SIMPLE EQUATIONS FOR PREDICTING ENTROPY OF AMMONIA-WATER MIXTURE

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Abstract   This work presents a set of three simple and explicit equations as a function of temperature, pressure, and mass fraction for calculation of the entropy of the ammonia-water mixture in saturated and super heated conditions. They are intended for use in the optimization and second law efficiency of absorption processes. The equations are constructed by the least square method for curve fitting using the valid available data in the literature. The presented equations are valid for the calculation entropy of the saturated liquid and vapor mixture within $-40 \leq T \leq 140$ºC, and the super heated vapor mixture within $0.1 \leq P \leq 10$ MPa and $T_{sat}(P) \leq T \leq 350$ºC, and the entire composition range. The obtained results are compared with available data in graphical and statistical forms, and comparisons reveal that the deviations are ±0.05 kJ/kg.K in the saturated liquid mixture, within -0.04 to $+0.06$ kJ/kg.K in the saturated vapor mixture, and within -0.08 to $+0.02$ kJ/kg.K in the super heated region.

Keywords   Ammonia-Water Mixture, Thermodynamic Properties, Entropy, Equation Fitting

چکیده   در این مقاله سه معادله ساده و صریح برحسب دما، فشار و کسر جرمی برای محاسبه انتروپی مخلوط آمونیاک-آب در شرایط اشباع و بخار فوق گرم ارائه می‌شود. این معادلات برای استفاده در بهینه سازی و بررسی بازدهی بر پایه قانون دوم در سیستم های جذبی در نظر گرفته می‌شود. معادلات بر اساس روش بهینه یابی کمترین مربعات برای برازش منحنی و با بکار بردن نتایج عددی معتبری که اخیراً ارائه شده، بدست آمده است. معادلات ارائه شده برای محاسبه انتروپی مخلوط آمونیاک-آب برای شرایط مایع و بخار اشباع در محدوده ۱۴۰°C ≤ T ≤ ۴۰-، برای بخار فوق گرم در ناحیه ۱۰۰ MPa≥ P ≤ ۰/۱، ۳۵۰°C≥ T ≤ T_sat(P) و غلظت آمونیاک از صفر تا یک (ترکیب مخلوط ازآب خالص تا آمونیاک خالص) معتبراست. نتایج عددی بدست آمده برای انتروپی از معادلات کنونی با نتایج عددی موجود در ادبیات فن بصورت ترسیمی وآماری مقایسه شده و ملاحظه می شود که انحراف برای مخلوط مایع اشباع برابر ۰/۰۵ kJ/kg.K±، برای مخلوط بخار اشباع بین ۰/۰۴ kJ/kg.K- تا ۰/۰۶+ و برای مخلوط بخار فوق گرم بین ۰/۰۸ kJ/kg.K- تا ۰/۰۲+ می‌باشد.

1. INTRODUCTION

The mixture of ammonia-water is of special interest as a working fluid in absorption cycles, refrigeration and waste heat recovery from power generation systems and other purposes. Recently, such mixtures have been proposed as a working fluid in future power generation plants based on the Kalina [1,2] cycle for increased efficiency in power generation, and solar assisted absorped refrigeration cycles [3,4]. Water and ammonia are natural fluids which do not harm the environment. Therefore, they are also considered as an alternative refrigerant to

replace chlorofluorocarbons in some refrigeration applications [5]. For design, simulation and optimization of such machinery, accurate description of the thermodynamic properties of the mixture for a wide range of pressure, temperature, and composition are needed. For this purpose, correlations for calculating thermodynamic properties of binary mixtures have been presented by researchers [6-11].

The mathematical forms of previous correlations are very complicated and require more computational efforts for calculation of the mixture thermodynamic properties. Up to now, for fast

calculation and industrial use, some simple correlations have been presented for determination of the enthalpy of ammonia- water mixture [12,13]. But there is not any simple function for fast calculation of the entropy of ammonia-water mixture.

Note that the entropy is a key thermodynamic property in second law and exergetic analysis of thermal systems. To fill this gap, a set of simple equations for fast calculation of the entropy of ammonia-water mixture has been presented in this paper. Required numerical data for the entropy of ammonia-water mixture to find the best fitted equations can be found in an article "A Helmholtz Free Energy Formulation of the Thermodynamic Properties of the Mixture{ Water + Ammonia}" proposed by R. Tillner-Roth and D. G. Friend [14] in 1998.

