



## HIGH-PRESSURE EQUATIONS OF STATE AND ELASTIC PROPERTIES OF THE LOWER MANTLE OF THE EARTH

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*"together we can and we will make a difference"*

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## ABSTRACT

In the present study, the elastic properties of the lower mantle of the earth have been studied. We have used a new equation of state on Eulerian finite theory based on  $n^{\text{th}}$  power of edge length by compression. Using the new equations of state, the pressure has been calculated density range varying from 3976.92 to 6628.2 kg m<sup>-3</sup> of lower earth's mantle. Along with this, the bulk modulus and its pressure derivative have computed at different pressure for the depth of lower mantle from 670 to 2891 km. We have also calculated the pressure dependence thermal expansivity using the Anderson-Grüneisen theory and other relation of  $\alpha$ . The results from this new equation of state (EOS) correspond well with the data reported by Stacey and Davis. Thus, the new expressions are capable to predict the elastic properties of Earth's minerals under high-pressure conditions. It can be used in geophysical applications.

**Keywords:** Thermal Expansivity, Isothermal Bulk Modulus, Pressure derivatives, Mine, High-pressure, equation of state, lower mantle.

## INTRODUCTION

Understanding the state of the earth's interior minerals and their density distribution under high pressure is a task that researchers are taking interest in more than ever before. The issues that arise with equations of state for the earth's interior differ in some ways from those that arise with high-pressure laboratory data. Since the composition of the earth's interior cannot be directly observed, one of the primary goals of minerals physics research is to infer composition from seismological evidence. The composition of Earth's lower mantle is primary (Mg, Fe) SiO<sub>3</sub> perovskite with a small amount of dissolved Al<sub>2</sub>O<sub>3</sub>, (Mg, Fe) O magnesiowustite, and a few percent CaSiO<sub>3</sub> perovskites, according to geophysical data. This composition is just simple enough to make a useful comparison and its properties with seismological data [1-2]. The seismological data based on the preliminary Reference Earth Model (PERM), is more precise than the laboratory data, according to Stacey and Davis [3]. Because of the pressure calibration, laboratory data is subject to uncertainty. Under extreme compression, the k-prime equation of state makes it easy to examine pressure, higher pressure derivatives of bulk modulus, and other elastic properties. The lower mantle pressure has been

found to be 23 GPa to 136 GPa between 670 km and 2891 km according to PREM Model [1].

The volume coefficient of thermal expansion of materials is a critical physical quantity that is connected with a number of thermoelastic properties [4], including the Anderson-Grüneisen parameter, bulk modulus, specific heats, and thermal pressure.

In this paper, we have studied the elastic properties of the lower mantle of the earth using the recently derived analytical equation of state based on the Eulerian finite strain [5]. The results for pressure, bulk modulus and its pressure derivative have compared to seismological data [3] derived from the Preliminary Reference Earth Model (PERM) using the Stacey relationship [6-8]. The thermal expansion volume coefficient has also been calculated for the lower mantle part of the earth and compared with the seismological data [3].

### High-pressure Theory and Analysis:

The physical acceptance of equations of state based on finite strain theory shows plausibility tests to the earth's interior with the PEM earth model [6]. The variation of pressure and bulk modulus both increase with increasing compression. The variation of pressure derivative is more sensitive to the precise forms of the equation than are under the compression.

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Majorly, the values of  $K'$  decrease with increasing compression. Stacey et. al. [3] reported that the variation of  $K$  with pressure is nonlinear such that the slope of curve  $K'$  decreases with the increase to be pressure. At the high compression limits, the volume tends to zero; the pressure and bulk modulus both tend to infinity, but their ratio ( $P/K$ ) provides the finite value. Stacey [7-8] has found in high compression limits the value  $K'$  attained a minimum constant value of  $K'$  which is denoted by  $K'_{\infty} > 0$ . There is a corresponding limit to  $K'$  and hold the following identity

$$\left(\frac{P}{K}\right)_{\infty} = \frac{1}{K'_{\infty}} \quad \dots(1)$$

Stacey [3] has been formulated a  $K$ -primed equation of state and expressed as follow

$$\frac{1}{K'} = \frac{1}{K'_0} + \left(1 - \frac{K'_{\infty}}{K'_0}\right) \frac{P}{K} \quad \dots(2)$$

