

Generating Correlations for Specific Volume, Enthalpy, and Entropy of Opteon: Utilizing a Novel Data Fitting Method

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Abstract

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 a distinctive method, appropriately named, Proportional Nodes Method, for correlating data on surfaces with two independent variables, focusing on precise estimations of correlations for boundary curves and nodal variation at selected points. The application of the proportional node method results in a lower average percentage deviation than the Chebyshev polynomial method (± 0.978 for the method utilizing Chebyshev polynomials and ± 0.5378 for the Proportional Nodes Method). This novel method exhibits lower complexity and generates correlations with superior simplicity and accuracy. Furthermore, the method effectively develops correlations for three properties—specific volume, enthalpy, and entropy of superheated Opteon, a widely-used refrigerant in automotive air-conditioners. The resulting data shows a satisfactory percentage deviation from the actual data ($< +0.22\%$ for a specific volume, $< +0.124$ for enthalpy and $< +0.125$ for entropy). In addition, correlations have been generated for the saturated vapour. This method's potential extends to developing correlations for non-overlapping data with two independent variables, making it a powerful tool for chemical process optimization.

1. Introduction

Numerous developing countries are progressively entering the automobile manufacturing industry to accelerate development. In this context, automotive air conditioning is no longer a luxury but a necessity. Crucial challenges in this domain involve the reduction of fuel consumption, greenhouse gas emissions, and the space occupied by the air conditioning system in the vehicle. Efficient air-conditioning systems can significantly mitigate fuel consumption and subsequent greenhouse gas emissions. The automotive air conditioning system, particularly the compressor, is a notable auxiliary component contributing to a vehicle's load, significantly affecting fuel consumption and CO₂ emissions. Hence, understanding its impact on fuel economy is vital to vehicle efficiency.

Designing, simulating, and optimizing an automotive air conditioning system involves several parameters, such as environmental conditions (air temperature and humidity), heat loads, refrigerant type, condenser and

evaporator design, vent configurations, temperature and pressure within the system components, and vehicle speed. Each of these factors, time-dependent in nature, must be carefully considered in the design process.

The choice of working fluid or refrigerant is crucial in determining the performance of a vehicle's refrigerating system. The design and simulation of the system depend on the properties of the chosen refrigerant and how accurately these properties can be determined for design and simulation. Recently, Opteon has been identified as a superior refrigerant for automotive air conditioning systems due to its environmentally friendly properties. Environmental concerns, spurred by global warming, have significantly influenced the choice of refrigerants used in all air conditioning systems. Recent studies highlight that a vehicle's A/C system can increase fuel consumption and various emissions considerably. Despite these challenges, it is crucial to design innovative automotive air conditioning systems focusing on efficiency, size, and resilience against harsh environmental conditions.

This paper introduces the "Proportional Nodes Curve Fitting Method," a new approach to developing correlations for surfaces. The method has been employed to create relationships for determining the specific volume, enthalpy, and entropy of Opteon at varying temperatures and pressures, hence demonstrating its utility in enhancing the design accuracy of automotive air conditioning systems.

2. Proportional Nodes Curve Fitting Method

It is generally accepted that the Chebyshev series provides a better way to represent polynomials than do power series for the function.

$$F(x) = \sum_{j=0}^L A_j P_j(x) \tag{1}$$

That is why a Chebyshev polynomial basis often provides a better representation for the polynomials than a power series basis). One advantage of using a Chebyshev polynomial over using the corresponding power term of the same degree to represent data for values $x \in [-1, +1]$ is that $T_j(x)$ oscillates j times between $x = -1$ and $x = +1$. Also, as j increases, the first and last zero crossings for $T_j(x)$ get progressively closer to, but never reach the interval endpoints $x = -1$ and $x = +1$. So, the set of Chebyshev polynomials provides "good coverage" for functions defined on the interval $[-1, +1]$ and the shape of a polynomial is usually better characterized by the coefficients when it is written in its Chebyshev series form than by the corresponding coefficients when it is written in its power series form [3].

However, the same argument cannot be extended to the double Chebyshev series represented by

$$H = \sum_{i=0}^K \sum_{j=0}^L A_{ij} P_i(x_1) P_j(x_2) \tag{2}$$

Because since the values of x_1 and x_2 must be in the range $(-1,1)$, a transformation from their original values is necessary.

To illustrate this, the values of enthalpies of ammonia-water solution from data provided by Macriss et al. [4] were used to calculate an appropriate surface equation. To calculate the coefficients of the double Chebyshev series of the first kind, use was made of the numerical algorithms group (NAG) subroutines [5]. The standard convention followed by this subroutine is that coefficients in the expansion in Equation (2) which have either i or j zero, are written as $0.5A_{ij}$ instead of simply A_{ij} and the coefficient with both i and $j =$ zero is written as $0.25A_{00}$. It should be noted that the maximum and minimum values are the endpoints of the ranges and when using a particular set of coefficients only values within such ranges should be applied. The process to calculate the enthalpy values for an ammonia-water solution is presented below.

