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A New Model to Study the Sound Velocity in Liquid Metals

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Highlights

- Computed sound velocities agree well with experimental data across all studied liquid metals.
- The model predicts first and second pressure derivatives of sound velocity at ambient conditions.
- The model captures variations in sound velocity and its derivatives with pressure and temperature

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Abstract

This study proposes a new relationship to investigate the behavior of sound velocity as a function of pressure in liquid metals. The suggested relation is applied in liquid metals like Sodium, Potassium, Rubidium, Cesium, Mercury and Bismuth. The computed sound velocity results for each liquid metal are found to be consistent with the experimental data across the entire pressure range, with root mean square deviations on the order of 10-4 in each case. The temperature effect is also introduced by considering the linear dependence of thermal pressure on temperature. The maximum average absolute percentage relative deviation (AARD %) of 0.45 is noted in the case of Bismuth across the entire pressure range at temperatures. The first and second pressure derivatives of sound velocity at ambient pressure and temperature are calculated and found to be in good agreement with the available data. Furthermore, the proposed relationship can predict the variation of the first pressure and temperature derivatives of sound velocity with pressure and temperature.

1. INTRODUCTION

The sound velocity is one of the most fundamental thermodynamic properties of liquid metals, and once the sound velocity data is accessible, many thermo-physical quantities, such as thermal pressure coefficient, Gruneisen parameter, isothermal bulk modulus, ratio of heat capacities, and adiabatic bulk modulus can be obtained from the fundamental thermodynamic associations. [1-6]. The significance of sound velocity lies in the fact that it can be measured more precisely than the equation of state (EOS), allowing for a more accurate study of the variation of thermo-physical properties of liquid metals in the pressure and temperature (P, T) domain based on sound velocity measurement.

The molecular structure and thermodynamics of liquid metals govern how sound velocity responds to changes in pressure and temperature. Increased pressure strengthens atomic interactions, enhancing resistance to compression and raising sound velocity. Conversely, temperature affects thermal expansion, reducing density and altering compressibility, which in turn influences sound velocity. Thermodynamically, sound velocity is linked to the adiabatic bulk modulus and density, following the equation $U_s = \sqrt{\frac{K_s}{\rho}}$, where K_s is the adiabatic bulk modulus and ρ is density.

The effect of pressure and temperature on sound velocity has been extensively studied using EOS in condensed matter [7-13]. This method, however, necessitates the handling of a greater number of parameters. Aside from this, some empirical or semi-empirical models have been proposed to investigate the effect of pressure or temperature on the sound velocity; however, no one has been found to represent

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the sound velocity as a function of pressure and temperature in liquid metals [14, 15]. Furthermore, the scarcity of higher order derivatives of sound velocity in the literature makes access to a wide range of thermos-physical properties in the entire (*P, T*) domain difficult. Furthermore, literature contains little information on acoustic parameters, such as Beyer's nonlinear parameters of liquid metals, which are related to sound velocity pressure and temperature derivatives.

As a result, a new model for representing sound velocity in the entire (*P, T*) domain in liquid metals is described in this study, allowing us to compute the higher pressure and temperature derivatives of sound speed in the entire (*P, T*) domain. Liquid sodium (Na), liquid potassium (K), liquid rubidium (Rb), liquid cesium (Cs), liquid mercury (Hg) and liquid bismuth (Bi) were considered for this study. The experimental data for these liquids were obtained from [16-18].

2. THEORY

We propose a Tait-like relation to study the effect of pressure on sound velocity at a given temperature *T*, which is given as:

$$\frac{U_S(P,T_0)}{U_S(P_0,T_0)} = 1 + \left\{\frac{1}{A} ln[1 + B(P - P_0)]\right\} \tag{1}$$

where $U_S(P,T_0)$ represents the sound velocity at pressure P and temperature T_0 and $U_S(P_0,T_0)$ represents the sound velocity at pressure P_0 and temperature T_0. Here A and B are constants.

