NATURENGS
MTU Journal of Engineering and Natural Sciences
https://dergipark.org.tr/tr/pub/naturengs
DOI: 10.46572/naturengs.950220

Research Article

A Simple Expression for the Refractive Index of Distilled Water

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(**Received:** 09.06.2021; **Accepted:** 19.09.2022)

ABSTRACT: Water is conceivably the most important material in the universe and essential to the functioning of all the known life forms. The refractive index is an important physical parameter that can be used to characterize and understand the properties of water. Therefore, accurate knowledge of the refractive index of water is of great importance. A simple expression for the real part of the refractive index of water was investigated and a new equation was proposed as a function of the temperature of distilled water between 0 and 100 ºC and wavelengths in the range of 200 to 1100 nm. Water is transparent in visible light and has a complex optical absorption property in the infrared and ultraviolet spectra. The refractive index highly depends on wavelength and temperature. The expression for the refractive index is helpful for different applications in biomedical optics. The proposed formula derived by using genetic programming methods has accurate terms, has a good agreement, and demonstrates increased performance with experimental measurements for calculations of knowledge of the refractive index of water at given ranges.

Keywords: Water, Temperature, Wavelength, Modelling, Refractive index.

1. INTRODUCTION

Water is an essential biological liquid. The liquid component of blood is about 90% water in plasma form. Human blood consists of approximately 54.3% of plasma. The water is more than half of the total blood volume. Water is presented in free and bound states with biomolecules in biological tissues. The water molecules can be combined with blood contents such as proteins, different concentrations of glucose, and other components. The substances were dissolved and transmitted into and out of a cell. Blood sample analysis is very important for the diagnosis of various diseases. The observed changes in the optical properties of water have advantages in medical and optical diagnostic techniques. The change in liquid refractive index, n, can be calculated by different experimental methods [1]. An expression overcomes the difficulties of determining the refractive index in less time for the given ranges.

The working principle, performance, and optimization of the sensors and new devices were determined and characterized by physics and responses in selected conditions of the elementary material. The knowledge of the refractive index of biological solutions and clinically relevant materials facilitates the design and optimization of new sensors [2]. In addition, determining

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the optical properties of water is an essential prerequisite to understanding the physical and chemical properties of aqueous environments [3]. In a laboratory, the refractive index was measured at a constant temperature. For real practical applications, the refractive index measurement as a function of temperature and wavelength simultaneously must fulfill some important requirements of the sensor research. The properties of different phases of water have been extensively investigated by scientists and engineers as a function of the wavelength (λ) or temperature (T) for several decades [3-7]. Measurement of the optical refractive index as an inherent characteristic of the substance is a formal investigation in research [8]. The refractive index represents the response of the electronic charge distribution to the disturbance brought about by the electric field component of incident electromagnetic radiation [9]. Water molecules are polar and if exposed to an electromagnetic wave, they will swing around and try to stay lined up with the alternating electric field. The properties of water play a role in understanding the electron charge transfer rates and behavior of aqueous solutions and determining the oxidation states of minerals and rocks used throughout science and industry [10]. These two parameters are the most known factors affecting the refractive index by modifications in the band gap energy and dielectric constant of water.

The structural and transport properties of the most abundant molecule on the earth's surface have been investigated to understand the material properties. In this article, the expression for the refractive index of distilled water formula as a function of wavelength and temperature has been studied using genetic programming in the given ranges. The genetic programming provided experimental data to calculate the desired parameter of given problems [11]. This is a powerful modeling technique for the simple expression of the water refractive index. The method adapted from the Darwinian evolution theory of natural selection has chromosomes and gene expression trees [12, 13]. The iterative process is used to generate an expression with a given accuracy. Genetic programming is a tool for predicting parameters in medicine, social sciences, and other disciplines. Genetic programming was explained in books and papers [13-18]. It aimed to be in the best fitness zone, minimize errors, simplify, and find the best predicted results [19]. A combination of these was investigated to increase the algorithm's performance to predict output parameters. The accuracy of the model was evaluated using statistical parameters such as root mean square error (RMSE), which is the best model with the lowest value or mean absolute error (MAE). The coefficient of correlation and explanations of these parameters have been provided in detail Ref. [19]. The correlation coefficient (R) was used to calculate the model performance. The calculated results of this study with these parameters were in good agreement with the experimental results.

