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Prediction of Thermophysical Properties of Helium Using Linear Prediction and Artificial Neural Networks

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Abstract

Thermophysical properties of helium are significant in practical applications. However, the values of properties vary under different circumstances, which may have bad impacts on practical productions and applications. In our study, computational models like Linear Prediction and Artificial Neural Networks (ANNs) are applied to predict the thermophysical properties of the chemical substances. By analyzing 50 data groups using Linear Prediction, General Regression Neural Network (GRNN) and Multilayer Feedforward Neural Network (MLFN) methods, 9 models were successfully established to predict the thermophysical properties of helium, including density, energy, enthalpy, entropy, isochoric heat capacity, isobaric heat capacity, viscosity, thermal conductivity and dielectric constant. Within permissible error range (30% tolerance), our models were proved to be robust and accurate which indicates that ANN models can be used to predict the thermophysical properties of helium.

Keywords: *helium, thermophysical property, artificial neural networks, linear prediction, General Regression Neural Network, Multilayer Feedforward Neural Network*

1. Introduction

Thermodynamics is a kind of natural science about heat and temperature including their connection with energy and work [1]. It defines macroscopic variables, such as internal energy, entropy and pressure that partially describe a body of matter or radiation. It states that the behavior of those variables is subject to general constraints which are common to all materials instead of the peculiar properties of particular materials. These general constraints are accurately expressed in the four laws of thermodynamics. Thermodynamics primarily explores the bulk behavior of the body rather than the microscopic behaviors of the very large numbers of its microscopic constituents [2]. In the field of the microscopic constituents, statistical mechanics can be applied to explain its laws.

In the field of electrochemistry, the direction and extent of the chemical reaction can be realized via researching on a thermodynamics system. However, the values of those thermodynamic variables of these electrochemical materials such as helium are difficult to obtain, which becomes a great obstacle of the related studies. Realizing that a quick and effective model to predict the properties is needed, we focused on finding a proper way to distinguish the structure characteristics of different gases and train the accurate Artificial Neural Networks (ANNs) with the help of the module of software in order to obtain an accurate Artificial Neural Network to predict the thermodynamics variables of helium.

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2. Artificial Neural Networks

Artificial Neural Networks (ANNs) [3-5] are computational models inspired by animals' central nervous systems that have the ability of machine learning and pattern recognition. They are usually showed as systems of interconnected "neurons" that can count different values from inputs via feeding information through the network. As the algorithm develops, this method is mature and has been adopted into the module of the software [6-12].

In our study, we aimed at establishing different ANN models based on the existing thermophysical properties of helium. With the aid of the models, the thermophysical properties of helium can be predicted accurately under different cases.

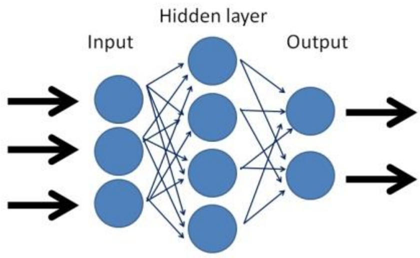

Figure 1. A Schematic View of Artificial Neural Network Structure

As can be seen from the figure above, the main structure of the Artificial Neural Network (ANN) is made up of the input layer and the output layer. The input variables are introduced to the network by the input layer [13]. Also, the response variables with predictions, which stand for the output of the nodes in this certain layer, provided by the network .Additionally, the hidden layer is included. The type and the complexity of the process or experimentation usually iteratively determine the optimal number of the neurons in the hidden layers [14].

3. Selection of Variables

In order to ensure the robustness and accuracy of the models, the temperature and pressure are regard as the independent variable in all models. Once a model is trained, all the other thermophysical properties are considered as the independent variables. Take the energy (*E*) prediction model as an example, once the energy prediction model was trained, all the other thermophysical properties as well as temperature and pressure were set to be the independent variables, which ensure the robustness and accuracy of the prediction model.

4. Training Process of Neural Networks

The ANN prediction model is constructed by the NeuralTools® software (Trial Version, Palisade Corporation, NY, USA) [15]. The General Regression Neural Networks (GRNN) [16-18] module and Multilayer Feedforward Neural Networks (MLFN) [19-21] module was selected as the training modules.

