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Simple model for the calculation of concentration and temperature dependent refractive index of different solutions

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Abstract: Simple analytical models for the calculation of concentration (c) and temperature (T) dependent refractive index i.e., $n(c,T)$ values of the six solutions namely, three electrolyte (KCl, $NaCl$, and $CaCl_2$), a polar (*glucose*), a non-polar (*ethyl acetate*), and a protein (*bovine serum albumin*) solutions have been proposed. The values of refractive index obtained using the proposed models have been compared with the corresponding values of the refractive index obtained using other reported models and the experimental values. A fairly good agreement between them has been obtained. Further, the proposed models require less number of concentration and temperature coefficients compared to the models reported in the literature, which makes it computationally simple in nature.

Keywords: Refractive index, electrolyte solution, polar solution, non-polar solution, protein solution, temperature, concentration

1. Introduction

Refractive index (n) plays a vital role in the estimation of physical properties of various kinds of solutions. The physical properties of the solutions change with the variation in the concentration (c) of the solution. Further, the concentration of the solution may be determined by computing the refractive index of a binary solution. However, the refractive index of any solution critically depends upon the various factors namely, concentration, temperature (T), wavelength and pressure [1-12] etc. The impacts of wavelength and pressure on the refractive index can be diminished by measuring at atmospheric pressure and at a fixed wavelength. However, the concentration and temperature dependence still plays a key role in the estimation of refractive index [1]. Several attempts have been reported in the literature [1-3, 8-9] for the estimation/measurement of the concentration and/or temperature dependence of the refractive index of different solutions. Moreover, the most commonly used Lorentz−Lorenz equation [6] for the estimation of concentration and temperature dependent refractive index values is unable to estimate the values of refractive index derivatives with respect to temperature and concentration very precisely. Therefore, for the precise calculation of refractive indices and the coefficient of its derivatives with respect to concentration and temperature, recently, polynomial expressions have been reported in [1] for different kinds of solutions. However, the polynomial expressions contain several concentration and temperature coefficients which are required to be estimated for each type of the solution, which make these expressions computationally complex in nature. Therefore, there is need of a simple model for the estimation of concentration and temperature dependent refractive index values.

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In this work, we have proposed simple exponential models for the estimation of concentration and temperature dependent refractive index values. As compared to the polynomial expressions reported in [1] where five coefficients are required, there is need of only three coefficients in the proposed models. The concentration and temperature dependent refractive index values of the different solutions have been calculated by utilizing both the polynomial expressions [1] and the proposed exponential models for the comparison purpose. It has been observed that the obtained values of the concentration and temperature dependent refractive index by utilizing the proposed models are very close to the experimental values compared to the values obtained by utilizing polynomial expressions reported in [1]. Therefore, the proposed exponential models for the calculation of refractive index at different values of concentration and temperature are simple in nature and provide very precise values compared to the models reported in the literature.

2. Computational Method

The exponential dependence of the energy gap on the concentration and temperature in alloy semiconductors materials have been reported elsewhere [13]. Further, the correlation between the energy gap and the refractive of semiconductors materials have extensively investigated and reported in the literature [14-18]. Therefore, based on the above analysis, simple exponential models have been proposed for the estimation of concentration and temperature dependent variations in refractive index values of the six solutions namely, three electrolyte (KCl, $NaCl$, and $CaCl_2$), a polar (*glucose*), a non-polar (*ethyl acetate*), and a protein (*bovine serum albumin*) solutions; by utilizing regression analysis to the experimental results and expressed as follows:

