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Application of the Novel Proportional Nodes Curve Fitting Method to develop Correlations for the Dynamic Viscosity of Ammonia-Water Solution

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Abstract

This study used the 'Proportional Nodes Method,' a novel curve fitting approach to correlate data for dynamic viscosity of ammonia-water solution. The approach integrates polynomial equations, generated at various temperatures, with those calculated at selected mole fraction nodes. These nodes are scaling factors that account for variations in dynamic viscosity at different temperatures at selected mole fractions. The polynomial equations provided a high degree of fitting accuracy, with R^2 values ranging from 0.999663 to 0.99985. The proportional nodes, computed systematically, were integrated into a robust and highly accurate polynomial model. This model exhibited minimal average percentage differences between predicted and actual viscosity values, indicating a high level of predictive accuracy. The Proportional Nodes Method offers a significant contribution to both academic research and industry. It provides a more precise and adaptive model for predicting the dynamic viscosity of ammonia-water solution, which is critical for optimizing and designing various industrial applications, including refrigeration systems.

1.0 Introduction

Data fitting gives the user a mathematical function that best fits to a series of data points while considering the constraints of the data. Curve fitting is a technique that is used to determine a mathematical equation that fits a given set of data points in such a way that the deviation of the points from the equation is minimized. In order to fit two or three-dimensional data, polynomial regression is used. Establishing precise data correlations is a fundamental necessity for effective design, simulation, and optimization of chemical processes. While several correlation-generating methods for data fitting exist, each brings a unique degree of complexity and accuracy.

This study introduces and evaluates the effectiveness of the 'Proportional Nodes Method,' a novel approach for curve fitting. The proportional nodes method was introduced by Mumah (2021). The method is applied to calculate dynamic viscosity of ammonia-water solution. The dynamic viscosity of ammonia-water solution is a key property necessary for design and optimization

purposes of refrigeration systems. Previous studies have employed polynomial equations to describe the viscosity of such solution based on temperature and composition (Kumar and Gardas, 2010). However, these models tend to lack adaptability to temperature changes, potentially leading to inaccuracies in predictive scenarios.

2.0 Methods

In this paper, we used data for dynamic viscosity of ammonia-water solution at various temperatures and mole fractions presented by Conde-Petit (2006) to demonstrate the effectiveness of the Proportional Nodes Method. The approach integrates polynomial equations, generated at all temperatures, with those calculated at selected mole fraction nodes. These nodes are scaling factors that account for variations in dynamic viscosity at different temperatures at selected mole fractions. These proportional nodes act as scaling factors that account for variations in dynamic viscosity at different temperatures for a selected mole fraction. This research addresses a significant gap in the literature by introducing a method that offers more precise and temperature-adaptive predictions for the dynamic viscosity of ammonia-water solution. By achieving R^2 values very close to 1 and minimal differences between predicted and actual values, this study validates the robustness and high reliability of the proposed model, presenting a significant contribution to both the academic community and relevant industries.

3.0 Results

In this study, the dynamic viscosity values of an ammonia-water solution presented by Conde-Petit (2006) were used. They are tabulated in Table 1, which clearly depict a decrease in dynamic viscosity as the temperature increases for various mole fractions. This is a common behavior observed in fluids where an increase in temperature tends to reduce the internal resistance to flow, thereby reducing the viscosity (Lide, 2005).

Table 1. Dynamic Viscosity of Ammonia-Water Solution for various temperatures and mole fraction

T (K)	Mole fraction (-)										
	0	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**0.9**	**1**
273.15	1.749E-03	2.122E-03	2.363E-03	2.301E-03	1.970E-03	1.500E-03	1.027E-03	6.492E-04	3.971E-04	2.478E-04	1.631E-04
283.15	1.328E-03	1.596E-03	1.771E-03	1.728E-03	1.490E-03	1.147E-03	7.982E-04	5.152E-04	3.233E-04	2.073E-04	1.367E-04
293.15	1.012E-03	1.201E-03	1.326E-03	1.297E-03	1.128E-03	8.811E-04	6.258E-04	4.144E-04	2.678E-04	1.769E-04	1.168E-04
303.15	7.819E-04	9.134E-04	1.002E-03	9.834E-04	8.651E-04	6.878E-04	5.004E-04	3.411E-04	2.274E-04	1.547E-04	1.023E-04

Generally, data are not depicted into 2 forms in published papers, but we have chosen to do so for a particular reason. The variation of dynamic viscosity of ammonia-water solution for various mole fractions and temperatures is shown in Figure 1.

