# Compressibility Factor of Low-Density Classical Real Gases with L-J Intermolecular Potential Modified by Jagla Type Ramp

**S. K. Suman**

*Assistant Professor, Department of Physics, Central University of Jharkhand*

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**Abstract:** *Analytical approach for the calculation of compressibility factor at different temperatures of some 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.*

**Keywords:** ***Compressibility factor, Lennard-Jones potential, Jagla potential.***

## 1. INTRODUCTION

Compressibility factor (Z) is an important physical property of a gaseous system [1]. When its value is less than 1, it simply indicates that the real gas has a lower pressure than an ideal gas and thus those molecules are more influenced by the attractive part of the potential than its repulsive part. If the temperature is very high, then the compressibility factor is greater than 1, and this indicates that the real gas has a higher pressure than an ideal gas and thus molecules of the real gas are more influenced by the repulsive part of the potential than its attractive part [2]. In this study we are considering the intermolecular potential as L-J 6-12 potential modified by Jagla type ramp [3].

## 2. THEORY

We are considering low density classical real gases so we may assume only binary interactions of the gas molecules in the calculation of compressibility factor. Therefore, writing the virial equation of state [4] by neglecting third and other higher virial coefficients, we have

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

Here the second virial coefficient for a classical real gas may be written as

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

……………….. (2)

where $N_A$ is Avogadro constant and the modified L-J 6-12 potential considered here is given by [5]

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

$$= c(r-\lambda) \text{ if } \lambda \le r \le \sigma$$

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

……………… (3)

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

## 3. NUMERICAL CALCULATION

Compressibility factors are calculated numerically for the gases Helium and Hydrogen using the above theory. Values of the parameters λ, σ and ε are taken from E. Albarrán-Zavala *et al.* [5]. For helium $\lambda$= 2.002807 x $10^{-10}$ m, $\sigma$= 2.477172 x $10^{-10}$ m, and $\varepsilon$= 1.260382 x $10^{-22}$ J. and for Hydrogen $\lambda$= 2.368190 x $10^{-10}$ m, $\sigma$= 2.861934 x $10^{-10}$ m, and $\varepsilon$= 5.513926 x $10^{-22}$ J.

Comparison of the obtained results with the data available in literatures are tabulated in the following tables-

**Table 1**

(Compressibility factor of He gas at T= 295.15 K)

| Pressure (N/m²) | Calculated Z | Experimental Z [6] | Percentage Difference |
|---|---|---|---|
| 1.00 X $10^6$ | 1.0045 | 0.996 | 0.85% |
| 1.40 X $10^6$ | 1.0063 | 1.01 | -0.37% |
| 1.80 X $10^6$ | 1.0081 | 1.01 | -0.19% |
| 2.20 X $10^6$ | 1.0099 | 1.01 | -0.01% |
| 2.60 X $10^6$ | 1.0117 | 1.01 | 0.17% |
| 3.00 X $10^6$ | 1.0134999 | 1.01 | 0.35% |
| 3.40 X $10^6$ | 1.0152999 | 1.02 | -0.46% |
| 3.80 X $10^6$ | 1.0170999 | 1.02 | -0.28% |
| 4.20 X $10^6$ | 1.0188999 | 1.02 | -0.11% |
| 4.60 X $10^6$ | 1.0206999 | 1.02 | 0.07% |
| 5.00 X $10^6$ | 1.0224999 | 1.02 | 0.25% |

**Table 2**

(Compressibility factor of $H_2$ gas at T= 300 K)

| Pressure in Bar | Calculated Z | Z (Bahtiyar A. Mamedov *et al.* [2]) | Percentage Difference |
|---|---|---|---|
| 5.00 X $10^6$ | 1.009 | 1.00916 | -0.01585477 % |
| 1.00 X $10^7$ | 1.018 | 1.01832 | 0.031424307 % |
| 1.50 X $10^7$ | 1.027 | 1.02748 | 0.046716238 % |
| 2.00 X $10^7$ | 1.036 | 1.03664 | 0.061737923 % |
| 2.50 X $10^7$ | 1.045 | 1.0458 | 0.076496462 % |
| 3.00 X $10^7$ | 1.054 | 1.05497 | 0.091945743 % |
| 3.50 X $10^7$ | 1.063 | 1.06413 | 0.106190033 % |
| 4.00 X $10^7$ | 1.072 | 1.07329 | 0.120191188 % |
| 4.50 X $10^7$ | 1.081 | - | - |
| 5.00 X $10^7$ | 1.09 | - | - |

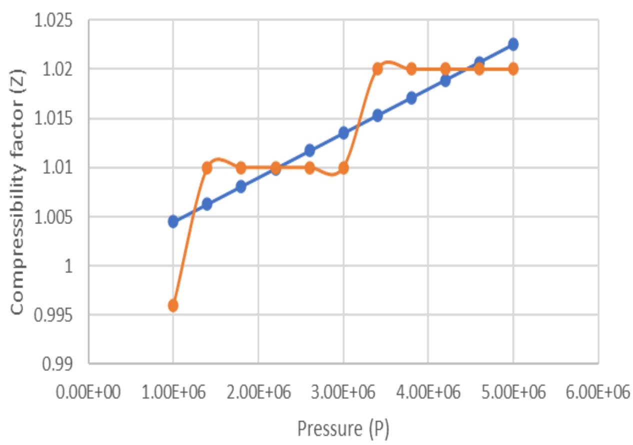


Figure 1
Blue and orange curves correspond to calculated and experimental values of Z respectively for Helium gas at 295.15K

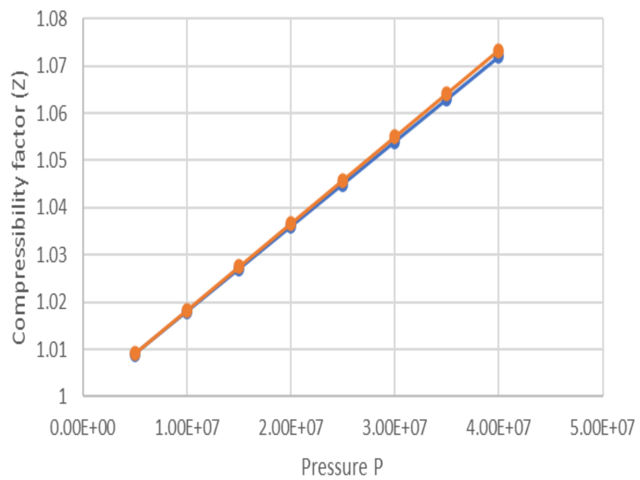


Figure 2
Blue and orange curves correspond to calculated values and the data from literature resprctively for hydrogen gas at 300 K

## 4. CONCLUSIONS

From the above tables we may conclude that the results obtained are in good agreement with the experimental data or the data available in literature. So, we may infer from this study that as far as the calculated value of compressibility factor of low-density classical real gases is considered, L-J intermolecular potential modified by Jagla type ramp may be assumed to be a good choice for the intermolecular potential for helium and hydrogen gases. Another very important information we get from the above data is that even at, near about room temperature the deviation in the calculated values of compressibility factor is more in case of helium gas than that of hydrogen gas, which may be due to more quantum effects in case of helium gas than that of hydrogen gas.

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