7th Thermal and Fluids Engineering Conference (TFEC)
May, 16-18, 2022
Partially Online Virtual and in Las Vegas, NV Conference

TFEC-2022- 40940

Classifying Thermal Conductivity of Fluids with Artificial Neural Networks

Andrew C. Jarrett[1], Ashwin Kodibagkar[2], Dugan Um[3], Tae-Youl Choi[1*], Denise P. Simmons[1]

[1]The University of North Texas, Denton, Texas 76207, USA
[2]School for the Talented and Gifted at Yvonne A. Ewell Townview Center, Dallas, TX 75203, USA
[3] Department of Engineering, Texas A&M Corpus Christi, Corpus Christi, TX 78412, USA

ABSTRACT

The objective of this paper is to discuss the capability of an Artificial Neural Network to classify the thermal conductivity of glycol concentrations in water. This was done by creating a COMSOL model of a micropipette thermal sensor in an infinite media and simulating a 500 µs laser pulse at the tip. Parameter approximation of the 2nd order heat transfer PDE permits concentration classification. The temperature profile dataset generated would then be fed into a trained ANN to classify the thermal conductivity, whose value would be used to distinguish the glycol concentration difference of up to 10%. Training of the ANN yielded an overall classification accuracy of 99.99% after 108 epochs.

KEY WORDS: Artificial Neural Networks, Classification, Temperature Profiles, Thermal Conductivity, Fluid Simulation, Heat Transfer

1. INTRODUCTION:

With the advancement of high heat flux devises there arises a need for more advanced thermal management techniques, including the utilization of micro and nano particles in fluids to dramatically increase the thermal conductivity [1]. With these methods for measuring and characterizing these nano fluids must be developed [2]. It has been shown that thermal conductivity of fluids can be optioned using a micropipette sensor. However, the process of obtaining the thermal conductivity based on a measured temperature profile was revealed as costly due to large computational time and limited computer resources [5]. Machine learning serves as an efficient alternative to numerical analysis [6].

Machine learning makes it possible to process large amounts of data to accomplish specific tasks, namely, to recognize patterns in the dataset [7]. This is useful in applications such as computer vision, speech processing, and game playing. [8] Artificial Neural Networks (ANN) work on pattern recognition and are trained with large data sets of known solutions [9]. Once the training is completed, the trained ANN can solve complex problems instantaneously with high accuracy [10]. This is based upon the concept of neurons in the brain, where nodes are connected to synapses with weighted values to make decisions [11]. Many ANN's use supervised training where the error from the known solutions is backpropagated through the system of neurons and the weights are adjusted by the errors between ground truth and ANN outcomes [12]. This process is iterated until an acceptable level of error is achieved [13].

Machine learning, especially artificial neural networks (ANN) have been used for various thermal prediction related tasks, including hybrid nanofluid thermal conductivity predictions and characterization of connective heat transfer rates [14] [15]. Artificial neural networks have also been used for an efficient prediction of supercritical CO2 heat transfer [16]. The use of artificial neural networks for thermal predictions is widespread and efficient in various tasks.

*Tae-youl.choi@my.unt.edu

Therefore, an ANN trained with the temperature profiles of known thermal conductivities can be proposed to predict parameters (i.e., thermal conductivity) of a model system including liquid or even a biological cell. Once trained, classification is instantaneous thereby solving the issues of computation time.

In order to obtain a large enough data set for training, a simulation model can be created in COMSOL to create transient temperature profiles of liquids with varying thermal properties. When training is complete, the ANN can be verified with real liquids. This is known as a sim-to-real approach, whereby the network is trained with a simulation dataset from a model and tested with experimental data [17].

2. METHODS

This section will cover the preparation of the training data, details of the simulation, as well as the method used to structure and train the neural network.