The next step is to generate polynomial equations for each curve. There are shown in Figures 2 to5. The polynomial equations and coefficient of determination, R^2, generated by Microsoft Excel as shown in Table 2, provided a high degree of fitting accuracy, as indicated by R^2 values very close to 1. These R^2 values range from 0.999663 to 0.99985, indicating that over 99.96% of the variation in dynamic viscosity can be explained by the variation in the mole fraction of ammonia

in the solution for a given temperature. This high degree of fit is consistent with the previous studies on the viscosity of ammonia-water mixtures (Kumar and Gardas, 2010).

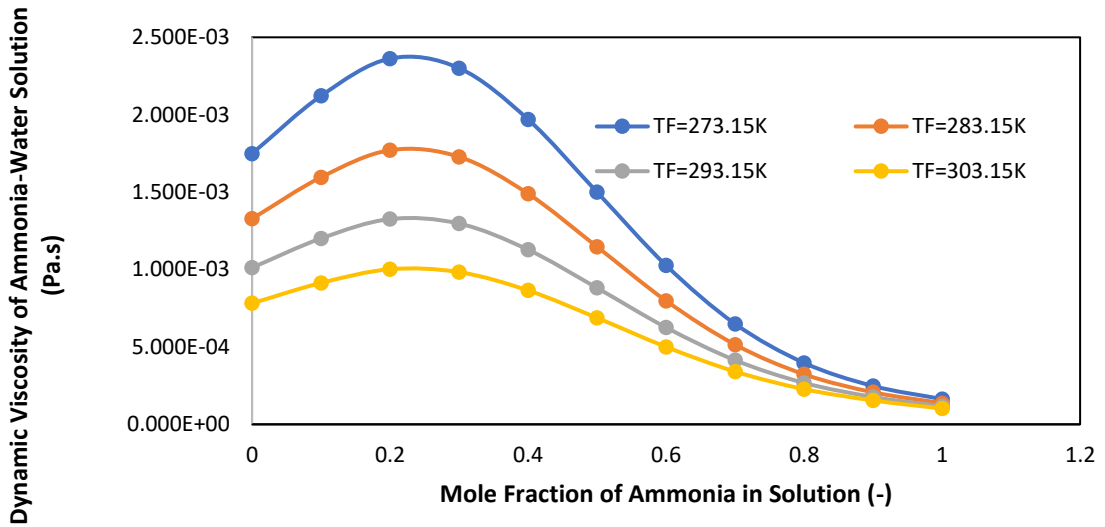

Figure 1. Variation of dynamic viscosity of ammonia-water solution for various mole fraction and temperatures