As far as the author has found in the literature, the Tillner-Roth and Friend formulation for thermodynamic properties of ammonia-water mixture have the-state-of-the-art accuracy. They used a two-fluid model and two individual equations for water and ammonia, respectively, and correlated the excess properties of the mixture concerned. They correlated the excess property of the Helmholtz free energy as a function of temperature, density, and mole fraction of ammonia. The International Association for the Properties of Water and Steam(IAPWS) [15] have demonstrated the significance of the development work down by Tillner-Roth and Friend for the calculation of power cycles operated with the ammonia-water mixture. From the viewpoint of mathematical structure, their formulation is very complicated and requires more computational time for thermodynamic property calculations and is suitable for scientific use not for simulation and industrial application.

In the present paper, three simple and explicit equations for fast calculation of the entropy of ammonia-water mixture necessary for second law and exergetic investigation of new power plants and absorption cycles have been developed. Equations are presented for calculation of entropy of saturated liquid, saturated vapor, and super heated vapor mixture. Mathematical structure of presented equations are simple and have been expressed as explicit functions in terms of easily measurable variables including temperature,

pressure, and ammonia mass fraction in the mixture. It is particularly well suited for computer-assisted design and optimization. The calculated results have been compared with Tillner-Roth and Friend data in graphical and statistical forms.

2. DERIVATION OF FUNCTIONS

The task of finding suitable equations to represent the entropy of the ammonia-water mixture are: a simple analytical form, fast evaluation, and a reasonable accuracy for simulation and industrial calculations. Initial numeric values for entropy from Tillner-Roth and Friend's equation of state [14] have been taken into consideration and also in the calculations of the present work. Based on this data, the equations with two variables for saturated vapor and liquid conditions and three variables for superheated vapor conditions are constructed in order to calculate the entropy of ammonia-water mixture. The least squares methods are used for finding the best fitted equations. Mathematical procedure for finding the best fitted equation to a given set of points is constructed by minimizing the sum of squares in the residuals of the points from the fitted equation. While there are methodical procedures for fitting equations to data, the process is also an art. The art of intuition is particularly needed in deciding upon the form of the equation, namely, the choice of independent variables to be included and the form in which these variables should appear. There are no fixed rules for knowing variables structure in the equation, but making at least a rough plot of the data will often provide some insight. It is possible, of course, to include all the terms that could possibly be imagined, evaluate the coefficients by the method of least squares, and then eliminate terms that provide little contributions. A requirement for keeping the equation simple is to choose the proper terms (polynomial, exponential, etc.) to include in the equations. Final evaluations of fitted equations are performed by goodness of fitting procedures.

In general, an approximating function of a thermodynamic quantity z depending on two independent variables u and v was sought in the

form of:

$$z(u,v) = \sum_{i=0}^{n} \left[\sum_{j=0}^{m_i} \alpha_{i,j} \psi_j(v) \right] \phi_i(u) \qquad (1)$$

where $\phi_i(u)$ and $\psi_j(v)$ are suitable functions which describe mathematical behavior of data points. For the data points $z(u,v_k)$ with $v_k = $ cte it is assumed that the best fitted equations have the form of:

$$z(u,v_k) = \sum_{i=0}^{n} \beta_i \phi_i(u) \qquad \text{for} \qquad v_k = \text{cte} \qquad (2)$$

where the β constants are calculated from the nonlinear least squares fitting method using respective entropy data from Ref.14. For m pairs of data points the sum of the squares of the offsets and minimization relations can be written as:

$$\sigma_k = \sum_{m} \left[z(u_m, v_k) \Big|_{\text{Ref.14}} - \sum_{i=0}^{n} \beta_i \phi_i(u_m) \right]^2 \qquad (3)$$

$$\frac{\partial \sigma_k}{\partial \beta_i} = 0 \quad , \ i = 0, 1, \dots n \qquad (4)$$

Similar procedures can be followed for the entropy data values for $v_k = $ cte (k = 1,2,…l) and then corresponding β constants are calculated. Next the b constants are fitted as a function in terms of v and could have the form of:

$$b_i = \sum_{j=0}^{m_i} \alpha_{i,j} \psi_j(v) \qquad (5)$$

Finally, the α constants are calculated by applying the nonlinear least squares method again [16]. After mathematical try-out the resulting best fitted equations for fast calculation of the entropy of ammonia-water mixture are arranged as below.