2.1 Training Data Preparation Training data was generated using a Partial Differential Equation (PDE) solver. COMSOL Multiphysics was chosen to calculate transient temperature profiles given a parameter – thermal conductivity for a model shown in Figure 1. Thermal conductivity (k) of the PDE in equation (1) below is the only parameter we used to evaluate the proposed ANN in terms of viability in the prediction of thermal conductivity:

$$\rho c_p \frac{\partial T}{\partial t} + \nabla \cdot (-k\nabla T) = Q \tag{1}$$

The model represents a micropipette thermal sensor (MTS) subjected to laser heating at the tip of the sensor. A section diagram of the MTS can be seen in figure 1B. The junction of the thermocouple was the inner core of bismuth, and a thin outer coating of nickel. The evolution of temperature depends upon thermal conductivity of the surrounding liquid – water and glycol mixture in the current study. A heat point source with a gaussian profile and a 500 µs pulse duration was set on the center of the MTS tip. The temperature profile was taken from the liquid 2.5 µm from the tip and saved for the training data set.

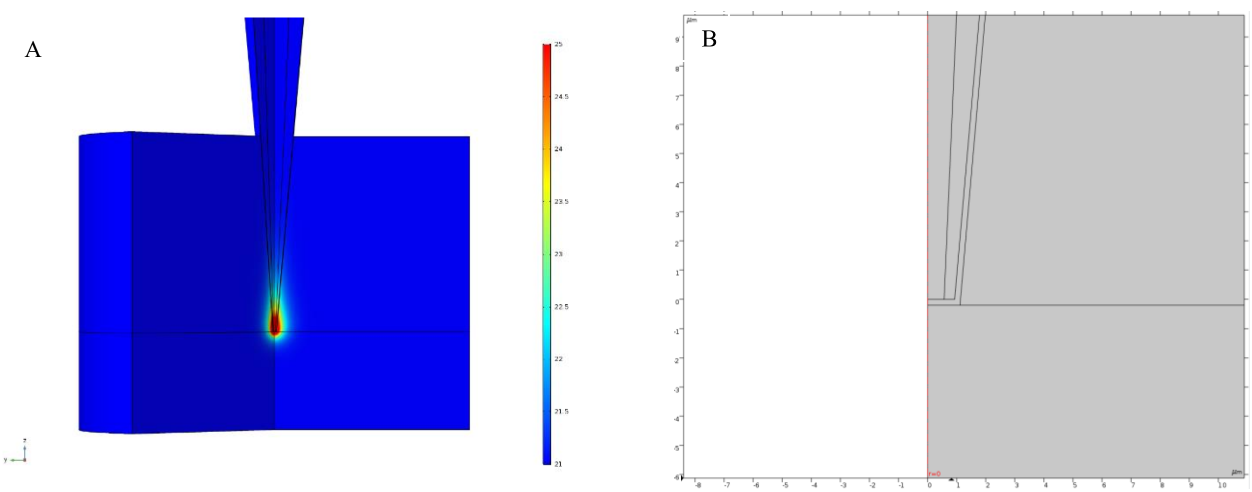

Figure 1: A) 3D cut away COMSOL Multiphysics simulation of MTS with temperature scale [18]. B) Section diagram of MTS and surrounding fluid

The concentration of glycol in water has a direct impact on the mixture's thermal properties. Specifically thermal conductivity decreases with the increase of glycol. Differences in thermal conductivity vs. the concentration can be seen in table 1, which separates the data and assigns each thermal conductivity range a label. Nine different labels were created for 10% changes in glycol concentrations. Next 100 temperatures vs. time data sets were generated for each of the classification labels, for a total of 900 sets to be used for training the ANN. Each data set had 126 data points to correspond to temperature sampling every 4 μs for a 500 μs duration. This data was normalized using the min-max method. Normalization allows for the data to be set on the same scale. This is important in machine learning when the range for the data is different and allows for faster convergence [19]. These normalized profiles can be seen in figure 2.