Table 1 Coefficients for calculating enthalpy of ammonia-water solution using Chebyshev polynomials

For temperature range $272.03449K \leq T < 360.92778K$ and NH_3 percentage mass fraction $0.0wt\% \leq x \leq 100.0wt\%$					
$A(1)$	$A(2)$	$A(3)$	$A(4)$	$A(5)$	$A(6)$
$3.2796x10^{+02}$	$4.1765x10^{+02}$	$7.2486x10^{+00}$	$1.4096x10^{+00}$	$1.3842x10^{+00}$	$8.0727x10^{-01}$
$A(7)$	$A(8)$	$A(9)$	$A(10)$	$A(11)$	$A(12)$
$3.6984x10^{+01}$	$1.8083x10^{+01}$	$3.7172x10^{+00}$	$1.3878x10^{+00}$	$5.7801x10^{-01}$	$2.6093x10^{-01}$
$A(13)$	$A(14)$	$A(15)$	$A(16)$	$A(17)$	$A(18)$
$2.5064x10^{+02}$	$-1.4995x10^{+00}$	$1.4144x10^{+00}$	$1.2629x10^{+00}$	$4.5639x10^{-01}$	$1.2939x10^{-01}$
$A(19)$	$A(20)$	$A(21)$	$A(22)$	$A(23)$	$A(24)$
$-6.7469x10^{+00}$	$3.2120x10^{+00}$	$1.3634x10^{+00}$	$4.7048x10^{-01}$	$4.8789x10^{-01}$	$3.9950x10^{-01}$
$A(25)$	$A(26)$	$A(27)$	$A(28)$	$A(29)$	$A(30)$

$-1.7843 \times 10^{+01}$	-2.8775×10^{-01}	2.9878×10^{-01}	2.9766×10^{-01}	2.1430×10^{-01}	2.3201×10^{-01}
A(31)	A(32)	A(33)	A(34)	A(35)	A(36)
$6.2351 \times 10^{+00}$	9.4842×10^{-01}	4.9746×10^{-01}	5.2922×10^{-01}	5.8257×10^{-01}	3.2683×10^{-01}
A(37)	A(38)	A(39)	A(40)	A(41)	A(42)
$2.4057 \times 10^{+00}$	$1.4490 \times 10^{+00}$	6.9218×10^{-01}	4.1905×10^{-01}	4.7021×10^{-01}	2.9575×10^{-01}

The derivation of the enthalpy of ammonia-water solution using Chebyshev polynomials is shown in the steps presented in sections 2.1 and 2.2)

2.1 Establishment of Parameters

For temperature range: $272.03449 \leq T < 360.92778 \text{ K}$ and ammonia percentage mass fraction $0.0 \text{ wt}\% \leq x \leq 100.0 \text{ wt}\%$, Table 1 provides 42 coefficients, A(1) to A(42), which are constants for a specific temperature range and ammonia fraction provided. Equation (3) and (4) present the transformation temperature and percentage mass fraction, U and V, respectively:

$$U = \frac{2.0T - (360.927778 + 272.038888)}{360.927778 - 272.038888} \quad (3)$$

$$V = \frac{2.0PC - 100}{100} \quad (4)$$

Using U, the X-values are computed as:

$$X_1 = \cos(\arccos U) \quad (5)$$

$$X_2 = \cos(2.0 \arccos U) \quad (6)$$

$$X_3 = \cos(3.0 \arccos U) \quad (7)$$

$$X_4 = \cos(4.0 \arccos U) \quad (8)$$

Using V, the Y-values are computed as:

$$Y_1 = \cos(\arccos V) \quad (9)$$

$$Y_2 = \cos(2.0 \arccos V) \quad (10)$$

$$Y_3 = \cos(3.0 \arccos V) \quad (11)$$

$$Y_4 = \cos(4.0 \arccos V) \quad (12)$$

$$Y_5 = \cos(5.0 \arccos V) \quad (13)$$

$$Z = 1.0 \quad (14)$$

From Y_1 to Y_5 using similar cosine transformations as the X-values.

2.2 Computations of Enthalpy of Ammonia-Water Solution Using Coefficients and Parameters

With coefficients A(1) to A(42) shown in Table 1 and the calculated X and Y values, equations A to G are derived as:

$$A = 0.25(Z)A(1) + 0.5A(2)X_1 + 0.5A(3)X_2 + 0.5A(4)X_3 + 0.5A(5)X_4 + 0.5A(6)X_5 \quad (15)$$

$$B = Y_1(0.5(Z)A(7) + A(8)X_1 + A(9)X_2 + A(10)X_3 + A(11)X_4 + A(12)X_5) \quad (16)$$

$$C = Y_2(0.5(Z)A(13) + A(14)X_1 + A(15)X_2 + A(16)X_3 + A(17)X_4 + A(18)X_5) \quad (17)$$

$$D = Y_3(0.5(Z)A(19) + A(20)X_1 + A(21)X_2 + A(22)X_3 + A(23)X_4 + A(24)X_5) \quad (18)$$

$$E = Y_4(0.5(Z)A(25) + A(26)X_1 + A(27)X_2 + A(28)X_3 + A(29)X_4 + A(30)X_5) \quad (19)$$

$$F = Y_5(0.5(Z)A(31) + A(32)X_1 + A(33)X_2 + A(34)X_3 + A(35)X_4 + A(36)X_5) \quad (20)$$

$$G = Y_6(0.5(Z)A(37) + A(38)X_1 + A(39)X_2 + A(40)X_3 + A(41)X_4 + A(42)X_5) \quad (21)$$

$$H_1 = A + B + C + D + E + F + G \quad (\% \text{ deviation} = \pm 0.978) \quad (24)$$

The average percentage deviation of the derived enthalpy from actual data presented by Macriss et al. is $\pm 0.978\%$.

3. Method for Correlations Generation

The Proportional Nodes Method was employed to derive a singular equation correlating the enthalpy of ammonia-water solution, as reported by Macriss et al (1964) within the temperature range of 273.15 K to 353.15 K. Table 2 showcases the enthalpy (kJ/kg) against varying concentrations of ammonia in the ammonia-water solution. The table establishes a relationship between temperature, represented in °C, and the ammonia concentration, given as weight percentages, ranging from 0.0 to 100.0 wt. %.

