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Prediction of thermophysical properties of oxygen using linear prediction and multilayer feedforward neural network

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ABSTRACT

Thermophysical properties of oxygen are of great importance in practical applications. However, the values of the properties differs from each other under different circumstances, which may have bad influence in practical productions and applications. In our study, we mainly used computational models like Artificial Neural Networks (ANNs) to predict the thermophysical properties of the chemical substances. We succeeded in establishing 9 models to predict the thermophysical properties of oxygen, namely density, energy, enthalpy, entropy, isochoric heat capacity, isobaric heat capacity, viscosity and dielectric constant, by analyzing 51 data groups using linear prediction and Multilayer Feedfoward Neural Network (MLFN) methods. Within permissible error range (30% tolerance), all the tested samples were corresponded with the actual value. Our models were proved to be robust and accurate which indicated that ANN models can be applied in predicting the thermophysical properties of oxygen.

Keywords: Oxygen, thermophysical property; Artificial Neural Networks, linear prediction, Multilayer Feedforward Neural Network.

INTRODUCTION

Thermodynamics [1] is a natural science studying heat and temperature and how they are related to energy and work. It defines macroscopic variables, such as internal energy, entropy, and pressure. It indicates that the behavior of those variables is subject to general constraints which are common to all materials rather than the peculiar properties of particular materials. The four laws of thermodynamics accurately express these general constraints. Thermodynamics mainly studies the bulk behavior of the body rather than the microscopic behaviors of the very large numbers of its microscopic constituents, like molecules [2-6]. Concerning the microscopic constituents, statistical mechanics can be used to explain its laws. behavior of the body rather than the microscopic behaviors of the very large numbers of its microscopic constituents, like molecules. What is more, statistical mechanics can be applied to explain the laws of the microscopic constituents.

Artificial Neural Networks

Artificial Neural Networks (ANNs) [7-9] are computational models inspired by animals' central nervous systems that are able to learn and recognize pattern. They are usually described as different kinds of interconnected "neurons" systems that can calculate different values from inputs via feeding information through the network. Relative methods such as non-linear approaches are growing more and more mature and has been packed into the module of the software as the algorithm develops [10-12].

In our study, we aimed at establishing different ANN models on the base of the current thermophysical properties of oxygen. With the help of the models, we can predict the themophysical properties of oxygen accurately under different circumstances.

An artificial neural network (ANN), also called neural network (NN), is a mathematical or computational model. By using concepts from an obviously disparate field, namely electric circuits and computer science [13], the model also indicates the possibilities of improved understanding of neural systems. And it is inspired by the structure and/or functional aspects of human biological neural networks.

A neural network consists of an interconnected group of artificial neurons. And a connectionist approach is taken to process information by the neural network. In most cases, an artificial neural network (ANN) is an adaptive system that is capable of adapting continuously to new data and learning from the accumulated experience [14-15]. Besides, the system can change its structure based on external or internal information that flows through the network during the learning phase. Apart from that, the system can also abstract essential information from data or model complex relationships between inputs and outputs.

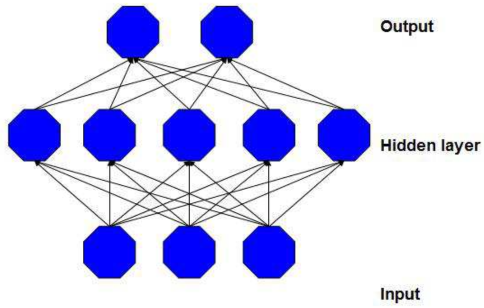

Figure 1. A schematic view of artificial neural network structure

The main structure of the artificial neural network (ANN) is made up of the input layer and the output layer, as can be seen from the figure above. It is the input layer that introduces the input variables into the network. [16]. Also, the network provides predictions for the response variables which stand for the output of the nodes in this certain layer. Besides, it also includes the hidden layers. The type and the complexity of the process or experimentation usually iteratively have a great influence on the optimal number of the neurons in the hidden layers [17].

EXPERIMENTAL SECTION

Selection of Variables

The temperature and pressure are set to be the independent variable in all models in order to ensure the robustness of the models,. When a model is being trained, all the other thermophysical properties are set to be the independent variables. Take the density (ρ) prediction model for an example, once the density prediction model is being trained, all the other thermophysical properties including temperature and pressure are considered as independent variables, thus ensuring the robustness of the prediction model.

Training Process of the Neural Network

The ANN prediction model is constructed by the Neural Tools® Software (Trial Version, Palisade Corporation, NY, USA) [18]. We chose the General Regression Neural Networks [19-21] (GRNN) module and Multilayer Feedforward Neural Networks [22-24] (MLFN) module as the training modules.

