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Using artificial neural network to predict velocity of sound in liquid water as a function of ambient temperature, electrical and magnetic fields

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Abstract

One of the main thermophysical properties of liquid water is velocity of sound. However, the effect of different externalities on velocity of sound in liquid water is not well known. Therefore, in current study, by designing an artificial neural network (ANN) velocity of sound in liquid water under different externalities is predicted. Selected externalities are ambient temperature from 272.65 K to 348.43 K, different electrical fields in range of 0 V/m to 4.03E + 9 V/m and magnetic fields in range of 0–10.0594 T. To prepare of reference dataset for entry to ANN, numerical and experimental data as macroscopic reference data are extracted from microscopic characteristic of water HB strength. In order to achieve an appropriate ANN, ANN architecture sensitivity analysis is conducted by using an iterative algorithm. Learning procedure in the selected feed-forward back propagation ANN is done by hyperbolic transfer functions. Also, Levenberg–Marquardt algorithm is utilized for the optimization process. ANNs output showed that the maximum MSE in prediction of velocity of sound is 0.00066. Also, the minimum of correlation coefficient in prediction of velocity of sound is 0.99131. Based on the ANNs outputs, weights and bias, an equation to predict of velocity of sound in liquid water under intended externalities is proposed. Also, according to weight sensitivity analysis input of electrical fields with 63% relative importance percentage has a grater impression on the response variable of velocity of sound in liquid water.

Keywords: Artificial neural network; Electrical field; Magnetic field; Velocity of sound; Temperature.

1. Introduction

The most abundant and vital liquid on our planet is water. So, it has been studied more than any other liquid by scholars. However, weird properties of water resulted to being a ‘‘complex fluid’’ with a lot of anomalies [1–3]. On the other hand, according to comprehensive application of liquid water at microscopic and macroscopic scales, it is necessary to understand of liquid water properties. Therefore, several numerical and experimental studies are conducted to cognition of liquid water properties in recent decade [4–7]. However, there are a lot of issues in field of liquid water properties which are not well known.

In this regard, environmental conditions are effective on liquid water properties. Ambient temperature, electrical field and magnetic field are some of the most important externalities which are impressive on liquid water properties. Several works related to study the effects of externalities on water are done by scholars [8–12]. While, these papers are only focused on effects of externalities on the hydrogen bonding (HB) strength of water in a restrict interval of their considered externalities. Hence, lack of study related to impression of different externalities on the thermophysical properties of liquid water is observable. Velocity of sound in liquid water is one of the important thermophysical properties in liquid water. So, velocity of sound in liquid water under different externalities is studied in the current paper. It is notable that, to access the velocity of sound in liquid water under different externalities, a lot of experiments or numerical simulations must be done, which are time consuming and expensive. Also, velocities of sound in liquid water under different externalities are complex and non-linear problem. Therefore, forecasting method according to available information such as soft computing

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and artificial intelligence tools including neural networks are proposed.

Although, there is no study in order to predict of velocity of sound in liquid water by using artificial neural network, however, there are several studies related to using soft computing (e.g. artificial neural networks) in context of acoustic and hydro-acoustic [13–17]. In this regard, Luo et al. [18] offered an artificial intelligent method to build a neural network model of multi-parameter sound velocity prediction. They focused sound velocity of marine sediment and showed an appropriate accordance of predicted and experimental data. Liu et al. [19] presented a more general predicting method to estimate of sound absorption coefficients at six central frequencies of a sandwich structure nonwoven absorber. They conducted their study by using general regression neural network (GRNN) as an estimation model to bridge the gap between the measured structural parameters of each absorber and its sound absorption coefficient. Novel biologically inspired method to classify of sound event that combines spike coding with a spiking neural network (SNN) is proposed by Dennis et al. [20]. They showed the superiority of spiking neural network versus conventional cross-entropy neural networks. Recently, Zhang et al. [21] in paper titled as “Sound quality prediction of vehicle interior noise and mathematical modeling using a back propagation neural network (BPNN) based on particle swarm optimization (PSO)” solve the complex non-linear problem between the subjective sound quality evaluation results by using a back propagation neural network.

