EOS has more sharpness in comparison to other SO-EOS. The results from the TO-GEOS, TO-BM-EOS and TO-Bardeen EOS are approximately similar to each other and corresponding well to experimental data in the case of MgO, CaO, and Al_2O_3. The GEOS (special case) for MgO has shown a close agreement with experimental data[18] in all of these. This indicates the validity of proposed EOS (special form of GEOS).

Next, we have examined Figure 2 a, 2b, and 2d.In Figure 2b, the experimental data by Speziale et al[19]are available up to 64.1 GPa for CaO. The third-order EOS of all cases shows corresponding to well with experimental data[19]. It's worthwhile to stress that SO-EOS of all cases has more deviations from TO-EOS and experimental data except SO-TPE-EOS. We have also found a similar trend but Figure 2 c is different from these. It should be pointed out that the SO-EOS of Bardeen, Birch-Murnaghan, and GEOS (special form) has been more deviated from the experimental reported by Marsh[18] and other TO-EOSs. However, the TO-EOS of Bardeen, MB, GEOS (Case IV) and SO-TPE-EOS generally agrees with experimental data. It reveals that the TO-GEOS (case-iv) and TO-Bardeen EOS have shown good agreement with experimental data[18]. Figure 2 d for Al_2O_3, the pressure has been calculated for the compression up to $V/V_0 = 0.7$ and the PV-curves for SO-EOS and TO-EOS has less diverge because of the low value of$K'_{T0} = 3.9$ in compared to other minerals. The PV-curve of SO-Third Power Eulerian EOS has close with experimental data[18] up to the compression$V/V_0 = 0.85$ after that it is deviated and the PV-curve for all TO-EOS and second order BM-EOS has shown the close agreement with experimental data[18].

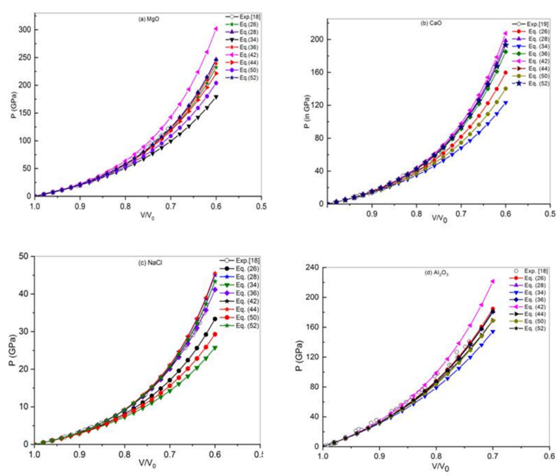

Fig 2. V/V_0as a function of pressure. The Comparison of four cases of second and third-order equations of state for(a) MgO (b) CaO (c) NaCl (d) Al_2O_3. The figures compare the calculated results (filled symbols) with the experiment data (open symbol)

The isothermal bulk have been calculated at different compression ranging from 1 to 0.6 at room temperature for MgO, CaO, NaCl, and Al_2O_3 using (i) Eq. (27) and (29); (ii) Eq. (35) and (37); (iii) Eq. (43) and (45); (iv) Eq.(51) and (53). The used input parameters[13–17] have been used.

