Morse oscillator equation of state: An integral equation theory based with virial expansion and compressibility terms

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A R T I C L E   I N F O

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A B S T R A C T

A number of interaction energy types are employed in the vibrations studies, especially in the spectroscopic analysis, such as the harmonic oscillator and Morse oscillator. In this research, a derivation of an analytical formula of equation of state of Morse oscillator is considered by employing the approximations used in the simple fluids theory. The compressibility formula of the pressure and the virial expansion formula of the pressure using the solutions of the main equation of the simple fluids theory with one of the approximations of the theory are employed for the purpose of the derivation. The virial coefficients of the total Morse oscillator pressure (the first order one, and the second order one) are found for Morse oscillator with respect to the fractional volume of the components, where we conclude that the first order term is proportional to the absolute temperature directly and depends on the diameter of the particles, while we concluded that the second order coefficient term is more complicated than the first order one with temperature, and also, depends on the three Morse oscillator parameters and the diameter of the particles. Besides, we conclude that the total pressure of Morse oscillator, generally, depends on the minimum energy of the well of Morse oscillator, the width parameter of Morse oscillator, and the equilibrium bond distance of the oscillator, in addition to their dependence on the absolute temperature of the components, and the diameter of the particles. The formula of the Morse oscillator equation of state which is found in this research can be applied to multiple materials described using Morse oscillator such as lots of dimers in the vibrations spectroscopy.

1. Introduction

For the study of vibrations in the quantum mechanics and their relations to the spectroscopic results, there are multiple types of the potentials, such as the harmonic oscillator potential an Morse oscillator potential which we focus on in this research. There are multiple used formulas of Morse oscillator, based on the zeros of the energy, such as the formula represented in the following equation (Abebe et al., 2021; Alqannas and Abdel-Khalek, 2019; Ikot et al., 2021; Morse, 1929; Okoia et al., 2020; Rong, 2003):

\[ V_{Morse} = E_0 e^{-2(r-r_0)^2} \left[ 1 - 2e^{(r-r_0)^2} \right] \]  \hspace{1cm} (1)

From equation (1), we note that the formula of Morse oscillator has three different parameters: \( E_0 \), which is the minimum energy of the well, \( r \) which represents the width parameter of Morse oscillator, and \( r_0 \) which represents the equilibrium bond of the oscillator (Pingk et al., 2021; Al-Raeie, 2021). In the following, we are going to show a method for deriving an equation of state of Morse oscillator (EOSMO) based on the integral equations theory using the mean spherical approximation. The integral equations theory is a significant theory for discussing thermodynamics of multiple spectrum of materials such as soft materials and simple fluids. For instance, Zhou et al. (2004) applied the integral equations theory for finding the depletion potential for the colloidal particle, Aguirre-Manzo and González-Mozuelos (2021) discuss the charged colloids with high charges with the salt in suspensions using the theory of the integral equations, Pérez-Molina et al. (2021) used the chaotic data with the theory of the integral equations for the estimation of the virial coefficients of the equation of state, Kalyuzhnyi et al. (2021) applied the theory of the integral equations with the numerical analysis techniques for the study of the mixtures of colloids, Hashimoto et al. (2019) use the theory of the integral equations with the atomic force microscopy data for the determination of the number density distribution of colloidal particles on a substrate, Filippov et al. (2019) used the theory of the integral equations for the dusty plasma mixtures, Munaöd and Saija (2019) studied the hertzian spheres in case of the low temperatures using the theory of the integral equations in the fluid...
and to the Monte-Carlo simulation, Herrera (2018) found some structural and thermodynamic properties of fluids described by hard sphere and Yukawa potential using the theory of the integral equations, Aranu-Lara showed some application of the integral equations theory to the colloidal fluids, Pizio et al. (2011) discussed a model for the simple fluids using the second order of the integral equations theory, Lukšić et al. (2011) applied the integral equations theory for the mixtures of the electrolytes and non-charged hard spheres for purpose of the determination of the structural properties and thermodynamics of these mixtures, Fukudome et al. (2014) showed a new formula for the direct correlation function for the hard sphere fluids, Wu et al. (2014) calculated the static structure factor for the charged spheres using the integral equations theory, Lomba et al. (2015) used the three dimensional integral equations approximation for discussing of fluids with confinement and applied in the case of theargon in zeolites, Miyata and Miyazaki (2016) discussed the one component fluids interacting via Lennard-Jones interaction for the study of the temperature derivative of the radial distribution function using the integral equations theory, Melnyk et al. (2016) found the structure factor of the fluids of the hard core type interacting via short range Yukawa potential using the integral equations theory and the simulation methods, Al-Raei (2022a) derived a state equation for London interaction. Also, Al-Raei (2021) applied the theory for the study of some soft materials, Zhou (2010) discussed the fluids with the honeycomb interaction with the integral equations theory. In the second section of this work, theoretical method of the derivation of the equation of state is illustrated, and in the third section, some discussions of the derived formula are illustrated, and in the last one, conclusions of the work are illustrated.

