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Modeling of Enthalpy Deviation Function of Refrigerants at Low Pressure

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ABSTRACT

In this paper, Enthalpy Deviation Function for refrigerant fluids are modeled in order to evaluate the performance of their correlation function. The studied refrigerants are R11, R123, R124, R134a, R143a, R152a, R141b, R142b, R227ea and R236ea. The studied corresponding state principle is the one suggested by Meng et al. The obtained results show that the correlation equation presented has a good ability to predict the studied thermophysical property of materials over a wide range of temperatures.

Keywords: Correlation function; Virial coefficients; Refrigerants; Enthalpy Deviation Function

Introduction

Refrigeration is a process of cooling or freezing a substance to a temperature lower than that of its surroundings and maintaining the substance in a cold state. Refrigeration can be accomplished by arranging heat transfer from a warm body through processes such as convection or thermal conduction. Refrigerant is a material used in the refrigeration process so that it vaporizes and cools as it passes through the throttling valve. The two main uses of refrigerants are refrigerators/freezers and air conditioners. Refrigerants must have suitable thermodynamic properties, including non-corrosion of mechanical components and non-toxic and flammable. In particular, refrigerants should not deplete the ozone layer and change the climate. For these reasons, some refrigerants that were previously widely used are now very limited in use such as chlorofluorocarbons (CFCs). Given the importance of refrigerants, much research has been done to determine the physicochemical properties and their effects on the environment so far. In this paper, enthalpy deviation function at low pressure for refrigerants fluids are predicted using their virial coefficients based on Corresponding State Principle.

Virial Coefficients

One of the important tools for the correlation and prediction of the thermodynamic properties of gases, liquids, and even solids over a wide range of temperatures and pressures is Equation of State (EOS). One of the oldest models for calculating the thermophysical properties of fluids is the virial equation of state (VEOS), which provides the required information with relatively good accuracy

$$Z = 1 + \sum_{n=2} B_n \rho^{n-1} \quad (1)$$

$$Z = 1 + \sum_{n=2} B_n \rho^{n-1} \quad (2)$$

$$OB_2^+ = \frac{B_2}{RT}$$

$$B_3^+ = (B_3 - B_2^2)/R^2T^2$$

where $Z$is the compressibility factor ($Z = pV_m/RT$), ρ is the density ($\rho = 1/V_m$) and B_n is nth-virial coefficient. It is clear that when the pressure or density becomes zero, the compressibility factor will be one, and this is the ideal gas equation, $Z = 1$, so the virial equation shows the deviation from the ideal state. The virial coefficients are related to intermolecular interactions by exact statistical-mechanical formulae. In this respect, nth-virial coefficient are related to molecular interactions in clusters of n molecules. For example, the second coefficient indicates the interaction between the pair of molecules and, as the same way, the third coefficient to

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the interaction of the three molecules in the cluster, and so on. Thus, the virial coefficients are the connection bridge between microscopic and macroscopic properties and show the non-ideal behavior of real fluids. From this view point, by accurately identifying the virial coefficients and how they depend on temperature and using VEOS, it can be easily to calculate the thermodynamic properties of fluids. Virial coefficients can be obtained using both experimental and theoretical methods.

Among the molecules whose virial coefficients have been studied so far, the virial coefficients of refrigerants have also been investigated due to their widespread industrial use. In this research, we use the Meng's correlation for the second virial coefficient of fluids [1]. Meng developed the well-known Tsonopoulos correlation for second virial coefficients based on the corresponding-states principle for nonpolar gases, polar haloalkanes and other nonhydrogen bonding polar gases. The correlated and developed equation as follows

$$B_r = \frac{BP_c}{RT_c} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) + f^{(2)}(T_r)$$

$$f^{(0)} = 0{,}1445 - \frac{0{,}330}{T_r} - \frac{0{,}1385}{T_r{}^2} - \frac{0{,}0121}{T_r{}^3} - \frac{0{,}000607}{T_r{}^8} \quad (3)$$

$$f^{(1)} = 0{,}0637 + \frac{0{,}331}{T_r{}^2} - \frac{0{,}423}{T_r{}^3} - \frac{0{,}008}{T_r{}^8}$$

$$f^{(2)} = \frac{a}{T_r{}^6}$$

in which, $T_r (= T/T_c)$ is the reduced temperature, P_c and T_c are the critical pressure and critical temperature respectively, ω is the acentric factor and *a* is proposed to be function of the reduced dipole moment μ_r. Table 1 gives their critical properties and other parameters of studied refrigerants.