Where  $K'_{\infty}$  is the value of  $K'$  in the limit of extreme compression (infinite pressure limit). The successive integration of eq. (2) yield the following expressions

$$\frac{K}{K_0} = \left(1 - K'_{\infty} \frac{P}{K}\right)^{\frac{K'_0}{K'_{\infty}}} \quad \dots(3)$$

$$\ln\left(\frac{P}{\rho_0}\right) = \left(1 - \frac{K'_0}{K'_{\infty}}\right) \frac{P}{K} - \frac{K'_0}{K'_{\infty}{}^2} \ln\left(1 - K'_{\infty} \frac{P}{K}\right) \quad \dots(4)$$

An expression for volume coefficient of thermal expansion ( $\alpha$ ) as a function of pressure have reported in the literature [9-10] and express as follow

$$\alpha = \alpha_0 \left[1 - K' \left(\frac{P}{K}\right)^l\right] \quad \dots(5)$$

Where  $l$  is a numerical arbitrary constant. In the calculation of  $\alpha$ , we have used the value of  $l = 1.13$ .

Eq. (5) gives  $\alpha = \alpha_0$  at  $P = 0$  and the limit of extreme compression, the  $\alpha$  tends to zero. The quantity  $\left[1 - K' \left(\frac{P}{K}\right)^l\right]$  tends to zero at infinite pressure. Thus the variation of  $\alpha$  decreases with increase in pressure and vanishes at limit of extreme compression.

The volume coefficient of thermal expansion of the minerals at high pressure usually related to their volume by Anderson-Grüneisen parameter ( $\delta_T$ ), which describes the degree of decrease in by compression [11] and expressed as follow

$$\frac{\alpha}{\alpha_0} = \left(\frac{V}{V_0}\right)^{\delta_T} = \left(\frac{\rho}{\rho_0}\right)^{-\delta_T} \quad \dots(6)$$

At the high temperature,  $\delta_T$  can be replaced by  $K'$  [11-12] and thus eq. (6) may be written as

$$\frac{\alpha}{\alpha_0} = \left(\frac{V}{V_0}\right)^{K'} = \left(\frac{\rho}{\rho_0}\right)^{-K'} \quad \dots(7)$$

Recently, Singh et.al. [5] has been formulated a generalized form of equations of state based on Eulerian finite strain theory and the corresponding expression for  $P$ ,  $K$  and  $K'$  given as follows

$$P = 3K_0 f (1 + nf)^{\frac{3}{n}+1} \left\{1 + \frac{3}{2}(K'_0 - (n + 2))f\right\} \quad \dots(8)$$

$$K = K_0 (1 + nf)^{\frac{3}{n}+1} \left\{1 + (3 + 2n)f + \frac{3}{2}\{K'_0 - (n + 2)\}\{2f + 3(n + 1)f^2\}\right\} \quad \dots(9)$$

$$K' = \frac{K_0}{K} (1 + nf)^{\frac{3}{n}+1} \left[ K'_0 + \frac{(2n+3)^2}{3} f + (5n + 6)\{K'_0 - (n + 2)\}f + \frac{9}{2}(n + 1)^2\{K'_0 - (n + 2)\}f^2 \right] \quad \dots(10)$$

$$\text{Where } f = \frac{1}{n} \left[ \left(\frac{\rho}{\rho_0}\right)^{n/3} - 1 \right] \quad \dots(11)$$

We have considered the four cases for the value of  $n = 1, 1.5, 2$  and  $3$  substituting in eq. (8), (9) and (10) respectively and obtained the  $P, K$  and  $K'$  relations in terms of finite strain  $f$ . We have also exploit the most prominent equations of state for a particular value of  $n$ . if  $n = 1$ , the First Power Eulerian EOS (Bardeen EOS); if  $n = 2$ , the Birch-Murnaghan EOS and if  $n = 3$ , the Third Power Eulerian EOS.