2. The method

The main equation in the study of the simple fluids using the integral equation theory is Ornstein–Zernike equation (OZE) which has two different terms: the first term is resulted from the direct correlation and the other is resulted from the indirect one, the OZE is worded via following formula (Al-Raei, 2022b,c):

$$\hat{h}^T = c^O + \tau \int d\vec{r} \left[ \rho^O_{\vec{r}} \right] \hbar^T$$  \hspace{1cm} (2)

Where the distance of the particles is $r$, the particle density number is $c^O$, and $\hbar^T$ correlation functions. From the formula of the equation (2), it is clear that the finding of solutions of this equation needs another equation which is resulted from multiple types of the approximations used in the simple fluids theory where some have linear form, some have exponential form, and others have natural logarithmic form. In this work, we employ the approximation namely MSA (mean spherical approximation) where this approximation is the basic approach of this study for finding the solutions and from these solutions, we derive our equation of state for Morse oscillator. The starting point of deriving the equation of state of Morse oscillator is from the general form of the pressure which has two terms as in the equation (3):

$$P_{\text{tot}}(T) = \frac{1}{2} (2P_{\text{vir}} + P_{\text{Com}})$$  \hspace{1cm} (3)

where the first term returns to the virial case, and the other returns to the compressibility one. Firstly, the treating of the virial terms is done, where this term is illustrated in the equation (4):

$$P_{\text{vir}}(T) \equiv P_{\text{vir}} = k_B T - \frac{2\pi}{3} \tau^2 \int_0^\infty d\vec{r} V'_{M_{\text{vir}}} \rho^O_{\vec{r}}$$  \hspace{1cm} (4)

where Boltzmann constant is $k_B$, the temperature is $T$, the radial distribution function is $\rho^O_{\vec{r}}$, and $V'_{M_{\text{vir}}}$ is the Morse potential derivation with respect to the distance which can be found in the following equation:

$$V'_{M_{\text{vir}}} = 2\sqrt{2q} e^{-2(r_{0} - r)} \left[ e^{2q(r_{0} - r)} + 2 \right]$$  \hspace{1cm} (5)

and by using the solutions of the equation (2) in the virial pressure equation, we find:

$$P_{\text{vir}}(T) \equiv k_B T - \frac{2\pi}{3} \tau^2 \int_0^\infty d\vec{r} V'_{M_{\text{vir}}} \rho^O_{\vec{r}}$$ \hspace{1cm} (6)

$$P_{\text{vir}}(T) = k_B T - \frac{2\pi}{3} \tau^2 \int_0^\infty d\vec{r} \left[ \left( \rho^O_{\vec{r}} \right) + \beta D_0 e^{-2(r_{0} - r)} + 2\beta D_0 e^{-2(r_{0} - r)} + 2\beta D_0 e^{-2(r_{0} - r)} \right]$$  \hspace{1cm} (7)

and by other form:

$$P_{\text{vir}}(T) = k_B T - \frac{2\pi \eta T}{3} \tau^2 \int_0^\infty d\vec{r} \left[ \left( \rho^O_{\vec{r}} \right) + \beta D_0 e^{-2(r_{0} - r)} + 2\beta D_0 e^{-2(r_{0} - r)} \right]$$  \hspace{1cm} (8)