$$n(c,T)_{NaCl} = 1.3736exp(0.132c - 9.58 \times 10^{-5}T) \quad (1)$$

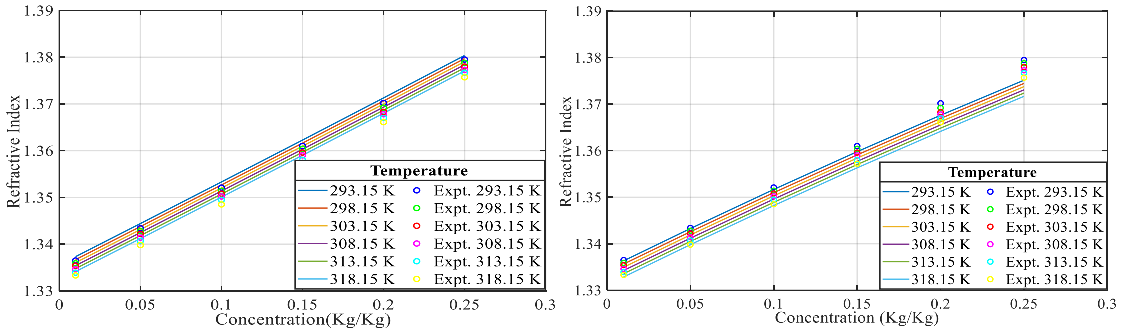
$$n(c,T)_{KCl} = 1.3678exp(0.1209c - 8.69 \times 10^{-5}T) \quad (2)$$

$$n(c,T)_{CaCl2} = 1.3628exp(0.1798c - 7.49 \times 10^{-5}T) \quad (3)$$

$$n(c,T)_{Glucose} = 1.3713exp(0.113c - 9.29 \times 10^{-5}T) \quad (4)$$

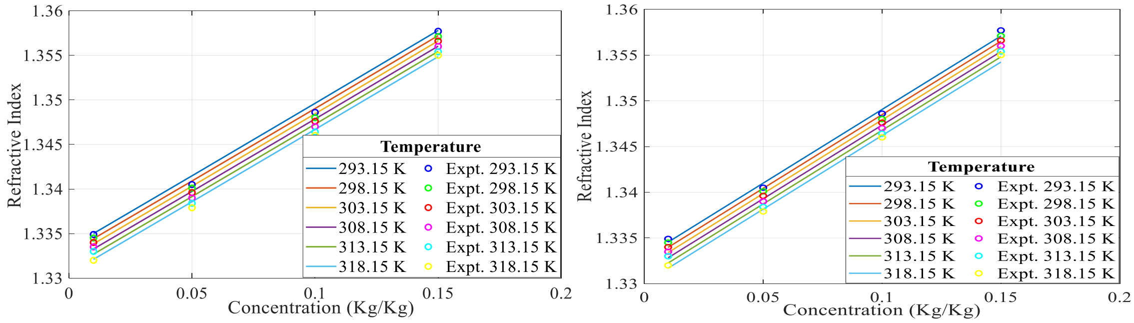
$$n(c,T)_{BSA} = 1.3742exp(0.124c - 9.89 \times 10^{-5}T) \quad (5)$$

$$n(c,T)_{Ethylacetate} = 1.3620exp(0.051c - 7.20 \times 10^{-5}T) \quad (6)$$



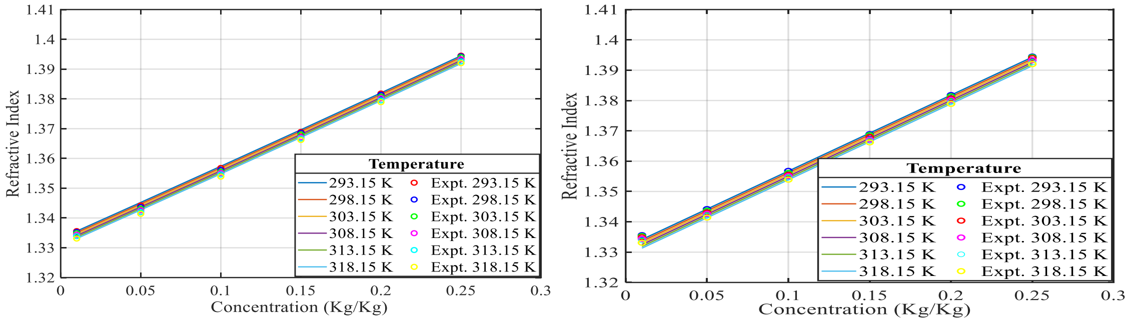
(a) (b)

Fig. 1 Concentration and temperature dependence of the refractive index of NaCl (a) proposed (b) reported [1] fits.