Table 1: Critical properties and other parameters of Refrigerants

Refrigerant	formula	T_c (K)	P_c (atm)	ρ_c (mol/L)	N	ω	μ_r	a
R11	$CFCl_3$	471.110	43.50001	4.032963	5	0.18875	3.97	0.00614
R123	$CHCl_2CF_3$	456.831	36.1390	3.596418	8	0.28192	31.84	-0.00091
R124	$CHClFCF_3$	395.425	35.76901	4.103316	8	0.28810	49.36	-0.00069
R134a	CF_3CFH_2	374.210	40.0620	5.017053	8	0.32684	121.17	-0.00740
R143a	CF_3CH_3	345.857	37.1180	5.128450	8	0.2615	169.91	-0.01703
R152a	CHF_2CH_3	386.411	44.5769	5.571450	8	0.27521	152.76	-0.01661
R141b	$CFCl_2CH_3$	477.5	41.5690	3.921	8	0.22	77.50	-0.00132
R142b	$CClF_2CH_3$	410.26	40.020	4.438	8	0.232	109.29	-0.00452
R227ea	CF_3CHFCF_3	375.95	29.598	3.41	11	0.354	43.85	0.00245
R236ea	$CF_3CHFCHF_2$	412.44	34.5619	3.70302	11	0.3794	25.90	-0.00078

Enthalpy Deviation Function

Deviation functions in thermodynamics represent the amount of deviation of fluids at different temperatures and pressures from the ideal state. For deviation function of enthalpy on the thermodynamic relations, we have

$$\mathrm{H_m^{id}(T.P) - H_m(T.P)} = \int_0^{\mathrm{P}} \left[\mathrm{T}\left(\frac{\partial \mathrm{V_m}}{\partial \mathrm{T}}\right)_{\mathrm{P}} - \mathrm{V_m} \right] \mathrm{dP} \quad (4)$$

This deviation can be written as the expansion by pressure in which expansion coefficients depend on virial coefficients as follows [2, 3]

$$H_m^{id}(T.P) - H_m(T.P) = \sum_{n=1} b_n P^n$$

$$b_1 = A_0 = T\frac{dB}{dT} - B \quad (5)$$

$$b_2 = \frac{1}{2}A_1 = \frac{1}{2R}\left(\frac{dC}{dT} - 2B\frac{dB}{dT}\right) + \frac{1}{RT}(B^2 - C)$$

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Therefore, non-ideality measurement can be calculated using virial coefficients. It is clear that deviation function of enthalpy is equal to zero when $P = 0$ and of course, at low pressure, second terms onwards can be ignored in the expansion.
In this work using the equations (3) and (5), enthalpy deviation function at low pressure for refrigerant fluids are calculated and modeled using their virial coefficients based on Corresponding State Principle.

Results and Discussion

In this paper, we chose 10 refrigerants R11, R123, R124, R134a, R143a, R152a, R141b, R142b, R227ea and R236ea in order to determine their enthalpy deviation function at low pressure. Figures 1-4 show the calculated deviation function of enthalpy for refrigerants versus temperature in different pressures 0.1, 0.5 and 1.0 atm and the results have been compared with experimental data from NIST [4]. As can be seen, there is a very good match between experimental and theoretical results.
In this regard, average absolute deviation (%AAD) as Eq. (6) were computed and the results are presented in Table 2. As is clear, there is little difference between theoretical and experimental results, and this shows a very good accuracy of the mentioned correlation and modeling in determining the studied thermophysical property that can be calculated through the virial coefficients.

$$\%AAD = \frac{1}{NP}\Sigma\left|\frac{(H_m^{id} - H_m)_{exp} - (H_m^{id} - H_m)_{calc}}{(H_m^{id} - H_m)_{exp}}\right| \times 100 \quad (6)$$

in which NP is the number of data points.