Here, the using of the dimensionless form of the parameters of the Morse oscillator those are given in the following equation:

$$\rho^* \equiv q \rho^{**}$$  \hspace{1cm} (9)

$$\rho^{**} \equiv \rho^{**} \tau^0$$  \hspace{1cm} (10)

$$\rho^{**} \equiv q \rho^{**}$$  \hspace{1cm} (11)

gives the virial term of the pressure as:

$$P_{\text{vir}}(T) = k_B T - \frac{2\pi \eta T}{3} \tau^2 \left[ \left( \rho^O_{\vec{r}} \right) + \beta D_0 e^{-2(r_{0} - r)} + \beta D_0 e^{-2(r_{0} - r)} + \beta D_0 e^{-2(r_{0} - r)} \right]$$  \hspace{1cm} (12)

where:

$$u_1 = K_1(q, r_0) \int_0^\infty d\rho \rho^3 e^{-2q\rho}$$  \hspace{1cm} (13)

$$u_2 = K_2(q, r_0) \int_0^\infty d\rho \rho^3 e^{-2q\rho}$$  \hspace{1cm} (14)

$$u_3 = K_3(q, r_0) \int_0^\infty d\rho \rho^3 e^{-2q\rho}$$  \hspace{1cm} (15)

$$u_4 = K_4(q, r_0) \int_0^\infty d\rho \rho^3 e^{-2q\rho}$$  \hspace{1cm} (16)

The integrating of the previous four equations can be done using the power-n with the exponential function integral which gives the following four results:

$$u_1 = \int_0^\infty \int_0^\infty \int_0^\infty d\rho^{**}$$ \hspace{1cm} (17)

$$u_2 = \int_0^\infty \int_0^\infty \int_0^\infty d\rho^{**}$$ \hspace{1cm} (18)

$$u_3 = \int_0^\infty \int_0^\infty \int_0^\infty d\rho^{**}$$ \hspace{1cm} (19)

$$u_4 = \int_0^\infty \int_0^\infty \int_0^\infty d\rho^{**}$$ \hspace{1cm} (20)

which gives the virial term of the pressure equation after returning to the dimensionless parameters as follows:
\[ P_{\text{C YM}}(r, T) = k_B r T \left( \frac{2\pi E_0}{3} r^2 \right) \left[ \frac{1}{3} - (1 - \beta E_0) \left( \frac{d^2}{q} + \frac{4d^2}{q^2} + \frac{3}{q^3} \right) \right] \]
\[ + (2\beta E_0 - 1) \left( \frac{1}{2} \right) \left( \frac{2}{4q} + \frac{3d^2}{4q^2} + \frac{3}{4q^3} \right) \right] e^{-2\alpha T} \]
\[ - 2\beta E_0 \left( \frac{d^3}{3q^3} + \frac{d^2}{2q^3} + \frac{2}{4q^3} \right) e^{-3\alpha T} \]
\[ + \beta E_0 \left( \frac{d^3}{4} + \frac{3d^2}{16q} + \frac{3d}{32q^2} + \frac{3}{128q^3} \right) e^{-\alpha T} \]  
where:
\[ \alpha = \frac{d}{3} r^{1/3} \]  
(22)

Then, the treatment of the compressibility pressure is done, where this term is given in the following equation: is given as follows:
\[ P_{\text{C YM}}(r, T) \equiv \int_{0}^{\infty} \frac{1}{r^2} dr \]  
(23)

with the help of the static structure factor as:
\[ \chi_T(k_B r T) = S_C(k) \Rightarrow (k_B r T \chi_T) = \frac{1}{1 - r \chi(k)} \]  
(24)

