Speed of Sound in Classical Real Gases with Intermolecular Potential as Lennard-Jones Potential Modified by Jagla Type Ramp

S. K. Suman

Ex Assistant Professor
Department of Physics, Central University of Jharkhand

Abstract: *Analytical approach for the calculation of speed of sound at atmospheric pressure in classical real gases with L-J potential modified by Jagla type ramp is presented in this paper. It is shown that the results are in good agreement with the data available in the literature.*

Key Words : *Speed of sound, Real gases, Lennard-Jones potential, Virial coefficients, Jagla potential.*

1. INTRODUCTION

We know that the speed of sound is very useful in the study of various properties of gases. They may be used in the engineering design of chemical processes. These data are essential for determining the energy necessary to bring the chemical reactants up to reaction temperature [1]. As we know that the various thermodynamic properties of real gases may be evaluated using virial equations of state. In this work, we evaluate the speed of sound, of some real gases for which the intermolecular potential is L-J potential modified by Jagla type ramp [2]. For this purpose, we numerically evaluate the first and second derivatives of the second virial coefficient of the gases under consideration. These values of first and second derivatives of the second virial coefficient of the gases under study are used to calculate the speed of sound of the classical real gases [3].

2. THEORY

We are assuming that the gases under consideration are low density classical real gases so that we may approximate the virial equation of state [4] up to the term containing second virial coefficient. Therefore, by neglecting third and other higher virial coefficients in virial equation of state, we have

$$Z = \frac{PV}{RT} = 1 + \frac{B(T)P}{RT} \quad \text{……… (1)}$$

Here the second virial coefficient B(T) for a classical real gas may be written as [5]

$$B(T) = -2\pi N_A \int_0^\infty r^2 [e^{-\varphi(r)/kT} - 1] dr \quad \text{……… (2)}$$

where N_A is Avogadro constant, k is Boltzmann's constant and the L-J 6-12 potential modified by Jagla ramp considered here is given by [6]

$$\varphi(r) = +\infty \text{ if } 0 \le r \le \lambda \quad \text{……… (3a)}$$

$$= c\,(r - \lambda) \text{ if } \lambda \le r \le \sigma \quad \text{……… (3b)}$$

$$= 4\,\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \text{ if } \sigma \le r \le +\infty \quad \text{……… (3c)}$$

$$\text{where } c = \frac{4\varepsilon}{(\lambda - \sigma)} \left[\left(\frac{\sigma}{\lambda}\right)^{12} - \left(\frac{\sigma}{\lambda}\right)^{6} \right] \quad \text{……… (4)}$$

Now the speed of sound of a real gas may be written in terms of the second virial coefficients as follows [3], [7]

$$c_0^2 = \frac{\gamma RT}{M}\left[1 + \frac{1}{V}\left((2B(T) + 2(\gamma - 1)T\frac{dB(T)}{dT} + \frac{(\gamma-1)^2}{\gamma}T^2\frac{d^2B(T)}{dT^2}\right) + \cdots\right] \quad \text{……… (5)}$$

where $\gamma = \frac{C_P}{C_V}$. .... (6)

Here M is molecular weight. R is gas constant.

3. NUMERICAL CALCULATION

In this work we numerically evaluate first and second derivatives of the second virial coefficients with respect to absolute temperature T for Argon and Neon, and then we calculate the speed of sound in these gases at atmospheric pressure by considering the intermolecular potential for these classical real gases as L-J potential modified by Jagla type ramp. In table 1 molecular weight and values of the parameters [6] for the potential $\varphi(r)$ are shown for the gases Argon and Neon. In table 2 numerically evaluated values of second virial coefficient and its first and second derivatives with respect to absolute temperature are given at different temperatures for Argon. In table 3 numerically evaluated values of second virial coefficient and its first and second derivatives with respect to absolute temperature are given at different temperatures for Neon. Speed of sound in Argon and Neon are finally numerically calculated using equation (5) and the values of the parameters given in table 1, table 2 and table 3 and finally these values are tabulated in table 4 and table 5 for Argon and Neon respectively. Value of γ at 1 atmosphere pressure for Argon and Neon are assumed to be 1.671 and 1.667 respectively for the temperature range 100 K to 400 K.