The data of thermodynamic and transport properties of helium are generated from the equations of state presented in the references below [22-24]. The properties are density (ρ), energy (E), enthalpy (H), entropy (S), isochoric heat capacity (C_v), isobaric heat capacity (C_p), thermal conductivity (λ), viscosity (η), and dielectric constant (D). All extensive properties are given on a molar basis. The references [22-24] should be consulted for information on the uncertainties and the reference states for E,H, and S. The training and testing results are shown as follows (Data source: *CRC Handbook of Chemistry and Physics* [25]):

Table 1. The Training Result of Density in Different ANN Models

ANN Model	Trained Samples	Tested Samples	RMS Error	Training Time	Finishing Reason
Linear Predictor	33	17	0.03	0:00:00	Auto-Stopped
GRNN	33	17	1.78	0:00:00	Auto-Stopped
MLFN 2 Nodes	33	17	6.88	0:00:58	Auto-Stopped
MLFN 3 Nodes	33	17	4.48	0:01:00	Auto-Stopped
MLFN 4 Nodes	33	17	2.91	0:01:14	Auto-Stopped
MLFN 5 Nodes	33	17	6.39	0:01:32	Auto-Stopped

According to the results presented by Table 1, we considered the Linear Predictor module is a better module to predict the values of density (RMS error: 0.03). 100% tested samples showed accurate results within permissible error range (30% tolerance). Therefore, there are totally 17 successful samples. The training results are shown as Figure 2:

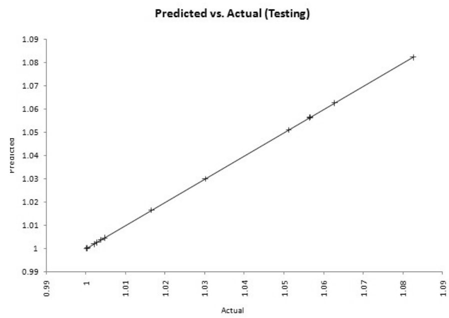

Figure 2. Comparison of the Predicted Values and Actual Values of Density during Testing Process

Table 2. The Training Result of Energy in Different ANN Models

ANN Model	Trained Samples	Tested Samples	RMS Error	Training Time	Finishing Reason
Linear Predictor	33	17	3.04	0:00:00	Auto-Stopped
GRNN	33	17	5886.08	0:00:00	Auto-Stopped
MLFN 2 Nodes	33	17	542.06	0:00:52	Auto-Stopped
MLFN 3 Nodes	33	17	490.03	0:00:47	Auto-Stopped
MLFN 4 Nodes	33	17	864.22	0:01:06	Auto-Stopped
MLFN 5 Nodes	33	17	1571.99	0:01:24	Auto-Stopped

According to the results presented by Table 2, we considered the Linear Predictor module is a better module to predict the values of energy (RMS error: 3.04). 94.1176%tested samples showed accurate results within permissible error range (30% tolerance). Therefore, there are totally 16 successful samples. The training results are shown as Figure 3:

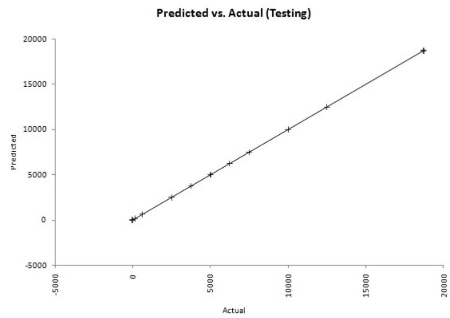

Figure 3. Comparison of Predicted Values and Actual Values of Energy during Testing Process

Table 3. The Training Result of Enthalpy in Different ANN Models

ANN Model	Trained Samples	Tested Samples	RMS Error	Training Time	Finishing Reason
Linear Predictor	33	17	7.92	0:00:00	Auto-Stopped
GRNN	33	17	89.12	0:00:00	Auto-Stopped
MLFN 2 Nodes	33	17	439.37	0:00:46	Auto-Stopped
MLFN 3 Nodes	33	17	159.59	0:00:48	Auto-Stopped
MLFN 4 Nodes	33	17	109.55	0:01:13	Auto-Stopped
MLFN 5 Nodes	33	17	273.35	0:01:17	Auto-Stopped