## RESULTS AND DISCUSSIONS

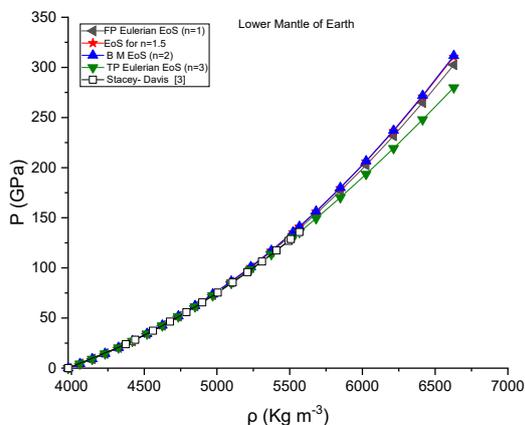
To evaluate the equations, we have computed the Pressure, isothermal bulk modulus, and its pressure derivative for the lower mantle. We have used eq. (8) to (10) for the values of  $n = 1, 1.5, 2$  and  $3$ . In order to calculate the volume coefficient of thermal expansion, we have used the eq. (5) and (7). The used input parameters in the calculations have been shown in Table I.

**TABLE I**

Values of used input parameters in calculations: density ( $\rho_0$ ) (in  $\text{Kg m}^{-3}$ ), volume coefficient of thermal expansion ( $\alpha_0$ ) (in  $10^{-6} \text{ K}^{-1}$ ), bulk modulus ( $K_0$ ) (in GPa), pressure derivative of bulk modulus ( $K'_0$ ) (dimensionless) at zero pressure ( $P = 0$ ) and pressure derivative of bulk modulus at infinite compression ( $K'_{\infty}$ ) (dimensionless).

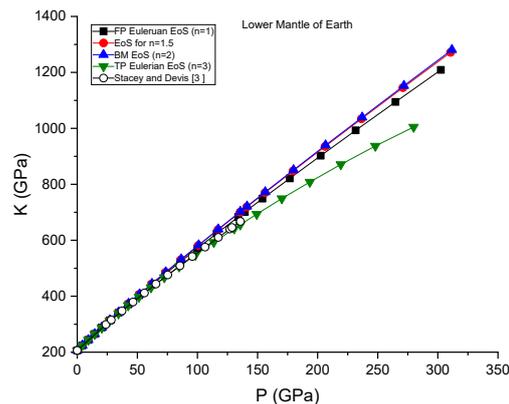
Parameters	$\rho_0$	$\alpha_0$	$K_0$	$K'_0$	$K'_\infty$
Lower mantle	3976.92	34.918	206.06	4.2	2.4

The pressure for the different values of n has been calculated density varying from 3976.92 to 6628.2 kg m<sup>-3</sup> of lower earth's mantle using the eq. (8). We have obtained a similar trend of the First Power Eulerian EOS for n=1, a new EOS for n= 1.5, Birch-Murnghan EOS for n=2 and Third Power Eulerian EOS for n=3 respectively. Which follows the basic thermodynamic conditions and Stacey criteria as compression ( $\frac{V}{V_0}$ ) → 0, the pressure P→∞. In Fig.1, the percentage deviation at the density  $\rho = 5567 \text{ Kg m}^{-3}$  has occurred 2.67, 3.89, 4.03 and 0.09 for the values of n = 1, 1.5, 2 and 3 respectively. Thus the Third Power Eulerian EOS for n=3 shows a very close agreement with Stacey and Davis results [3] in comparison to other values of n. Other EOS shows very minute deviations i.e. the present model of EoS (Eq. 8) shows similarity with the data reported by Stacey and Davis [3].