• The entropy of ammonia-water mixture in saturated liquid phase can be expressed in terms of temperature, T, and ammonia mass fraction in the

mixture, x, and have the polynomial form of:

$$s_1(x,T) = \sum_{i=1}^{3} \left(\sum_{j=0}^{5} a_{ij} T^j \right) x^i \qquad (6)$$

range of validity:

$-40 \leq T \leq 140°C$ and $0 \leq x \leq 1$

• The entropy of ammonia-water mixture in saturated vapor phase is expressed as a function of the entropy of saturated vapor of their pure components (i.e. s_{g,H_2O} and s_{g,NH_3}), ammonia mass fraction in the saturated vapor mixture, x, and the departure function for entropy from ideal mixture, $\Delta s^r(x,T)$, and can be written as:

$$s_g(x,T) = x s_{g,NH_3}(T) + (1-x) s_{g,H_2O}(T) -$$
$$\frac{\overline{R}}{M_{mix}} \left[\xi \ln(\xi) + (1-\xi) \ln(1-\xi) \right] + \Delta s^r(x,T) \qquad (7)$$

range of validity:

$-40 \leq T \leq 140°C$ and $0 \leq x \leq 1$

Where ξ and M_{mix}, are the mole fraction of ammonia and molar mass of mixture respectively and are defined as:

$$\xi = \frac{x(M_{H_2O}/M_{NH_3})}{(1-x-x.M_{H_2O}/M_{NH_3})} \qquad (8)$$

$$M_{mix} = (1-\xi)M_{H_2O} + \xi M_{NH_3} \qquad (9)$$

$$R_{mix} = \frac{\overline{R}}{M_{mix}} \qquad (10)$$

The entropy of saturated vapor of pure water and ammonia can be expressed as a function of their temperature, T, in polynomial forms as:

$$s_{g,H_2O}(T) = \sum_{i=0}^{3} a_i T^i \qquad (11)$$

$$s_{g,NH_3}(T) = \sum_{i=0}^{5} b_i T^i \qquad (12)$$

In Equation 7 the third terms on the right hand side indicate the entropy change of mixing for the ideal binary mixture and the fourth term, i.e. $\Delta s^r(x,T)$, is the entropy departure function of the real mixture from an ideal binary mixture. By applying the best fitting technique in the case of the entropy departure function, $\Delta s^r(x,T)$, the rational equation produces the best fit and can be written as:

$$\Delta s^r(x,T) = \left(x \sum_{i=0}^{4} c_i T^i + x^2 \sum_{i=0}^{4} d_i T^i - x^3 \sum_{i=0}^{4} (c_i - d_i) T^i \right) \Big/ (1 - 0.96x) \qquad (13)$$

A rational equation can follow curves that are not essentially polynomial. Graphical investigation of Entropy-Concentration data from Ref. 14 for saturated vapor of ammonia-water mixture (i.e. Figure 2) show that there might be a vertical asymptote near the $x = 1$. So, a suitable rational equation can be eligible for departure function (13) for the best curve fitting. Note that the rational equations are not associated with physical parameters of the data. Instead, they provide a simple and flexible empirical model that we can use for the entropy departure function.

- The entropy of the ammonia-water mixture in superheated vapor phase with considering a gaseous phase as an ideal mixture of real components, which is expressed as a function of the entropy of their pure component in superheated vapor (i.e. s_{H_2O} and s_{NH_3}) and ammonia mass fraction in the mixture, x, which can be written as:

$$s_{mix}(x,P,T) = x s_{NH_3}(P,T) + (1-x) s_{H_2O}(P,T) - \left(\frac{\overline{R}}{M_{mix}} \right) [\xi \ln(\xi) + (1-\xi)\ln(1-\xi)] \qquad (14)$$

range of validity:

$0.1 \le P \le 10\text{MPa}$, $T_{sat}(P) \le T \le 350°C$ and $0 \le x \le 1$

In Equation 14 the entropy of both superheated ammonia vapor, s_{NH_3}, and water vapor, s_{H_2O} in terms of temperature, T, and pressure, P, with using the best fitting technique can be calculated from:

$$s_{NH_3}(P,T) = \sum_{i=0}^{3} a_i (\ln(P))^i + \ln\left[\frac{T+273.15}{T_0+273.15} \right] \sum_{i=0}^{4} b_i P^i +$$

$$\left[\sum_{i=0}^{4} c_i P^i \right](T - T_0) +$$

$$\frac{1}{2}\left[\sum_{i=0}^{4} d_i P^i \right]\left[(T+273.15)^2 - (T_0 - 273.15)^2 \right] \qquad (15)$$

$$s_{H_2O}(P,T) = \sum_{i=0}^{8} a_i P^i + \sum_{i=1}^{4} \left(\sum_{j=0}^{5} b_{ij} P^j \right) T^i \qquad (16)$$