The data we used were generated from the equations of state presented in the references below [25-27]. The properties tabulated 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). The references [25-27] should be consulted for information on the uncertainties and the reference states for E,H, and S. The training results are shown as follows (Data source: *CRC Handbook of Chemistry and Physics* [28]).

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	34	17	0.02	0:00:00	Auto-Stopped
GRNN	34	17	4.92	0:00:00	Auto-Stopped
MLFN 2 Nodes	34	17	3.61	0:02:44	Auto-Stopped
MLFN 3 Nodes	34	17	1.65	0:04:12	Auto-Stopped
MLFN 4 Nodes	34	17	3.07	0:03:31	Auto-Stopped
MLFN 5 Nodes	34	17	4.18	0:04:24	Auto-Stopped

According to the training results shown on Table 1, linear prediction is considered to be the best model in predicting the values of density (RMS error: 0.02). 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 follows:

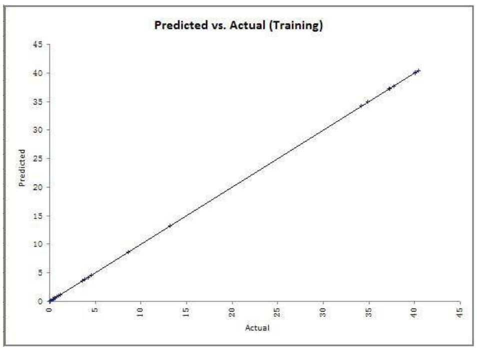

Figure 2. A comparison of the predicted values and actual values of density (Training)

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	34	17	23.64	0:00:00	Auto-Stopped
GRNN	34	17	621.89	0:00:00	Auto-Stopped
MLFN 2 Nodes	34	17	260.72	0:01:13	Auto-Stopped
MLFN 3 Nodes	34	17	386.50	0:01:07	Auto-Stopped
MLFN 4 Nodes	34	17	667.63	0:01:37	Auto-Stopped
MLFN 5 Nodes	34	17	961.86	0:01:22	Auto-Stopped

According to the training results shown on Table 2, linear prediction is considered to be the best model in predicting the values of energy (RMS error: 23.64). 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 follows:

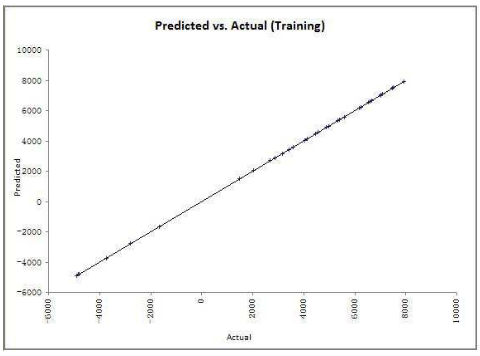

Figure 3 A comparison of the predicted values and actual values of energy (Training)

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	34	17	18.14	0:00:00	Auto-Stopped
GRNN	34	17	344.82	0:00:00	Auto-Stopped
MLFN 2 Nodes	34	17	149.52	0:00:42	Auto-Stopped
MLFN 3 Nodes	34	17	53.60	0:01:04	Auto-Stopped
MLFN 4 Nodes	34	17	391.37	0:01:24	Auto-Stopped
MLFN 5 Nodes	34	17	723.67	0:01:48	Auto-Stopped

According to the training results above, linear prediction is considered to be the best model in predicting values of enthalpy (RMS error: 18.14). 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 follows:

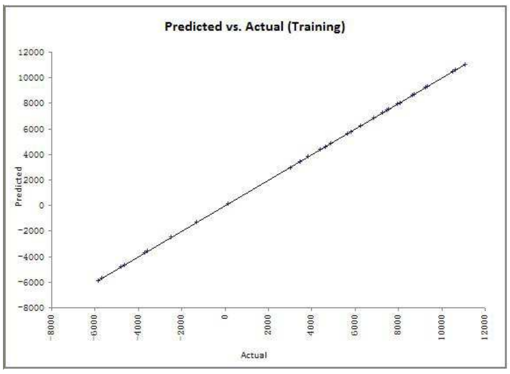

Figure 4. A comparison of the predicted values and actual values of enthalpy (Training)

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	34	17	6.29	0:00:00	Auto-Stopped
GRNN	34	17	3.25	0:00:00	Auto-Stopped
MLFN 2 Nodes	34	17	0.89	0:00:50	Auto-Stopped
MLFN 3 Nodes	34	17	2.77	0:01:09	Auto-Stopped
MLFN 4 Nodes	34	17	0.65	0:01:33	Auto-Stopped
MLFN 5 Nodes	34	17	0.40	0:01:28	Auto-Stopped

According to the training results on Table 4, MLFN model with 5 nodes is considered to be the best model in predicting the values of entropy (RMS error: 0.40). 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 follows:

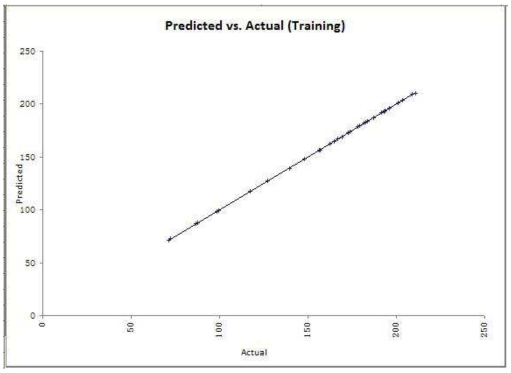

Figure 5. A comparison of the predicted values and actual values of entropy (Training)

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	34	17	0.35	0:00:00	Auto-Stopped
GRNN	34	17	0.96	0:00:00	Auto-Stopped
MLFN 2 Nodes	34	17	0.10	0:01:08	Auto-Stopped
MLFN 3 Nodes	34	17	0.20	0:01:43	Auto-Stopped
MLFN 4 Nodes	34	17	0.31	0:01:32	Auto-Stopped
MLFN 5 Nodes	34	17	0.38	0:02:18	Auto-Stopped

According to the training results shown on Table 5, MLFN model with 2 nodes is considered to be the best model in predicting the values of isochoric heat capacity (RMS error: 0.10). 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 follows:

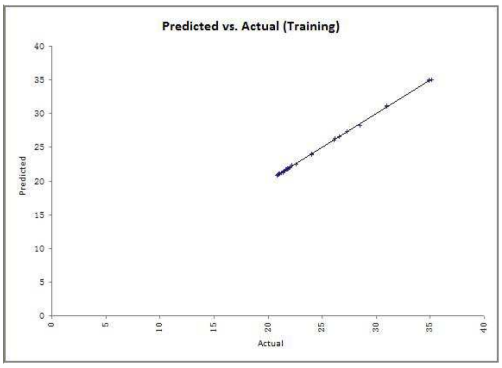

Figure 6. A comparison of the predicted values and actual values of isochoric heat capacity (Training)

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	34	17	4.36	0:00:00	Auto-Stopped
GRNN	34	17	5.14	0:00:00	Auto-Stopped
MLFN 2 Nodes	34	17	7.78	0:01:47	Auto-Stopped
MLFN 3 Nodes	34	17	10.43	0:01:59	Auto-Stopped
MLFN 4 Nodes	34	17	9.33	0:02:31	Auto-Stopped
MLFN 5 Nodes	34	17	14.71	0:02:38	Auto-Stopped

According to the training results shown on Table 6, linear prediction is considered to be the best model in predicting the values of isobaric heat capacity (RMS error: 4.36). 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 follows:

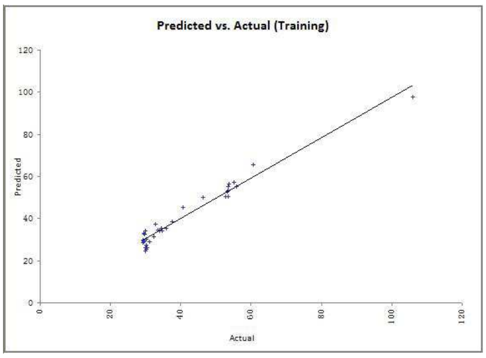

Figure 7. A comparison of the predicted values and actual values of isobaric heat capacity (Training)

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	34	17	64.94	0:00:00	Auto-Stopped
GRNN	34	17	78.99	0:00:00	Auto-Stopped
MLFN 2 Nodes	34	17	25.02	0:01:30	Auto-Stopped
MLFN 3 Nodes	34	17	77.05	0:01:09	Auto-Stopped
MLFN 4 Nodes	34	17	79.85	0:02:03	Auto-Stopped
MLFN 5 Nodes	34	17	77.03	0:02:21	Auto-Stopped

According to the training results above, MLFN model with 2 nodes is considered to be the best model in predicting the values of viscosity (RMS error: 2.55). 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 follows:

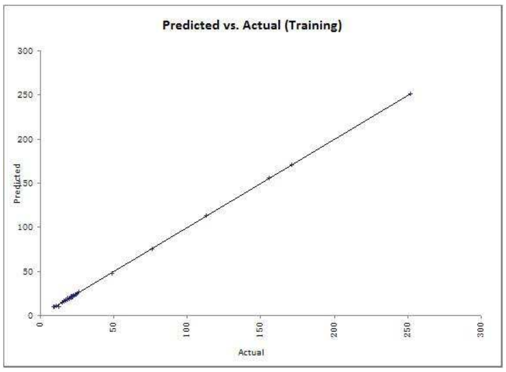

Figure 8. A comparison of the predicted values and actual values of viscosity (Training)