With \( k \) is the amplitude of the wave vector, and the previous formula becomes:
\[ (\chi_T k_B r T)^{-1} = -4\pi T \int_{0}^{\infty} r^2 e^{2\alpha T} dr + 1 \]  
(25)

using the solutions of the equation (2) in the compressibility equation, we find
\[ (\chi_T k_B r T)^{-1} = 4\pi T \int_{0}^{\infty} r dr + 8\pi \beta E_0 \int_{0}^{\infty} r dr \]  
(26)

and if we use the Morse oscillator dimensionless parameters, the equation (26) is written as:
\[ (\chi_T k_B r T)^{-1} = \frac{4\pi T}{3} + 8\pi \beta E_0 u_6 - 4\pi \beta E_0 u_5 + 1 \]  
(27)

where:
\[ u_5 = K_5(q, r_0) \int_{0}^{\infty} \rho^2 e^{-2\alpha \rho^2} d\rho \]
\[ u_6 = K_6(q, r_0) \int_{0}^{\infty} \rho^2 e^{-\alpha \rho^2} d\rho \]  
(28)

The integrating of the previous two equations can be done using the power-n with the exponential function integral which gives the following two results:
\[ u_5 = e^{2\alpha r^2} \left[ \frac{r^2}{2q^2} - \frac{r}{q^2} - \frac{1}{4q^4} \right] \]  
(30)

\[ u_6 = e^{\alpha r^2} \left[ \frac{r^2}{q^2} - \frac{2r}{q^2} - \frac{2}{4q^4} \right] \]  
(31)

By substituting the integrals in the equation (27), we find the compressibility in the following equation:
\[ (\chi_T k_B r T)^{-1} = 1 + \frac{4}{3} \pi T d^3 - 8\pi \beta E_0 e^{-2\alpha T} \left( \frac{d^2}{q} + \frac{2d}{q^2} + \frac{2}{q^3} \right) \]
\[ + 4\pi \beta E_0 e^{-2\alpha T} \left( \frac{d^2}{2q} + \frac{d}{2q^2} + \frac{1}{4q^3} \right) \]  
(32)

And we find that the compressibility term of the pressure is given in the following equation:
\[ P_{\text{C YM}}(r, T) = T k_B \int_{0}^{\infty} \left[ \frac{1 + 4\pi T d^3}{3} - 8\pi \beta E_0 e^{-2\alpha T} \left( \frac{d^2}{q} + \frac{2d}{q^2} + \frac{2}{q^3} \right) \right] d\tau \]  
(33a)

By using the power-n integrals, we find:
\[ P_{\text{C YM}}(r, T) = T k_B \int_{0}^{\infty} \left[ \frac{2\pi d^3 d^3}{3} - 4\pi \beta E_0 e^{-2\alpha T} \left( \frac{d^2}{q} + \frac{2d}{q^2} + \frac{2}{q^3} \right) \right] d\tau \]  
(33b)

By substituting the equation (21) and the equation (33b) in the general formula of pressure, we find that:
\[ P(r, T) \equiv \int_{0}^{\infty} \frac{2\pi d^3}{9} \left[ (1 - \beta E_0) \left( \frac{d}{q^2} + \frac{4d^2}{q^2} + \frac{3}{q^3} \right) \right] e^{-\alpha T} \]
\[ + (2\beta E_0 - 1) \left( \frac{1}{2} \right) \left( \frac{2}{4q} + \frac{3d^2}{4q^2} + \frac{3}{4q^3} \right) e^{-2\alpha T} \]
\[ - 2\beta E_0 \left( \frac{d}{3q^3} + \frac{d^2}{2q^3} + \frac{2}{4q^3} \right) e^{-3\alpha T} \]
\[ + \beta E_0 \left( \frac{d}{4} + \frac{3d}{16q} + \frac{3d}{32q^2} + \frac{3}{128q^3} \right) e^{-\alpha T} \]  
(34)

and in simpler form:
\[ P(r, T) = k_B \int_{0}^{\infty} \left[ \frac{2\pi d^3}{9} \left[ (1 - \beta E_0) \left( \frac{d}{q^2} + \frac{4d^2}{q^2} + \frac{3}{q^3} \right) \right] e^{-\alpha T} \]
\[ + (2\beta E_0 - 1) \left( \frac{1}{2} \right) \left( \frac{2}{4q} + \frac{3d^2}{4q^2} + \frac{3}{4q^3} \right) e^{-2\alpha T} \]
\[ - 2\beta E_0 \left( \frac{d}{3q^3} + \frac{d^2}{2q^3} + \frac{2}{4q^3} \right) e^{-3\alpha T} \]
\[ + \beta E_0 \left( \frac{d}{4} + \frac{3d}{16q} + \frac{3d}{32q^2} + \frac{3}{128q^3} \right) e^{-\alpha T} \]  
(35)

