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Presentation of the Soft-Core Double Yukawa Potential for Noble Gasses using in sillico

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ABSTRACT

The understanding of the intermolecular pair potential is important for determining the physical and chemical properties of the matter. The new data for noble gasses was calculated with Soft-Core Double Yukawa Potential (SCDY). We studied the effect of the Soft- Core potential on the phase behavior with Hartree-Fock-Dispersion (HFD) Potential. This model had a steep repulsion exponential term and double Yukawa potential which represents correctly the radial dependence of repulsive and long range energy respectively. The method was analyzed using sigma plot (SP-13) software. In order to find a correlation between variables Spearman correlation coefficient was used. Results showed that high content values for Ne-Ne, Ar-Ar, Kr-Kr, Xe-Xe of the pair potential which were fitted with HFD-B Potential. This work was used the Yukawa potential and evaluation of it's the parameters to present potential. The results were accurate and in according to previous studies. In conclusion, was summarized that potential was adjusted in two forms of (HFD and SCDY) potentials.

Keywords: Yukawa potential; Noble gasses; Soft- Core potential; Long range energy.

INTRODUCTION

The Prediction and interpretation of most phenomena involving atoms and molecules depend on knowledge of the intermolecular pair potential. Such knowledge is important for determining the physical and chemical properties of the matter. Although the exact nature of these forces is very complicated, there are no conceptual difficulties. There are many empirical potential functions in making use of them, but the problem is that it is often difficult to find a sufficiently flexible form for the potential without introducing so many adjustable parameters. In this paper a new Soft- Core Double Yukawa (SCDY) Potential was used for Neon, Argon, Krypton and Xenon and fitted with Hartree-Fock-dispersion (HFD) at both Short and long range. The potential form chosen to represent the Noble Gasses interaction is the HFD form used by Aziz and Chen[1] which is a variation of the original HFD potential of Aldrich's et al. [2]. It has been applied successfully to other systems[3, 4].

Several different representations of an LJ-like fluid in terms of a hard-core plus two Yukawa fluid (HC2YF) have been proposed in the literature [5-8]. The one we use here is very similar to that recently given by Kalyuzhnyi and Cummings[9] The

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numbers of new proposed potential functions for the noble gases interactions are numerous [10-12].

The potentials to be considered explicitly here are of the Hartree-Fock-dispersion (HFD) and the Exchange-Coulomb (XC) types. The HFD potential [2, 13] can be written in the form:

$$E_{int} = \Delta E_{SCF} + \Delta E_{Corr} \quad (1)$$

Where ΔE_{SCF}, is the (SCF) Hartree-Fock interaction energy of the rare-gas dimmer and ΔE_{Corr} is a semi empirical estimate of the correlation energy given by

$$\Delta E_{Corr} = - (C_6/R^6 + C_8/R^8 + C_{10}/R^{10}) F(R), \quad (2)$$

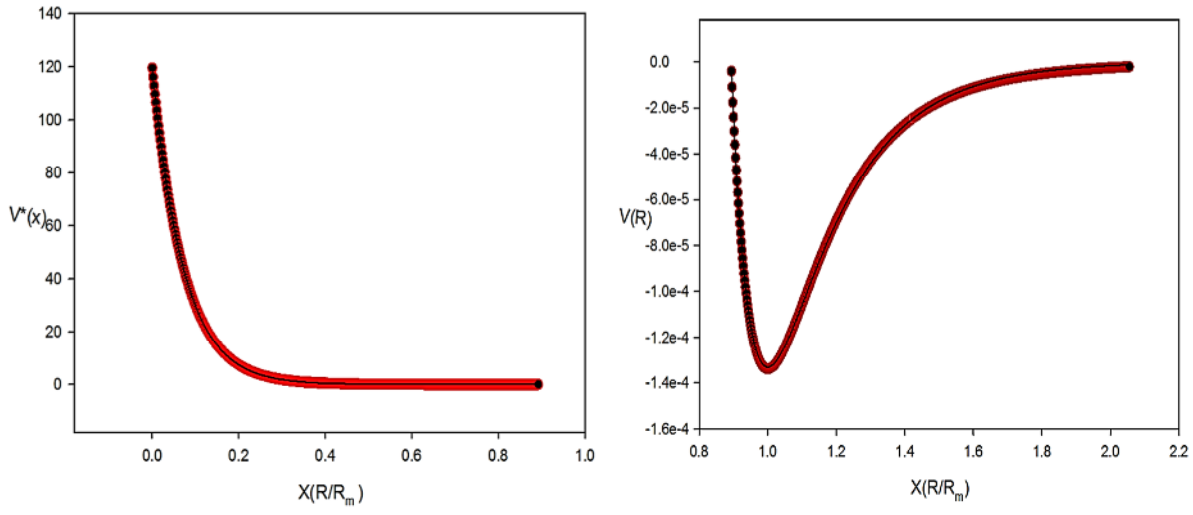
$F(R) = \exp [-(1.28R_mR^{-1}-1)2]$, $R \leq 1.28R_m$;
$F(R) = 1$, $R \geq 1.28R_m$,
In some applications (1) initial values for these parameters are obtained by fitting abinitio results for ΔE, and F(R) in (2) is replaced by:
$F(R) = \exp [-(DR_mR^{-1} -1)^2]$, $R \leq DR_m$;
$F(R) = 1$, $R \geq DR_m$, (3)