One important motivation in the development of this paper is calculation of the entropy of ammonia-water mixture in different phases which are desirable to be very fast and stable in case simulations of refrigeration systems. The traditional method based on equation of state cannot meet such requirements because of unavoidable iteration calculation. Therefore, Equation 6 for calculating the entropy of saturated liquid mixture, and Equations 11-12 and 15-16 for calculating the entropy of saturated and superheated pure components were developed based on entropy data from ref. 14. For this purpose, fitting equations procedures have been used for the best curve fitting by applying simple functional forms without the help of equations of state and are of completely mathematically nature [17].

As explained previously by Equations 1-5, the calculated respective coefficients of Equations 6, 11-13 and 15-16 by best fitting procedures, which are given in Tables 1-4. The molar gas constant, $\overline{R}$, and the molar mass of ammonia and water used in the mixture model are given as:

$\overline{R} = 8.314471 \quad \text{kJ/kmol.K}$

$M_{NH_3} = 17.03026 \quad \text{kg/kmol}$

$M_{H_2O} = 18.015268 \quad \text{kg/kmol}$

i	j	a_{ij}	i	j	a_{ij}
0	0	$+2.1713\times10^{-2}$	2	0	$+1.2675\times10^{-1}$
0	1	$+1.5910\times10^{-2}$	2	1	$+2.4487\times10^{-2}$
0	2	-5.0981×10^{-5}	2	2	-3.9966×10^{-4}
0	3	$+3.2942\times10^{-7}$	2	3	$+3.5886\times10^{-6}$
0	4	-1.0652×10^{-9}	2	4	-2.3771×10^{-8}
0	5	0	2	5	$+5.5948\times10^{-11}$
1	0	$+7.8243\times10^{-1}$	3	0	$+5.7267\times10^{-1}$
1	1	-6.6703×10^{-3}	3	1	-1.6800×10^{-2}
1	2	$+2.0955\times10^{-4}$	3	2	$+2.1541\times10^{-4}$
1	3	-2.5047×10^{-6}	3	3	-1.5282×10^{-6}
1	4	$+1.7901\times10^{-8}$	3	4	$+1.0844\times10^{-8}$
1	5	-4.6583×10^{-11}	3	5	-2.3703×10^{-11}

TABLE 2. Coefficients of Equations 11-13.

i	a_i	b_i	c_i	d_i
0	$+9.1536\times10^{0}$	$+6.0973\times10^{0}$	$+2.5846\times10^{0}$	-2.2119×10^{0}
1	-2.6289×10^{-2}	-1.2755×10^{-2}	-1.2182×10^{-2}	$+3.3271\times10^{-4}$
2	$+1.0505\times10^{-4}$	$+3.0495\times10^{-5}$	$+1.4634\times10^{-4}$	$+2.4253\times10^{-5}$
3	-2.2033×10^{-7}	-5.0194×10^{-7}	-1.5161×10^{-6}	-3.5006×10^{-7}
4	-	$+9.6447\times10^{-9}$	$+7.6718\times10^{-9}$	$+5.7461\times10^{10}$
5	-	-6.1023×10^{-11}	-	-

TABLE 3. Coefficients of Equation 15.

i	a_i	b_i	c_i	d_i
0	$+1.1575\times10^{1}$	$+1.8427\times10^{0}$	$+1.4240\times10^{-4}$	$+2.1976\times10^{-6}$
1	-7.4094×10^{-1}	$+3.8662\times10^{-3}$	-1.4327×10^{-5}	$+1.3328\times10^{-8}$
2	$+4.2991\times10^{-2}$	-1.1763×10^{-6}	$+4.5920\times10^{-9}$	-4.4223×10^{-12}
3	-2.4442×10^{-3}	$+3.1511\times10^{-10}$	-1.2068×10^{-12}	$+1.1440\times10^{-15}$
4	0	-2.0715×10^{-2}	$+7.9319\times10^{-17}$	-7.5156×10^{-20}