3. Results and discussion

The equation (35) is the basic equation of this study where the equation can be reworded using the fractional volume of the components, which is illustrated in the following equation:
\[ \nu = d^3 \frac{\pi}{6} \]  
(36)

and the equation (35) becomes:
\[ P_{\text{C YM}}(v, T) = \pi T \nu^2 + \Gamma_1 \nu \]  
(37)

where:
\[ \Gamma_1 = k_B \frac{6d^3}{T} \]  
(38)
\[ \Gamma_2(T) = \frac{-16E_0}{\pi d^6} [(1 - \beta E_0) \frac{d^4}{1} + \frac{3d^2}{q^2} + \frac{6d}{q^3} + 6e^{-4\pi r}] \\
+ (2\beta E_0 - 1) \left[ \frac{d^4}{4} + \frac{3d^2}{4q^2} + \frac{3}{8q^4} \right]e^{-2\pi r} \\
- \frac{2\beta E_0}{3} \left[ \frac{d^4}{3} + \frac{2d^2}{3q^2} + 2\frac{2}{27q^4} \right]e^{-3\pi r} \\
+ \beta E_0 \left( \frac{d^4}{4} + \frac{3d^2}{16q^2} + \frac{3}{32q^4} + \frac{3}{128q^8} \right) \\
+ \frac{8\beta T}{\pi d^5} \left[ \frac{d^4}{2} - \frac{4E_0}{\pi d^6} e^{-\pi r} \frac{d^2}{q} + \frac{2\pi r}{q^2} + \frac{2}{q^3} \right] \\
+ \frac{12E_0}{\pi d^6} e^{-2\pi r} \left( \frac{d^2}{q} + \frac{d}{q^2} + \frac{1}{2q^3} \right) \]  

(39)

It is noted from the equation (35), and the equation (37) that the total pressure of Morse oscillator is function to the fractional volume via square function. Also, we see from the two equations (35), and (37) that the total pressure of Morse oscillator depends on the absolute temperature, the fractional volume of the components, the depth of Morse potential, the bond distance of Morse potential, the components' diameter, and the well width parameter. Besides, it can be seen that the pressure is proportional to the square of the Morse potential well depth. In addition to that it is seen from the equation (38) that the first order virial expansion coefficient of the Morse potential does not depend on the three Morse oscillator parameters, and this first order coefficient is function to the inverse of the cube of the diameter of the component and to the linear function of the temperature. While the second order virial coefficient of Morse oscillator (from the equation (39)), depends on the Morse bond distance, the well depth of Morse potential, and the width parameter of Morse potential, and also to the diameter of the components, and temperature. Besides, it can be seen from the equation (39) that the second order virial coefficient is function to an exponential function with the width of the Morse potential and the bond distance of Morse oscillator, while this coefficient is a square function to the depth of the Morse potential. Further applications of the equation of the total pressure derived from this work can be applied to significant molecules and dimers, for instance: the dimer of phosphorus (Jia et al., 2018; Peng et al., 2018), the nitrogen gasous, hydrogen chloride, carbon monoxide, hydrogen sulphide, and Bohr fluoride (Jia et al., 2019; Jiang et al., 2019; Wang et al., 2019, and Jia et al., 2020), and for water (Wang et al., 2021), where we can use the fittings parameters resulted from the previous studies for simulating our equation of state of Morse oscillator for further numerical results.

4. Conclusions

In this research, an analytical formula of the Morse oscillator equation of state for systems described by Morse potential in the vibrational case was derived. The mean spherical approximation for low density simple fluid for deriving the Morse oscillator equation of state. The general formula of pressure which includes the virial expansion term and the compressibility term was applied.