TEORETICAL METHOD

Our data were analyzed using sigma plot (SP-13) software. The One-Sample Kolmogorov Smirnov Test was used to test for normality of distributed of data parameters. The correlation is measured in terms of coefficient, which takes into consideration the co variation between the two variables (V* (x) and X (R/R_m), one time in the HFD-B potential and the other in the Soft- Core Double Yukawa (SCDY) potential separately. In order to find a correlation between variables Spearman correlation coefficient was used.

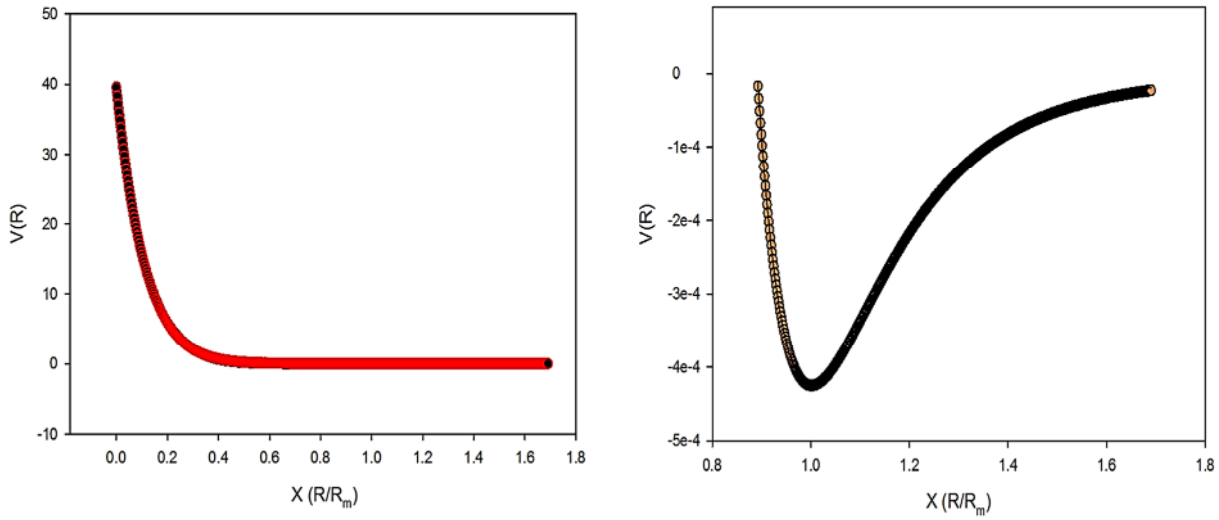
RESULTS AND DISCUSSION

They have been validated through comparison with experimental second virial data, gas transport properties, spectroscopic information and differential scattering cross sections, but their weak points is the difficulty to find a sufficiently flexible form. The Soft-core Double Yukawa potential, constructed in this work, represented an additional fine tuning of the original HFD potential for Ne-Ne, Ar-Ar ,Kr-Kr, Xe-Xe (see Fig 1-4) to the repulsive