First and second derivatives of Equation (1) with respect to pressure are given as:

$$\frac{1}{U_S(P_0,T_0)}\left[\frac{dU_S(P,T)}{dP}\right]_{T_0} = \frac{B}{\{A[1+B(P-P_0)]\}} \tag{2}$$

$$\frac{1}{U_S(P_0,T_0)}\left[\frac{d^2U_S(P,T)}{dP^2}\right]_{T_0} = \frac{-B^2}{\{A[1+B(P-P_0)]^2\}}. \tag{3}$$

Applying the initial condition of pressure $P = P_0$ to Equations (2) and (3), we get

$$\left[\frac{1}{U_S(P_0,T_0)}\right] U_S'(P_0,T_0) = \frac{B}{A} \tag{4}$$

$$\left[\frac{1}{U_S(P_0,T_0)}\right] U_S''(P_0,T_0) = -\frac{B^2}{A}. \tag{5}$$

From Equations (4) and (5), we get:

$$A = -\frac{U_S''(P_0,T_0)}{U_S'(P_0,T_0)} \tag{6}$$

$$B = -\frac{U_S''(P_0,T_0)U_S(P_0,T_0)}{[U_S'(P_0,T_0)]^2}. \tag{7}$$

The experimental results suggest that the sound velocity in liquids increases with pressure. Consequently, the sound velocity first pressure derivative will always be positive. Thus, *B/A* is positive from Equation (4) meaning that either both are positive, or both are negative. It is observed that the second derivative of sound velocity is negative. Therefore, one can easily conclude from Equations (6) and (7) that both A and B are positive.

In the present study, the thermal effect is considered in the same way as it is considered in [8]

$$P(T) = P(T_0) + P_{th} \tag{8}$$

where P_{th} is the thermal pressure and can be written in simplest form as

$$P_{th} = \alpha(0,T_0)\, B_T(0,T_0)\, (T - T_0) = \xi\, (T - T_0) \tag{9}$$

where $\alpha(0,T_0)$ and $B_T(0,T_0)$ are the volume expansion coefficient and the isothermal bulk modules, respectively, at $P = 0$ and $T = 0$.

To take into account the thermal effect, Equations (1) - (3) can be written as

$$\frac{U_S(P,T)}{U_S(P_0,T_0)} = 1 + \left\{\frac{1}{A} ln\left[1 + B\left(P - P_0 - \xi(T - \ T_0)\right)\right]\right\} \tag{10}$$

$$\left[\frac{dU_S(P,T)}{dP}\right]_T = \frac{B\, U_S(P_0,T_0)}{\{A[1+B(P-P_0-\xi(T-T_0))]\}} \tag{11}$$

$$\left[\frac{dU_S(P,T)}{dT}\right]_P = \frac{-B\, \xi\, U_S(P_0,T_0)}{\{A[1+B(P-P_0-\xi(T-T_0))]\}} \tag{12}$$

where ξ is the thermal pressure coefficient and taken as pressure and temperature independent for present study.

3. METHODOLOGY

In liquid metals, the variation of sound velocity in entire (P, T) domain can be computed using Equation (8) provided $U_S(P_0,T_0)$, A, B, and ξ are known at reference temperature, T_0. The best fit values of A and B at reference temperature, T_0 are obtained from Equation (1) by using a nonlinear fitting toolbox in MATLAB. The experimental data of sound velocity at T_0 in liquid metals was taken from the references [15-17]. However, the best fit value of ξ is obtained by applying the Whale optimization algorithm in the entire (P, T) domain in which experimental data velocity as a function of pressure and temperature is available. Once the values of A, B, and ξ are known, the sound velocity and its first pressure and temperature derivatives can be easily computed using Equations (10)-(12) at any pressure and temperature combination. It will be appropriate to mention here that the value of ξ is taken as pressure and temperature is independent. Although it appears to be a very wild approximation at first, the close agreement between computed and experimental sound velocity across the entire pressure and temperature ranges gives confidence to this approximation.

