



Original Research Article

Thermal Conductivity and Anisotropy of Intermolecular Potential Energy in Refrigerant Fluids R125, R134a, R12, R14 and R141b

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ABSTRACT

Refrigerant fluids are widely used to reduce temperature in heat transfer systems and study of the thermal conductivity of these fluids is of great importance in design of heat transformers, pumps and refrigeration cycles. The main goal of this work is intended to serve as the assessment of corresponding states correlation of thermal conductivity in terms of pair interaction potential energy for R125, R134a, R12, R14 and R141b refrigerants, considering the anisotropy of potential interactions. In order to present a concise theoretical model for calculation of thermal conductivity, we first applied the extended Chapman-Enskog formalism and calculated the collision integrals and thermal conductivity values for R125, R134a, R12, R14 and R141b dilute fluids and subsequently, made a comparison between the computed results and the most accurate available experimental data. In this respect, the efficiency of intermolecular potential parameters to reproduce thermal conductivity values of R125, R134a, R12, R14 and R141b refrigerants was assessed. In the next step, the effect of non-spherical potential energy functions and the contribution of internal degrees of freedom for the thermal conductivity of the mentioned refrigerants fluids have been formulated and led to more accurate computational results. Finally, we have shown that the present theoretical model provide a good overall account of the experimental thermal conductivity of these compounds, considering the stated uncertainty in the measurements.

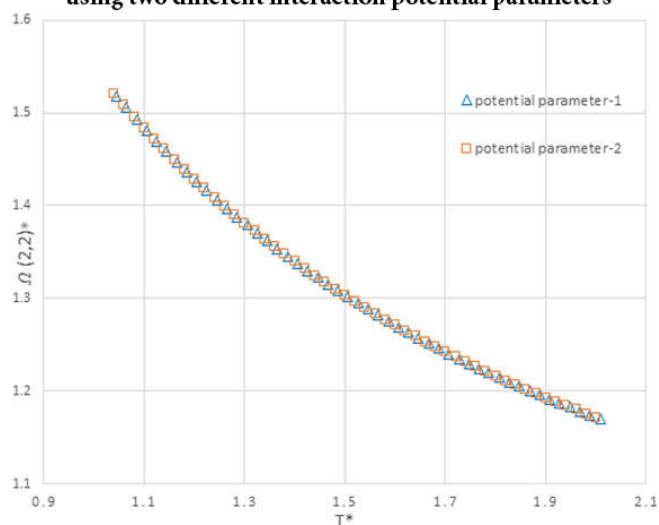
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GRAPHICAL ABSTRACT
The corresponding states behavior of collision integrals using two different interaction potential parameters


1. Introduction

Refrigerants have been recognized as the fluid compounds that can absorb and dissipate heat very well and are widely used in versatile areas of industry, such as refrigerators, air conditioners, chemical industries, and the automotive industry, [1]. Moreover, the environmental aspects of refrigerants are increasingly being taken into consideration to minimize their negative impacts on stratospheric ozone layer and greenhouse gases effect which have provided a better insight into the significance of determination of thermal conductivity in refrigerants.

Intermolecular forces and their consequent energy transfer mechanism have distinguished differences in solid, gas, and liquid phases at the microscopic scale. The thermal conductivity of liquids is usually analyzed for various phenomena, including heat transfer processes and higher thermal conductivity will result in higher heat transport coefficient [2]. A suitable refrigerant should have high thermal conductivity for rapid heat transfer in the evaporators and condensers [3]. Although many scientific and industrial phenomena

require the knowledge of thermal conductivity, the thermal conductivity values especially for refrigerants, are often unreliable and a number of theories based on material properties, including heating capacity, density, etc., have been proposed extensively to interpret this type of transport properties[4]. One of the most profound and concise theories for determination of thermal conductivity is the Chapman-Enskog theory, which is based on solving collision integrals and using the intermolecular interaction potentials. In this route, numerous researches have been carried out to obtain the thermal conductivity of refrigerants with versatile approaches. Papari and coworkers calculated the carbon dioxide system's interaction potential using the inversion technique to obtain thermal conductivity. The accuracy of thermal conductivity was reported to be 3% in the 250K <T< 2000K temperature range [5]. Moghaddasi et al. separately obtained the interaction potential of polyatomic gases, including sulfur hexafluoride [4], carbon tetrafluoride [5] and nitroxide [6], using the inversion technique, and determined transport properties. Percentage error of thermal