Figure 3 show the isothermal bulk modulus (K_T) versus pressure for SO and TO of BM-EOS, Bardeen EOS,TPE-EOS and GEOS (special form). In Figure 3, the isothermal increases with the increase in pressure. In Figure 3 a for MgO, the results from Eq. (29) and (53) for TO-BM-EOS and TO-GEOS (case-iv) have shown the better agreement with theoretical results reported by Karki et al[20]. At the pressure range above the 10 GPa other Eq. (27) and (45) for TO-Bardeen EOS and TO-TPE-EOS show the diverge from the results[20]. In case of results obtained by all SO-EOS represented much diverge from the results reported by Karki et al [20]. From Figure 3 b for CaO, we have found the results from Eq. (29), (53), (43) and (45) for TO-BM- EOS, TO-GEOS (Case IV), SO-TPE-EOS and TO-TPE-EOS have been shown the good agreement with the experimental results reported by Speziale et al [19], while, the isothermal bulk modulus obtained from Eq. (27), (35), (51), and (37) have been much diverge by experiment data [19]. The results for NaCl and $Al_2O_3$are carried out by using Eq. (27), (35), (43), and (51) for SO-EOS and Eq. (29), (37), (45), and (53) for TO-EOS. The isothermal bulk moduli (K_T) as a function of pressure for NaCl and Al_2O_3 have shown in Figure 3 c and 3d. In case of NaCl, the results from Eq. (29), (45), (53), and (43) for TO-BM-EOS, TO-TPE-EOS, TO-GEOS (case-iv) and SO-TPE-EOS are very close while others are divert. In case of Al_2O_3, the results form Eq. (27), (29), (37), and (53) for SO and TO-BM-EOS,TO-GEOS (case-iv) are very close to each other because of low values of $K'_{T0} = 3.9$, other EOSs are more diverted.

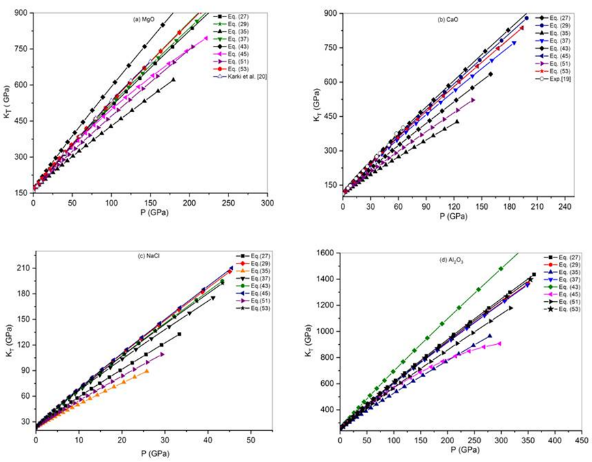

Fig 3. K_T as a function of pressure. The Comparison of four cases of second and third order equations of states for (a) MgO (b) CaO (c) NaCl (d) Al_2O_3. The figures compare the calculated results (filled symbols) with other theoretical and experimental results (open circle symbol)

The percentage deviations of pressures have calculated at available experimental data of the highest isothermal compression (V/V_0)and reported in Table 2. From the examine the Table 2, we have found that the third-order GEOS (Case IV) shows the consistency of the results between 1.06 to 3.87 percentage deviations of pressures corresponding to the highest compression for which experimental data are available [18,19]. The results of others SO-EOS and TO-EOS show more variation in the percentage deviations in comparison to the GEOS (Case IV). Thus, the special case of Generalized Equation of State (GEOS) shows the more validity in comparison to others prominent equations of state.

4 Conclusions

Noticeably, GEOS plays a crucial role and is capable of producing prominent equations of states. Additionally, the GEOS model produces similar results to other models and matches well with experimental data [18,19]. As a result, it demonstrates the validity and justification of the proposed research. Obviously, it shows that the alternative methods developed recently reported by Katsura and Tange [13], Singh et al [6–8] and Myhill [21] lead to identical results from comparable approximations. Therefore, the GEOS may be appropriate for the extension of the research and geophysical applications. The major feature of this GEOS is that follows the basic laws of thermodynamics under high pressure and hence allows extrapolation to regions for which experimental data are not available. GEOS may prove to be useful for planning high-pressure experiments on the compression behavior of earth-forming minerals, solids, and nanomaterials. It could be also modified to incorporate thermal pressure in high-temperature applications. From an extension point of view, the expression for elastic modulus with compression can be derived using GEOS. The variation of vibrational frequencies with compression can also be expressed as a Taylor series expansion in Eulerian finite strain, whose volume derivative can be used to calculate the Gruneisen parameter [22,23].

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