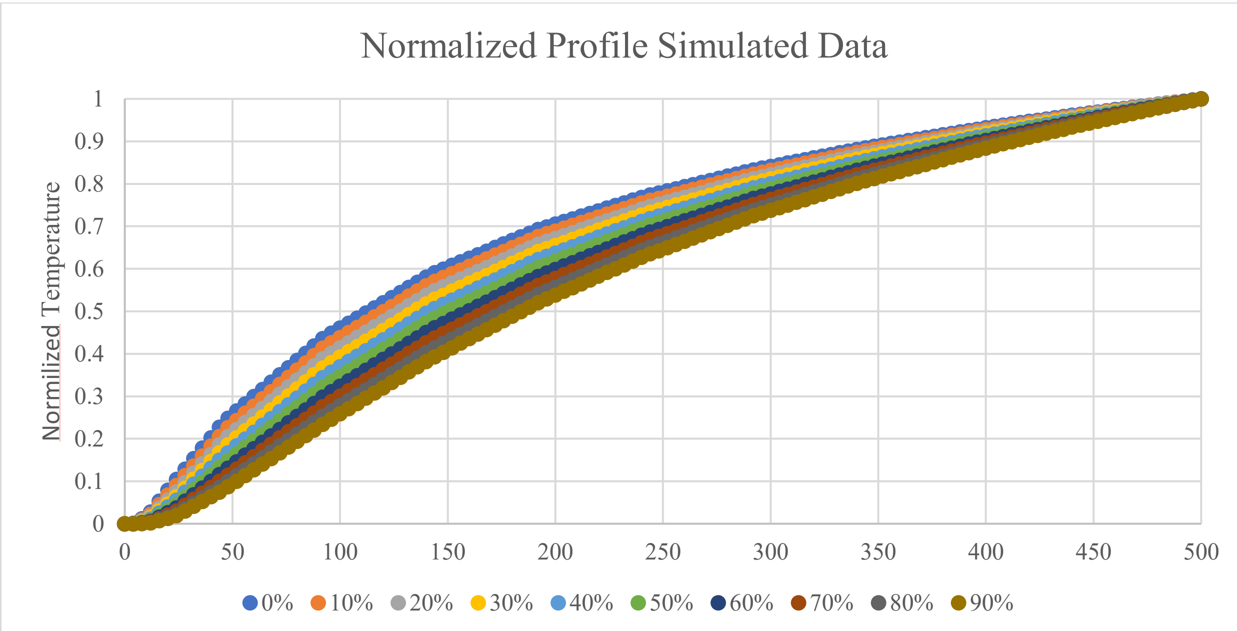

Figure 2: Normalized temperature profiles of propylene glycol concentrations

Table 1: Classification based on thermal conductivity range and glycol concentration

Glycol %	Thermal Conductivity Range	Classification Label
0% - 10%	.608 - .542	[1 0 0 0 0 0 0 0 0]
10% - 20%	.541 - .484	[0 1 0 0 0 0 0 0 0]
20% - 30%	.483 - 432	[0 0 1 0 0 0 0 0 0]
30% - 40%	.431 - .385	[0 0 0 1 0 0 0 0 0]
40% - 50%	.384 - .342	[0 0 0 0 1 0 0 0 0]
50% - 60%	.341 - .303	[0 0 0 0 0 1 0 0 0]
60% - 70%	.302 - .268	[0 0 0 0 0 0 1 0 0]
70% - 80%	.267 - .238	[0 0 0 0 0 0 0 1 0]
80% - 90%	.237 - .214	[0 0 0 0 0 0 0 0 1]

2.2 Training ANN with simulated data: Once the training data was prepared, a neural network is created and trained. MATLAB has developed a tool for creating single hidden layer ANNs for neural pattern recognition (NPR) in the Deep Learning Toolbox. The NPR function was used to generate and train the network using the default scaled conjugate gradient method (SCGM). This method is similar to he gradient descent method where the gradient of the cost function with respect to weights is calculated and subtracted from each weight set to reach a minimum. The difference comes in through the learning rate. In SCGM the learning rate is varied based on the slope of the gradient [20]. Therefore, if the gradient is large, the learning rate increases and decreases if the gradient is small. This allows for faster and more accurate learning when compared to traditional gradient descent in which the learning rate is constant.