conductivity was about 5% to 10% in the 220K <T< 300K temperature range. They also obtained the intermolecular potential of 15 mixtures from 9 environmentally friendly refrigerants, including R227ea, RC318, R125, R134a, R152a, R143a, R32, R236ea, R236f, using the inversion technique, and then calculated the mixture's conductive properties. The measurement accuracy of these mixtures in the 200K<T< 1000K range was reported to be 15% [6].

Mohammad Aghaei et al. determined the intermolecular potential of a number of nitrogen mixtures using the inversion method [7]. They used the Schreiber approach to calculate thermal conductivity at low density [8] and the average absolute deviation (AAD) of thermal conductivity was reported to be around 7%. They also obtained the intermolecular potential of some binary mixtures of equal moles using the inversion technique, and then calculated thermal conductivity of the mixtures. The AAD of thermal conductivity values obtained via the Schreiber method were respectively 4.52%, 7.98%, 12.01%, and 13.7%. In the same year, Sung Bo et al. calculated intermolecular potential using the inversion method. They calculated the mixture's thermal conductivity in the 273.15K to 3273.15K range in low density. Their thermal conductivity measurement accuracy was reported as 5% [9].

Regarding the interaction of molecules with no spherical symmetry, the potential function depends not only on the intermolecular distance but also on the relative orientation of the two molecules. For such molecules, there is an additional contribution to the interaction potential energy of the system called anisotropy, which originates from the internal energies, including vibrational and rotational degrees of freedom. Qualitatively, anisotropy is

interpreted as dependency of interaction energy on the relative orientation of interacting species [10]. It is noteworthy that up to our knowledge, there is no exact quantitative definition that provides a measure for the anisotropic aspects of potential interactions and its effects on transport properties. Hence, in this research we have attempted to investigate the internal degrees of freedom contribution on the thermal conductivity of some widely used refrigerants and formulated the anisotropic effect of potential interactions. It should be mentioned that since in most cases, the experimental measurement of thermal conductivity for refrigerant fluids is a complicated and time-consuming procedure, theoretical modeling in this area has attracted tremendous attractions among experimentalists [11-14].

This research has been intended to obtain an accurate and appropriate theoretical model to calculate the thermal conductivity of R125, R134a, R12, R14 and R141b in low density range. First, the thermal conductivity collision integrals were obtained using the Chapman-Enskog method followed by the contribution of internal degrees of freedom computations, and then they obtained results were compared with the most accurate available experimental data. In the next step, the specific heat capacity values are parameterized using the least squares methods and the Eucken formalism and then accuracy of obtained correlated model was investigated in comparison the experimental thermal conductivity data.

2. Formulation of internal degrees of freedom contribution of thermal conductivity: anisotropic potential energy effect

The kinetic theory of gases investigates the macroscopic properties of gases according to their motion and intermolecular interaction. Many researchers have attempted to develop

kinetic theories, including Boltzmann, who proposed an equation for atom velocity and position distribution function for a nonequilibrium dilute gas. Chapman and Enskog solved this equation, and presented the following results for Boltzmann equation of dilute monoatomic gases [15]:

$$\theta = \pi - 2b \int \frac{r^{-2} dr}{r_m \left(1 - \left(\frac{b^2}{r^2} \right) \left[\frac{2u(r)}{m\omega^2} \right] \right)^{\frac{1}{2}}} \quad (1)$$

$$Q^{(l)}(E) = 2\pi \left[1 - \frac{1+(-)^l}{2(1+l)} \right]^{-1} \int_0^\infty (1 - \cos^l \theta) b db \quad (2)$$

$$\Omega^{(l,s)}(T) = \left[(s+l)! (k_B T)^{s+2} \right]^{-1} \int_0^\infty \left(Q^{(l)}(E) \times e^{\left(\frac{-E}{k_B T} \right)} \right) E^{s+l} dE \quad (3)$$