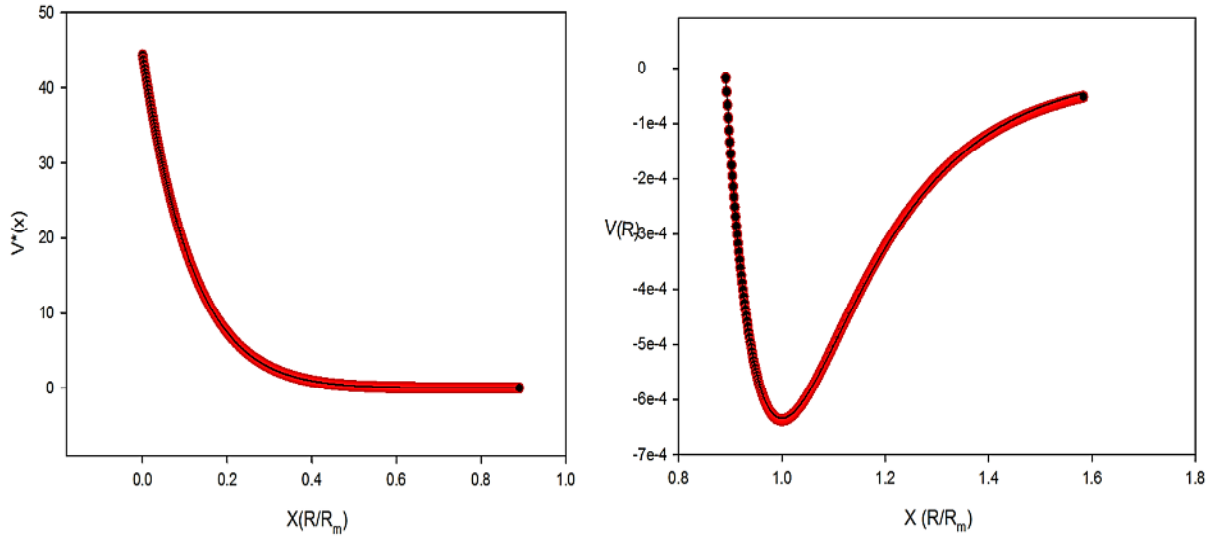
(a) (b)

Fig. 1. (a) potential HFD fitted with Double Yukawa Potential in the short range for Neon (Ne); **(b)** potential HFD fitted with Double Yukawa Potential in the long range for Neon (Ne).



(a) (b)

Fig. 2. (a) potential HFD fitted with Double Yukawa Potential in the short range for Argon (Ar); **(b)** potential HFD fitted with Double Yukawa Potential in the long range for Argon (Ar).

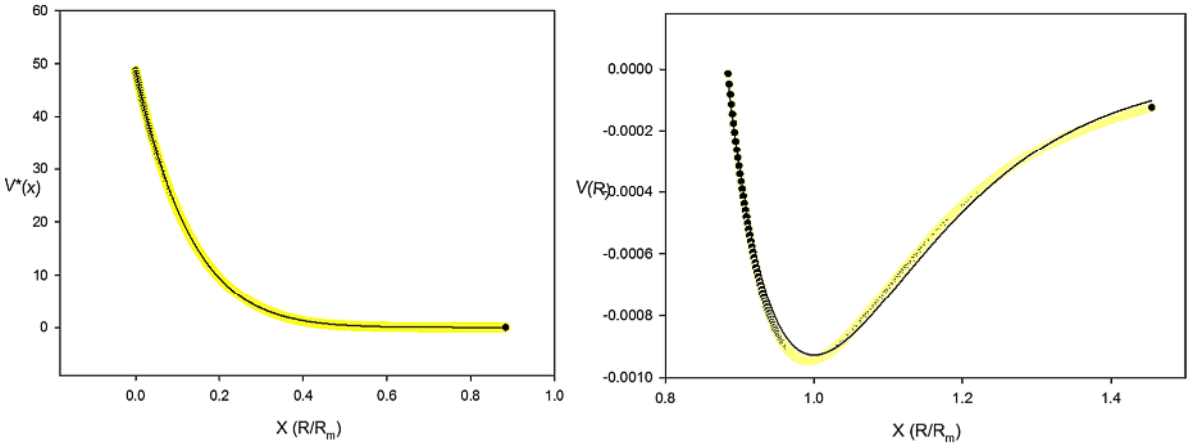


(a) (b)