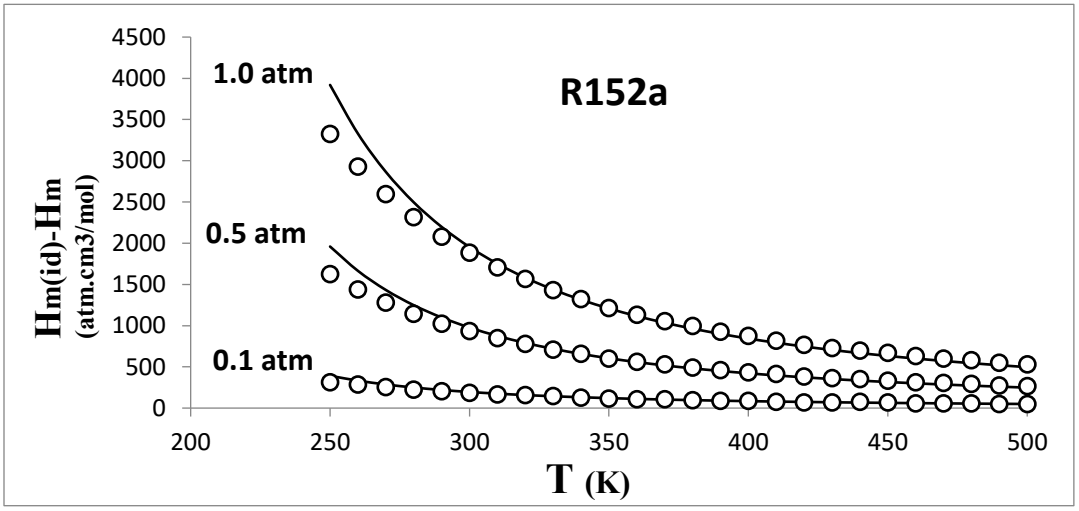


Fig. 1. Deviation function of enthalpy for R152a in different pressures, (—) This work; (○) Experimental data

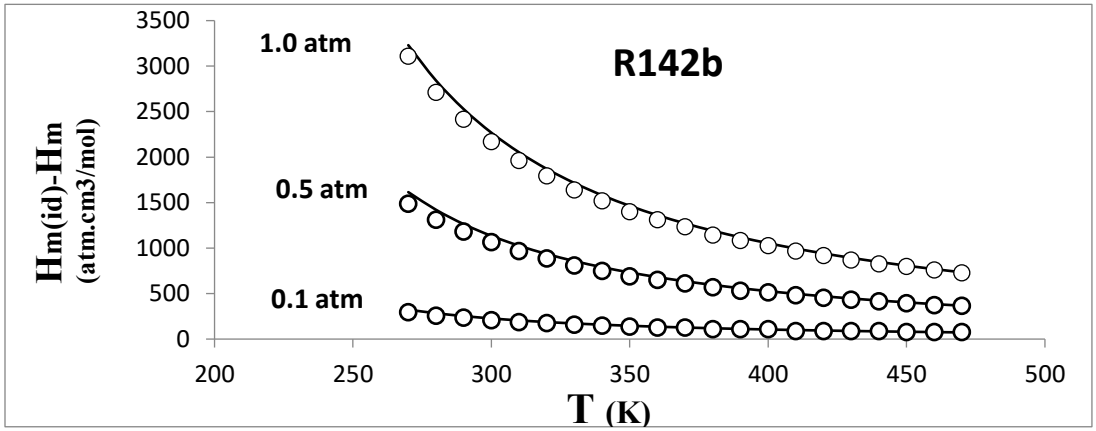


Fig. 2. Deviation function of enthalpy for R142b in different pressures, (—) This work; (○) Experimental data