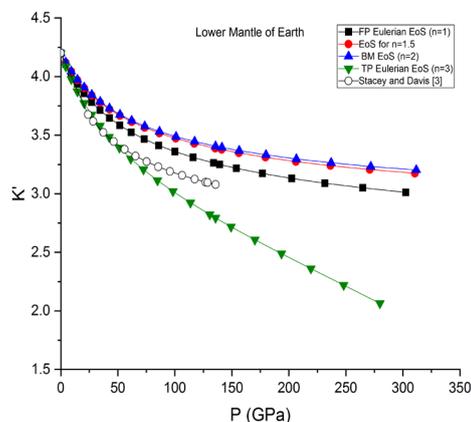
**Fig.1** Compression curves for different values of n of the equations of state for nth powered length. The figures compare the calculated results (filled symbols) with Seismic data reported by Stacey and Davis (open symbols).

We have calculated the fundamental elastic property isothermal bulk modulus using the eq. (9) for different values of n and obtained results have shown in Fig.2. The percentage deviation at the depth of 2891 km and pressure 135.75 GPa have been found 5.06, 7.74, 8.08 and 1.72 for the values of n =1, 1.5, 2 and 3 respectively.



**Fig.2** Pressure dependence of bulk modulus. The filled and color symbols are calculated results and open symbols show seismic data reported by Stacey and Davis (open symbols).

From the geophysical point of view, the first pressure derivative of the isothermal bulk modulus is a parameter that is necessary for the accurate inversion of the seismic data into composition, structure, and texture of the earth, as well as for determining the thermal properties of the earth's interior [14] and the isothermal empirical equation of state of the materials in the earth's interior [4]. The results for pressure derivative  $K'_T$  obtained from the eq. (10) for the values of n =1, 1.5, 2 and 3 respectively and compared with the data reported by Stacey and Davis [3]. The results have been shown in Fig. 3. The percentage deviation at 135.75 GPa have been found 5.53, 9.66, 10.26 and 9.27 for the values of n =1, 1.5, 2 and 3 respectively. The first power Eulerian EOS shows the less deviation in compare to other equations of state. Although, the present model of EoS (Eq. 10) shows significant consistency with the data reported by Stacey and Davis [3].



**Fig.3** Pressure dependence of  $K'_T$  plot. The filled and color symbols are calculated results and open

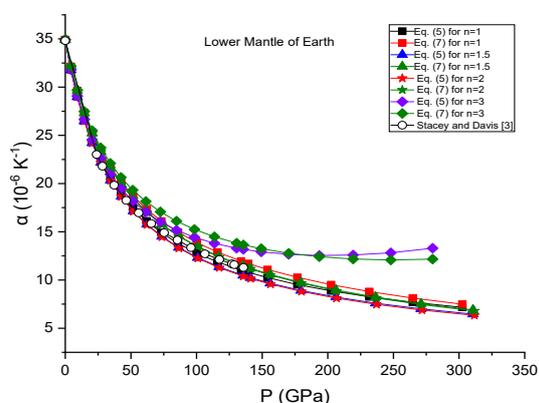
symbols show seismic data reported by Stacey and Davis (open symbols).

**TABLE II**

Percentage deviation of calculated volume thermal expansivity at depth 2831km (pressure 135.75 GPa) of lower mantle earth in comparison to the results of Stacey and Davis [3].

$\alpha$ for n=1		$\alpha$ for n=1.5		$\alpha$ for n=2		$\alpha$ for n=3	
Eq. (5)	Eq. (7)	Eq. (5)	Eq. (7)	Eq. (5)	Eq. (7)	Eq. (5)	Eq. (7)
4.36	3.68	9.35	0.66	10.09	1.27	16.72	20.86

In order to calculate the value of  $\alpha$ , substituting the value of  $K'$  in eq. (5) and (7), from the eq. (10) for the values of  $n = 1, 1.5, 2$  and  $3$  respectively. Thus we have obtained the eight results for  $\alpha$  at different pressure shown in Fig.4. The percentage deviation of  $\alpha$  at pressure 135.75 GPa for the lower mantle of the earth has been shown in Table II. The results for  $\alpha$  as a function of pressure reveal that a close agreement data obtained by eq. (5) and (7) for the value  $n = 1$ , eq. (7) for  $n = 1.5$  and  $2$ , with data extracted by Stacey and Davis using the seismological data [3].