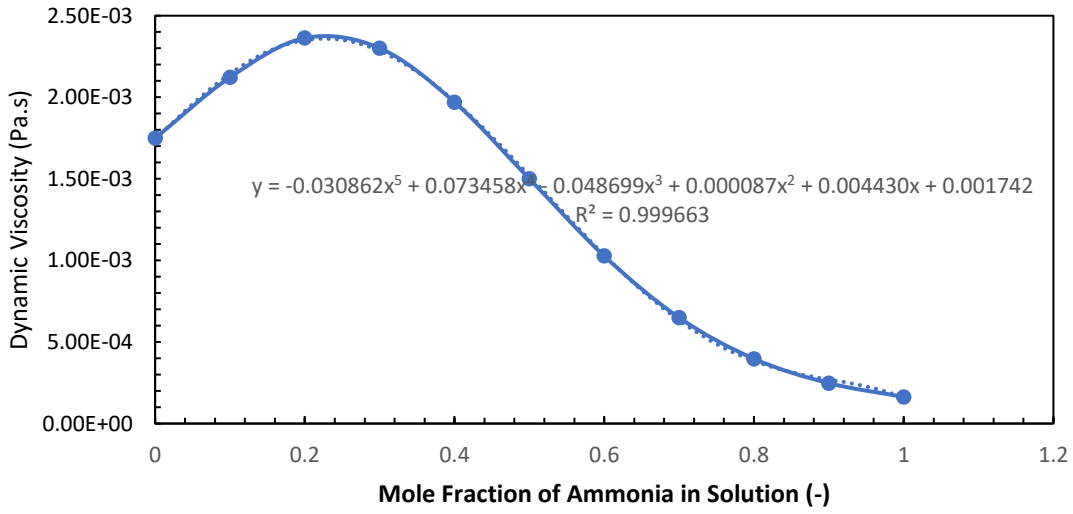

Figure 2. Equation at T = 273.15K

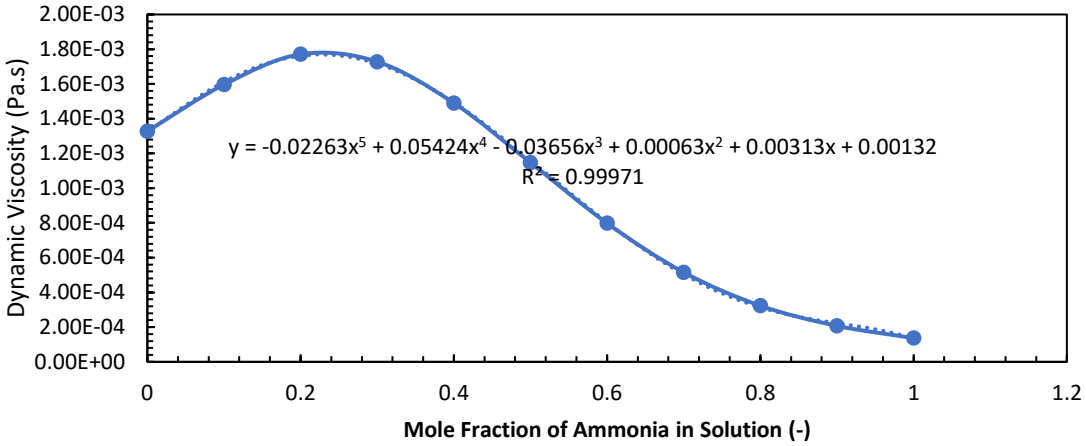

Figure 3. Equation at T = 283.15K

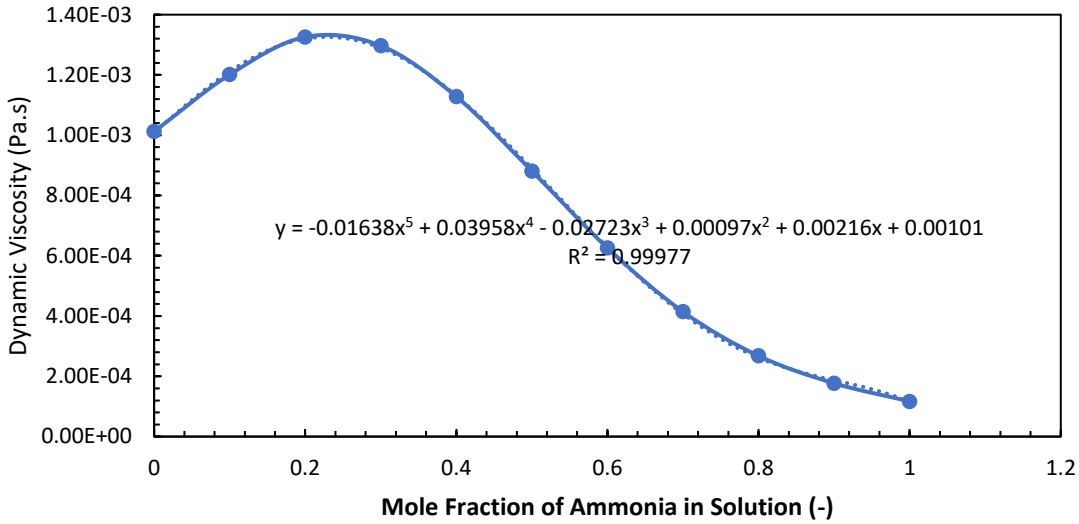

Figure 4. Equation at T = 293.15K

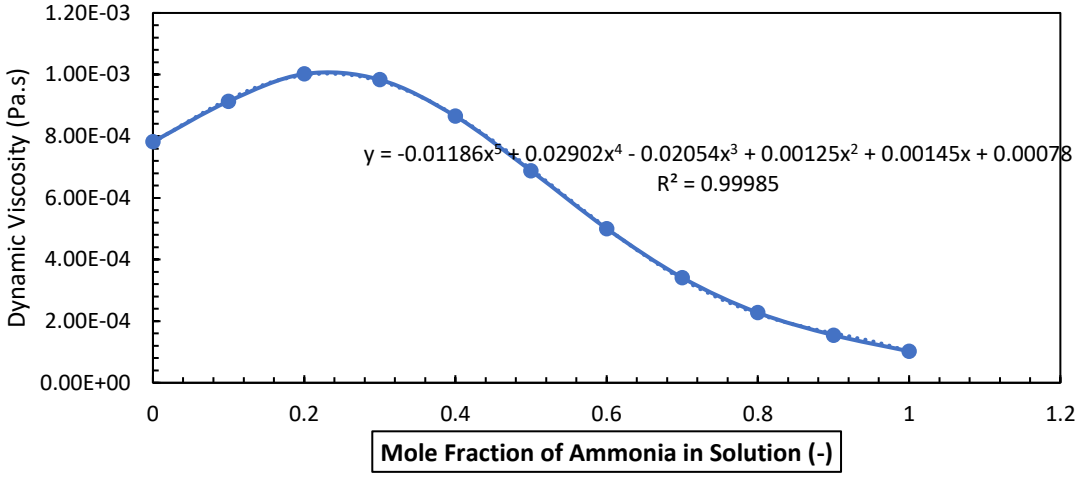

Figure 5. Equation at T = 303.15K

The equations generated for each temperature show that a fifth-order polynomial was used to fit the data. The choice of a fifth-order polynomial, as maintained across different temperatures, is guided by the R^2 values as per the analysis. It is observed that the coefficients of the polynomials change with temperature, which is a logical outcome, considering that temperature is a fundamental factor affecting viscosity.

In this study, the novel concept of 'proportional nodes' was introduced to account for variations in the dynamic viscosity of the ammonia-water solution at different temperatures. To illustrate this method, the mole fraction with the greatest difference in dynamic viscosity was considered, which, for demonstration purposes, was assumed to be at 0.2 moles. That is the reason a graphical illustration is necessary. Generally, a computer program can be generated to determine the exact mole fraction. Table 3 highlights that as temperature increases, the dynamic viscosity decreases consistently, affirming the inverse relationship between temperature and viscosity, commonly observed in fluid dynamics (Holman and Gajda, 2001).