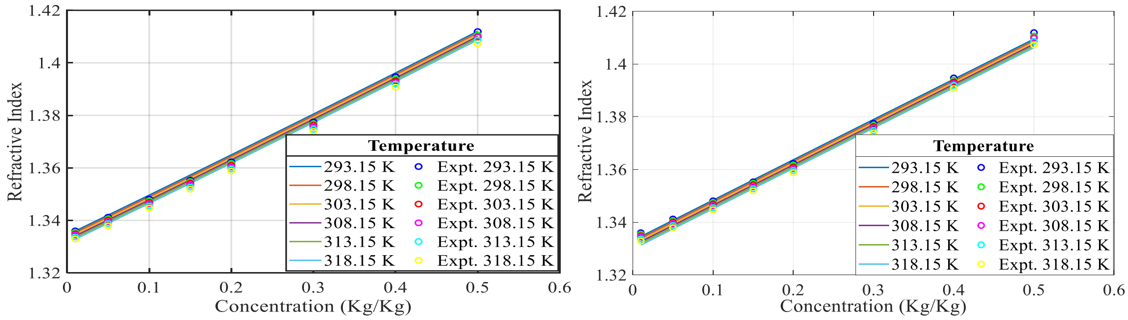
(a) (b)

Fig. 2 Concentration and temperature dependence of the refractive index of KCl (a) proposed (b) reported [1] fits.



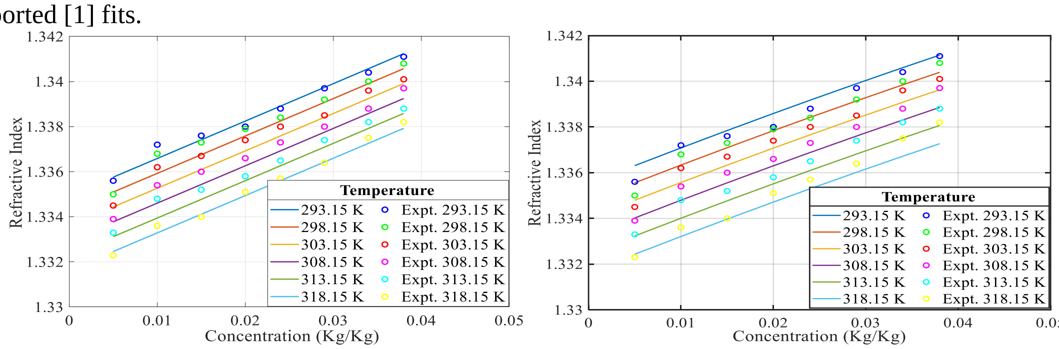
(a) (b)

Fig. 3 Concentration and temperature dependence of the refractive index of $CaCl_2$ (a) proposed (b) reported [1] fits.



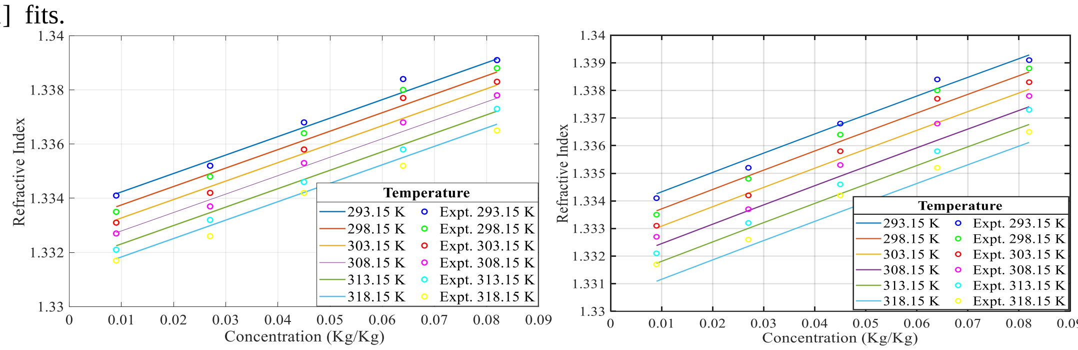
(a) (b)

Fig. 4 Concentration and temperature dependence of the refractive index of glucose (a) proposed (b) reported [1] fits.