According to the results presented by Table 3, we considered the linear predictor module is a better module to predict the values of enthalpy (RMS error:7.92). 100 % tested samples showed accurate results within permissible error range (30% tolerance). Therefore, there are totally 17 successful samples. The training results are shown as Figure 4:

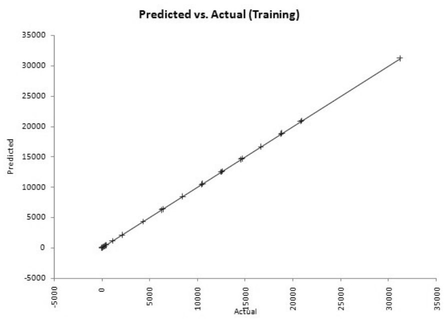

Figure 4. Comparison of the Predicted Values and Actual Values of Enthalpy during Testing Process

Table 4. The Training Result of Entropy in Different ANN Models

ANN Model	Trained Samples	Tested Samples	RMS Error	Training Time	Finishing Reason
Linear Predictor	33	17	10.46	0:00:00	Auto-Stopped
GRNN	33	17	15.96	0:00:00	Auto-Stopped
MLFN 2 Nodes	33	17	3.52	0:00:43	Auto-Stopped
MLFN 3 Nodes	33	17	8.79	0:00:50	Auto-Stopped
MLFN 4 Nodes	33	17	5.53	0:00:59	Auto-Stopped
MLFN 5 Nodes	33	17	14.25	0:01:21	Auto-Stopped

According to the results presented by Table 4, we considered the MLFN 2 Node module is a better module to predict the values of entropy (RMS error: 3.52). 94.1176% tested samples showed accurate results within permissible error range

(30% tolerance). Therefore, there are totally 16 successful samples. The training results are shown as Figure 5:

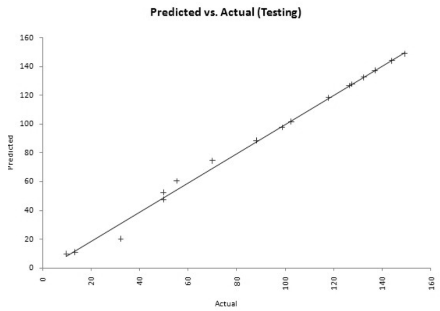

Figure 5. Comparison of the Predicted Values and Actual Values of Entropy during Testing Process

Table 5. The Training Result of Isochoric Heat Capacity in Different ANN Models

ANN Model	Trained Samples	Tested Samples	RMS Error	Training Time	Finishing Reason
Linear Predictor	33	17	0.31	0:00:00	Auto-Stopped
GRNN	33	17	0.48	0:00:00	Auto-Stopped
MLFN 2 Nodes	33	17	1.30	0:01:51	Auto-Stopped
MLFN 3 Nodes	33	17	1.28	0:01:39	Auto-Stopped
MLFN 4 Nodes	33	17	1.98	0:01:39	Auto-Stopped
MLFN 5 Nodes	33	17	1.66	0:01:51	Auto-Stopped

According to the results presented by Table 5, we considered the Linear Predictor module is a better module to predict the values of isochoric heat capacity (RMS error: 0.31). 100% tested samples showed accurate results within permissible error range (30% tolerance). Therefore, there are totally 17 successful samples. The training results are shown as Figure 6:

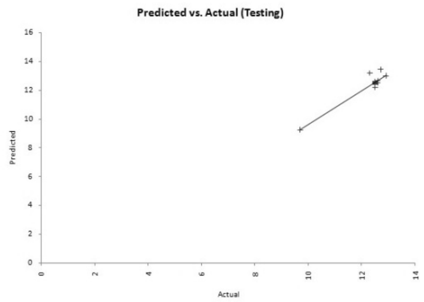

Figure 6. Comparison of the Predicted Values and Actual Values of Isochoric Heat Capacity during Testing Process

Table 6. The Training Result of Isobaric Heat Capacity in Different ANN Models

ANN Model	Trained Samples	Tested Samples	RMS Error	Training Time	Finishing Reason
Linear Predictor	33	17	1.69	0:00:00	Auto-Stopped
GRNN	33	17	1.89	0:00:00	Auto-Stopped
MLFN 2 Nodes	33	17	0.50	0:00:55	Auto-Stopped
MLFN 3 Nodes	33	17	1.62	0:01:11	Auto-Stopped
MLFN 4 Nodes	33	17	0.88	0:01:16	Auto-Stopped
MLFN 5 Nodes	33	17	1.96	0:01:50	Auto-Stopped