The cost function used in this is the cross-entropy loss function (CELF) [21]. This loss function is based upon the concept of entropy or the uncertainty in possible outcomes. When the probability of the ANN classifying the correct output is high the loss of the function is minimized.

$$L_{CE} = -\sum_{i=1}^{n} t_i \log(p_i) \tag{3}$$

A network diagram is shown below in Figure 3. The 126 input nodes correspond to the temperatures at 4 µs time intervals. The different sized hidden layers were generated from 25 to 150. Next, the output was a vector of 9 nodes to represent the different classification labels.

The normalized data were randomized and separated into 70% training, 15% validation, and 15% testing data sets. Training data sets are used with optimization methods such as gradient descent. Validation sets provides a way to evaluate the model during training. This prevents overfitting of the data by early stopping. The final testing data is used to evaluate the trained model.

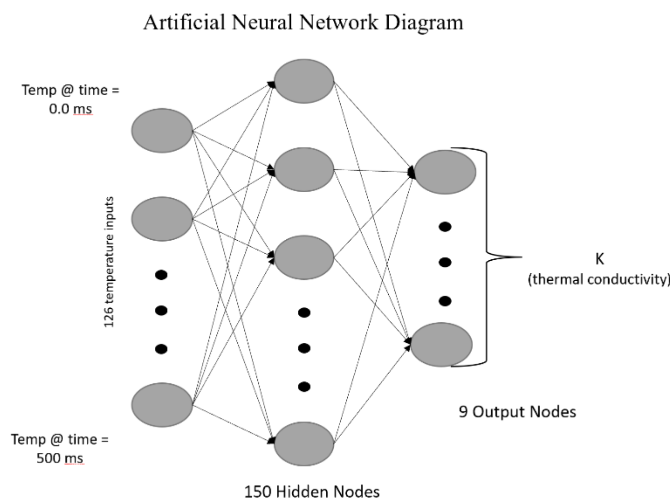

Figure 3: Neural Network Diagram

2.3 Evaluating the Network: The network can be evaluated by using the respected confusion matrix. This matrix is a visual way to view the performance of the network. It shows the number of true positives (TP), true negatives (TN), false positives (FP), and false negatives (FN) produced by the network from the training, validation, and testing data. Most confusion matrixes are shown from binary machine learning models, meaning only two outputs. In this study the confusion matrix generated is from a multiclass machine learning model, where there were 9 outputs.

There are several metrics that can be utilized from the confusion matrix such as: Accuracy, Precision, and F1-Score [22].

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} \tag{3}$$

$$Percision = \frac{TP}{TP+FP} \tag{4}$$

$$F1\ Score = \left(\frac{2*TP}{2*TP+FP+FN}\right) \tag{5}$$

In the case of the multiclass model, each of the metrics can be found by the individual classification or by the total TP, FP, and NP of the model. When the total is taken it is known as the micro F1 or micro average F1 score. Since no one output is of more importance the total F1 score will be found and used to evaluate the network. In multiclass models the accuracy, precision, and micro F1 score are all equal.

3. RESULTS

3.1 Training Results for the ANN: The first part of the study was to determine the number of nodes that would yield the lowest error in classification. This was done by finding the average micro F1 score for each of the hidden layer configurations, shown in table 2. All the networks performed similar to each other with a 99% accuracy or above. The configuration with 100 nodes after training for 109 epochs yielded a 100% accuracy for training, validation, and testing data. This training epoch had a validation performance of .00852 from the CEF.