Table 2 Enthalpy of ammonia-water solution (kJ/kg)

T °C	Concentration of ammonia in ammonia-water solution (Wt. %)										
	0.0	10.0	20.0	30.0	40.0	50.0	60.0	70.0	80.0	90.0	100.0
273.15	0.0	-78.1582	-153.869	-213.083	-247.659	-254.739	-235.18	-195.646	-139.87	-73.76	.0000
283.15	41.7575	-35.661	-110.732	-169.323	-203.292	-209.843	-190.53	-149.921	-93.864	-27.429	46.416
293.15	83.5793	7.4289	-67.0239	-125.105	-158.529	-164.52	-144.66	-103.497	-46.909	19.7389	93.418
303.15	125.4576	51.2286	-21.9246	-79.5219	-112.728	-118.276	-97.675	-55.8394	.8776	67.2383	141.0732
315.15	167.3867	95.4158	24.1818	-32.7687	-65.9047	-71.1427	-49.8034	-7.3235	49.2770	115.1723	189.4842
323.15	209.3632	139.5391	70.4100	14.4206	-18.4622	-23.4771	-1.6450	41.3719	98.1312	163.9905	238.7873
333.15	251.3856	183.3273	116.0783	61.3432	29.0685	24.2785	46.3285	89.8681	147.5133	214.2274	289.1536
343.15	293.4547	226.9985	161.4135	107.8953	76.2957	71.8268	94.2586	138.6905	197.8959	266.2408	340.7888
353.15	335.5736	271.5703	208.2552	155.1415	123.2303	119.2488	143.3902	189.8730	250.189	319.9510	399.5855

A plot of the data is necessary for this method. This data can be represented as shown in Figure 1.

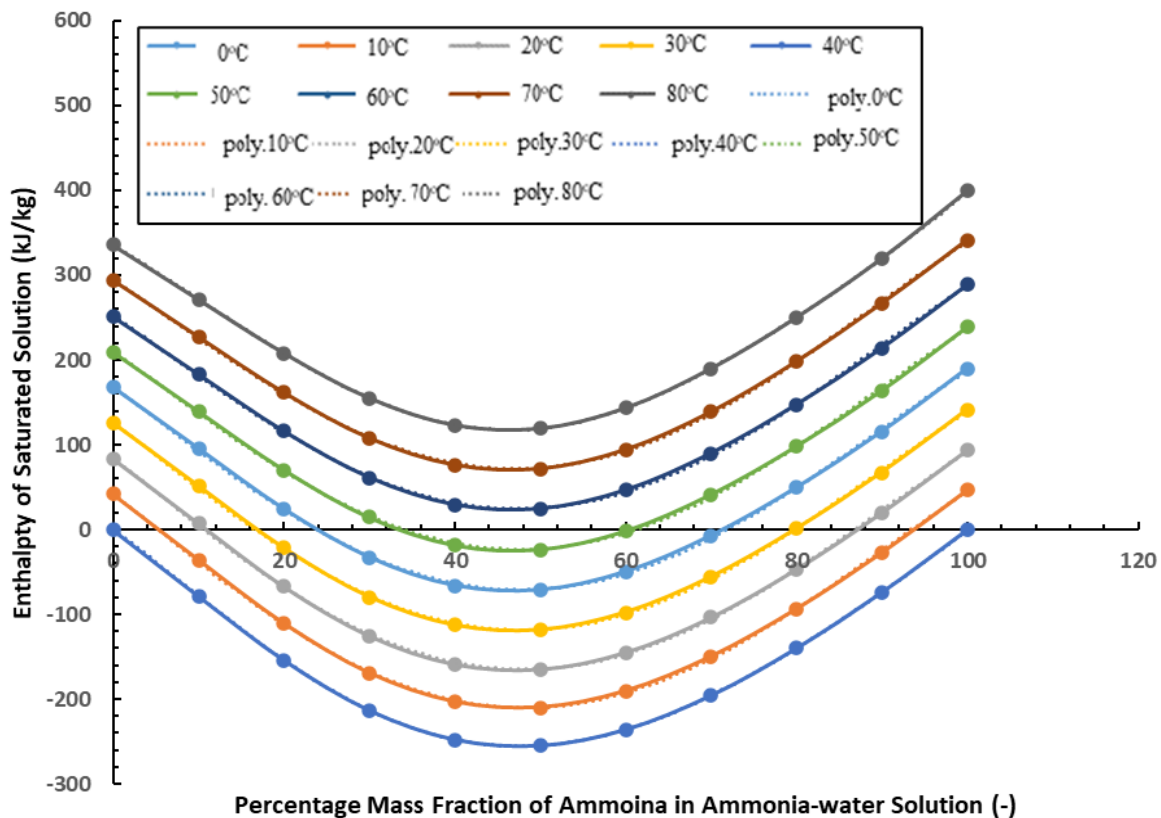


Fig. 1 Variation of Enthalpy of ammonia-water solution for various percentage mass fraction and temperatures

To further elucidate the data in Table 2, a graphical representation is paramount. Hence, the data from Table 2 has been illustrated in Figure 1. Such visualization is pivotal, especially when employing the Proportional Nodes Method, as it aids in discerning the mass fraction where the maximum difference in enthalpy exists across the entire temperature spectrum. Scrutinizing Figure 1 reveals that this maximal spread is evident at approximately 100.0 wt %. Although the disparity in enthalpy is not overtly discernible in the current figure, it's noteworthy that when variations in spread across weight percentages are profound, computerization can assist in accurately pinpointing the exact concentration where the maximum spread arises.

The enthalpy correlations of the ammonia-water solution across various temperatures, as provided in Table 3, are polynomial equations with a fourth-degree power term as the highest order. Each of these correlations is supported by a high coefficient of determination (R^2) ranging from 0.99938749 to 0.99963307, suggesting a very good fit of the data.