(a) (b)

Fig. 5 Concentration and temperature dependence of the refractive index of BSA (a) proposed (b) reported [1] fits.



(a) (b)

Fig. 6 Concentration and temperature dependence of the refractive index of ethyl acetate (a) proposed (b) reported [1] fits.

where c and T represent respectively the concentration of the solution and the temperature (in Kelvin). In the present analysis, the different values of T such as 293.15 K, 298.15 K, 303.15 K, 308.15 K, 313.15 K, and 318.15 K, and different range of values for c have been taken from [1] for the comparison purpose.

3. Results and Discussions

3.1. Concentration and temperature dependence of the refractive index

In order to investigate the variation in refractive index values of the different considered solutions with respect to concentration and temperature values, the proposed Eqs. (1) – (6) have been utilized. Moreover, for the comparison purpose the values of refractive index corresponding to different values of concentration and temperature for the different solutions have been calculated and plotted in Figs. (1) – (6); and by utilizing the proposed models and the expressions reported in [1] alongwith the experimental data reported in Table 2 - Table 5 of [1]. From Figs. 1 and 2, it is observed that compared to the values of refractive index calculated from the proposed exponential models the values of refractive index calculated from the polynomial expressions reported in [1] are relatively close to the experimental values for the lower values of concentration; while, for the higher values of concentration there is large deviation from the experimental values.

Further, with the increase in temperature the refractive index values calculated using polynomial expressions deviates significantly from the experimental values compared to that obtained from the proposed exponential models. On the other hand, there is no any significant difference between the two plots obtained by utilizing the polynomial expressions and the exponential models in Figs. 3 and 4. This is mainly due to the fact that with the increase in temperature the variation in the refractive index values of the $CaCl_2$ and glucose solutions are less compared to that in the NaCl and KCl solutions.

Moreover, in Figs. 5(b) and 6(b), the refractive index values calculated by utilizing polynomial expressions are generally overestimated for the lower value of temperature and as the temperature increases this trend changes and the calculated values of the refractive index are underestimated. This shows that the reported polynomial expressions are unable to estimate the precise values of the refractive index for the BSA and ethyl acetate solutions. While, the calculated values of the refractive index for the BSA and ethyl acetate solutions by utilizing proposed exponential models have uniform nature of variation with respect to the variation in temperature. Therefore, it is concluded that the concentration and temperature dependent values of the refractive index for the different solutions obtained from the proposed exponential models are very close to the experimental values compared to the values obtained from the polynomial expressions reported in [1]. Further, since, the proposed models consist of fewer coefficients compared to polynomial expressions reported in [1], therefore it is computationally simple in nature.

3.2. Temperature and concentration dependence of the refractive index

The variations in refractive index values of the above six solutions with respect to the variation in temperature at different concentrations have been investigated and plotted in Figs. (7)(a) – (12)(a) using the Eqs. (1) - (6). Further, for the comparison purpose the values of the refractive index calculated from the polynomial expressions reported in [1] have also been shown in Figs. (7)(b) – (12)(b).