Table 2. Equations and coefficient of determination for dynamic viscosity at each temperature

Mole Fraction of Ammonia in Solution	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
273.15K	1.749E-03	2.122E-03	2.363E-03	2.301E-03	1.970E-03	1.500E-03	1.027E-03	6.492E-04	3.971E-04	2.478E-04	1.631E-04
Generated Equation 1 and R^2 from Microsoft Excel	$\eta = -0.030862x^5 + 0.073458x^4 - 0.048699x^3 + 0.000087x^2 + 0.004430x + 0.001742$ $R^2 = 0.999663$										
283.15K	1.328E-03	1.596E-03	1.771E-03	1.728E-03	1.490E-03	1.147E-03	7.982E-04	5.152E-04	3.233E-04	2.073E-04	1.367E-04
Generated Equation 2 and R^2 from Microsoft Excel	$\eta = -0.02263x^5 + 0.05424x^4 - 0.03656x^3 + 0.00063x^2 + 0.00313x + 0.00132$ $R^2 = 0.99971$										
293.15K	1.012E-03	1.201E-03	1.326E-03	1.297E-03	1.128E-03	8.811E-04	6.258E-04	4.144E-04	2.678E-04	1.769E-04	1.168E-04
Generated Equation 3 and R^2 from Microsoft Excel	$\eta = -0.01638x^5 + 0.03958x^4 - 0.02723x^3 + 0.00097x^2 + 0.00216x + 0.00101$ $R^2 = 0.99977$										
303.15K	7.819E-04	9.134E-04	1.002E-03	9.834E-04	8.651E-04	6.878E-04	5.004E-04	3.411E-04	2.274E-04	1.547E-04	1.023E-04
Generated Equation 4 and R^2 from Microsoft Excel	$\eta = -0.01186x^5 + 0.02902x^4 - 0.02054x^3 + 0.00125x^2 + 0.00145x + 0.00078$ $R^2 = 0.99985$										

Table 3. Dynamic Viscosity Values of Ammonia-water Solution at 0.2 wt fraction for Various Temperatures

Temperature (K) (y Value)	Dynamic Viscosity (Pa.s) (x value)
273.15	2.363E-03
283.15	1.771E-03
293.15	1.326E-03
303.15	1.002E-03

The procedure for calculating the proportional nodes for each temperature is shown in Table 4.

The equation of the proportional nodes is gotten by applying Microsoft Excel. The details are extracted from Table 4 and is shown in Table 5.

Table 4. Procedure for calculating the proportional nodes

Temperature (K) (y value)	Dynamic viscosity (Pa.s) (X value)	Values of proportional nodes (x values)	
273.15=E	2.363E-03 =A	(A-A)/(A-D)	0.0000
283.15=F	1.771E-03 = B	(A-B)/(A-D)	4.35E-01
293.15=G	1.326E-03 = C	(A-C)/(A-D)	7.62E-01
303.15=H	1.002E-03 = D	(A-D)/A-D)	1.0000

Table 5. Proportional nodes data

Temperature (K)	Nodes
273.1500	0.0000
283.1500	4.35E-01
293.1500	7.62E-01
303.1500	1.0000

The Microsoft Excel plot of Table 5.is shown in Figure 6.

$$Nodes = -0.0004925\,T^2 + 0.3170978\,T - 49.8684211 \quad (1)$$
$$R^2 = 0.9999679$$

The proportional nodes were computed using a methodical procedure, as outlined in Table 4. These nodes were then utilized to generate a second-degree polynomial as seen in Equation (1), with an impressive R^2 value of 0.9999679. This polynomial represents how the viscosity changes as the temperature changes for a specific mole fraction, essentially acting as a scaling factor.

We have the equations of each line as shown in Table 2 and the proportional nodes equation. It must be stressed that for this method, the power of the polynomial should be maintained for each temperature. In addition, the Trendline Option (Microsoft Excel) should also be maintained for each process.

Therefore, the dynamic viscosity at any point within the temperature range is given by Equation (2).