θ is the dispersion angle, $Q^{(l)}(E)$ is transfer collision level, b is the collision parameter, E is the relative kinetic energy of colliding particles, and ω is the relative velocity of the colliding particles. l and s in Ω represent weight factors related to the molecular collision transfer mechanism.

Transport properties are calculated simply using collision integral values without reduced units [15].

$$\Omega^{*(l,s)} = \Omega^{(l,s)} / \pi \sigma^2 \quad (4)$$

σ is the distance parameter and represents intermolecular distance at zero potential.

The equation used for calculating heat transport of dilute gases is as follows [16]:

$$\lambda = \frac{75}{64} \left(\frac{KT}{\pi m} \right)^{\frac{1}{2}} \frac{f_\lambda}{\sigma^2 \Omega_{(2,2)}^*(T^*)} \quad (5)$$

$$f_\lambda = 1 + \frac{1}{42} (8E^* - 7)^2 \quad (6)$$

where f_λ is the corrective heat transport coefficient, $\Omega^{(2,2)*}$ is the reduced collision integral relative to the hard sphere collision integral, T^* is the reduced temperature equal to $\frac{KT}{\epsilon}$, and σ is the potential distance parameter. Also, E^* is obtained using the following equation [16]:

$$E^* = \frac{\Omega_{(2,3)}^*}{\Omega_{(2,2)}^*} \quad (7)$$

Since the Boltzmann equation only considers binary collisions, results from the theory of transport properties can be used for dilute gases. However, this theory is invalid for high densities with triple collisions.

Najafi et al. presented reduced viscosity collision integrals as corresponding states $\Omega^{(2,2)*}$, which uses Aziz' potential. According to (T^*) , the correlation equation of corresponding states of collision integrals $\Omega^{(2,2)*}$ follows this equation [15]:

$$\Omega^{(2,2)*}(T^*) = \exp \sum_0^6 a_i (\ln \ln T^*)^i \quad (8)$$

The expansion coefficients are as follows:

$$\begin{aligned} a_0 &= 4.369 \times 10^{-1} \pm 7.8 \times 10^{-4} \\ a_1 &= -4.505 \times 10^{-1} \pm 1.3 \times 10^{-3} \\ a_2 &= 5.326 \times 10^{-2} \pm 8.1 \times 10^{-4} \\ a_3 &= 3.519 \times 10^{-2} \pm 9.2 \times 10^{-4} \\ a_4 &= -1.751 \times 10^{-2} \pm 4 \times 10^{-4} \\ a_5 &= 2.772 \times 10^{-3} \pm 7 \times 10^{-5} \\ a_6 &= -1.529 \times 10^{-4} \pm 4.3 \times 10^{-6} \end{aligned}$$

Thermal conductivity is heat transfer occurring due to molecular collision and the metric unit of thermal conductivity is $\frac{W}{m.K}$. In the case of thermal conductivity in the polyatomic gases, the effects of internal degrees of freedom cannot be ignored. In fact, since the internal degrees of freedom of polyatomic molecules involve transporting energy in gases, the Chapman-Enskog theory can only be employed to predict the translational proportion of thermal conductivity, whereas, this transport property depends upon both the translational and the internal contributions to the heat flux. [16]:

$$\lambda^\circ = \lambda_{tr}^\circ + \lambda_{int}^\circ \quad (9)$$

In which inelastic collisions and the exchange of energy between internal degrees of freedom are accounted.