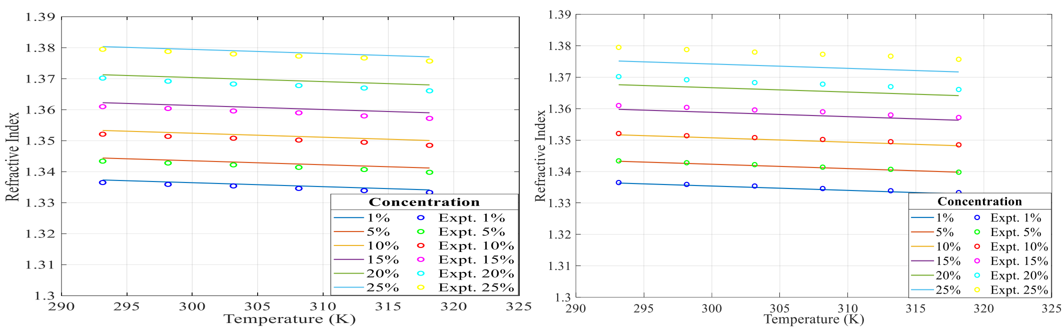
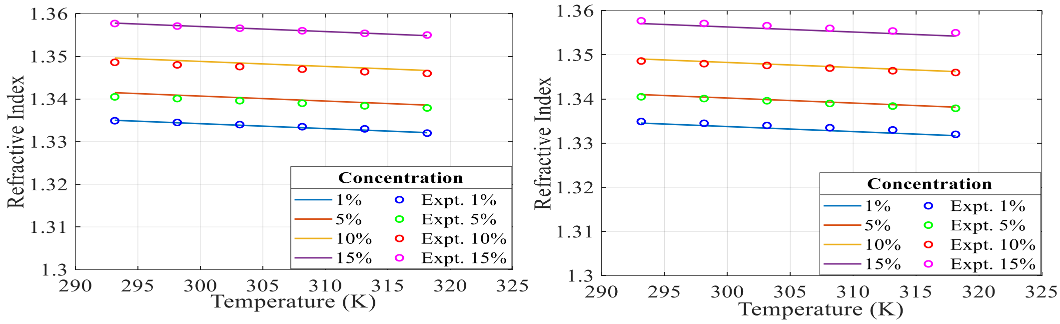
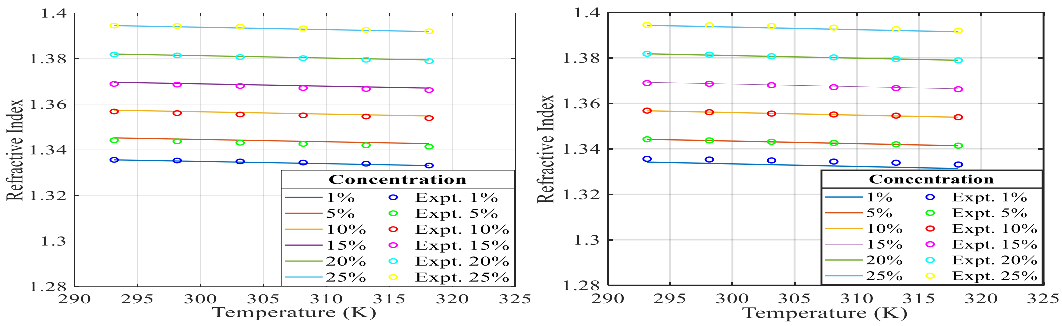


Fig. 7 Temperature and concentration dependence of the refractive index of NaCl (a) proposed (b) reported [1] fits.



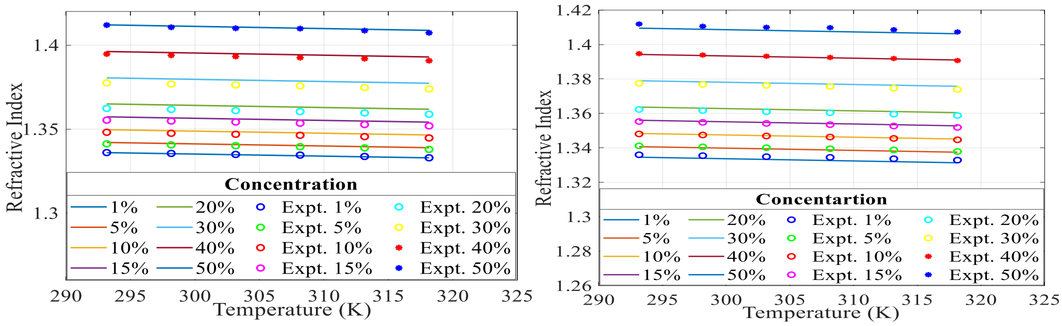
(a) (b)

Fig. 8 Temperature and concentration dependence of the refractive index of KCl (a) proposed (b) reported [1] fits.