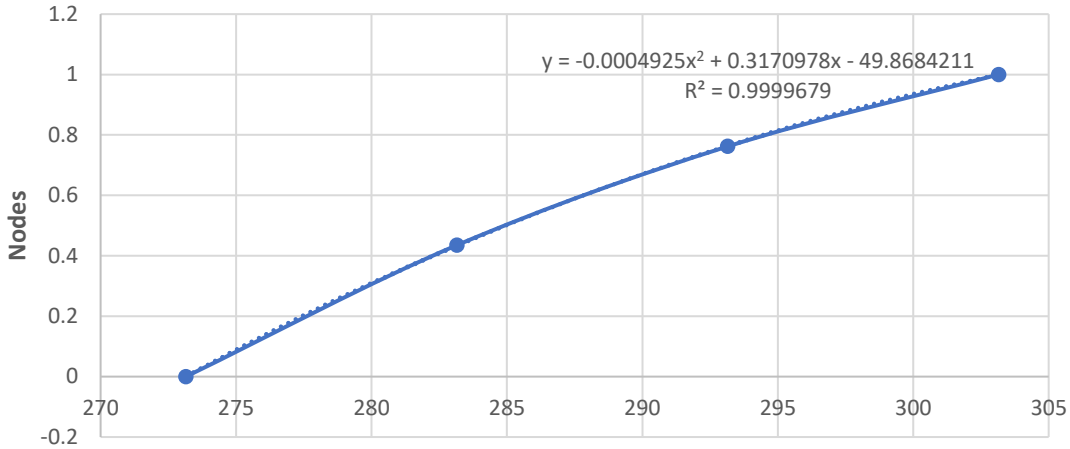

Figure 6. Plot of Nodes data

η (Pa.s)= (Equation of enthalpy at point where nodes =0) - [(Equation of enthalpy at point where nodes =1) – (Equation of enthalpy at point where nodes =0)] x Nodes Equation* (2)

* Please note that the sign is minus and not plus because dynamic viscosity decreases as temperature increases.

The dynamic viscosity of ammonia water solution can be represented by;

$$\eta\ (Pa.s) = y = (-0.030862X^5 + 0.073458X^4 - 0.048699X^3 + 0.000087X^2 + 0.00443X + 0.001742)-((-0.030862X^5 + 0.073458X^4 - 0.048699X^3 + 0.000087X^2 + 0.00443X + 0.001742)-(-0.01186X^5 + 0.02902X^4 - 0.02054X^3 + 0.00125X^2 + 0.00145X + 0.00078))x\ Nodes \quad (3)$$

or

$$\eta\ (Pa.s)=(-0.030862X^5 + 0.073458X^4 - 0.048699X^3 + 0.000087X^2 + 0.00443X + 0.001742)-((-0.030862X^5 + 0.073458X^4 - 0.048699X^3 + 0.000087X^2 + 0.00443X + 0.001742)-(-0.01186X^5 + 0.02902X^4 - 0.02054X^3 + 0.00125X^2 + 0.00145X + 0.00078))\ (-0.0004925T^2 + 0.31709775T - 49.868421081) \quad (4)$$

Simplifying;

$-0.030862x^5 + 0.073458x^4 - 0.048699x^3 + 0.000087x^2 + 0.004430x + 0.001742$
-
There is a bracket here

$-0.030862x^5 + 0.073458x^4 - 0.048699x^3 + 0.000087x^2 + 0.004430x + 0.001742$ - $(-0.01186x^5 + 0.02902x^4 - 0.02054x^3 + 0.00125x^2 + 0.00145x + 0.00078)$	$* (-0.0004925T^2 + 0.31709775T - 49.868421081$

Subtracting first the coefficients in the bracket;

-0.030862	0.073458	-0.048699	0.000087	0.004430	0.001742
-					
-0.01186	0.02902	-0.02054	0.00125	0.00145	0.00078
=					
-0.01900	0.04444	-0.02816	-0.00116	0.00298	0.00096

Thus

$-0.030862x^5 + 0.073458x^4 - 0.048699x^3 + 0.000087x^2 + 0.004430x + 0.001742$
-
There is a bracket here

$-0.01900x^5 + 0.04444x^4 - 0.02816x^3 - 0.00116x^2 + 0.00298x + 0.00096$	$* (-0.0004925T^2 + 0.31709775T - 49.868421081)$