**Fig.4** Pressure dependence of thermal expansion plot for the lower mantle. The filled and color symbols are calculated results and open symbols show seismic data reported by Stacey and Davis (open symbols).

**CONCLUSIONS**

The results obtained from the proposed equation of state are nearly similar to Stacey and Davis models [3, 6-8]. The main feature of this model is fewer input parameters are required which are easily available in experimental studies. The proposed equation of state is capable to produce the prominent equation of state

for different values of  $n$ . The current study follows the basic thermodynamic laws and Stacey criteria at high pressure. These studies may, therefore, be useful for future planning high-pressure experiments on the compression behavior of the earth forming minerals, solids, etc.

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**REFERENCES**

- [1]. Anderson, D. L. (1989). Theory of the Earth. Blackwell scientific publications.
- [2]. Dziewonski, A. M., & Anderson, D. L. (1981). Preliminary reference Earth model. Physics of the earth and planetary interiors, 25(4), 297-356. [https://doi.org/10.1016/0031-9201\(81\)90046-7](https://doi.org/10.1016/0031-9201(81)90046-7)
- [3]. Stacey, F. D., & Davis, P. M. (2004). High pressure equations of state with applications to the lower mantle and core. Physics of the Earth and Planetary interiors, 142(3-4), 137-184. <https://doi.org/10.1016/j.pepi.2004.02.003>
- [4]. O.L. Anderson, Equation of state of solids for Geophysics and Ceramic Science, Oxford University Press, Oxford, (1995).
- [5]. Singh, S. P., and Singh, Dharmendra. (2021). A New formulation of Equation of State and the Study of Elastic Properties of Alkaline Earth Oxides under High Pressure. Acta Phys. Pol. A Vol 140, No.2, (2021)
- [6]. Stacey, F. D., Brennan, B. J., & Irvine, R. D. (1981). Finite strain theories and comparisons with seismological data. Geophysical surveys, 4(3), 189-232. <https://doi.org/10.1007/BF01449185>
- [7]. Stacey, F. D. (2000). The K-primed approach to high-pressure equations of state. Geophysical Journal International, 143(3), 621-628. <https://doi.org/10.1046/j.1365-246X.2000.00253.x>

- [8]. Stacey, F. D. (1995). Theory of thermal and elastic properties of the lower mantle and core. *Physics of the Earth and Planetary Interiors*, 89(3-4), 219-245. [https://doi.org/10.1016/0031-9201\(94\)03005-4](https://doi.org/10.1016/0031-9201(94)03005-4)
- [9]. Sunil, K., & Sharma, B. S. (2017). Thermoelastic properties of the earth lower mantle. *International Journal of Modern Physics B*, 31(14), 1750108. <https://doi.org/10.1142/S0217979217501089>
- [10]. Sunil, K., Singh, P. K., & Sharma, B. S. (2012). Analysis of Thermal Expansivity of Solids Under High Pressures. *Modern Physics Letters B*, 26(22), 1250146. <https://doi.org/10.1142/S0217984912501461>
- [11]. Anderson, O. L. (1967). Equation for thermal expansivity in planetary interiors. *Journal of Geophysical Research*, 72(14), 3661-3668. <https://doi.org/10.1029/JZ072i014p03661>
- [12]. Birch, F. (1968). Thermal expansion at high pressures. *Journal of Geophysical Research*, 73(2), 817-819. <https://doi.org/10.1029/JB073i002p00817>
- [13]. Duffy, T. S., & Anderson, D. L. (1989). Seismic velocities in mantle minerals and the mineralogy of the upper mantle. *Journal of Geophysical Research: Solid Earth*, 94(B2), 1895-1912. <https://doi.org/10.1029/JB094iB02p01895>