Fig. 3. (a) potential HFD fitted with Double Yukawa Potential in the short range for Krypton (Kr); (**b**) potential HFD fitted with Double Yukawa Potential in the long range for Krypton (Kr).

as well as adjusted with studies Rol [14] The other parameter, including of B1, B2, ϵ determined with these HFD potentials [14] and the spectroscopic data of Freeman et al [15]. The HFD potential is also preferred to regarding the reproduction of the high temperature viscosity data of Goldblatt and Wageman [16]

We introduced a new intermolecular potential model, incorporating Soft-Core potential in Yukawa functional form for noble gases. This model has a steep repulsion exponential term and double Yukawa potential which represent correctly the radial dependence of repulsive and long range energy, respectively (see fig 1-4).



(a) (b)

Fig. 4. (a) potential HFD fitted with Double Yukawa Potential in the short range for Xenon (Xe); **(b)** potential HFD fitted with Double Yukawa Potential in the long range for Xenon (Xe).

The most crucial advantage of the Soft-Core Double Yukawa potential (SCDY) is that its parameters are not directly related to the thermodynamic and transport properties of the gases, so, the temperature range of this potential could be extended. In addition, parameters in the long range potential are lower than accurate experimental potentials [10-12].Unless indicated otherwise, atomic units are used for all quantities in this work. Double Yukawa form for noble gases are as follows:

U_{DY} =-ε*((1+B2)*exp(-B1*(x-1))-(1+B1)*exp(-B2*(x-1)))/(x*(B2-B1))

And the form of the HFD-B is:

U(r)= ϵ U *(X)

Where:

U*(x)=A* exp(-a*x+ß*x^2)- F(X) $\sum^{2}_{j=0}$ C_{2j+6}/x^{2j+}

With:

F(x)=exp[-(D/x-l)2], X<D

F(x)=1 X≥D

Parameters denoted which in addition to C_6, C_8 and C_{l0} (see table 1) are directly varied in the determining of the potential[17, 18] The parameters for the Soft-core Double Yukawa potential were determined by fitting the HFD-B potential, which is fine tuned to Rol's data via the function G, see (table 1). Spearman correlation coefficients between long range SCDY potential V*(x) and X(R/Rm) and long range HFD-B potential V*(x) and X(R/Rm) for each gasses were very strong and significant, also were approximately similar (table3).

Table 1. Parameters for the HFD-B2 potential

	Ne	**Ar**	**Kr**	**Xe**
A*	8.957096944* IO^5	8.7265.0990*10^4	6.96664509*104	54249.1966*10^4
a*	13.8638	8.9611	8.3432	7.4007
ß*	-0.1346	-2.8156	-3.0586	-4.1356
B1	14.4828	13.5231	4.5976	7.5157
B2	4.0830	4.3940	12.9250	7.5157
ϵ/k(^{o}K)	42.0093	133.7784	200.2406	292.8551
R_m(^{o}A)	3.091	3.756999	4.011	4.3656

Table 2. Parameters for the SCDY potential

	Ne	**Ar**	**Kr**	**Xe**
A*	8.957096944* IO^5	8.7393327*10^4	6.97353915*10^4	5.44087277*10^4
a*	13.86434671	9.03228328	8.38802216	7.52958289
ß*	-0.12993822	-2.371328323	-2.79611543	-3.390428
c_6	1.21317545	1.0930995	1.06136003	1.00555220
c_8	0.53222749	0.51568309	0.56845577	0.58359858
c_{10}	0.24570703	0.32521242	0.42605480	0.47378306
D	1.36	1.107	1.2080	1.114
$\epsilon/k(^oK)$	42.25	143.235	201.3	282.8
$R_m(^oA)$	3.091	3.756999	4.011	4.3656

Table 3. Spearman correlation coefficient**s**

P-value	**R Double Yukawa SCDY****	**P-value**	**R Double Yukawa HFD-P***	**P-value**	**R long Range SCDY potential***	**P-value**	**R long Range HFD-B potential****	**Row**
0.000	-0.755	0.000	-0.644	0.000	0.962	0.000	0.969	NEO
0.000	-0.777	0.000	-0.783	0.000	0.778	0.000	0.788	XEO
0.000	-0.762	0.000	-0.810	0.000	0.908	0.000	0.974	ARG
0.000	-0.767	0.000	-0.843	0.000	0.868	0.000	0.873	KRI