The internal degrees of freedom contribution can be parameterized using the least squares regression methods, based on the following correlation equation:

$$\lambda_{int} = \sum_{i=0}^4 a_i(T)^i \quad (10)$$

For polyatomic fluids since these molecules have rotational and vibrational energies in addition to the kinetic energy of translation of the center of mass, these forms of internal energies may be exchanged in collision. In the other word, to evaluate the effects of internal degrees of freedom on thermal conductivity, Eucken proposed the following equation, considering the heat capacity values [16]:

$$\lambda = \eta \frac{R}{M} \left[\frac{c_v}{R} + \frac{9}{4} \right] \quad (11)$$

According to the Eucken equation, in order to determine thermal conductivity, first, viscosity should be examined using the following Chapman-Enskog equation [15]:

$$\eta^0 = 5 \sqrt{\frac{mkT}{\pi}} \Omega^{(2,2)*} \quad (12)$$

Next, the following mathematical correlation model is used to parameterize heat capacity in terms of temperature, via Eucken's formalism:

$$c_v = \sum_{i=0}^4 a_i(T)^i \quad (13)$$

3. Results and Discussion

3.1. Corresponding states behavior of collision integrals: Interaction potential energy parameters

Thermal conductivity of materials depends on pair molecular potential. To use the paired intermolecular potential function, a specific potential model with the corresponded parameters including $\frac{\epsilon}{k}$ and σ , should be defined. $\frac{\epsilon}{k}$ is the parameter for measuring the energy or depth of a hypothetical potential and σ it is a parameter for measuring the length or diameter of a collision in nm. These parameters are adjustable and the results of calculations performed with several sets of parameters can be analyzed comparatively

with experimental data to find the optimal parameters for the studied fluids.

In this study, we have investigated the accuracy of two sets of intermolecular potential energy parameters in the R12, R14, R125, R134a, and R141b refrigerants to reproduce the thermal conductivity of these refrigerants in the dilute density ranges. It should be mentioned that the aforementioned energy and distance potential parameters have been driven from the inversion of thermophysical properties and quantum chemical approaches which have been reported in Table 1 for R125, R134a, R12, R14 and R141b materials.

Figure 1 gives a comparative presentation for the corresponding states behavior of the computational values of the reduced collision integrals in terms of the reduced temperature for all studied refrigerants.

In this respect, we first converted the temperature to the reduced temperature and then calculated the reduced collision integral as a function of reduced temperature and correlated all calculated data for all refrigerants according to Equation 8. It should be noticed that two abovementioned sets of potential parameters have been employed to evaluate the corresponding states principle for collision integrals.

3.2. Assessment on the internal contribution of thermal conductivity

As mentioned earlier, in order to calculate thermal conductivity of dilute refrigerants as polyatomic fluids, the contribution of internal degrees of freedom should not be neglected. To this end, we first employed a polynomial expansion equation, followed by a parameterization process using the least squares correlation method (Eq. 10).

Table 1. The Interaction potential energy parameters of R125, R134a, R12, R14 and R141b [15,17-20]

Interaction Potential Energy Parameters				
Refrigerant	Set-1		Set-2	
	nm(σ)	$\frac{\epsilon}{k}$ (K)	nm(σ)	$\frac{\epsilon}{k}$ (K)
R125	0.5190	249.00	0.5150	250.00
R134a	0.5067	277.74	0.5187	289.70
R12	0.5275	307.90	0.5186	297.24
R14	0.4543	164.44	0.4035	257.60
R141b	0.5493	370.44	0.5070	421.10