4. THE WHALE OPTIMIZATION ALGORITHM (WOA)

The WOA is a recently introduced meta-heuristic optimization method that replicates the hunting behavior of humpback whales. The size of a full-grown humpback whale is comparable to that of a school bus. The bubble-net feeding method [18] is a novel way of humpback whale hunting. Humpback whales prefer to feed on krill or small fish at the water's surface. Humpback whales dive to a depth of 12 meters, then start ejecting bubbles in a spiral pattern that encircles prey, then follow the bubbles to the surface to catch it [18]. Humpback whales are known to remove prey from other people's bubble nets and to work in groups of at least two individuals. Humpback whales have a unique eating behavior known as bubble-net feeding. The mathematical model of encircling prey, the bubble net hunting method, and the search for prey are all described in the original publication [19].

5. PROBLEM FORMULATION

Before performing an optimization process, an objective function must be developed in order to extract the optimal value of ξ from the set of experimental data of sound velocity over the whole pressure and temperature range [20]. The Root Mean Square Error (RMSE) is employed as the objective function in this paper to quantify the difference in calculated and measured sound velocity. Using Equation (10), the difference between the experimental and estimated values of sound velocity can be represented as follows:

$$f(P,T) = U_{SE}(P,T) - U_S(P_0,T_0)\left[1 + \left\{\frac{1}{A} ln[1 + B(P - P_0 - \xi(T - T_0))]\right\}\right] \quad . \tag{13}$$

As a result, for any given set of measurements, the objective function that adds RMSE is defined as

$$RMSD = \sqrt{\frac{1}{N}\sum_1^N \{f(P,T)\}^2} \tag{14}$$

where N is the number of measured results and $U_{SE}(P,T)$ is the experimentally measured sound velocity at pressure, P and temperature, T.

The objective function provided in Equation (14) is used to monitor the selection of the best-fit value for ξ. The objective function is summed during the WOA optimization process to be minimized regarding the parameter, ξ range. The literature survey [3, 13-15] was used to determine the upper and lower bounds of ξ.

6. CALCULATIONS AND RESULTS

Equation (1) has been applied in liquid metals studied to compute the sound velocity as a function of pressure at reference temperature, T_0. The best-fit values of constants A and B, pressure range studied, the reference temperature and the root mean square deviation in each liquid are mentioned in Table 1. Figure 1 shows the close agreement between computed sound velocity across the entire pressure range at reference temperature and experimental values for all liquid metals. Even though the fit in the instance of liquid Bi is quite poor, the maximum percentage error (MPE) remains well within experimental uncertainty.

To estimate the sound velocity with pressure at different temperatures in each liquid metal, the best value of ξ in Equation (10) is obtained by minimizing the objective function of Equation (14) using the WOA. The range of the thermal pressure coefficient, ξ is set between 10^{-5} and 10^{-3}. The optimized value of ξ along with the final score of the objective function in each liquid metal are reported in Table 2. The final score of the objective function is found to be of the order of 10^{-3} in each liquid except Bi where it is of the order of 10^{-2}.

Table 1. *Input parameters, best fit values of A and B and RMSD for the Equation (1)*

Liquid Metal	T_0 (K)	P_0 (GPa)	$U(P_0,T_0)$(km/s)	A	B (GPa^{-1})	RMSD
Na	422.05	0.025	2.529	1.106	0.4579	0.0018
K	423.25	0.025	1.873	0.9811	0.8613	0.00123
Rb	423.25	0.025	1.249	0.9776	1.092	0.00152
Cs	423.25	0.025	0.975	1.089	1.571	0.00123