The total confusion matrixes for each of the network configurations are shown in figure 4. The column on the far right of the plot shows precision of each class, or the percentage of the classes that were correctly identified. While the bottom row shows the recall of the examples or the percentage of examples that were correctly identified as positive. The bottom right corner shows the overall accuracy of the ANN, which should be noted is equal to the Micro F1 score as discussed in the method.

Table 2: Hidden layer size and resulting average RMSE

Hidden Layer Size	Average Micro F1
25	.9988
50	.9933
75	.9988
100	**1.00**
125	.9988
150	.9977

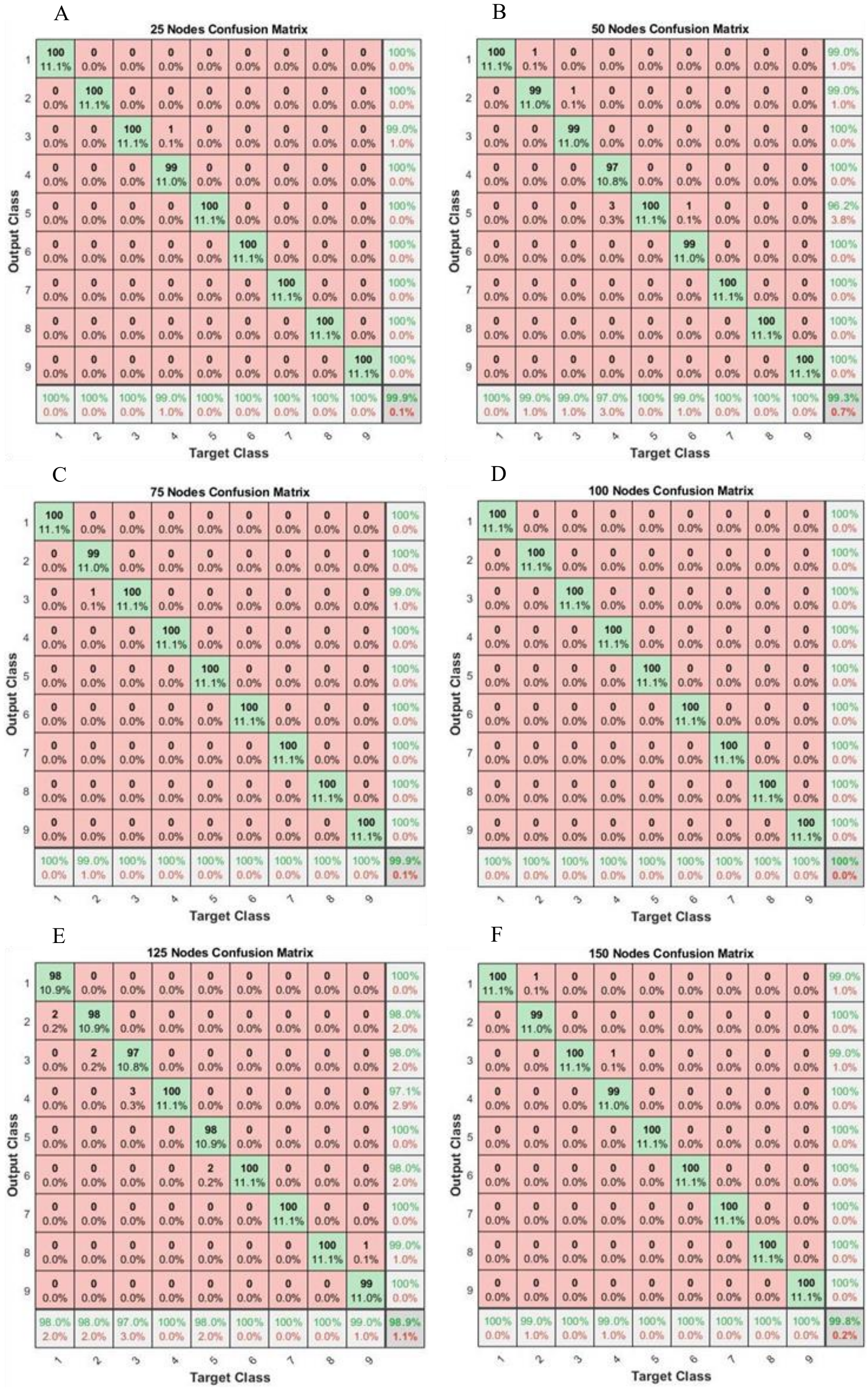

Figure 4: Total data confusion matrix for varying hidden layer size. The green diagonal represents the data sets the network got correct. The far-right column shows the precision for each class, while the bottom row shows the recall. (A) 25 Hidden Nodes (B) 50 Hidden Nodes (C) 75 Hidden Nodes (D) 100 Hidden Nodes (E) 125 Hidden Nodes (F) 150 Hidden Nodes

4. CONCLUSION:

In the proposed study, it was found that the Artificial Neural Network can accurately classify the thermal conductivity of different glycol concentrations. Training data was created by COMSOL, a PDE solver. The model was an MTS in an infinite media where all parameters were held constant except for the thermal conductivity. The simulation consisted of heating the tip of the MTS with a 500 μs laser pulse, and the temperature profile was collected. MATLAB was used to generate the ANN model and randomize the data sets into training, validation, and testing. Different network arrangements were tested by varying number of nodes in the hidden layer from 25-150. Training of the network consisted of SCGM. Once the network was trained, validation and test sets were fed into the trained ANN.