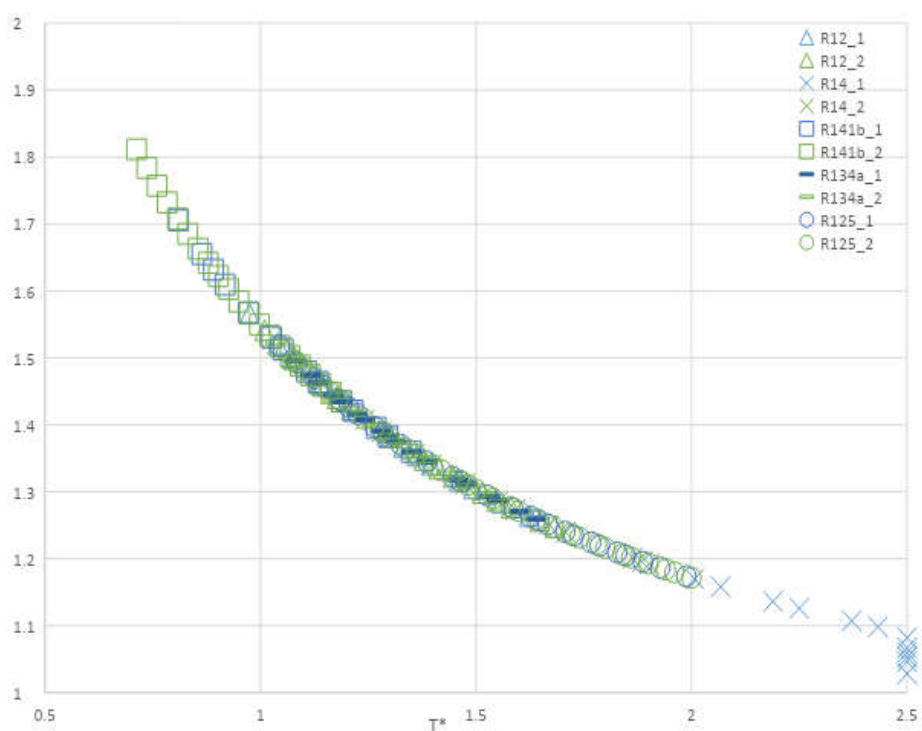


Fig. 1. Corresponding states of reduced thermal conductivity collision integrals using two sets of interaction potential parameters for R125, R134a, R12, R14 and R141b refrigerants

In fact, in this parameterization procedure, we provide a mathematical demonstration of the relationship between the internal contribution of the calculated thermal conductivity data and the corresponded temperature data. In Table 2, the obtained values of adjusted parameters on the basis of our proposed mathematical function of Eq. 10 for the internal contribution of thermal conductivity have been reported for all mentioned refrigerants. It should be noticed that the formulation was performed using two sets of potential energy parameters. In Tables 1-5 in supplementary data section, we have listed the calculated values of translational and internal contribution of thermal conductivity together with the corresponded experimental data, as well as deviation percent, using two sets of interaction potential parameters

through our proposed mathematical model for R125, R134a, R12, R14 and R141b refrigerants. Table 3 shows the obtained average absolute deviation (AADs) of thermal conductivity for two sets of potential parameters in R125, R134a, R12, R14 and R141b refrigerants. Based on the analysis of deviation plots, the lowest AAD values in R125, R134a, R12, R14 and R141b refrigerants are 2.57, 1.29, 0.011, 0.063, and 0.006, respectively. In Figure 2, we have illustrated the percentages deviation of calculated thermal conductivity values, with the experimental values, using the obtained equation of internal degrees of freedom proportion of the total thermal conductivity together with the optimized potential parameters for all surveyed refrigerants.

Table 2. Regression analysis of internal contribution of thermal conductivity in term of temperature, using two sets of interaction potential parameters in R125, R134a, R12, R14 and R141b refrigerants

		a_0	a_1	a_2	a_3	a_4
R125	Potential Parameter-1	0.72	-7.95e-03	3.23e-05	-5.70e-08	3.72e-11
	Potential Parameter-2	0.64	-7.04e-03	2.86e-05	-5.04e-08	3.29e-11
R134a	Potential Parameter-1	-0.22	2.35e-03	-9.11e-06	1.61e-08	-1.06e-11
	Potential Parameter-2	1.28	-1.38e-02	5.52e-05	-9.74e-08	6.41e-11
R12	Potential Parameter-1	8.29e-04	-1.62e-05	1.91e-07	-2.74e-10	1.39e-13
	Potential Parameter-2	8.46e-04	-1.66e-05	1.92e-07	-2.74e-10	1.39e-13
R14	Potential Parameter-1	0.017	-1.97e-04	9.71e-07	-1.57e-09	9.38e-13
	Potential Parameter-2	0.017	-1.90e-04	9.55e-07	-1.56e-09	9.30e-13
R141b	Potential Parameter-1	4.01e-03	-4.16e-05	1.85e-07	-1.79e-11	-3.25e-13
	Potential Parameter-2	3.94e-03	-4.04 e-05	1.83e-07	-1.64e-11	-3.31e-14