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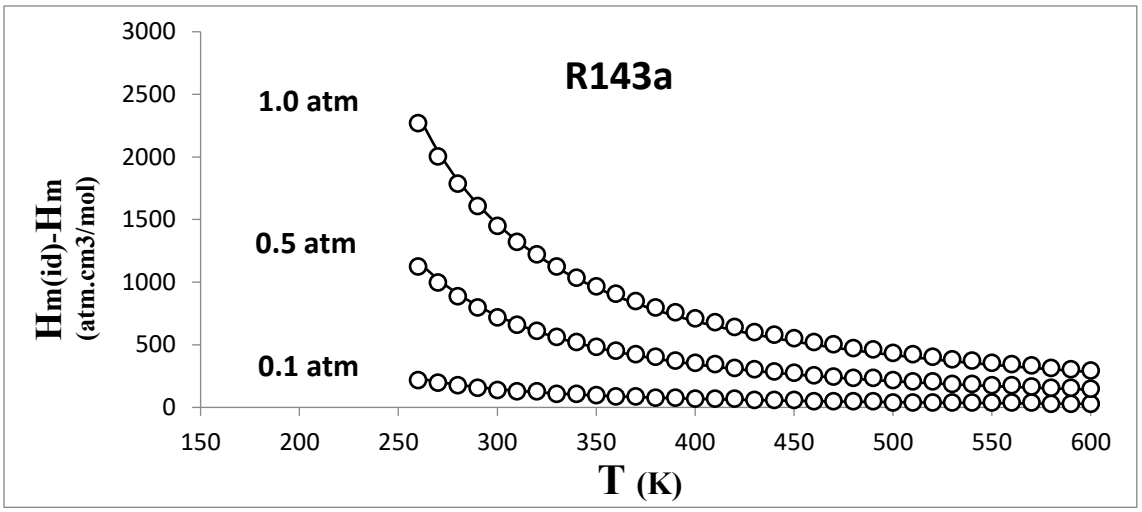


Fig. 3. Deviation function of enthalpy for R143a in different pressures, (—) This work; (○) Experimental data

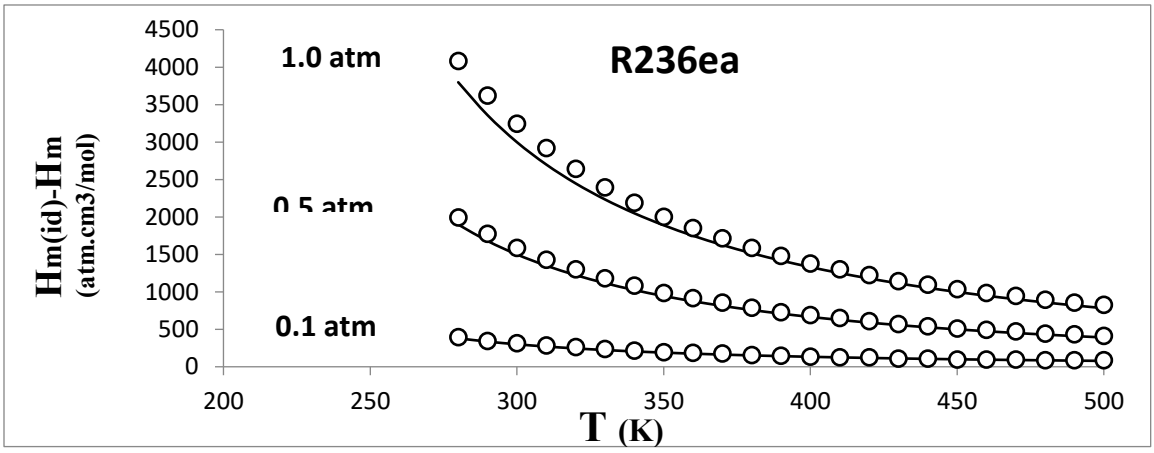


Fig. 4. Deviation function of enthalpy for R236ea in different pressures, (—) This work; (○) Experimental data

Table 2. Temperature range and %AAD in deviation function of studied Refrigerants

Refrigerant	NP	Temp. Range (K)	%AAD		
			$P = 0.1$	$P = 0.5$	$P = 1.0$
R11	31	300-600	3.65	3.97	4.76
R123	30	310-600	3.94	3.24	3.68
R124	21	270-470	2.83	1.08	0.63
R134a	21	250-450	3.13	1.77	1.57
R143a	38	230-600	5.75	3.58	3.43
R152a	26	250-500	5.91	5.43	4.87
R141b	20	310-500	5.50	4.95	4.17
R142b	21	270-470	6.18	4.55	3.30
R227ea	22	260-470	3.38	2.98	3.88
R236ea	23	280-500	5.25	4.47	5.23

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Conclusion

In this paper, Deviation function of enthalpy at low pressure for refrigerants fluids was calculated and modeled in order to evaluate the performance of their correlation equation in low pressure and wide range of temperature. For this purpose, 10 refrigerants were selected and studied. A review of the figures, tables and results shows that the modeling and correlation equation presented has a good ability to predict enthalpy deviation function of materials over a wide range of temperatures.

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