ISSN 2394-3777 (Print)
ISSN 2394-3785 (Online)
Available online at www.ijartet.com

International Journal of Advanced Research Trends in Engineering and Technology (IJARTET)
Vol. 4, Special Issue 21, August 2017

Importance of differential equations and its use in the field of Chemistry

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Abstract: In Chemistry and Engineering fields, many industrial processes and functions are determined by differential equations. Though the mathematical principles are same in all cases, the utility and relevance of these equations may differ in different topics and contain various parameters and units. The current study highlights the importance of the usage of differential equations to determine various thermodynamic physical properties of the binary mixtures such as excess molar volume, isentropic compressibility, partial molar volume, acoustic impedance, inter molecular free length, deviation in ultrasonic speed of sound etc.

Keywords: Differential equations; Thermodynamics, Partial molar volume, isentropic compressibility

I. INTRODUCTION

All Mathematics has been used as a powerful tool for problem solving in engineering and chemical research fields. Especially in chemistry field and chemical engineering, analytical mathematical solutions of problems have been limited. Mostly the problems in heat conduction, mass transfer, diffusion etc. are solved by using mathematical equations.

In general, modeling of the variation of a physical quantity, such as temperature, pressure, displacement, velocity, stress, strain, current, voltage, or concentration of a pollutant, with the change of time or location, or both would result in differential equations. Similarly, studying the variation of some physical quantities on other physical quantities would also lead to differential equations. In fact, many engineering subjects, such as mechanical vibration or structural dynamics, heat transfer, or theory of electric circuits, are founded on the theory of differential equations [1]

"Differential equations are extremely important in the history of mathematics and science, because the laws of nature are generally expressed in terms of differential equations. Differential equations are the means by which scientists describe and understand the world" [2]

An equation with a derivative such as $dy/dx + y = x$ is known as a differential equation. The derivative dy/dx is of the first order and hence it is the first order differential equation.

The mathematical description of various processes in chemistry and physics is possible by describing them with the help of differential equations which are based on simple model assumptions and defining the boundary conditions [3, 4]. In many cases, first-order differential equations are completely describing the variation dy of a function $y(x)$ and other quantities. If y is a quantity depending on x, a model may be based on the following assumptions: The differential decrease of the variable y is proportional to a differential increase of the other variable, here x, i.e. $-dy \sim dx$. This decrease $-dy$ should depend on the function y itself: $-dy \sim ydx$, and together with a so far unknown constant a, results in the equation

$dy = -\,aydx$

Thus follows the ordinary linear homogeneous first-order differential equation:

$dy/dx + ay = 0$

The characteristics of an ordinary linear homogeneous first-order differential equation are: (i) there is only one independent variable, i.e. here x, rendering it an ordinary differential equation, (ii) the depending variable, i.e. here y, having the exponent 1, rendering it a linear differential equation, and (iii) there are only terms containing the variable y and its first derivative, rendering it a homogeneous first-order differential equation [5]. One should understand the Order, Degree, Linear and Non-Linear terms in Differential equations. [7] proposed a principle in which another NN yield input control law was created for an under incited quad rotor UAV which uses the regular limitations of the under incited framework to create virtual control contributions to ensure the UAV tracks a craved direction. Utilizing the versatile back venturing method, every one of the six DOF are effectively followed utilizing just four control inputs while within the sight of un demonstrated flow and limited unsettling influences. The current study is on the usage of differential equations in the field of chemistry and its research purposes.

II. DISCUSSIONS

The experimental values of Ultrasonic velocity and density of binary mixtures at different temperatures with respective mole fractions (x1) are used to calculate the following relations:

a) The density values were used to calculate excess molar volumes V E using the following equation:

$$V^E = \frac{x_1M_1 + x_2M_2}{\rho_m} - \left\{\frac{x_1M_1}{\rho_1} + \frac{x_2M_2}{\rho_2}\right\} \text{----(1)}$$

V E(cm3·mol−1) is excess molar volume, where ρm is the density of the mixture and (x1,M1,ρ1) and (x2, M2, ρ2) are the mole fraction, the molecular weight, and the density of pure components 1 and 2, respectively. A graph (parabolic) can be plotted with the calculated VE values with respect to mole fraction x1 values. The increase or decrease in the volume on mixing the liquids can be taken as a criterion and measure of molecular interaction.

b) The isentropic compressibility(Ks) was calculated using the Laplace relation (it is a second order partial differential equation)

$$K_s = U^{-2}\rho^{-1} \text{--------(2)}$$

Where u is the ultrasonic velocity and ρ the density.

c) The deviation in isentropic compressibility, ΔKS obtained using the relation,

$$\Delta KS\ (TPa{-}1) = K_S12 - \varphi 1 K_S1 - \varphi 2 K_S2 \text{ ----(3)}$$

Where KS12 is the experimental isentropic compressibility of the mixture, and φ1, φ2 and KS1, KS2 are the volume fractions and isentropic compressibility respectively of the pure components.
Where φi is the ideal state volume fraction and is defined by the relation:

$$\phi_i = \frac{x_iV_i}{\sum_{i=1}^{Z} x_iV_i} \text{--------(4)}$$

d) Deviation in Ultrasonic speed of sound (Δu) calculated by using the following relation

$$\Delta_u = u \quad (x_1u_1 \mid x_2u_2) \text{-------(5)}$$

Where U is the experimental ultrasonic speed for the mixture, x1, u1, x2, u2 are the mole fractions and ultrasonic speed of the pure components 1 & 2 respectively.