Table 3. Average absolute deviation of calculated thermal conductivity values with experimental data, applying two sets of interaction potential parameters in the R125[19-26], R134a[20,21,27], R12[28-32], R14[33-45] and R141b[17,46-58] refrigerants

	Potential Parameter-1	Potential Parameter-2
R125	2.057	2.917
R134a	1.290	3.386
R12	0.022	0.011
R14	0.069	0.063
R141b	0.030	0.006

It can be obviously seen that all obtained deviations are in the range between -0.06 and 0.12 that corroborate the reliability of our

proposed theoretical model in the estimation of thermal conductivity values in these dilute fluids.

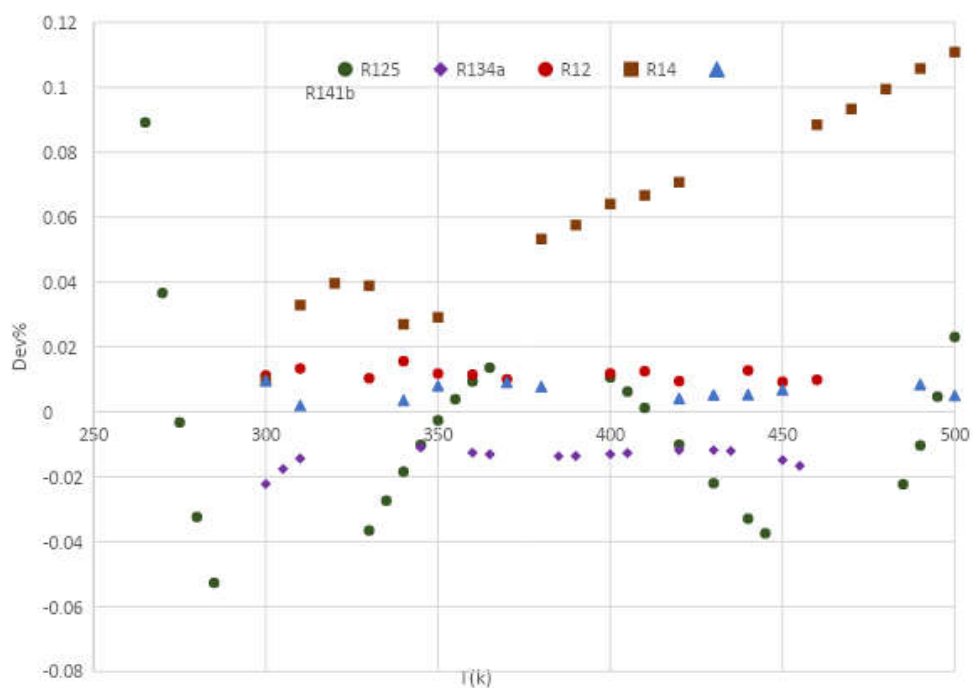


Figure 2. Percent deviation of calculated thermal conductivity based on the formulation of internal degrees of freedom contribution, with the experimental ones, in R125[19-26], R134a[20,21,27], R12[28-32], R14[33-45] and R141b[17,46-58] refrigerants

As discussed earlier, the contribution of internal degrees of freedom in calculation of thermal conductivity of anisotropic potential systems can be investigated via the heat capacity values using Eucken equation, Eq.12. To this end, we correlated the calculated heat

capacity values as a function of temperature, based on Eq.13, using the regression optimization method. In fact, we employed the method of least-squares regression to obtain the most reliable parameters of Eq.13 to the accompanying heat capacity and temperature

data points, considering two potential parameters sets for all surveyed refrigerants, which have been reported in Table 4. In continuation, thermal conductivity values have been calculated based on the obtained viscosity and heat capacity data using Eucken formalism, and then, their percent deviation with the corresponded experimental data was investigated to evaluate the accuracy of each potential energy parameter sets and the heat capacity correlative functions (which have been reported in Tables 6-10 of supplementary data).