Based on cited literature, lack of study related to predict of velocity of sound in liquid water under different externalities and necessity of study in this context is detectable. As a result, novelty of present paper is study and prediction of velocity of sound in liquid water under different externalities by using artificial neural network (ANN). To this accomplishment, influence of different electrical fields, magnetic fields and different ambient temperatures on velocity of sound in liquid water are predicted.

The following sections are organized as follows. Influences of external fields on water HB and velocity of sound in liquid water vs. water HB strength are reviewed in Section 2. Then, in Section 3, theoretical and computational procedures based on ANN architectures are provided. The results of ANN training procedure and predicted results are presented and discussed in Section 4. Finally, Section 5 is given for the conclusions.

2. Influences of external fields on water HB

Gases, liquid and solid are three phases of water. Water environmental condition (e.g. ambient temperature and pressure) and external fields have key role in existence of these different phases. So that, these factors are impressive on the molecular structure of water, especially on the average number of hydrogen bonding (nHB) and strength of HB in water. It is also notable that, according to continuum models of water, it has a space-filling hydrogen bond network. The strength of covalent bonding between oxygen-hydrogen bonding in an individual water molecule in liquid phase at 298.15 K is 492 kJ $mol^{-1,}$ while the hydrogen bonding between one molecule oxygen atoms to hydrogen atom of another water molecule has an averaged strength of 23.3 kJ mol^{-1} [22,23].

These are different definition for strength of HB in water. In this regard, one of the useful definitions for strength of HB in liquid water is the energy required to break and completely separate of bond as sum of maximum four hydrogen bonds per molecule [22]. We use this dentition to determine of strength of HB in liquid water in the current study. So that, averaged number of hydrogen bonding (n_{HB}) of each an individual water molecule is multiply by its related strength is intended as HB strength of an individual water molecule.

On the other hand, length and angle of HB are two affective parameters on the HB strength. These parameters are dependent on polarization shifts in different hydrogen-bonded environments. Small change of HB length and angle resulted to significant variations in strength of HB. On the other words, stronger HB is predicted under lower HB length. Therefore, it can be conclude that, external fields are impressive on HB strength by change of HB length and angle and consequently, are effective on the strength of donor and acceptor atom in HB.

Ambient temperature is one of the most important effective externalities on the water molecules. Water molecules clusters and strength of HB are under influence of temperature difference. So that super-cooled water, ambient water, supercritical water and gaseous water are obtainable. In the present paper, we are interested on the ambient water. Ambient water is ubiquitous phase of water which forms in temperature interval of 273.15–373.15 K. Importance of ambient water resulted to several theoretical and experimental studies related to investigate of impression of temperature difference on the strength of HB [24–26]. In these studies, scholars used X-ray Raman spectroscopy (XRS) and X-ray absorption spectroscopy (XAS) to study the effects of temperature difference on the HB strength [27,28]. On the other hand, average number of hydrogen bonding (n_{HB}) is another efficient parameter to study the change of one water molecules due to its surrounding effects. In this regards, several studies related to the influence of temperature on the n_{HB} by using molecular simulations are conducted [8,9,23]. According to these studies, one can be concluded that, tendency of individual water molecules to enhancement of n_{HB} is decreased by water temperature increment.

On the other hand, bipolar structure of water molecules and delocalization of electrons between water molecules resulted to capability of water interaction with external field including magnetic, electric and electromagnetic fields. Enhancement of HB strength in direction of external electrical field is predictable [29]. The reason of this fact is related to polarizability of water molecule. In addition, increase of HB and diminish of water cluster size with impose of electrical filed is detectable [30,31]. However, Suresh et al. [10] indicated that electrical fields can only enhance the HB structure