Spearman correlation coefficient between long range SCDY potential V(x) and X(R/Rm)
** Spearman correlation coefficient between long range HFD-B potential V*(x) and X(R/Rm)
* Spearman correlation coefficient between short and long range HFD-B potential V*(x) and X(R/Rm)
** Spearman correlation coefficient between short and long range SCDY potential V*(x) and X(R/Rm)

CONCLUSIONS

The predictive ability of the potentials considered in this work, with respect to the various properties of xenon, relevant to testing a two-body potential, was summarized that distribution of v(x) parameter in two forms of (HFD-B AND SCDY) potentials was not normal .As a general result, the transport properties can be determined for higher temperatures than those cited in this paper. As explained earlier, analysis of transport properties through a potential model for the intermolecular potential can improve the accuracy and range of validity of potential function. Therefore, this potential must be checked a new and simple pair potential function (soft-core double Yukawa potential) for noble gases by calculation of the transport properties.

REFERENCES

[1] R.A. Aziz, H. Chen, An accurate intermolecular potential for argon, The Journal of Chemical Physics, 67 (1977) 5719-5726.

[2] R. Ahlrichs, R. Penco, G. Scoles, Intermolecular forces in simple systems, Chemical Physics, 19 (1977) 119-130.

[3] R.A. Aziz, M. Slaman, The argon and krypton interatomic potentials

revisited, Molecular Physics, 58 (1986) 679-697.
[4] R.A. Aziz, F.R. McCourt, C.C. Wong, A new determination of the ground state interatomic potential for He2, Molecular Physics, 61 (1987) 1487-1511.
[5] C. Jedrzejek, G. Mansoori, Equation of state of a hard core fluid with a two-Yukawa tail: toward a simple analytic theory, DOI (1980).
[6] S. Foiles, N. Ashcroft, Variational theory of phase separation in binary liquid mixtures, The Journal of Chemical Physics, 75 (1981) 3594-3598.
[7] J. Konior, C. Jedrzejek, Monte Carlo and the WCA type perturbation theory for a hard-core with two-Yukawa-tails fluid, Molecular Physics, 63 (1988) 655-667.
[8] E. Rudisill, P. Cummings, Gibbs ensemble simulation of phase equilibrium in the hard core two-Yukawa fluid model for the Lennard-Jones fluid, Molecular Physics, 68 (1989) 629-635.
[9] Y.V. Kalyuzhnyi, P. Cummings, Phase diagram for the Lennard-Jones fluid modelled by the hard-core Yukawa fluid, Molecular Physics, 87 (1996) 1459-1462.
[10] A. Janzen, R. Aziz, An accurate potential energy curve for helium based on ab initio calculations, The Journal of chemical physics, 107 (1997) 914-919.
[11] R.A. Aziz, A highly accurate interatomic potential for argon, The Journal of chemical physics, 99 (1993) 4518-4525.
[12] R.A. Aziz, M. Slaman, The repulsive wall of the Ar–Ar interatomic potential reexamined, The Journal of chemical physics, 92 (1990) 1030-1035.
[13] J. Hepburn, G. Scoles, R. Penco, A simple but reliable method for the prediction of intermolecular potentials, Chemical Physics Letters, 36 (1975) 451-456.
[14] P. Rol, as cited in RA Aziz, Inert Gases, 34 (1984).
[15] D. Freeman, K. Yoshino, Y. Tanaka, Vacuum ultraviolet absorption spectrum of the van der Waals molecule Xe2. I. Ground state vibrational structure, potential well depth, and shape, The Journal of Chemical Physics, 61 (1974) 4880-4889.
[16] M. Goldblatt, W. Wageman, High temperature viscosity ratios for xenon, Physics of Fluids (1958-1988), 14 (1971) 1024-1025.
[17] R.A. Aziz, M. Slaman, On the Xe-Xe potential energy curve and related properties, Molecular Physics, 57 (1986) 825-840.
[18] R.A. Aziz, M. Slaman, The Ne-Ne interatomic potential revisited, Chemical Physics, 130 (1989) 187-194.