2. MATERIAL AND METHODS

Common computing techniques were used to propose new expressions and solve real-life problems. The latest and high-performance computers and advanced techniques could solve problems and determine parameters for scientists and computer programmers. The genetic programming technique created the water refractive index expression in this study. The variables consist of temperature and wavelength as input and refractive index for output. The function sets used were +, −, *, /, √, exp(x), x^2, x^2, $x^{1/3}$, with seven head sizes and three genes were used for the proposed simple expression of calculating the $n(T, \lambda)$. The number of training samples was 70% of the total samples (155), and 25% for validation, with 5% for testing. The training data were used to implement and build a model for the sake of the remastered version and the validation data was used to validate the results with the renewed model. 5% of the data points in all the data are excluded from the dataset and are used to test the proposed expressions. Validation and test data were chosen randomly and equally spaced in these data sets.

Table 1. The genetic programming parameters used for the proposed model.

Statistical Coefficient	Training	Validation
R^2	0.93510	0.94291
Mean Squared Error (MSE)	3.1 10^{-5}	3.4 10^{-5}
Mean Absolute Error (MAE)	0.00531	0.00483
Relative Absolute Error (RAE)	0.25895	0.28174
Root Mean Squared Error (RMSE)	0.00617	0.00584
Correlation Coefficient	0.96700	0.97103

The correlation coefficient, R^2, showed the flawless fit of the data and how it is greater than 0.93 in Table 1. These values demonstrated that the proposed model's performance is highly accurate. The correct number of training and test data depends on the task, the desired performance, the input features, the noise in the training data, the noise itself, the complexity of the model, and so on. The bigger the dataset, it is that much more preferred to train it. The employed computational method has the potential to save costs while broadening accessibility.

3. RESULTS AND DISCUSSION

The change in refractive index in water is not attributable to temperature because it is not linear [9, 10]. The expression for the refractive index was collected from the literature [9, 20-22]. The performance of genetic programming by comparing the experimental and the predicted values are given in Fig. 1. It is observed that the critical trends in formulation proposed by the genetic programming formula for the refractive index in overall performance are successful. There are different formulations for determining the water refractive index but no direct, explicit formulations related to temperature and wavelength.

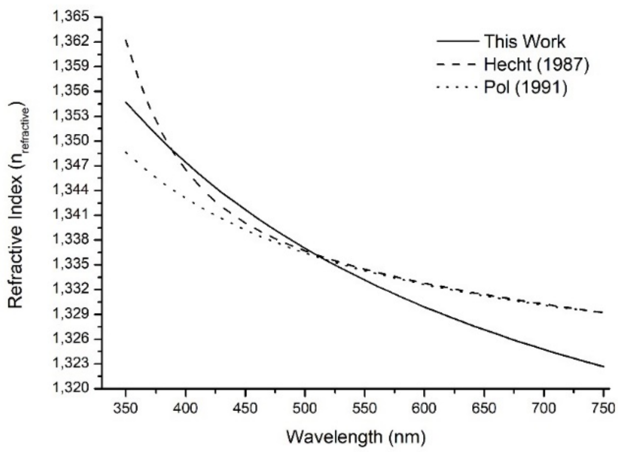

Figure 1. The comparison of equations for the refractive index of water.