Table 3 Correlation of enthalpy for ammonia-water solution for various temperatures

T (K)	Equation of saturated enthalpy (kJ/kg) and coefficient of determination at each temperature
273.15	$H = -0.00001108x^4 + 0.00204055x^3 - 0.01044078x^2 - 8.31398994x + 1.39561958$; $R^2 = 0.99958045$
283.15	$H = -0.00001107x^4 + 0.00203831x^3 - 0.01052219x^2 - 8.24243298x + 43.16174406$; $R^2 = 0.99957946$
293.15	$H = -0.00001133x^4 + 0.00208797x^3 - 0.01385550x^2 - 8.09955034x + 85.01857972$; $R^2 = 0.99956644$
303.15	$H = -0.00001169x^4 + 0.00216637x^3 - 0.01991402x^2 - 7.85679173x + 126.93420420$; $R^2 = 0.99949195$
313.15	$H = -0.00001202x^4 + 0.00224577x^3 - 0.02695787x^2 - 7.55103479x + 168.85774266$; $R^2 = 0.99938749$
323.15	$H = -0.00001226x^4 + 0.00230944x^3 - 0.03339303x^2 - 7.23911668x + 210.74380350$; $R^2 = 0.99935122$
333.15	$H = -0.00001246x^4 + 0.00236717x^3 - 0.03912627x^2 - 6.95245637x + 252.57648042$; $R^2 = 0.99946227$
343.15	$H = -0.00001291x^4 + 0.00247074x^3 - 0.04691931x^2 - 6.65169400x + 294.39386224$; $R^2 = 0.99963307$
353.15	$H = -0.00001317x^4 + 0.00256076x^3 - 0.05514505x^2 - 6.31602523x + 336.55414266$; $R^2 = 0.99939592$

The process of deriving proportional nodes is particularly vital in understanding the variances in enthalpies across the temperature spectrum. As depicted in Figure 1, the enthalpy values appear to be uniformly spread. Table 4 provides the enthalpy values at a 50 wt % concentration for varying temperatures.

Table 4 Enthalpy values of ammonia-water solution at 50 wt % for various temperatures

Temperature (K)	Saturated enthalpy of ammonia-water solution (kJ/kg)
273.15	-254.7629
283.15	-209.8433
293.15	-164.5206
303.15	-118.2756
313.15	-71.1427
323.15	-23.4771
333.15	24.2785
343.15	71.8268
353.15	119.2488

Using the data from Table 4, the method for computing the proportional nodes for each temperature is detailed in Table 5. The nodes, representing a normalized scale for enthalpy values, are calculated with respect to the highest and lowest enthalpy values.

Table 5 Procedure for calculating the proportional nodes

Temperature (K)	Saturated Enthalpy of Ammonia Water Solution	Values of Proportional Nodes
273.15	-254.7629 = A	(A-A)/(A-I) 0
283.15	-209.8433 = B	(A-B)/(A-I) 0.120102
293.15	-164.5206 = C	(A-C)/(A-I) 0.241282
303.15	-118.2756 = D	(A-D)/(A-I) 0.364928
313.15	-71.1427 = E	(A-E)/(A-I) 0.490948
323.15	-23.4771 = F	(A-F)/(A-I) 0.618392
333.15	24.2785 = G	(A-G)/(A-I) 0.746077
343.15	71.8268 = H	(A-H)/(A-I) 0.873207
353.15	119.2488 = I	(A-I)/(A-I) 1

Table 6 provides the data on proportional nodes for various temperatures. The equation for nodes as a function of temperature is also provided, which was generated using Microsoft Excel.

Table 6 Proportional nodes data

Temperature (K) - y-axis	Nodes - x-axis
273.15	0
283.15	0.120102
293.15	0.241282
303.15	0.364928
313.15	0.490948
323.15	0.618392

333.15	0.746077
343.15	0.873207
353.15	1

The Microsoft Excel plot is shown in Figure 2.

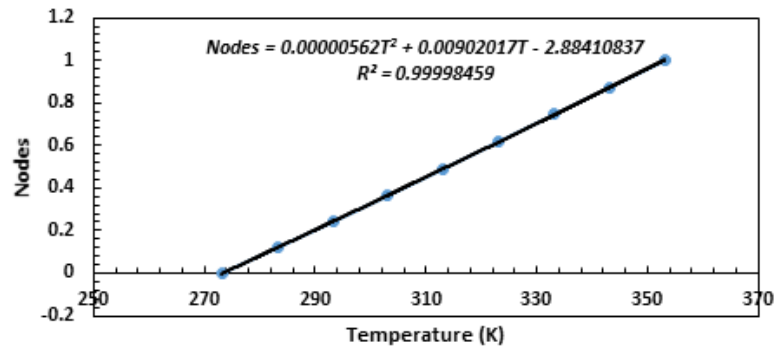


Fig. 2 Plot of data from table 6

The nodal equation, derived using Microsoft Excel, establishes a relationship between the temperature and nodes. The foundational equation is denoted by the following:

$$Node = 0.00000562T^2 + 0.00902017T - 2.88410837 \tag{24}$$

The conceptual foundation posits that the saturated enthalpy at any temperature point within a predefined range can be ascertained using:

$$H = H_0 + (H_1 - H_0)x \text{ Nodes} \tag{25}$$

Here, H_0 represents the enthalpy equation when nodes equal 0, taken at 273.15 K:

$$H_0 = -0.00001108x^4 + 0.00204055x^3 - 0.01044078x^2 - 8.31398994x + 1.39561958 \tag{26}$$

Conversely, H_1 signifies the enthalpy equation when nodes equal 1, observed at 353.15 K:

$$H_1 = -0.00001317x^4 + 0.00256076x^3 - 0.05514505x^2 - 6.31602523x + 336.55414266 \tag{27}$$