According to the results presented by Table 6, we considered the MLFN 2 Node module is a better module to predict the values of isobaric heat capacity (RMS error: 0.50). 100% tested samples showed accurate results within permissible error range (30% tolerance). Therefore, there are totally 17 successful samples. The training results are shown as Figure 7:

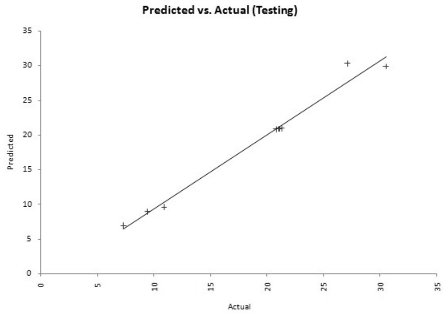

Figure 7. Comparison of the Predicted Values and Actual Values of Isobaric Heat Capacity during Testing Process

Table 7. The Training Result of Viscosity in Different ANN Models

ANN Model	Trained Samples	Tested Samples	RMS Error	Training Time	Finishing Reason
Linear Predictor	33	17	0.61	0:00:00	Auto-Stopped
GRNN	33	17	0.54	0:00:00	Auto-Stopped
MLFN 2 Nodes	33	17	0.30	0:00:45	Auto-Stopped
MLFN 3 Nodes	33	17	0.26	0:00:55	Auto-Stopped
MLFN 4 Nodes	33	17	0.40	0:00:57	Auto-Stopped
MLFN 5 Nodes	33	17	4.87	0:01:20	Auto-Stopped

According to the results presented by Table 7, we considered the MLFN 3 Nodes module is a better module to predict the values of viscosity (RMS error: 0.26). 100% tested samples showed accurate results within permissible error range (30% tolerance). Therefore, there are totally 17 successful samples. The training results are shown as Figure 8:

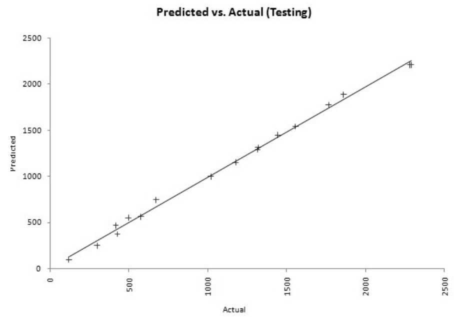

Figure 8. A Comparison of the Predicted Values and Actual Values of Viscosity (Testing)

Table 8. The Training Result of Thermal Conductivity in Different ANN Models

ANN Model	Trained Samples	Tested Samples	RMS Error	Training Time	Finishing Reason
Linear Predictor	33	17	54.39	0:00:00	Auto-Stopped
GRNN	33	17	76.41	0:00:00	Auto-Stopped
MLFN 2 Nodes	33	17	41.57	0:00:35	Auto-Stopped

MLFN 3 Nodes	33	17	71.61	0:00:37	Auto-Stopped
MLFN 4 Nodes	33	17	82.56	0:00:42	Auto-Stopped
MLFN 5 Nodes	33	17	130.84	0:01:03	Auto-Stopped

According to the results presented by Table 8, we considered the MLFN 2 Nodes module is a better module to predict the values of thermal conductivity (RMS error: 41.57). 100% tested samples showed accurate results within permissible error range (30% tolerance). Therefore, there are totally 17 successful samples. The training results are shown as Figure 9:

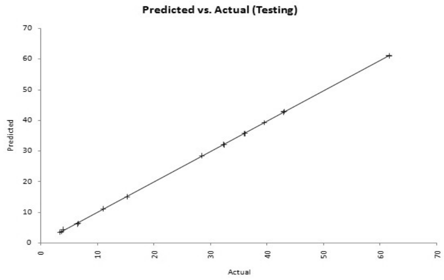

Figure 9. Comparison of the Predicted Values and Actual Values of Thermal Conductivity during Testing Process