Or;

$$\eta\ (Pa.s) = (-0.030862x^5 + 0.073458x^4 - 0.048699x^3 + 0.000087x^2 + 0.004430x + 0.001742) - (-0.01900x^5 + 0.04444x^4 - 0.02816x^3 - 0.00116x^2 + 0.00298x + 0.00096) * (-0.0004925T^2 + 0.31709775T - 49.868421081) \quad (5)$$

To prove that this equation satisfactory represent the data, the Percentage Difference for values from correlation and actual values, $[(\eta_{actual} - \eta_{calculated})/\eta_{actual}] * 100.0)$, is calculated and from these values, the average percentage difference (Sum of Percentage Difference/Number of Points) calculated. The values are presented in Table 6.

The average percentage difference for the surface (Sum of percentage deviation/Number of points) is calculated from values in Table 6 and presented in Table 7.

The very low average percentage difference for the surface proves that the Equation (5) satisfactorily represents the final expression for calculating the dynamic viscosity of the ammonia-water solution at any given temperature and mole fraction for the selected temperature range

Table 6. Percentage difference for dynamic viscosity values from correlations and actual values

Mole Fraction of ammonia in Ammonia in Solution	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
273.15K	1.749E-03	2.122E-03	2.363E-03	2.301E-03	1.970E-03	1.500E-03	1.027E-03	6.492E-04	3.971E-04	2.478E-04	1.631E-04
Calculated value from Proportional Nodes Method 273.15	0.001741086	0.002143045	0.002348	0.002283	0.001975	0.001517	0.001032	0.000632	0.000383	0.00027	0.000156
Percentage Difference $[(\eta_{actual} - \eta_{calculated})/\eta_{actual}]*100.0$	0.452487	-0.99175	0.634786	0.782269	-0.25381	-1.13333	-0.48685	2.649415	3.550743	-8.95884	4.353158
Generated Equation 1 and R^2 from Excel	$\eta = -0.030862x^5 + 0.073458x^4 - 0.048699x^3 + 0.000087x^2 + 0.004430x + 0.001742$ $R^2 = 0.999663$										
Mole Fraction of Ammonia in Solution	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
283.15K	1.328E-03	1.596E-03	1.771E-03	1.728E-03	1.490E-03	1.147E-03	7.982E-04	5.152E-04	3.233E-04	2.073E-04	1.367E-04
Calculated value from Proportional Nodes Method 283.15K	0.001326272	0.001615056	0.001766	0.00172	0.001497	0.001162	0.000803	0.000504	0.000314	0.000223	0.000132
Percentage Difference $[(\eta_{actual} - \eta_{calculated})/\eta_{actual}]*100.0$	0.13012	-1.19398	0.282326	0.462963	-0.4698	-1.30776	-0.60135	2.173913	2.876585	-7.57356	3.438186
Generated Equation 2 and R^2 from Excel	$\eta = -0.02263x^5 + 0.05424x^4 - 0.03656x^3 + 0.00063x^2 + 0.00313x + 0.00132$ $R^2 = 0.99971$										
Mole Fraction of Ammonia in Solution	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
293.15K	1.012E-03	1.201E-03	1.326E-03	1.297E-03	1.128E-03	8.811E-04	6.258E-04	4.144E-04	2.678E-04	1.769E-04	1.168E-04
Calculated value from Proportional Nodes Method 293.15K	0.001006214	0.001207676	0.001316	0.001286	0.001128	0.000887	0.000627	0.000406	0.000261	0.000186	0.000113
Percentage Difference $[(\eta_{actual} - \eta_{calculated})/\eta_{actual}]*100.0$	0.571739	-0.55587	0.754148	0.848111	0	-0.66962	-0.19175	2.027027	2.539208	-3135.16	3.253425
Generated Equation 3 and R^2 from Excel	$\eta = -0.01638x^5 + 0.03958x^4 - 0.02723x^3 + 0.00097x^2 + 0.00216x + 0.00101$ $R^2 = 0.99977$										
Mole Fraction of Ammonia in Solution	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
303.15K	7.819E-04	9.134E-04	1.002E-03	9.834E-04	8.651E-04	6.878E-04	5.004E-04	3.411E-04	2.274E-04	1.547E-04	1.023E-04
Calculated value from Proportional Nodes Method 303.15K	0.000780914	0.000920907	0.001	0.00098	0.000868	0.000694	0.000503	0.000337	0.000224	0.000161	0.0001
Percentage Difference $[(\eta_{actual} - \eta_{calculated})/\eta_{actual}]*100.0$	0.126103	-0.82187	0.199601	0.345739	-0.33522	-0.90142	-0.51958	1.201994	1.495163	-4.0724	2.248289
Generated Equation 4 and R^2 from Excel	$\eta = -0.01186x^5 + 0.02902x^4 - 0.02054x^3 + 0.00125x^2 + 0.00145x + 0.00078$ $R^2 = 0.99985$										