Incorporating the node equation:

$$Node = 0.00000562T^2 + 0.00902017T - 2.88410837 \tag{28}$$

Equation (25) expands to the more comprehensive equation (29):

$$H = H_0 + (H_1 - H_0) \times 0.00000562T^2 + 0.00902017T - 2.88410837 \tag{29}$$

After simplifying and subtracting the coefficients of H_0 and H_1 , we derive the following enthalpy equation:

$$\begin{aligned}
 H = & (-0.00001108x^4 + 0.00204055x^3 - 0.01044078x^2 - 8.31398994x + 1.39561958) \\
 & + [(-0.00001317x^4 + 0.00256076x^3 - 0.05514505x^2 - 6.31602523x + 336.55414266) \\
 & - (-0.00001108x^4 + 0.00204055x^3 - 0.01044078x^2 - 8.31398994x + 1.39561958)] \\
 & * 0.00000562T^2 + 0.00902017T - 2.88410837
 \end{aligned} \tag{30}$$

Simplifying equation (30) results to equation (31):

$$\begin{aligned}
 H = & (-0.00001108x^4 + 0.00204055x^3 - 0.01044078x^2 - 8.31398994x + 1.39561958) \\
 & + [(-0.00000209x^4 + 0.000526x^3 - 0.0447x^2 + 1.997965x + 335.1585) \\
 & * 0.00000562T^2 + 0.00902017T - 2.88410837]
 \end{aligned} \tag{31}$$

The directionality of the dependent variable relative to the independent variables, as they increase or decrease, dictates whether a plus or minus is applied in the above formulation.

An intriguing observation arises when comparing this approach with the Chebyshev method. The former manifests a higher degree of simplicity and precision, marking a notable advancement in the field.

As a case study, this methodology was applied to the superheated properties of Opteon. The relevant data, encapsulating dynamic viscosity, heat capacity, heat capacity ratio (C_p/C_v), and thermal conductivity, were extracted from the 2015 report [7]. The properties considered in this study are dynamic viscosity, heat capacity, heat capacity ratio (C_p/C_v), and thermal conductivity.

4. Application of Proportional Nodes Method to Generate Correlations for Opteon

As the global automotive industry gravitates towards more eco-friendly alternatives, Opteon (R-1234yf), a non-ozone depleting and low global warming potential (GWP) refrigerant, is establishing its prominence. The main differentiating factor lies in Opteon's composition: it is a hydrofluoroolefin (HFO) refrigerant with one double bond between a set of carbon atoms, compared to conventional hydrofluorocarbon (HFC) refrigerants. Consequently, Opteon YF's GWP is less than 1, whereas HFC-134a refrigerant has a GWP of 1,300 [6].

Opteon's low toxicity, zero ozone-depleting potential, and low GWP, combined with its slow flame propagation, make it a safe and environmentally friendly option. Furthermore, it meets global regulations for lower GWP and possesses similar thermodynamics to HFC-134a, providing comparable energy efficiency and capacity. Opteon YF (R-1234yf) therefore offers an optimal balance of properties and performance for automobile air conditioning applications [7].

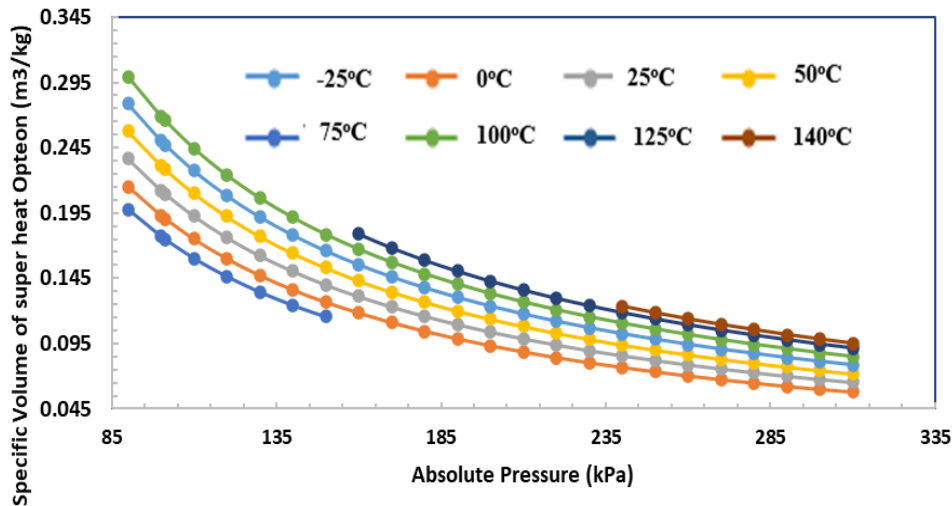


Fig. 3 Variation of specific volume for superheated Opteon (HFO-1234yf) vapour at various temperatures and pressures (Data from Perry's Chemical Engineers' Handbook [7])