Table 9. The Training Result of Dielectric Constant in Different ANN Models

ANN Model	Trained Samples	Tested Samples	RMS Error	Training Time	Finishing Reason
Linear Predictor	33	17	0.00003	0:00:00	Auto-Stopped
GRNN	33	17	0.00012	0:00:00	Auto-Stopped
MLFN 2 Nodes	33	17	0.00032	0:01:07	Auto-Stopped
MLFN 3 Nodes	33	17	0.01000	0:01:32	Auto-Stopped
MLFN 4 Nodes	33	17	0.01000	0:01:48	Auto-Stopped
MLFN 5 Nodes	33	17	0.01000	0:02:02	Auto-Stopped

According to the results presented by Table 9, we considered the Linear Predictor module is a better module to predict the values of dielectric constant (RMS error: 0.00). 100% tested samples showed accurate results within permissible error range (30% tolerance). Therefore, there are totally 17 successful samples. The testing results are shown in Figure 10:

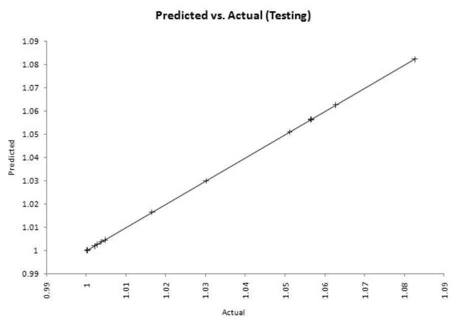

Figure 10. A Comparison of the Predicted Values and Actual Values of Dielectric Constant during Testing Process

5. Results and Discussion

According to the training results above, the best model of each thermophysical property could be obtained as Table 10:

Table 10. The Best Model of Each Thermophysical Property

	Density	Energy	Enthalpy	Entropy	Isochoric heat capacity	Isobaric heat capacity	Viscosity	Thermal conductivity	Dielectric constant
Best Model	Linear Prediction	Linear Prediction	Linear Prediction	MLFN 2 nodes	Linear Prediction	MLFN 2 nodes	MLFN 3 nodes	MLFN 2 nodes	Linear Prediction

On the basis of the results shown in table 10, we found that different thermophysical properties of helium should be developed by different ANN models, which can ensure the robustness of the prediction model. Every model corresponds with the requirement of the accuracy.

According to previous studies [26-30], we found out the similar researches on the gases' thermophysical properties. Vesovic and his co-workers [26] has developed a model using a pseudoradial distribution function to predict the viscosity of dense gas mixtures. Todd B. and his co-workers [27] provided an estimation method to obtain the thermophysical properties of different simple gases, which was based on the existing data and statistical analysis. Gardas and his co-workers [28] have developed a prediction method of thermophysical and transport properties of ionic liquids, which is based on group contribution methods. Roman Balabin and Ekaterina [29] compared six popular approaches of calibration models to predict the density of gasoline based a spectral data. Gy. Bohács and Z. Ovádi [30] have developed a procedure model to predict the quality parameters of gasoline on the basis of 350 commercially available gasoline samples. C. Laroche together with O. Vizika [31] used network modeling to calculate transport properties of porous media on the basis of interpretation of mercury invasion capillary pressure curves.

These previous studies are successful and can be used for references to our study, which have different advantages respectively by using different prediction models or calculation methods. However, there is still no report of prediction of the helium's thermophysical properties by using linear prediction and Artificial Neural Networks. Compared to the previous researches above, using Linear Prediction and ANN models to predict the relative properties is more convenient and easy to operate. What's worth mentioning is that using ANN models to predict such properties with the new distinction method of helium is easy to understand for operators.

In the field of electrochemistry, thermophysical properties of helium are of great significance in practical application. Different from other studies, we focused our research on the gases, which is hard to be described by the existing equations or calculation methods. Our study shows that Linear Prediction and ANN models are accurate models to predict the thermophysical properties of helium.

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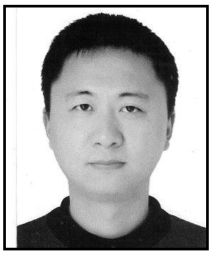

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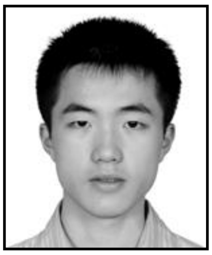

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