Based on the Morse oscillator equation of state derived in this research, it is shown that the Morse oscillator pressure depends on the absolute temperature of the components, the depth of the Morse oscillator potential well, the bond distance of Morse potential, the diameter of particle of the described system, and the compact factor. We found that the pressure of the Morse oscillator depends on the fractional volume via square function. In addition and based on the Morse oscillator equation of state derived in this research. The first two order terms of the virial Morse oscillator pressure were found, where, it was shown that the first order virial coefficient does not depend on the three Morse oscillator parameters, while only the second order virial coefficient is dependent on the three Morse oscillator parameters in addition to its dependence on the absolute temperature of the components and the diameter of the components.

We believe that the Morse oscillator equation of state which was derived in this research can be applied generally for the study for lots of systems described by the Morse oscillator interaction such as the diatomic molecules, for instance: the hydrogen chloride and the hydrogen fluoride, where this equation can be applied for the numerical calculations, however, in this work we focus on the finding of the equation of state of Morse oscillator rather than the calculating of the numerical values.

Declarations

Author contribution statement

Marwan Al-Raeei: Conceived and designed the experiments; performed the experiments; analyzed and interpreted the data; contributed reagents, materials, analysis tools or data; wrote the paper.

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References

Abebe, O.J., Oberen, O.P., Okorie, U.S., Ikot, A.N., 2021. Spin and pseudospin symmetries of the Dirac equation for the generalised Morse potential and a class of Yukawa potential. Pramana J. Phys. 95, 126.
Aguirre-Manzo, I.A., González-Moruelo, P., 2021. A self-consistent Ornstein–Zernike jelly for highly charged colloids (microgels) in suspensions with added salt. J. Phys. Condens. Matter 33 (27).
Al-Raeei, M., 2021. The use of classical and quantum theoretical Physics methods in the study of complex systems and their applications in condensed matter Physics and quantum information theory. Damascus, the Syrian Arab Republic, PhD thesis.
Al-Raeei, M., 2022a. An equation of state for London dispersion interaction with thermodynamic inconsistent terms. Results Chem. 4.
Al-Raeei, M., 2022b. Bulk modulus for Morse potential interaction with the distribution function based. Chem. Thermodyn. Therm. Anal. 6, 10006.
Al-Raeei, M., 2022c. Morse potential specific heat with applications: an integral equations theory based. BMC Chem. 16.
Alqarnas, H.S., Abdel-Khalek, S., 2019. Physical and nonclassical properties of the interaction between a four-level atom and field in coherent state of Morse potential. Opt. Quantum Electron. 51, 50.
Filippov, A.V., Reshetnyak, V.V., Starostin, A.N., Tkachenko, L.M., Fortov, V.E., 2019. Investigation of dusty plasma based on the Ornstein–Zernike integral equation for a multicomponent fluid. JETP Lett. 110 (10), 659–666.
Fukudome, T., Mitarai, D., Irima, M., 2014. An analytical expression for the direct correlation function of a hard-sphere liquid derived from the extended scaled particle theory. J. Mol. Liq. 200 (PA), 95–103.
Hashimoto, K., Amano, K.-, Nishi, N., Sakka, T., 2019. Integral equation theory based method to determine number density distribution of colloidal particles near a substrate using a force curve from colloidal probe atomic force microscopy. J. Mol. Liq. 294.
Herrera, J.N., 2018. Thermodynamic and structural properties of fluids with a hard-sphere plus multi-Yukawa interaction potential. J. Mol. Liq. 270, 25–29.
Iiko, A.N., Okorie, U.S., Rampho, G.J., Amadi, P.O., 2021. Approximate analytical solutions of the Klein–Gordon equation with generalized Morse potential. Int. J. Thermophys. 42, 10.
Jia, C.-S., Wang, C.-W., Zhang, L.-H., Peng, X.-L., Tang, H.-M., Zeng, R., 2018. Enthalpy of gaseous phosphorus dimer. Chem. Eng. Sci. 183, 26–29.
Jia, C.-S., Zhang, L.-H., Peng, X.-L., Luo, J.-X., Zhao, Y.-L., Liu, J.-Y., et al., 2019. Prediction of entropy and Gibbs free energy for nitrogen. Chem. Eng. Sci. 202, 70–74.
Jia, C.-S., Li, J., Liu, Y.-S., Peng, X.-L., Jia, X., Zhang, L.-H., et al., 2020. Predictions of thermodynamic properties for hydrogen sulfide. J. Mol. Liq. 315.