Hg	513	0.72	1.49	1.723	0.2028	0.00909
Bi	568	1.12	1.891	3.818	0.3964	0.00521

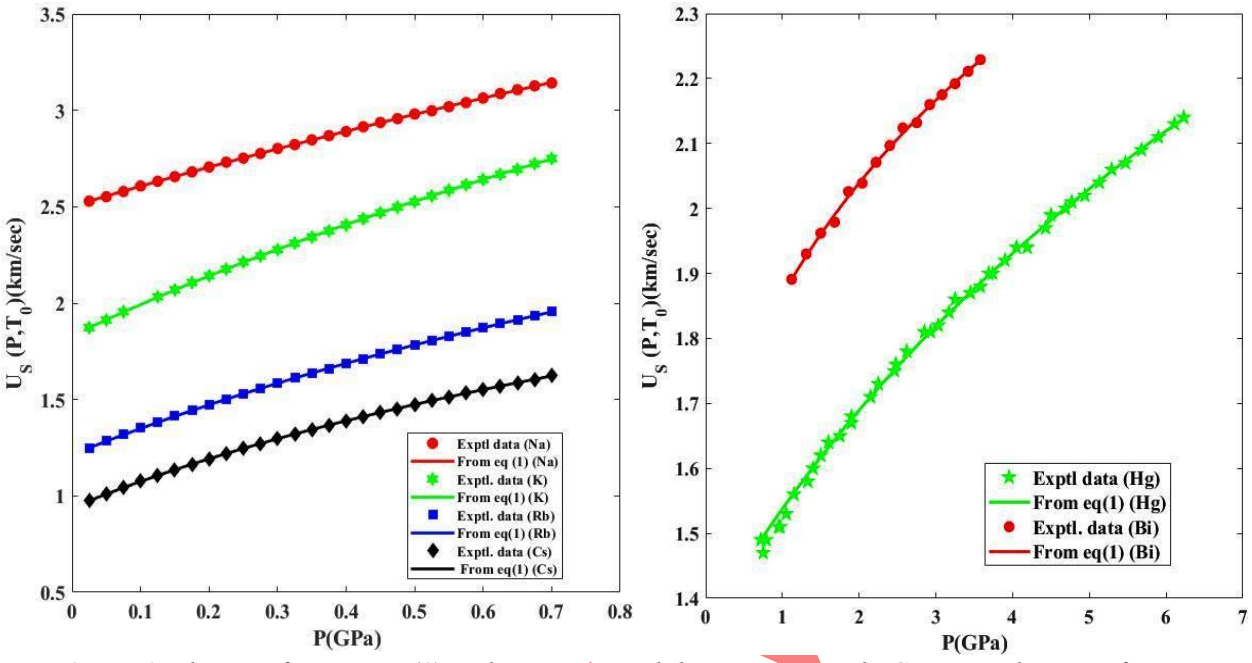

Figure 1. *The Fit of Equation (1) with experimental data in Na, K, Rb, Cs, Hg and Bi at reference temperature*

The optimized value of ξ is used to compute the sound velocity in the entire pressure and temperature range in each liquid metal. The computed value of %AARD over the entire pressure and temperature range in case of each metal is also reported in Table 3. The maximum %AARD is obtained as 0.45 in the case of Bi which is clear from the higher value of objective function in this case. However, the value of ξ obtained here is around one order smaller than the values calculated from the definition of thermal pressure coefficient $\xi = \alpha_P/K_T$, where α_P is the isobaric thermal expansion coefficient and K_T is the isothermal compressibility. The maximum percentage error (MPE) in each liquid metal is largely within the experimental uncertainty in the sound velocity measurement. The scatter plots in Figure 2 are chosen to demonstrate the kind of MPE obtained in entire pressure and temperature range in case of liquid Sodium and liquid Bismuth. In liquid Sodium, the %AARD is found to be minimum of 0.07 while in liquid Bismuth it is maximum of 0.45. The higher AARD% in bismuth suggests a larger deviation between computed and experimental values compared to other metals. This deviation may be due to unique electronic properties of bismuth, particularly its semi-metallic nature and bonding characteristics. In contrast, other metals like sodium and potassium exhibit significantly lower AARD%, reflecting a better fit. Despite this, the computed sound velocities remain within experimental uncertainties. Table 2 shows that the value of ξ generally decreases with decreasing metal melting point, except for mercury, which exhibits a relatively high ξ value despite having the lowest melting point among the metals studied. Mercury's strange behavior may be due to a relativistic effect on the core electrons [16], and as a result, it exhibits anomalous electronic properties when compared to other transition metals.