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	34	17	1.45	0:00:00	Auto-Stopped
GRNN	34	17	2.20	0:00:00	Auto-Stopped
MLFN 2 Nodes	34	17	7.01	0:01:17	Auto-Stopped
MLFN 3 Nodes	34	17	6.64	0:01:54	Auto-Stopped
MLFN 4 Nodes	34	17	6.77	0:02:44	Auto-Stopped
MLFN 5 Nodes	34	17	8.51	0:02:45	Auto-Stopped

According to the training results shown on Table 8, linear prediction is considered to be the best model in predicting the values of thermal conductivity (RMS error: 1.45). 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 follows:

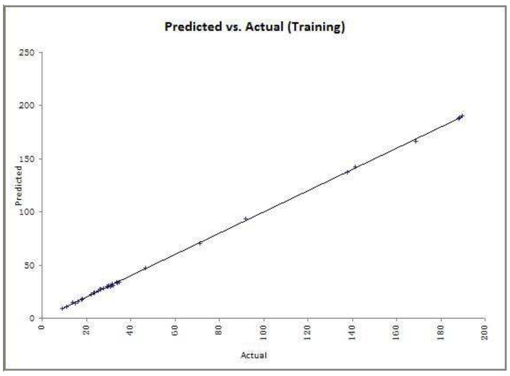

Figure 9. A comparison of the predicted values and actual values of thermal conductivity (Training)

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	28	17	0.00	0:00:00	Auto-Stopped
GRNN	28	17	0.02	0:00:00	Auto-Stopped
MLFN 2 Nodes	28	17	0.00	0:01:54	Auto-Stopped
MLFN 3 Nodes	28	17	0.01	0:02:26	Auto-Stopped
MLFN 4 Nodes	28	17	0.02	0:02:41	Auto-Stopped
MLFN 5 Nodes	28	17	6.05	0:02:58	Auto-Stopped

According to the training results shown on Table 9, MLFN model with 2 nodes is considered to be the best model in predicting 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 training results are shown as follows:

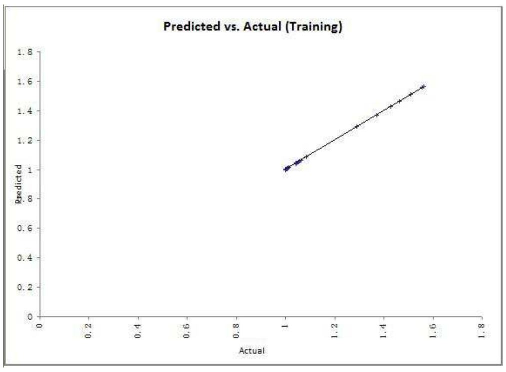

Figure 10. A comparison of the predicted values and actual values of dielectric constant (Training)

RESULTS AND DISCUSSION

Results of Each Thermophysical Property

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

Table 10: The best model of each thermophysical property of oxygen

	Density	Energy	Enthalpy	Entropy	Isochoric heat capacity	Isobaric heat capacity	Viscosity	Thermal conductivity	Dielectric constant
Best Model	Linear Prediction	Linear Prediction	Linear Prediction	MLFN 5 nodes	MLFN 2 nodes	Linear Prediction	MLFN 2 nodes	Linear Prediction	MLFN 2 nodes

Based on the results shown in Table 10, it is obvious that different ANN models can develop different thermophycical properties of oxygen, thus ensuring the robustness of the prediction model. Also, every model corresponds with the requirement of the accuracy.

Comparison with Other Researches

For comparison, we have done the same research with nitrogen, the results are shown as follows:

Table 11: The best model of each thermophysical property of nitrogen

	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 9 nodes	GRNN	MLFN 5 nodes	Linear Prediction

According to the two tables above, we found that in the two elementary substances, the density, energy and enthalpy can be predicted effectively by Linear Prediction. However, other models of thermophysical properties are different. The results indicated that we cannot combine the two substances into the same prediction method together in our research results. We'll do further studies to find out the main difference between the models of oxygen and nitrogen.

CONCLUSION

Thermophysical properties of oxygen are important in practical application. In our study, We succeeded in establishing 9 models to predict the thermophysical properties of oxygen, namely density, energy, enthalpy, entropy, isochoric heat capacity, isobaric heat capacity, viscosity, thermal conductivity and dielectric constant, by analyzing 51 data groups using Linear Prediction and MLFN methods. Within permissible error range (30% tolerance), all the tested samples were corresponded with the actual value. Our models were proved to be robust and accurate which indicated that ANN models can be applied in predicting the thermophysical properties of oxygen. In addition, we found that the method of Linear Prediction and Multilayer Feedforward Neural Network can also predict the values correctly even some of the data are missing.

For further study, we'll pay our attention to modify the models and apply such method to predict other properties of elementary substances. What's more, we'll apply such method to predicting other air elemental such as hydrogen and helium. We'll do more researches to find out the main difference among different models of elementary substances.

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