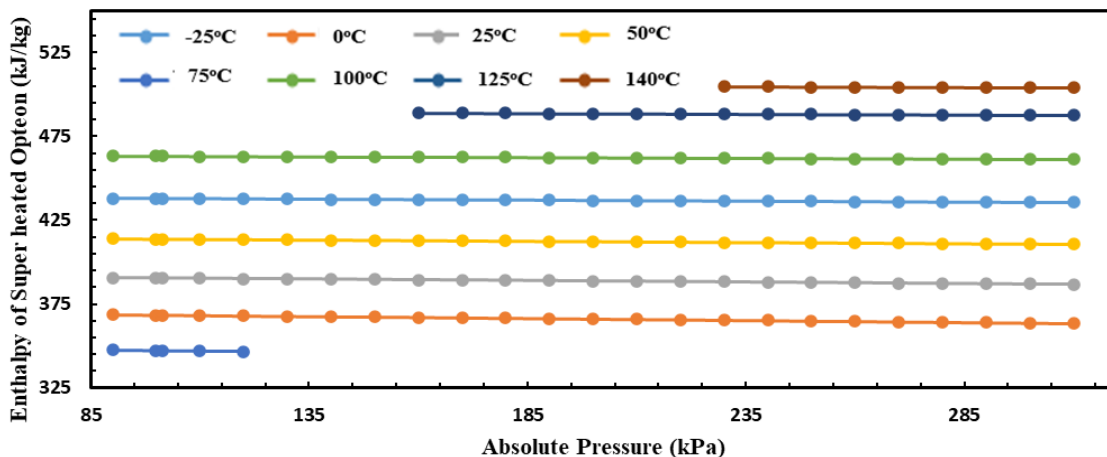


Fig. 4 Variation of enthalpy (kJ/kg) for superheated Opteon (HFO-1234yf) vapour at various temperatures and pressures (Data from Perry's Chemical Engineers' Handbook [7])

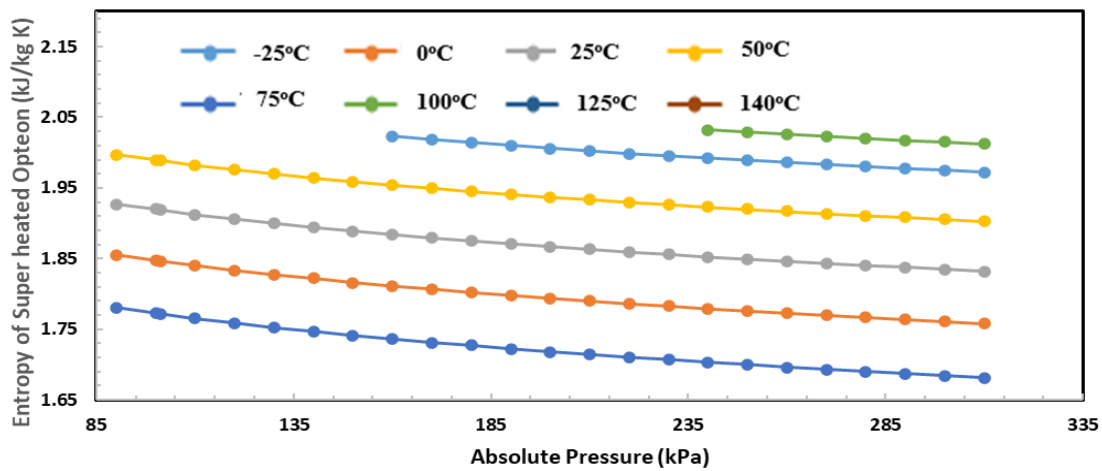


Fig. 5 Variation of entropy (kJ/(kg K)) for superheated Opteon (HFO-1234yf) vapour at various temperatures and pressures (Data from Perry's Chemical Engineers' Handbook [7])

Table 6 Correlations for saturated vapour

Temperature range: -20°C ≤ T < 3140°C; Absolute pressure range; 90 ≤ P ≤ 310 kPa

$T = -2.44041923E-04P^2 + 2.34318478E-01P - 4.99161955E+01$

Specific Volume
 $V = -9.47202541E-09P^3 + 8.08769745E-06P^2 - 2.52405209E-03P + 3.44616273E-01; R^2 = 0.9967045$
 $V = -1.22608642E-06T^3 + 2.44521600E-05T^2 - 1.93625801E-03T + 5.65714745E-02; R^2 = 0.9964033$

Enthalpy
 $H = 4.54538656E-07P^3 - 4.65426237E-04P^2 + 2.20373773E-01P + 3.25799318E+02; R^2 = 0.9961735$
 $H = -5.56785807E-04T^2 + 6.50916578E-01T + 3.63286756E+0; R^2 = 0.99883352$

Entropy
 Over the temperature and pressure ranges, Entropy, S, is approximately 1.59.

Table 7 Details of correlation for a specific volume of superheated Opteon vapour

Temperature (T, °C)*	Absolute Pressure, (P, kPa)*	Correlations for Specific Volume (V - m ³ /kg, P = Absolute Pressure, kPa; T = °C)
-30°C ≤ T < -25°C	90	Temperature range for equations: -20°C ≤ T < 0°C $V = (aP^5 + bP^4 + cP^3 + dP^2 + eP + f) - (gT^2 + hT + i) / (0.0265)$ ‡ where $a = -0.000000000000557$ $b = +0.000000000660384$ $c = -0.00000031644394$ $d = +0.000078197850662$ $e = -0.010486430338533$ $f = +0.716035219239089$ $g = 0.0000269542$ $h = -0.0325336927$ $i = -0.0002695417$
-25°C ≤ T < -20°C	90 ≤ P ≤ 120	
-20°C ≤ T < -15°C	90 ≤ P ≤ 150	
-15°C ≤ T < -10°C	90 ≤ P ≤ 180	
-10°C ≤ T < -5°C	90 ≤ P ≤ 220	
-5°C ≤ T < 0°C	90 ≤ P ≤ 260	Average percentage deviation: ±0.14456 Temperature range for equations: 0.0°C ≤ T ≤ -115°C $V = (aP^5 + bP^4 + cP^3 + dP^2 + eP + f) + [(gP^5 + hP^4 + iP^3 + jP^2 + kP + l) / (mT^4 + nT^3 + oT^2 + pT + q)]$