The wavelength dependence of the water refractive index in the visible region was used to compare the results of the proposed expression given in the literature [23-25] as

$$n(\lambda) = A + \frac{B}{\lambda^2} - \frac{C}{\lambda^4} + \frac{D}{\lambda^6} \tag{1}$$

$$n(\lambda) = 1.31848 + \frac{6.662}{\lambda - 129.2} \tag{2}$$

where λ is a wavelength, the coefficients are A = 1.3199, B = 6.788 10^3, C = 1.132 10^9 and D = 1.11 10^{14} in Eqn. 1. The water was transparent at visible wavelengths. In Fig. 1, we compare the refractive index of water as a function of wavelengths in the visible range of the spectrum at room temperature. The refractive index values are decreased with increasing wavelengths and our proposed formula's results show good agreement. The results of these equations have been obtained for a room temperature environment and the temperature was not included in Eqn. 1 and Eqn. 2. Water refractive index's temperature and wavelength dependence are critical for biomedical optical applications. The goal of this study is to obtain the simple expression for water refractive index as a function of temperature and wavelength

$$n_{refractive}(\lambda,T)=1.28900+\frac{16.45262\,\lambda+\lambda^{4/3}+11.86573\,\lambda-108.85351}{\lambda\,(\lambda+T-9.173768)} \tag{3}$$

where λ is a wavelength, and T is the temperature. This expression is valid in the range from 200 nm to 1100 nm, and the temperature ranges from 0 °C to 100 °C.

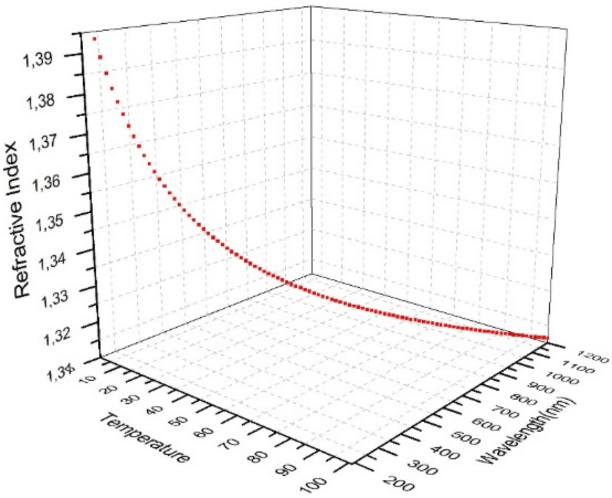

Figure 2. The synergistic effects of each parameter in refractive index, n(λ, T).

The data shows that the water refractive index decreases with the increase in both wavelength and temperature in Fig 2. The water refractive index was directly calculated and we overcame this limitation by using our proposed expression, which agreed with our experimental and predicted results. The Cauchy formula was used to determine the water refractive index dependency on temperature and wavelength. The coefficients in Eqn.1 were temperature-dependent and in the form of A(T), B(T), C(T) and D(T). There were variable coefficients for each temperature value and the variables were determined by curve fitting methods in Ref. [22].

In addition, the electronic band gap of water has been inferred from using the formula of its refractive index, *n*, which can be obtained by genetic programming. According to the single-oscillator model, the Penn model, the refractive and the electronic gap E_g are correlated as

$$n^2 = 1 + \frac{(\hbar\omega)^2}{{E_g}^2} \tag{4}$$

where ω is the frequency [26], this correlation between n and E_g holds for materials. Measurements of the band gap of water by light are not practicable under some conditions; therefore, establishing the correlation between the band gap and the refractive index is a crucial step in inferring band gaps from measured dielectric constants [27]. The image below compares the experimental and predicted values of Fig. 3 and Fig. 4.