e) In an attempt to explore the nature of the interactions, various thermodynamic parameters like intermolecular free length, Lf [6]; acoustic impedance, Z; of the binary mixtures have been calculated using the following equations:

$$L\_f = K\,\rho\text{^}(1/2) \text{------(6)}$$

Where Lf is the intermolecular free length, K is the isentropic compressibility and ρ is the density.
Acoustic impedance calculated by using the relation

$$Z = u\rho \qquad \text{------(7)}$$

Where Z is the acoustic impedance, is the Ultrasonic speed of sound and ρ is the density.

f) Excess molar free length Lf^E calculated by using the relation

$$L_f^E = L_f - (x_1L_{f1} + x_2L_{f2}) \text{---(8)}$$

Where is excess molar free length, Lf is intermolecular free length of the mixture, x1, x2, Lf1 & Lf2 are the mole fraction and intermolecular free length for pure components 1 & 2 respectively.

g) Deviation in acoustic impedance calculated by using the relation

$$\Delta z = z - (x_1z_1 + x_2z_2) \text{------(9)}$$

Where Δz is the deviation in acoustic impedance, z is the acoustic impedance of the mixture, x1,x2, z1,z2 are the mole fraction and acoustic impedances of pure components 1 & 2 respectively.

2.1 Partial Molar volume (PMV)

Behaviour of the mixtures is further analysed by calculating the partial excess molar volumes of the components. Vm_1^E and Vm_2^E for each binary mixture are calculated with respect to their mole fractions at different temperatures
The partial molar volumes, $V^o m1$ of component 1 and $V^o m2$ of component-2 in the mixture over entire composition range are calculated using the following relations.

$$\bar{V}^o{}_{m,1} = V_m^E + V_{m,1}^* + x_2\left(\frac{\partial V_m^E}{\partial x_1}\right)_{T,P} \text{......(10)}$$

$$\bar{V}^o{}_{m,2} = V_m^E + V_{m,2}^* - x_1\left(\frac{\partial V_m^E}{\partial x_1}\right)_{T,P} \text{..... (11)}$$

Where V^*m1, V^*m2 are molar volumes of pure components-1 and 2. The derivative of $\partial V_m^E/\partial x_1$ obtained by using below equations.

$$\bar{V}^{o}{}_{m,2} = V^{*}_{m,2} + x_1^2 \sum_{i=0}^{n} A_i (1-2x_1)^i + 2x_1x_2^2 \sum_{i=1}^{n} A_i (1-2x_1)^{i-1} \qquad \ldots\ldots (12)$$

$$\bar{V}^{o}{}_{m,1} = V^{*}_{m,1} + x_2^2 \sum_{i=0}^{n} A_i (1-2x_1)^i + 2x_1x_2^2 \sum_{i=1}^{n} A_i (1-2x_1)^{i-1} \qquad \ldots\ldots (13)$$

The Excess Partial Molar Volumes, $V^E{}_{m1}$, $V^E{}_{m2}$over the whole composition range are calculated by using the below relation [8].

$$\bar{V}^{o,E}{}_{m,1} = \bar{V}^{o}{}_{m,1} - V^{*}_{m,1} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(14)$$

$$\bar{V}^{o,E}{}_{m,2} = \bar{V}^{o}{}_{m,2} - V^{*}_{m,2} \quad \ldots\ldots. (15)$$

$$\bar{V}^{o,E,\infty}{}_{m,2} = \bar{V}^{o,\infty}{}_{m,2} - V^{*}_{m,2} \ldots\ldots\ldots.(16)$$

$$\bar{V}^{o,E,\infty}{}_{m,1} = \bar{V}^{o,\infty}{}_{m,1} - V^{*}_{m,1} \quad \ldots\ldots. (17)$$

The values of excess partial molar volume of at infinite dilution $V^{oE\infty}{}_{m1}$, $V^{oE\infty}{}_{m2}$ for the selected binary systems at different temperatures can be calculated to know the strength of molecular interactions.

2.2 Redlich-Kister equation

The variation of V^E, Ks^E, Δz, Δu and LfE with mole fraction were fitted to the Redlich–Kister Equation of the type:

$$Y^E = x_i x_2 \{a0 + a1(x_1 - x_2) + a2(x_1 - x_2)^2\} \quad \ldots\ldots. (18)$$

Where Y^E is for V^E, Δks, Δu, Δz & LfE in the polynomial degree. The values of a0, a1 and a2 are the coefficients of the polynomial equation and it can be obtained by the method of least-squares. The standard deviations are calculated by using the equation:

$$\sigma(Y^E) = \frac{\{\sum_{i=1}^{n} (Y^E_{obs} - Y^E_{cal})\char`^2\}^{1/2}}{n-m} \quad \ldots\ldots\ldots\ \ldots..(19)$$

Where n is the total number of experimental points and m is the number of coefficients.

An equation containing two or more independent variables and partial derivatives with respect to these variables is called a partial differential equation. It is rarely possible to write a complete solution of the equation. Boundary conditions are used to get the required solution through differential equations. Starting point of the problem solving will be the physical problem involving the solution through partial derivatives. The above equations can be used to calculate and obtained solution shall be interpreted to know the behavior of the intermolecular interactions between the ionic and organic solvent liquid binary mixtures in thermodynamic excess properties.

III. CONCLUSION

In this paper, the usage of differential equations to find the excess thermodynamic properties of binary mixtures at the various temperatures is highlighted. The principle procedure is to consider the boundary conditions as a first step in the operational method and handling the non-homogeneous equation on the right side with minimum effort. Mathematical modelling is the fast and consistent method to determine various unknown parameters with the set boundary conditions. Computer aided modelling technology and software is necessary to ease the solution for the complex equations in chemistry and also general scienceMaintaining the Integrity of the Specifications

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