Figure 3 depicts the deviation plot of the calculated thermal conductivity values with the

most accurate available experimental data in the temperature range between 250-500 K, considering the anisotropic effect of interactions, via employing Eucken formalism in conjunction with the optimized potential parameters for each refrigerant. As it is clear the obtained deviation percent values are scattered in a reliable range between -0.05% to 0.07%, that is considered as the experimental uncertainty of this property. In Table 5, we have listed the average absolute deviation of calculated thermal conductivity values with the experimental data, considering two sets of potential energy parameters in all refrigerants.

Table 4. The calculated values of parameters for the heat capacity correlation equation, using two sets of interaction potential parameters in R125, R134a, R12, R14 and R141b refrigerants.

		a_0	a_1	a_2	a_3	a_4
R125	Potential Parameter-1	373.50	-2.15	5.91e-03	-7.95e-06	4.27e-09
	Potential Parameter-2	387.30	-2.23	6.11e-03	-8.23e-06	4.36e-09
R134a	Potential Parameter-1	-0.22	-0.22	-4.86e-03	6.59e-06	-3.54e-09
	Potential Parameter-2	-178.70	1.97	-5.24e-03	7.11e-06	-3.82e-09
R12	Potential Parameter-1	-1.75	0.38	-3.28e-04	-1.27e-07	2.34e-10
	Potential Parameter-2	-1.48	0.37	-2.95e-04	-1.55e-07	2.48e-10
R14	Potential Parameter-1	55.57	-0.36	2.42e-03	-4.66e-06	3.04e-09
	Potential Parameter-2	68.18	-0.37	2.58e-03	-5.10e-06	3.38e-09
R141b	Potential Parameter-1	44.17	-0.23	2.10e-03	-2.66e-06	1.25e-09
	Potential Parameter-2	44.59	-0.22	2.17e-03	-2.78e-06	1.32e-09

Table 5. Average absolute deviation of the calculated thermal conductivity, according to Eucken formalism, with the experimental data for two sets of interaction potential parameters in R125[19-26], R134a[20,21,27], R12[28-32], R14[33-45] and R141b[17,46-58] refrigerants.

	Potential Parameter-1	Potential Parameter-2
R125	0.086	0.016
R134a	1.163	0.055
R12	0.010	0.007
R14	0.004	0.065
R141b	0.029	0.026