The highest accuracy ANN configuration was with a hidden layer of 100 nodes, which attained an overall classification accuracy of 100.00% from training, validation, and test data sets. However, these were only verified with simulated data. To further prove the method an experimental study must be performed to which propylene glycol solutions are tested with a fabricated MTS. The temperature profile measured will be fed into the trained ANN for classification. This experiment will the show the ability of the sim to real approach for this method.

ACKNOWLEDGMENT

This work was supported by National Science Foundation (award number: 1906553).

REFERENCES

[1] S. Murshed, K. Leong and C. Yang, "Enhanced thermal conductivity of TiO2—water based nanofluids," *International Journal of Thermal Sciences,* vol. 44, no. 4, pp. 367-373, 2005.

[2] G. Paul, M. Chopkar, I. Manna and P. Dasc, "Techniques for measuring the thermal conductivity of nanofluids: A review," *Renewable and Sustainable Energy Reviews,* vol. 14, no. 7, pp. 1913-1924, 2010.

[3] R. Shrestha, R. Atluri, D. Simmons, D. Kim and T. Choi, "Thermal Conductivity of a Jurkat Cell Measured by a Transient Laser Point Heating Method," *International Journal of Heat and Mass Transfer,* vol. 160, p. 120161, 2020.

[4] M. Frank, D. Dimitris and C. Vassilis, "Machine-Learning Methods for Computational Science and Engineering," *Computation,* vol. 8, no. 15, 2020.

[5] J. Lee, J. Kang, W. Shim, H. Chung and T. Sung, "Pattern Detection Model Using a Deep Learning Algorithm for Power Data Analysis in Abnormal Conditions," *Electronics,* vol. 9, no. 1140, 2020.

[6] O. Abiodun, A. Jantan, A. Omolara, K. Dada, A. Mohamed and H. Arshad, "State-of-the-art in artificial neural network applications: A survey," *Heliyon,* vol. 4, no. 11, 2018.

[7] M. Najafabadi, F. Villanustre, T. Khoshgoftaar, N. Seliya, R. Wald and E. Muharemagic, "Deep Learning Applications and Challenges in Big Data Analytics," *Journal of Big Data,* vol. 2, no. 1, 2015.

[8] C. Carmichael, "A Study of the Accuracy, Completeness, and Efficiency of Artificial Neural Networks and Related Inductive Learning Techniques," *Iowa State University Digital Repository,* 2001.