Table 1

S.N.	Gas	M	λ	σ	ε/k
1.	Argon	39.948 g/mol	3.145084 x10^{-10} m	4.746780 x10^{-10} m	89.1935 K
2.	Neon	20.179 g/mol	2.027787x10^{-10} m	2.571497x10^{-10} m	45.7158 K

Table 2

(Numerically evaluated values for Argon)

S.N.	T	B(T) in cm^3 / mol	$\frac{dB(T)}{dT}$ in cm^3 / (mol.K)	$\frac{d^2B(T)}{dT^2}$ in cm^3 / (mol.K^2)
1.	100 K	-187	3.52	-0.1074
2.	120 K	-133.1	2.058333	-0.04875
3.	140 K	-99.8	1.342857	-0.025969388
4.	160 K	-77.2	0.94375	-0.015390625
5.	200 K	-48.7	0.535	-0.00665
6.	240 K	-31.5	0.345833	-0.0034375
7.	280 K	-20.1	0.239286	-0.002002551
8.	320 K	-11.9	0.175	-0.001269531
9.	360 K	-5.8	0.133333	-0.000848765
10.	400 K	-1.1	0.105	-0.0006

Table 3

(Numerically evaluated values for Neon)

S.N.	T	B(T) in cm^3 / mol	$\frac{dB(T)}{dT}$ in cm^3 / (mol.K)	$\frac{d^2B(T)}{dT^2}$ in cm^3 / (mol.K^2)
1.	100 K	-4.8	0.27	-0.0063
2.	120 K	-0.4	0.175	-0.0034
3.	140 K	2.6	0.128571	-0.00204
4.	160 K	4.8	0.09375	-0.00133
5.	200 K	7.6	0.055	-0.00065
6.	240 K	9.4	0.0375	-0.00035
7.	280 K	10.6	0.025	-0.00022

8.	320 K	11.5	0.01875	-0.00014
9.	360 K	12.1	0.013889	-9.3 x 10^{-5}
10.	400 K	12.6	0.01	-6.9 x 10^{-5}

Table 4

(Numerically evaluated speed of sound in Argon at P= 1 atm)

S.N.	T	Numerically evaluated speed of sound	Speed of sound [8], [9]	% difference
1.	100 K	182.11 m/s	183.51 m/s	-0.762901204
2.	120 K	203.3 m/s	202.43 m/s	0.429778195
3.	140 K	220.12 m/s	219.38 m/s	0.337314249
4.	160 K	235.1 m/s	234.95 m/s	0.063843371
5.	200 K	261.25 m/s	263.13 m/s	-0.714475734
6.	240 K	287.56 m/s	288.45 m/s	-0.308545675
7.	280 K	310.32 m/s	311.67 m/s	-0.433150448
8.	320 K	333.6 m/s	333.24 m/s	0.108030248
9.	360 K	352.1 m/s	353.49 m/s	-0.393221873
10.	400 K	371.5 m/s	372.62 m/s	-0.300574312

Table 5

(Numerically evaluated speed of sound in Neon at P=1 atm)

S.N.	T	Numerically evaluated speed of sound	Speed of sound [8], [9]	% difference
1.	100 K	263.01 m/s	262.2434 m/s	0.292323849
2.	120 K	287.12 m/s	287.3076 m/s	-0.065295871
3.	140 K	309.11 m/s	310.3315 m/s	-0.393611348
4.	160 K	330.921 m/s	331.7488 m/s	-0.249526147
5.	200 K	371.671 m/s	370.8726 m/s	0.215276081
6.	240 K	407.5 m/s	406.2335 m/s	0.311766509
7.	280 K	437.01 m/s	438.7477 m/s	-0.396059056
8.	320 K	470.34 m/s	469.0102 m/s	0.283533279
9.	360 K	499.01 m/s	497.4332 m/s	0.316987286
10.	400 K	525.5 m/s	524.3167 m/s	0.22568421

4. DISCUSSIONS AND CONCLUSIONS

From the above tables we may infer that the values of speed of sound in both the gases Argon and Neon are in very good agreement with the data available in literature. This means that the L-J potential modified by Jagla type ramp is a good choice of intermolecular potential for the gases Argon and Neon.

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