Table 7. Values of percentage deviation for various temperatures and mole fractions

	Mole Fraction										
Temp (K)	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
273.15	0.452487	-0.99175	0.634786	0.782269	-0.25381	-1.13333	-0.48685	2.649415	3.550743	-8.95884	4.353158
283.15	0.13012	-1.19398	0.282326	0.462963	-0.4698	-1.30776	-0.60135	2.173913	2.876585	-7.57356	3.438186
293.15	0.571739	-0.55587	0.754148	0.848111	0	-0.66962	-0.19175	2.027027	2.539208	-5.14415	3.253425
303.15	0.126103	-0.82187	0.199601	0.345739	-0.33522	-0.90142	-0.51958	1.201994	1.495163	-4.0724	2.248289
	Average percentage difference for the surface ±0.2614293										

4.0 Discussion

Equation (5) satisfactorily represents the correlation for calculating the dynamic viscosity of the ammonia-water solution at any given temperature and mole fraction for the selected temperature range. It incorporates the polynomial equations at the extreme temperatures (273.15K and 303.15K), as well as the proportional nodes equation. The resulting equation is less complex and offers a robust and highly accurate model for predicting the dynamic viscosity of an ammonia-water solution under varying conditions.

The R^2 values associated with each generated equation (as shown in Table 6) are consistently very close to 1, ranging from 0.999663 to 0.99985. This is an indication of the model's exceptional ability to accurately predict the dynamic viscosity of ammonia-water solution under different conditions. These R^2 values further substantiate the validity and reliability of the derived model, reflecting its strong alignment with actual observations (Motulsky and Ransnas, 1987). The inverse relationship between temperature and viscosity, as indicated in our results, is consistent with existing literature on fluid dynamics (Bergman et al., 2011). For example, it has been previously established that an increase in temperature generally corresponds to a decrease in viscosity due to the increased kinetic energy of the molecules, resulting in a reduced internal resistance to flow (Incropera and DeWitt, 2002).

The average percentage differences between the actual and calculated dynamic viscosity values for various mole fractions and temperatures are tabulated in Table 7. These percentage differences are generally very low, affirming the strong correspondence between the model's predictions and the actual measured data. Notably, the deviations are not systematic and fluctuate around zero, indicating no apparent bias in the model's predictions.

5.0 Conclusion

This study provides a comprehensive and highly accurate model for predicting the dynamic viscosity of an ammonia-water solution under varying temperatures and mole fractions. The innovative concept of 'proportional nodes,' introduced in this study, allows for temperature-adaptive predictions, a significant advantage over standard polynomial fitting techniques. The R^2 values, close to 1, and the minimal percentage differences between actual and calculated values at various conditions, demonstrate the model's exceptional predictive capability and reliability. Overall, this study makes a noteworthy contribution to the understanding and calculation of the correlation for dynamic viscosity of ammonia-water mixtures, promising implications for various applications where such data arrangement for mixtures exist.

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