Furthermore, the results for the first and second derivatives of the sound velocity from Equations (4) and (5) at pressure, P_0 and temperature, T_0, are obtained and compared with the existing data in Table 3. The agreement is also very good in this case. Furthermore, Equations (9) and (10) can predict the pressure and temperature variations of the first pressure and temperature derivatives of sound velocity, which is useful for studying non-linear Bayer's parameters. [21, 22]. Moreover, the proposed model predicts that the first pressure derivative of sound velocity remains positive, indicating an increase in sound

velocity with pressure. The second derivative is negative, suggesting a decreasing rate with increase in presure. Similarly, the temperature derivative varies based on the thermal expansion coefficient, showing that metals with higher thermal expansion (such as alkali metals) experience a more pronounced temperature effect on sound velocity.

Table 2. *The AARD% in Equation (8), the minimized objective function, Equation (12) and best fit value of ξ in Equation (8)*

Liquid	Temperature Range (K)	Pressure Range (GPa)	%AARD	ξ ($\times 10^{-4}$)	Objective function (x 10^{-3})	T_m (K)
Na	382.55-422.05	0.025-0.700	0.027	3.119	2.436	371
K	357.55-423.25	0.025-0.700	0.035	2.559	3.039	337
Rb	333.25-423.25	0.025-0.700	0.267	1.393	3.859	312
Cs	322.85-423.25	0.025-0.700	0.35	1.367	3.818	302
Hg	296-513	0.720-6.230	0.343	26.63	8.8	234
Bi	568-973	1.12-4.16	0.449	5.361	10.5	544

Table 3. *Comparison of first and second derivatives of the sound velocity in liquid metals*

Liquid	P_0 (GPa)	T(K)	$U_S'(P_o,T)$ (Calc) ($kms^{-1}GPa^{-1}$)	$U_S'(P_o,T)$ [3] ($kms^{-1}GPa^{-1}$)	$U_S''(P_O,T)$ (Calc) $kms^{-1}GPa^{-2}$	$U_S''(P_O,T)$ [3] $kms^{-1}GPa^{-2}$
Na	0.025	422.05	1.05	1.01	- 0.48	- 0.40
K	0.025	423.25	1.64	1.68	- 1.41	- 1.40
Rb	0.025	423.25	1.39	1.44	- 1.52	- 1.60
C	0.025	423.25	1.49	1.50	- 2.19	- 2.80
Hg	0.720	513.00	0.176	--	- 0.036	- 0.036
Bi	1.12	568	0.2	--	- 0.079	--