i	a_i	i	j	b_{ij}	i	j	b_{ij}
0	$+7.0751\times10^{0}$	1	0	$+6.5556\times10^{-3}$	3	0	$+1.1559\times10^{-8}$
1	-4.1431×10^{-3}	1	1	$+7.0450\times10^{-6}$	3	1	$+4.4989\times10^{-11}$
2	$+3.8106\times10^{-6}$	1	2	-1.9181×10^{-10}	3	2	-4.5240×10^{-15}
3	-2.5381×10^{-9}	1	3	$+2.6552\times10^{-13}$	3	3	$+2.0802\times10^{-18}$
4	$+9.5459\times10^{-13}$	1	4	-2.3718×10^{-17}	3	4	-1.9338×10^{-22}
5	-2.1065×10^{-16}	1	5	$+1.3882\times10^{-21}$	3	5	$+9.6783\times10^{-27}$
6	$+2.6684\times10^{-20}$	2	0	-9.0999×10^{-6}	4	0	-6.8293×10^{-12}
7	-1.7898×10^{-24}	2	1	-2.6507×10^{-8}	4	1	-2.8631×10^{-14}
8	$+4.9037\times10^{-29}$	2	2	$+1.7636\times10^{-12}$	4	2	$+3.7044\times10^{-18}$
-	-	2	3	-1.1250×10^{-15}	4	3	-1.4148×10^{-21}
-	-	2	4	$+1.0287\times10^{-19}$	4	4	$+1.3312\times10^{-25}$
-	-	2	5	-5.5110×10^{-24}	4	5	-6.3223×10^{-30}

3. DISSCUSION

Presented functions by Equations 6-7 and 14 provide reliable information on the entropy of ammonia-water mixture in saturated liquid, saturated vapor, and superheated vapor for the entire composition range from pure water to pure ammonia. By these equations the entropy of ammonia-water mixture can be explicitly determined with knowing the temperature, pressure, and composition of the mixture. For the saturated phase, presented equations cover the mixture temperature form -40 to +140°C. While, for superheated vapor phase, the presented equation covers the mixture pressure from 0.1 to 10 MPa and temperature from $T_{sat}(P)$ to 350ºC. Although the presented functions are of completely mathematical nature, they allow the determination of the entropy of ammonia water mixture with accuracy acceptable for industrial use. Also, the numerical solution of present equations is simpler than that of the formulation recently adopted by the IAPWS [15] based upon the fundamental equations of state for the Helmholts free energy developed by Tillner-Roth and Friend. The graphical comparison of the calculated entropy of ammonia water mixture in saturated liquid, saturated vapor, and superheated vapor phases with data from Tillner-Roth and Friend [14] are shown in Figures 1-3.

The variations of the entropy of saturated liquid and vapor mixtures in terms of their composition at different temperatures are shown in Figures 1 and 2 respectively. Figure 3 represents the variations of the entropy of super heated vapor mixture in terms of their temperature at various isobars for ammonia mass fractions x = 0.4 and 0.8. As it is evident from graphical inspection of these figures, the comparison of calculated data from the present work and those from Ref. 14 show good conformity. For more evaluation, the goodness-of--fitting are investigated in detail for the fitted equations.

After using graphical methods to evaluate the goodness of fit (i.e. Figures 1-3), it should be examine mathematically. For this purpose the sum
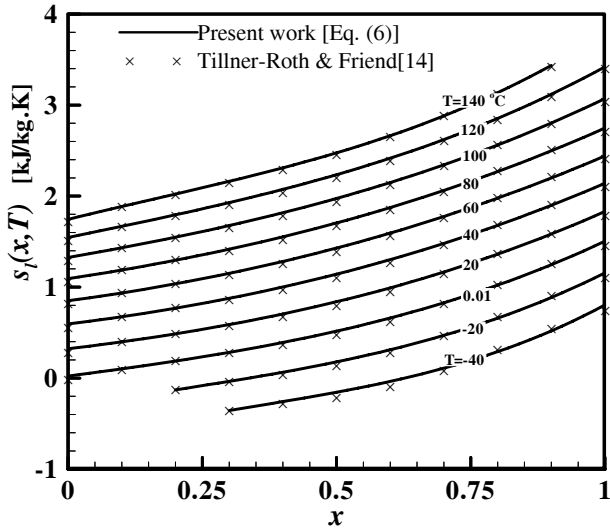
Figure 1. Entropy-Concentration diagram for saturated liquid of ammonia-water mixture at a various temperature.
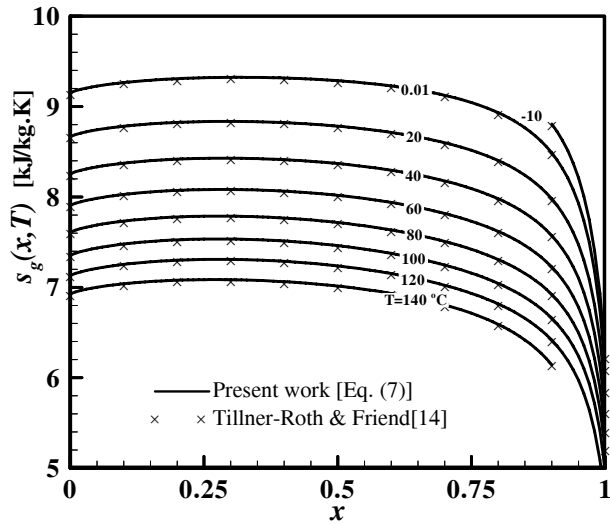