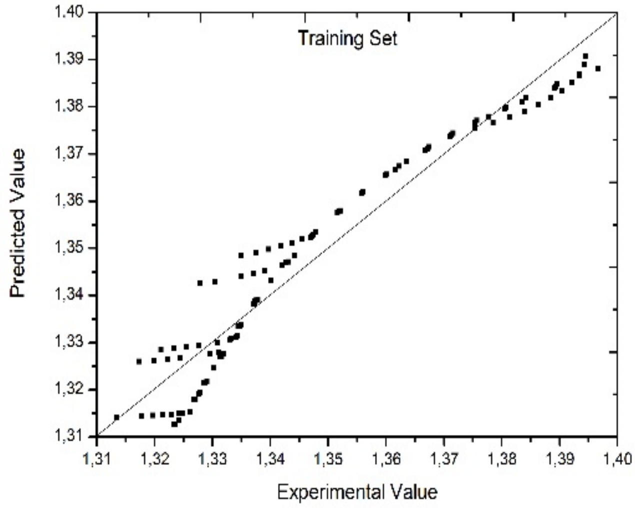

Figure 3. The values of water refractive index for the training dataset.

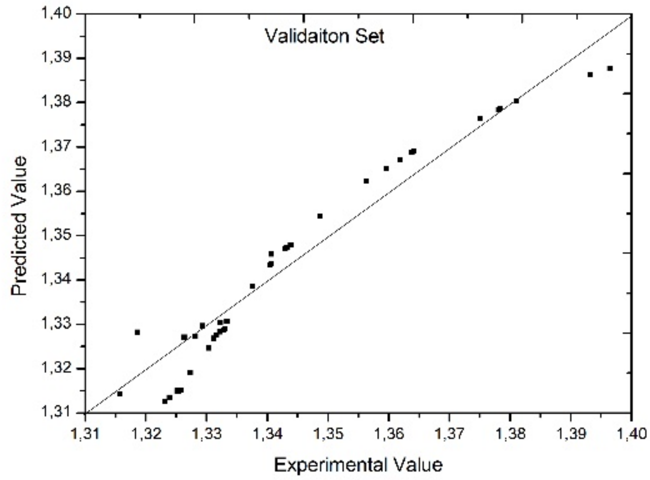

Figure 4. The values of water refractive index for validation dataset.

The refractive index of water decreasing with the temperature and wavelength can be easily shown in the proposed formula. Therefore, comparing the difference between test and reference substance is preferable to achieve reliable changes in the result. The water content of substances generally characterizes the refractive indices and the entire spectra exhibit additional strong features due to solvents in its contents. The effect of temperature on the refractive index is much smaller than that of solution or solvent alone. The index difference corresponds to distilled water and different liquids or water with various soluble additives dissolved inside. The sources of differences at low and high values on experimental and predicted uncertainties in the wavelength and temperature data caused values. It can be noted from Fig. 3 and Fig 4 the good agreement between our theoretical predictions with the experimental results. The results shown in such a figure suggest that our predicted formula and our results were almost ideal.

4. CONCLUSIONS

In this study, we proposed a simple expression for water refractive index as a function of wavelength and temperature. The genetic programming works well and provides optimized parameters of real parts of the refractive index. For optimizing and adjusting the parameters of new methods and techniques at given temperatures, the refractive index of water can be used as a reference. It allows us to compare all the parameters with one another in calibration and measurement. The predictive capacity of the program is 93.51% of the training and 94.29% of the validation results. The proposed equations are user-friendly. The proposed formulation's statistical parameters (R2, MAPE, and RMS) show high potential for predicting the refractive index and using the results for diagnostic purposes. This study also developed and analyzed a simple linear refractive index formula of distilled water as a reference liquid for parameters. The results have potential in the future of biomedical device applications. The water-related science has a broad area, and these types of studies and results are essential for researchers. The optical properties of materials are necessary to determine and improve the prospects of device performance. The knowledge of such quantities presented here is expected for designing optical devices and their applications.

Acknowledgments
This work was not supported by any institution or organization.

Conflict of Interest
All authors declare that they have no conflicts of interest.

Author Contribution
REO. and MO. verified the analytical methods and REO. performed the computations. REO wrote the manuscript with support from MO. The authors contributed to the final version of the manuscript.

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