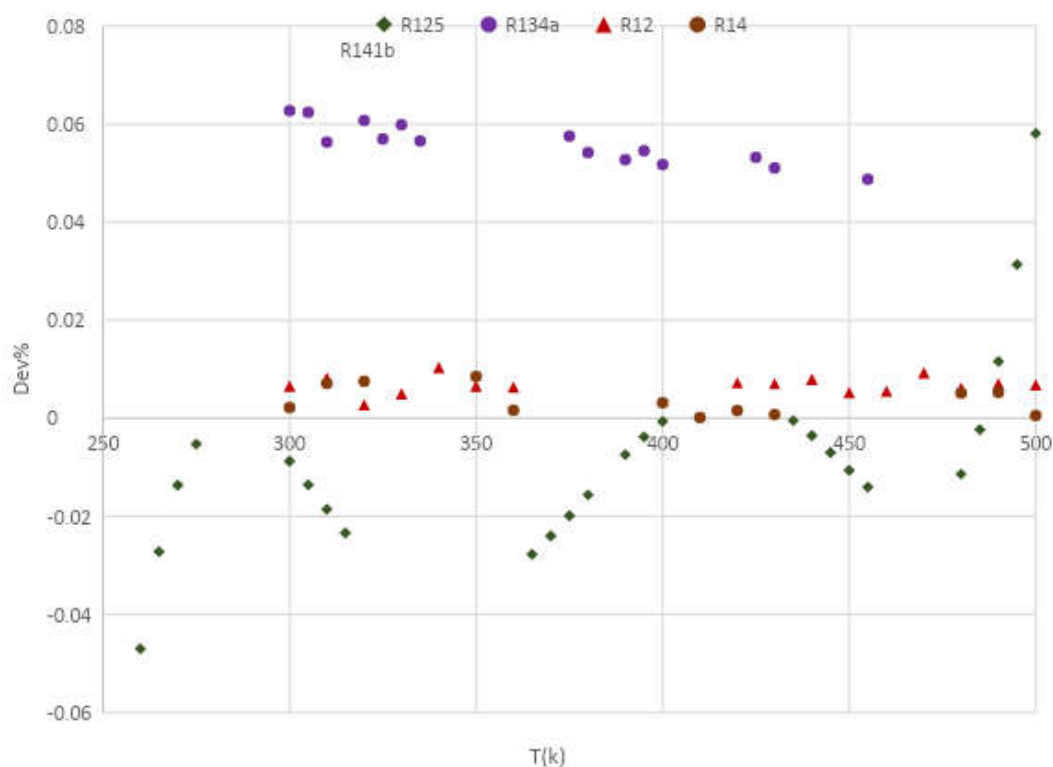


Figure 3. The deviation plot of the calculated thermal conductivity, according to Eucken formalism, with the experimental data for the optimized sets of interaction potential parameters in R125[19-26], R134a[20,21,27], R12[28-32], R14[33-45] and R141b[17,46-58] refrigerants

4. Conclusion

The main goal of this study was concentrated on determining of the thermal conductivity of refrigerant fluids in low density range using statistical thermodynamics formalisms. To this end, a reliable correlative model was presented to determine thermal conductivity values, according to the Chapman-Enskog theory and the Eucken equation, and then the accuracy of our proposed computational model was assessed in comparison with the available experimental data.

In the first stage, the corresponding states of collision integrals were investigated using two sets of intermolecular potential parameters in the R125, R134a, R12, R14 and R141b refrigerants. To extend calculations to thermal conductivity to polyatomic molecules such as our surveyed refrigerants, the theory of transport properties must account for inelastic collisions and the exchange of energy between translational and internal degrees of freedom. Therefore, we determined the translational and internal contribution of thermal conductivity separately and compared the obtained values with the most accurate available experimental data. The internal proportion of thermal conductivity was parameterized according to the least squares regression method. On the basis of our obtained comparative results, we introduced the most accurate potential parameter set to determine the thermal conductivity of each refrigerants at low-density with the following obtained average absolute deviations: 2.57, 1.29, 0.011, 0.063, and 0.006 in R125, R12, R14, and R141b fluids, respectively.

In the next step, based on Eucken approach in thermal conductivity of polyatomic gases, the heat capacity values were parameterized and thermal conductivity of mentioned dilute refrigerants were calculated using two sets of potential parameters of intermolecular

interaction in the R125, R134a, R12, R14 and R141b. The analysis of deviation plots revealed the most accurate sets of intermolecular potential parameters to predict thermal conductivity of studied refrigerants with the following AAD results: 0.069, 0.055, 0.007, 0.004, and 0.026 in R125, R12, R14, and R141b, respectively as it is clear all average absolute deviations are in the experimental uncertainty of this property, validating the reliability of our suggested theoretical model. Hence, we can claim that the comparison of our obtained correlation model with previously reported works that have been performed by the inversion of thermophysical properties clearly substantiates the validity of our proposed method.

Owing to the difficulties associated with the experimental determination of thermal conductivity of fluids and so, the availability of few experimental data, there is a need to search for computational models to supplement the experimental data. Moreover, any such calculation procedure should have a profound statistical mechanical basis such as Chapman-Enskog theory which was widely used in our proposed calculational procedure.

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