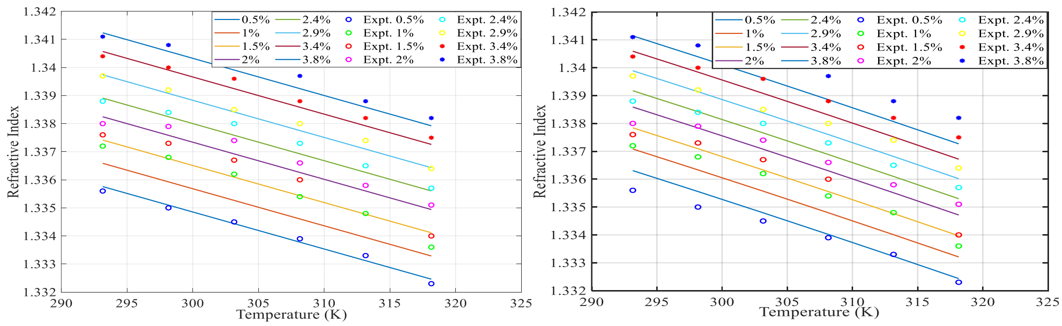
(a) (b)

Fig. 9 Temperature and concentration dependence of the refractive index of $CaCl_2$ (a) proposed (b) reported [1] fits.



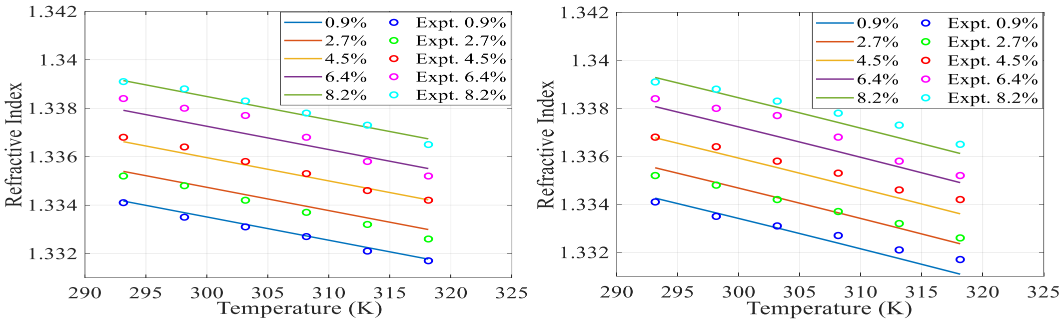
(a) (b)

Fig. 10 Temperature and concentration dependence of the refractive index of glucose (a) proposed (b) reported [1] fits.



(a) (b)

Fig. 11 Temperature and concentration dependence of the refractive index of BSA (a) proposed (b) reported [1] fits.



(a) (b)

Fig. 12 Temperature and concentration dependence of the refractive index of ethyl acetate (a) proposed (b) reported [1] fits.

In this section, the same six solutions have been considered and the range of concentration and temperature values are also same as considered in section 3.1. The purpose of the study considered in this section, is to observe the rate of variations in refractive index values with respect to the variation in temperature and the rate of variations in refractive index values with respect to the variation in concentration for the same solutions. It has been observed that, in all the considered solutions the rate of variations in refractive index values with respect to the variation in temperature is lower than the rate of variations in refractive index values with respect to the variation in concentration. Further, it has also been observed that with the increase in the concentration, refractive index values of the different solutions increases while with the increase in the temperature it decreases.

4. Conclusions

In order to calculate concentration and temperature dependent refractive index values and the coefficient of its derivatives with respect to concentration and/or temperature precisely for the different kind of solutions; simple exponential models have been proposed for the six solutions namely, three electrolyte (KCl, $NaCl$, and $CaCl_2$), a polar (*glucose*), a non-polar (*ethyl acetate*), and a protein (*bovine serum albumin*) solutions. Further, for the comparison purpose the concentration and temperature dependent refractive index values of the considered solutions have been calculated using the proposed exponential models and the polynomial expressions reported in the literature. It has been observed that the refractive index values obtained using the proposed exponential models for the different solutions are very close to the experimental values compared to the values obtained by utilizing polynomial expressions. Further, the polynomial expressions require five coefficients while in the proposed models there is need of only three coefficients. Therefore, the proposed exponential models for the calculation of refractive index at different values of concentration and temperature require fewer coefficients and hence computationally simple in nature and provide very precise values compared to the models reported in the literature. This validates the superiority of the proposed models and similar expressions can be obtained for the estimations of concentration and temperature dependent refractive index values of other kind of solutions.

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