Figure 2. Entropy-Concentration diagram for saturated vapor of ammonia-water mixture at various temperatures.
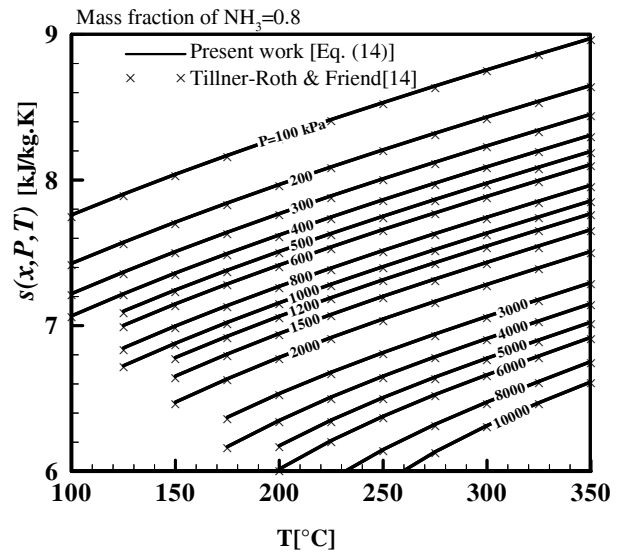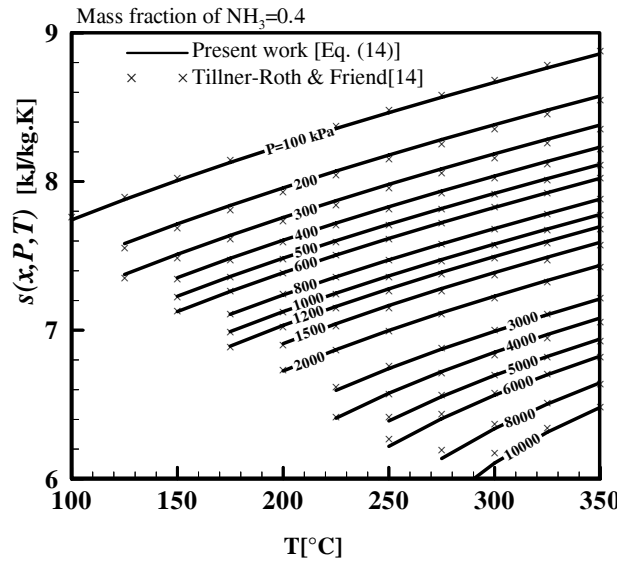

Figure 3. Entropy-Temperature diagram for super heated vapor of ammonia-water mixture at various pressures for ammonia mass fraction 0.4 and 0.8.

of squares due to error (SSE), the mean square error (MSE), and the root mean square error (RMSE) have been used to obtain data from fitted equations. The SSE measures the total deviation of the calculated values from the fit to the values of

Ref. 14 and can be written as:

$$SSE = \sum_{i=1}^{n} (s_{cal,i} - s_{Ref.14,i})^2 \tag{17}$$

A value closer to 0 indicates that the model has a smaller random error component, and that the fit will be more useful for prediction. The RMSE is an estimate of the standard deviation of the random
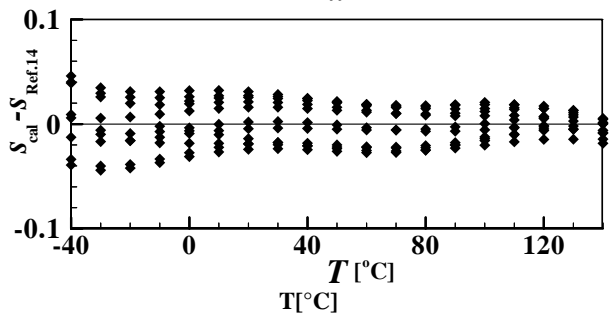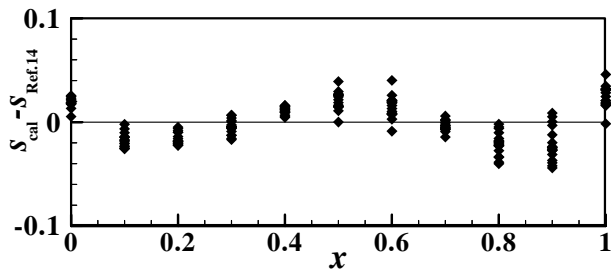
Figure 4. Deviations between the calculated entropy of saturated liquid mixture from Equation 6 and those values calculated from Ref. 14.
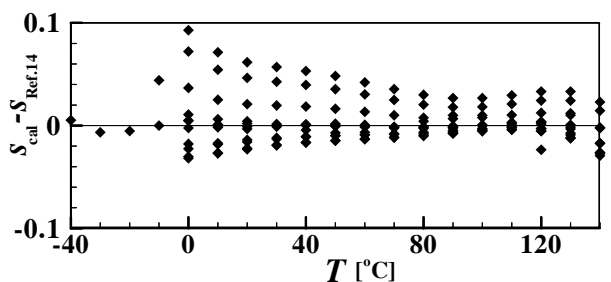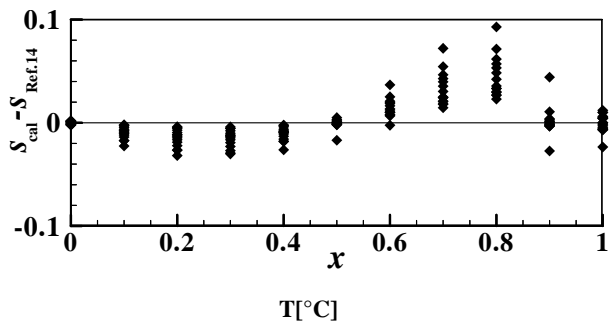

Figure 5. Deviation between the calculated entropy of saturated vapor mixture and those values calculated from Ref. 14.

component in the data, and is defined as:

$$RMSE=(MSE)^{1/2}=\left(\sum_{i=1}^{n}(s_{cal,i}-s_{Ref.14,i})^2\Big/n\right)^{1/2}$$

(18)

Just as with the SSE, a RMSE value closer to 0 indicates a fit that is more useful for prediction. Figures 4-6 shows the deviation between calculated data for the entropy in different phases from the fitted equations and values calculated from helmholtz free energy formulation by Tillner-Roth and Friend [14]. To prove that these assessments are still conservative, Figure 4 shows deviations between the calculated entropy of saturated liquid mixture from Equation 6 and highly accurate results from Ref. 14 which cover the range -40 ≤ T ≤ 140°C and 0 ≤ x ≤ 1. With very few exceptions, all of these data are represented within s_{cal}-$s_{Ref.14}$ = ±0.05 kJ/kg.K. Deviation between the calculated entropy of saturated vapor mixture and those values from Ref. 14 are depicted in Figure 5. Deviations for this entropy remain within -0.04 to +0.06 kJ/kg.K. In Figure 6 entropy of the superheated vapor mixture are plotted for P, T, and x. Most data are represented within -0.08 to +0.02 kJ/kg.K.

The presented equation by Tillner-Roth and Friend [14] is based on a fundamental equation of state for the Helmholtz free energy and the independent variables are volume, temperature, and a mole fraction of ammonia. From the viewpoint of mathematical structure, their complicated formulation is written as a sum of so called 105 polynomial and exponential terms and a set of four nonlinear complicated equations which can be used for phase equilibrium calculations. The calculation speeds of entropy of saturated liquid mixture, for example, from Equation 6 which have only 23 terms, are more than 10000 times faster than those of the Tillner-Roth and Friend equation of state while the mean deviation of the fast calculation is only within s_{cal}-$s_{Ref.14}$ = ±0.05 kJ/kg.K.