$0^{\circ}\text{C} \leq T < 115^{\circ}\text{C}$	$90 \leq P \leq 310$	<p>where</p> $a = -0.000000000000557$ $b = + 0.00000000660384$ $c = - 0.00000031644394$ $d = +0.000078197850662$ $e = - 0.010486430338533$ $f = + 0.716035219239089$ $g = -0.000000000000266$ $h = +0.00000000310291$ $i = -0.000000145690276$ $j = + 0.000035238892493$ $k = -0.004618771760001$ $l = + 0.314225759727231$ $m = -0.0000000002$ $n = + 0.0000000761$ $o = -0.0000119903$ $p = + 0.0094123592$ $q = + 0.0005937998$ <p>Average percentage deviation: ± 0.218</p>
$15^{\circ}\text{C} \leq T < 120^{\circ}\text{C}$	$120 \leq P \leq 310$	<p>Temperature range for equations: $115^{\circ}\text{C} < T \leq 140^{\circ}\text{C}$</p> $V = (aP^5 + bP^4 + cP^3 + dP^2 + eP + f) + (gT^3 + hT^2 + iT + j)(0.0071) \ddagger$
$120^{\circ}\text{C} \leq T < 130^{\circ}\text{C}$	$160 \leq P \leq 310$	
$130^{\circ}\text{C} \leq T < 135^{\circ}\text{C}$	$200 \leq P \leq 310$	
$135^{\circ}\text{C} \leq T < 140^{\circ}\text{C}$	$240 \leq P \leq 310$	<p>where</p> $a = -0.000000000000823$ $b = + 0.00000000970675$ $c = - 0.000000462134216$ $d = + 0.000113436743155$ $e = - 0.0151052020985$ $f = + 1.03026097896632$ $g = +0.000005216667$ $h = - 0.002045678571$ $I = + 0.306418147619$ $J = - 16.117326857135$ <p>Average percentage deviation: ± 0.13399</p>

* These are the ranges for which data have been provided.

‡ Only the equation at $T = 0^{\circ}\text{C}$ is used and the nodes equation is multiplied by the difference between the highest and lowest values of V in the range at the absolute pressure selected for the nodes equation.

† Only the equation at $T = 115^{\circ}\text{C}$ is used and the nodes equation is multiplied by the difference between the highest and lowest values of V in the range at the absolute pressure selected for the nodes equation.

Table 9 Details of correlation for enthalpy of superheated Opteon vapour

Temperature (T, °C)*	Absolute pressure, (P, kPa)*	Correlation for enthalpy (H = Enthalpy in kJ/kg; P = Absolute Pressure, kPa; T = °C)
$-30^{\circ}\text{C} \leq T < -25^{\circ}\text{C}$	90	For temperature range for equations: $0^{\circ}\text{C} \leq T \leq -140^{\circ}\text{C}$ $H = (aP^2 + bP + c) + ((dP^2 + eP + f)(gT^2 + hT + i))$
$-25^{\circ}\text{C} \leq T < -20^{\circ}\text{C}$	$90 \leq P \leq 120$	
$-20^{\circ}\text{C} \leq T < -15^{\circ}\text{C}$	$90 \leq P \leq 150$	where
$-15^{\circ}\text{C} \leq T < -10^{\circ}\text{C}$	$90 \leq P \leq 180$	
$-10^{\circ}\text{C} \leq T < -5^{\circ}\text{C}$	$90 \leq P \leq 220$	$a = +0.00000350$ $b = - 0.03163108$ $c = + 346.36536117$
$-5^{\circ}\text{C} \leq T < 0^{\circ}\text{C}$	$90 \leq P \leq 260$	
$0^{\circ}\text{C} \leq T < 115^{\circ}\text{C}$	$90 \leq P \leq 310$	$d = +0.0000038017$ $e = +0.0201991839$
$115^{\circ}\text{C} \leq T < 120^{\circ}\text{C}$	$120 \leq P \leq 310$	
$120^{\circ}\text{C} \leq T < 130^{\circ}\text{C}$	$160 \leq P \leq 310$	$f = +160.4475341865$ $g = +0.0000040445$ $h = + 0.0054354710$
$130^{\circ}\text{C} \leq T < 135^{\circ}\text{C}$	$200 \leq P \leq 310$	
$135^{\circ}\text{C} \leq T < 140^{\circ}\text{C}$	$240 \leq P \leq 310$	$i = + 0.1594405594$ <p>Average percentage deviation: ± 0.124</p>

*These are the ranges for which data have been provided.

The variations of specific volume, enthalpy and entropy for various temperatures and pressures for Opteon is shown in Figs. 3 to 5 respectively.

5. Results

Microsoft Excel was employed to generate the various components of the correlations due to its comprehensive suite of data management capabilities that allow users to easily import, explore, clean, analyze, and visualize data. The Proportional Nodes Method was used to derive correlations for various properties using actual data. For saturated vapour, the correlations are presented in Table 6. They are derived for specific volume, enthalpy and entropy of saturated Opteon using actual property data. For superheated vapour, the correlations presented in Tables 7 to 10. They are also derived for using actual property data. These are the same data used to generate Figs. 3 to 5.

6. Discussion

A comparison was made between the data produced using the Proportional Nodes Method and those generated by the Chebyshev Curve fitting method. The application of the proportional node method results in a lower average percentage deviation than the Chebyshev polynomial method (± 0.978 for the method utilizing Chebyshev polynomials and ± 0.5378 for the Proportional Nodes Method). This novel approach is also less complex while resulting to simpler and more accurate correlations. This method was further applied to develop correlations for three properties—specific volume, enthalpy, and entropy—of Opteon, a refrigerant used in automotive air-conditioners. As can be seen on Table 6, the R^2 values of the correlations of the properties for saturated vapour of Opteon are very close to 1.0 and so can be considered very accurate equations for each property. As illustrated in Tables 7 to 10, a single correlation can be used for each thermodynamic property, and the data derived from these correlations show a satisfactory percentage deviation from the actual data ($< \pm 0.22\%$ for a specific volume, $< \pm 0.124$ for enthalpy and $< \pm 0.125$ for entropy).