Jiang, R., Jia, C.-S., Wang, Y.-Q., Peng, X.-L., Zhang, L.-H., 2019. Prediction of enthalpy for the gases CO, HCl, and BF. Chem. Phys. Lett. 715, 186–189.

Kalyuzhnyi, Y.V., Nezbeda, I., Cummings, P.T., 2021. Integral equation theory for mixtures of spherical and patchy colloids. 2. Numerical results. Soft Matter 17 (12), 3513–3519.

Lomba, E., Bores, C., Sánchez-Gil, V., Noya, E.G., 2015. A three dimensional integral equation approach for fluids under confinement: argon in zeolites. J. Chem. Phys. 143 (16).

Lukić, M., Hribar-Lee, B., Pizio, O., 2011. Structural and thermodynamic properties of the restricted primitive model electrolyte in a mixture with uncharged hard spheres: a grand canonical Monte Carlo simulation and integral equation study. Mol. Phys. 109 (6), 893–904.

Melnik, R., Nezbeda, I., Trokhymchuk, A., 2016. Structure factor of a hard-core fluid with short-range Yukawa attraction: analytical FMSA theory against Monte Carlo simulations. Mol. Phys. 114 (16–17), 2523–2529.

Miyata, T., Miyazaki, S., 2016. Accuracy of temperature-derivative of radial distribution function calculated under approximations in Ornstein-Zernike theory for one-component Lennard-Jones fluid. Chem. Phys. Lett. 658, 224–229.

Morse, P.M., 1929. Diatomic molecules according to the wave mechanics. II. Vibrational levels. Phys. Rev., 57–64.

Munah, S., Saija, F., 2019. Monte Carlo simulation and integral equation study of hertzian spheres in the low-temperature regime. J. Chem. Phys. 151 (13).

Okoia, P.O., Edelh, C.O., Magu, T.O., 2020. Relativistic treatment of the Hellmann-generalized Morse potential. Rev. Mex. Fis. 66 (1), 1–13.

Peng, X.-L., Jiang, R., Jia, C.-S., Zhang, L.-H., Zhao, Y.-L., 2018. Gibbs free energy of gaseous phosphorus dimer. Chem. Eng. Sci. 190, 122–125.

Pérez-Molina, M., Pérez-Polo, M.F., Chica, J.G., Varó, E.F., 2021. An equation of state based on the intermolecular potential and the radial distribution function to estimate the virial coefficients by using PVT chaotic data. Fluid Phase Equilib. 546.

Pingak, R.K., Johannes, A.Z., Ngara, Z.S., Bukit, M., Nitti, F., Tambaru, D., Ndii, M.Z., 2021. Accuracy of Morse and Morse-like oscillators for diatomic molecular interaction: a comparative study. Results Chem. 3.

Pizio, O., Sokolowska, Z., Sokolowski, S., 2011. Microscopic structure and thermodynamics of a core-softened model fluid from the second-order integral equations theory. Condens. Matter Phys. 14 (1).

Rong, Z., 2003. Comparison of the Morse and Deng-Fan potentials for X-H bonds in small molecules. Mol. Phys. 101, 2285–2294.

Wang, C.-W., Wang, J., Liu, Y.-S., Li, J., Peng, X.-L., Jia, C.-S., et al., 2021. Prediction of the ideal-gas thermodynamic properties for water. J. Mol. Liq. 321.

Wang, J., Jia, C.-S., Li, C.-J., Peng, X.-L., Zhang, L.-H., Liu, J.-Y., 2019. Thermodynamic properties for carbon dioxide. ACS Omega 4 (21), 19193–19198.

Wu, C., Chan, D.Y.C., Tabor, R.F., 2014. A simple and accurate method for calculation of the structure factor of interacting charged spheres. J. Colloid Interface Sci. 426, 80–82.

Zhou, S., 2010. A theoretical investigation on the honeycomb potential fluid. J. Chem. Phys. 133 (13).

Zhou, S., Zhang, X., Xiang, X., Xiang, H., 2004. Integral equation method for the determination of the depletion potential between two colloidal particles. Chin. J. Chem. Phys. 17 (1), 38–44.