The number of data, n, used for the equation fitting, together with the sum of squares due to error, the mean square error, and the root mean square error are summarized in Table 5. These deviations enable one to estimate the accuracy of the equations. The precision of a particular set of data is evident from its band of deviations. The
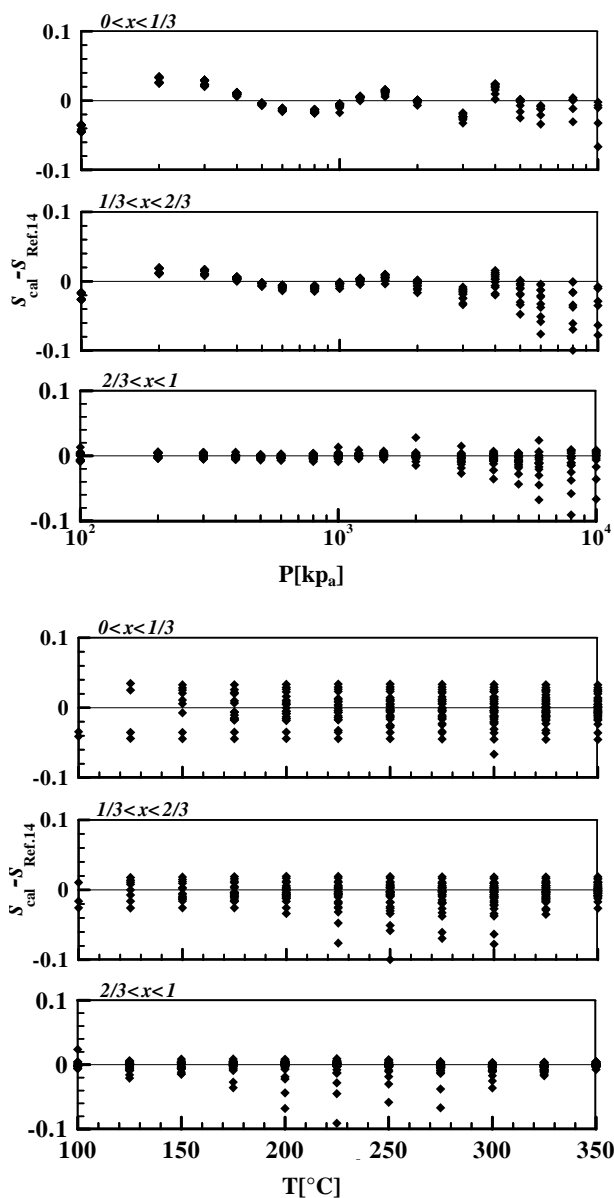
Figure 6. Deviation between the calculated entropy of super heated vapor mixture and those values calculated from Ref. 14.

suitability of the equations can be evaluated and compared using the chi-square method. Because of simplicity and known distributional properties and determination of confidence intervals for initial reference data, the root mean square error of approximation is the preferred inferential approach to assessing the model fit.

TABLE 5. The-Goodness-of-Fit Statistics.

Equation	n	SSE	MSE	RMSE
1	200	0.0853	0.00043	0.0207
2	169	0.0763	0.00045	0.0213
9	867	0.3445	0.00040	0.0199

4. CONCLUSIONS

The fitted equations for the calculation of the entropy of ammonia-water mixture are intended for use in the design, optimization, and second law efficiency of absorption refrigeration cycles. The presented equations have a simple mathematical form, while also having relevant accuracy in comparison with other complicated correlations. The comparison reveals that the deviations for entropy are ±0.05 kJ/kg.K in the saturated liquid mixture, within −0.04 to +0.06 kJ/kg.K in the saturated vapor mixture, and within −0.08 to +0.02 kJ/kg.K in the super heated region. These models can be implemented with ease in all types of language and program that require the calculation of the entropy of ammonia-water mixture. As well as avoiding iterative calculation, the merit of the fast approximation functions consist in their simplicity, which facilitates their incorporation in any computer code.

5. NOMENCLATURE

a,b,c,d	Coefficient
M	Molar Mass
MSE	Mean Square Error
n	Number of Data
P	Pressure [kPa]
R	Gas Constant [kJ/kg.K]
RMSE	Root Mean Square Error
$\overline{R}$	Universal Gas Constan [kJ/kmol.K]
s	Specific Entropy [kJ/kg.K]
SSE	Sum of Square Error
T	Temperature [°C]
x	Liquid or Overall Mass Fraction of Ammonia

| σ | Sum of the Squares of the Offsets |
| ξ | Liquid or Overall Mole Fraction of Ammonia |

Subscripts

cal	Calculated Value from Present Work
g	Saturated Vapor
H_2O	Water (Pure Component)
l	Saturated Liquid
mix	Mixture
NH_3	Ammonia (Pure Component)
r	Residual
Ref. 14	Calculated Value from Reference [14]

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