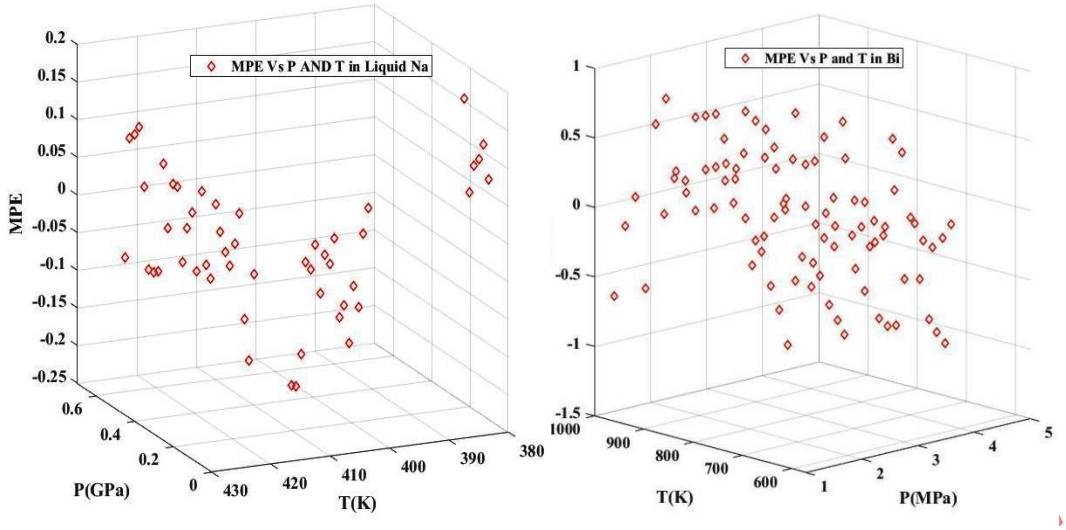

Figure 2. *Maximum percentage error involved in Equation (8) across the entire pressure and temperature range*

6.1. Comparison with Existing Model

The proposed approach provides an effective framework for modeling the variation of sound velocity in liquid metals across a range of pressures and temperatures using a straightforward parameterized equation. While this study validates the model by comparing its results with experimental data, a more detailed comparison with other approaches—including equation of state (EOS)-based models, as well as empirical and semi-empirical models—has been presented in Table 4 to further enrich the discussion. In contrast to conventional EOS methods, which often require multiple parameters and complex calculations, the proposed model relies on just three parameters, offering a balance between computational simplicity and accuracy. The study demonstrates that a simple parameterized approach can accurately model sound velocity in liquid metals. Future work could explore refining as a function of pressure and temperature, incorporating electronic structure calculations for metals like mercury and bismuth. Additionally, extending the model to other liquid systems, such as molten salts and alloys, would be beneficial.

Table 4*. Comparison with Other Models*

Model Type	*Equation Type*	*Number of Parameters*	*Remark*
Empirical (Linear Pressure Model) [3]	$U_s(P) = U_s(P_o) + C_1(P - P_o)$	1 ($C1$)	Pros: Simple, easy to fit Cons: Fails at high pressures
Semi- Empirical (Birch's Law-Based Model) [10]	$U_s = a + b\,\rho$ ρ: *density*	2 (a,b)	Pros: Captures density effects Cons: Requires density data
EOS (Murnaghan's Model) [2]	$U_s = \frac{K_o}{n}\left[\left(\frac{V_o}{V}\right)^n - 1\right]$	3 ($K_o V_o, n$)	Pros: Thermodynamic basis Cons: Complex, and needs high- precision data

Gruneisen Model [8]	$U_s^2 = \frac{\gamma P}{\rho}$	2-3 (depends on γ)	Pros: Useful for high pressure Cons: γ function is material-dependent
Present Model (Tait-like Equation)	$\frac{U_S(P,T)}{U_S(P_0,T_0)} = 1 + \left\{\frac{1}{A}\ln\left[1 + B\left(P - P_0 - \xi(T - T_0)\right)\right]\right\}$	3 (A, B, ξ)	Pros: Accurate for entire (P, T) domain, only 3 parameters Cons: Assumes ξ is independent of P, T

7. CONCLUSION

The above discussions clearly indicate that the present model is successful in representing the sound speed in entire pressure and temperature range in all liquid metals of study. The kind of AARD% obtained in each case demonstrates the success of the present model. Further, the first pressure and temperature derivatives of the sound velocity are computed first time in liquid metals, which are important to study the thermos-physical properties. The values of these derivatives show the slow variation of sound velocity in liquid Hg and liquid Bi with pressure and temperature. The novelty of this model is that only three parameters (A, B, and ξ) are required to represent the sound velocity over the pressure and temperature range of interest.

CONFLICTS OF INTEREST

No conflict of interest was declared by the authors.

LCIENCE STATEMENT

MATLAB software (R2023a, The MathWorks, Inc., Natick, Massachusetts, United States) was used under a licensed agreement provided by UPES.

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