[9] M. Fauth, F. Wörgötter and C. Tetzlaff, "The Formation of Multi-synaptic Connections by the Interaction of Synaptic and Structural Plasticity and Their Functional Consequences," *PLOS Computational Biology,* 2015.

[10] P. Cunningham, M. Cord and S. Delany, "Supervised Learning," in *Machine Learning Techniques for Multimedia*.

[11] N. Christiansen, P. Voie, O. Winther and J. Høgsberg, "Comparison of Neural Network Error Measures for Simulation of Slender Marine Structures," *Journal of Applied Mathematics,* 2014.

[12] H. Adun, I. Wole-Osho, E. Okonkwo, O. Bamisile, M. Dagbasi and S. Abbasoglu, "A Neural Network-Based Predictive Model for the Thermal Conductivity of Hybrid Nanofluids," *International Communications in Heat and Mass Transfer,* vol. 119, 2020.

[13] R. Romero-Méndez, P. Lara-Vázquez, F. Oviedo-Tolentino, F. P.-G. H. Durán-García and A. Pacheco-Vega, "Use of Artificial Neural Networks for Prediction of the Connective Heat Transfer Coefficient in Evaporative Mini-Tubes," *Ingeniería, Investigación y Tecnología,* vol. 17, no. 1, 2016.

[14] B. Zhu, X. Zhu, J. Xie, J. Xu and H. Liu, "Heat Transfer Prediction of Supercritical Carbon Dioxide in Vertical Tube Based on Artificial Neural Networks," *Journal of Thermal Science,* vol. 30, p. 1751–1767, 2021.

[15] W. Zhao, J. Queralta and W. T, "Sim-to-Real Transfer in Deep Reinforcement," *IEEE Symposium Series on Computational Intelligence,* pp. 737-744, 2020.

[16] A. Jarrett, T.-Y. Choi and D. Um, "Artificial Neural Network for Real-Time Characterization of Cancer Cell Thermal Properites," in *UKC 2020*, 2020.

[17] J.-M. Jo, "Effectiveness of Normalization Pre-Processing of Big Data to the Machine Learning Performance," *The Journal of the Korea institute of electronic communication sciences,* vol. 14, no. 3, pp. 547-552, 2019.

[18] L. Bottou, "Large-Scale Machine Learning with Stochastic Gradient Descent," in *COMPSTAT*, Paris, 2010.

[19] K. Murphy, Machine Learning, Cambridge: MIT, A Probabilistic Perspective.

[20] I. Markoulidakis, I. Rallis, I. Georgoulas, G. Kopsiaftis, A. Doulamis and N. Doulamis, "Multiclass Confusion Matrix Reduction Method and Its Application on Net Promoter Score Classification Problem," *Technologies,* vol. 9, no. 81, 2021.

[21] H. Kurt and M. Kayfeci, "Prediction of thermal conductivity of ethylene glycol–water solutions by using artificial neural networks," *Applied Energy,* vol. 86, no. 10, pp. 2244-2248, 2009.

[22] S. S. Sablani, O.-D. Baik and M. Marcotte, "Neural networks for predicting thermal conductivity of bakery products," *Journal of Food Engineering,* vol. 52, no. 3, pp. 299-304, 2002.

[23] K. Kasza, A. Rowat, J. Liu, T. Angelini, C. Brangwynne, G. Koenderink and D. Weitz, "The cell as a material," *Curent Opinion in Cell biology,* vol. 19, no. 1, pp. 101-107, 2007.

[24] R. Shrestha, R. Atluri, D. P. Simmons, D. S. Kim and T. Y. Choi, "A micro-pipette thermal sensing technique for measuring the thermal conductivity of non-volatile fluids," *Review of Scientific Instruments,* vol. 89, 2018.

[25] L. Huang, J. Qin, Y. Zhou, L. Liu and L. Shao, "Normalization Techniques in Training DNNs: Methodology, Analysis and Application," 2020.