The method can also be extended to the dataset beyond the endpoints. In this situation, only the equation of the endpoint data involved will be used, and a new nodes equation should be derived. This new dataset must include the data used to derive the endpoint equation and the proportional node value at this point must be 0.0.

It should be further noted that the set of data used to derive the nodes equation does not rely only on spread, but also on its distribution. In the case of unevenly spread data ($> 100\%$ across the x-axis), the set of y-axis data at the centre of the x-axis should be used to calculate the nodes equation.

However, these conclusions cannot be generalized for all datasets, as the accuracy of the correlations is contingent upon the accuracy of the equations of the endpoints and nodes, and the requirement that the data should not be overlapping. If R^2 , the coefficient of determination, is less than 0.9, the method should not be applied.

Table 10 Details of correlation for the entropy of superheated Opteon vapour

Temperature (T, °C)*	Absolute pressure, (P, kPa)*	Correlation for entropy (S = Entropy in kJ/(kg K); P = Absolute Pressure, kPa; T = °C)
$-30^\circ\text{C} \leq T < -25^\circ\text{C}$	90	Temperature range for equations: $-20^\circ\text{C} \leq T < 0^\circ\text{C}$ $S = (aP^3 + bP^2 + cP + d) - (eT^2 + fT + g)(0.097) \ddagger$
$-25^\circ\text{C} \leq T < -20^\circ\text{C}$	$90 \leq P \leq 120$	where
$-20^\circ\text{C} \leq T < -15^\circ\text{C}$	$90 \leq P \leq 150$	$a = -0.0000000032873$
$-15^\circ\text{C} \leq T < -10^\circ\text{C}$	$90 \leq P \leq 180$	$b = +0.0000030032707$
$-10^\circ\text{C} \leq T < -5^\circ\text{C}$	$90 \leq P \leq 220$	$c = -0.0012366856061$
$-5^\circ\text{C} \leq T < 0^\circ\text{C}$	$90 \leq P \leq 260$	$d = +1.7922994382189$
		$e = -0.00002455$
		$f = +0.03262151$
		$g = +0.99950926$
		Average percentage deviation: ± 0.11874
		Temperature range for equations: $0^\circ\text{C} \leq T \leq -115^\circ\text{C}$ $S = (aP^3 + bP^2 + cP + d) + ((eP^3 + fP^2 + gP + h) * (iT^2 + jT + k))$
		where
		$a = -0.0000000032873$
		$b = +0.0000030032707$

$0^{\circ}\text{C} \leq T < 115^{\circ}\text{C}$	$90 \leq P \leq 310$	$c = -0.0012366856061$ $d = +1.7922994382189$ $e = -0.0000000007337$ $f = +0.0000004792473$ $g = -0.0000505094909$ $h = +0.3363073231551$ $i = -0.0000063446$ $j = +0.0093958728$ $k = +0.001182183$
		Average percentage deviation: ± 0.12390
$115^{\circ}\text{C} \leq T < 120^{\circ}\text{C}$	$120 \leq P \leq 310$	Temperature range for equations: $115^{\circ}\text{C} < T \leq 140^{\circ}\text{C}$
$120^{\circ}\text{C} \leq T < 130^{\circ}\text{C}$	$160 \leq P \leq 310$	
$130^{\circ}\text{C} \leq T < 135^{\circ}\text{C}$	$200 \leq P \leq 310$	
		$S = (aP^3 + bP^2 + cP + d) + (eT + f)(0.067)^{\ddagger}$
		where
$135^{\circ}\text{C} \leq T < 140^{\circ}\text{C}$	$240 \leq P \leq 310$	$a = -0.000000004021$ $b = +0.000003482518$ $c = -0.001287195097$ $d = +2.128606761374$ $e = 0.0401706$ $f = -4.6217479$
		Average percentage deviation: ± 0.09549

* These are the ranges for which data have been provided.

\ddagger Only the equation at $T = 0^{\circ}\text{C}$ is used and the nodes equation is multiplied by the difference between the highest and lowest values of S in the range at the absolute pressure selected for the nodes equation.

\dagger Only the equation at $T = 115^{\circ}\text{C}$ is used and the nodes equation is multiplied by the difference between the highest and lowest values of S in the range at the absolute pressure selected for the nodes equation.

7. Conclusion

Accurate correlations of data remain essential for the design, simulation, and optimization of chemical processes. This paper introduces a novel method for correlating non-overlapping data for surfaces, namely, data with two dependent variables. The method hinges on precise estimations of correlations for boundary curves and the variation of nodes at selected points of other curves within the boundary. A comparison was made between the data produced using the proposed method and those generated by the Chebyshev curve fitting method. The application of the proportional node method results in a lower average percentage deviation than the Chebyshev polynomial method (± 0.978 for the method utilizing Chebyshev polynomials and ± 0.5378 for the Proportional Nodes Method). This new approach is less complex, yielding simpler and more accurate correlations. Its efficacy has been demonstrated in developing correlations for three properties—specific volume, enthalpy, and entropy—of Opteon, a refrigerant used in automotive air conditioners. The derived data exhibited a satisfactory percentage deviation from the actual data ($< \pm 0.22\%$ for a specific volume, $< \pm 0.124$ for enthalpy and $< \pm 0.125$ for entropy). In addition, correlations have been generated for the saturated vapour. In essence, the presented method offers a promising approach to developing correlations for non-overlapping data with two dependent variables. Future work could explore its applicability in other contexts and with different types of data.

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Conflict of Interest

Authors declare that there is no conflict of interests regarding the publication of the paper.

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