# A GUI Based Property Package for Thermo-physical Properties of Cryogenic Fluids

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## Abstract

❖ In recent years, Deep Learning and Artificial Neural Networks (ANNs) have emerged as powerful tools for modeling complex relationships in data-driven applications, including fluid property prediction [1]. The present work explores the possibility of utilizing the capabilities of ANN to predict the thermo-physical properties of cryogenic fluids. The module named "CRYOProp" will be capable of predicting various thermodynamic and transport properties of cryogenic fluids, such as density, viscosity, thermal conductivity, and specific heat, as a function of temperature, pressure, composition, and other relevant parameters. The present work highlights the lessons learned and limitations during this development.

## Introduction

❖ A need always arises for the cryogenic fluid properties, especially for quantum fluids like helium and hydrogen, calculations of properties of mixtures such as mixed refrigerant, air, LNG, hydrogen-deuterium tritium, helium-neon mixtures, and He-3-He-4 mixtures that are either used as refrigerant or need separation.

❖ At present, there are various property routines from where one can get the thermo-physical properties e.g. RefProp®, Hepak®, GasPack®, CoolProp®, etc.

❖ Properties of the quantum fluids like helium and hydrogen are also estimated using the above property modules. At lower temperatures, there are deviations observed in these modules, when compared with experimental data e.g. thermal conductivity of n-hydrogen.

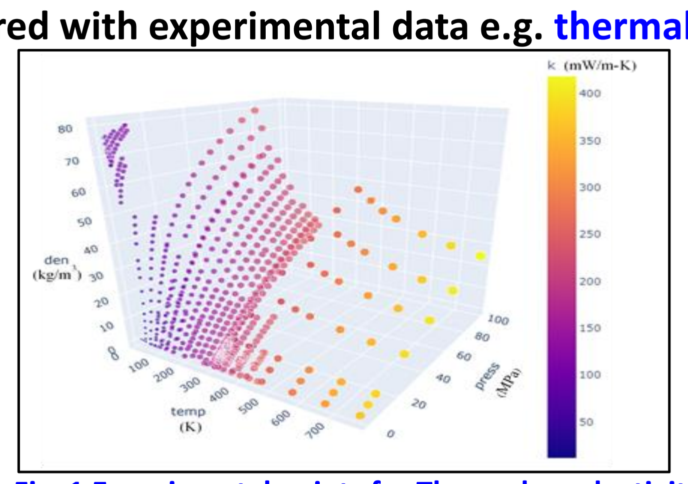


Fig. 1 Experimental points for Thermal conductivity

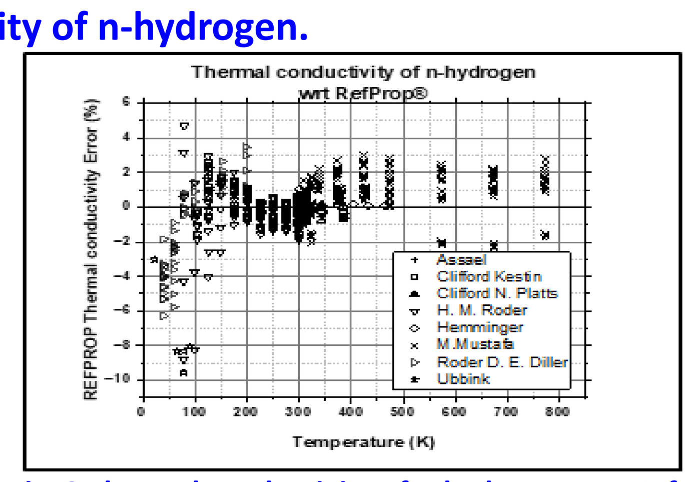


Fig. 2 Thermal conductivity of n-hydrogen wrt RefProp®

## Objective

❖ In the present work, the thermal conductivity of n-hydrogen has been predicted at a lower temperature level i.e. 15 K to 30 K using the concept of transfer learning of ANN.

❖ The experimental subcooled thermal conductivity data points are taken from Roder [2] and Charignon [3] to train the ANN model.

## Methodology

❖ In the present work, Excel input data of thermo-dynamic fluid properties derived from CoolProp® [4] have been provided to train the base model and experimental data of thermal conductivity for n-Hydrogen has been added to a pre-trained neural model.

❖ To train the base model, density and temperature have been provided in the input layer, and thermal conductivity is predicted at the output layer.

❖ As part of the work, a GUI has also been developed for the ease of users to estimate the thermo-physical and transport properties of cryogenic fluid. A GUI interface has been shown in Fig. 4.

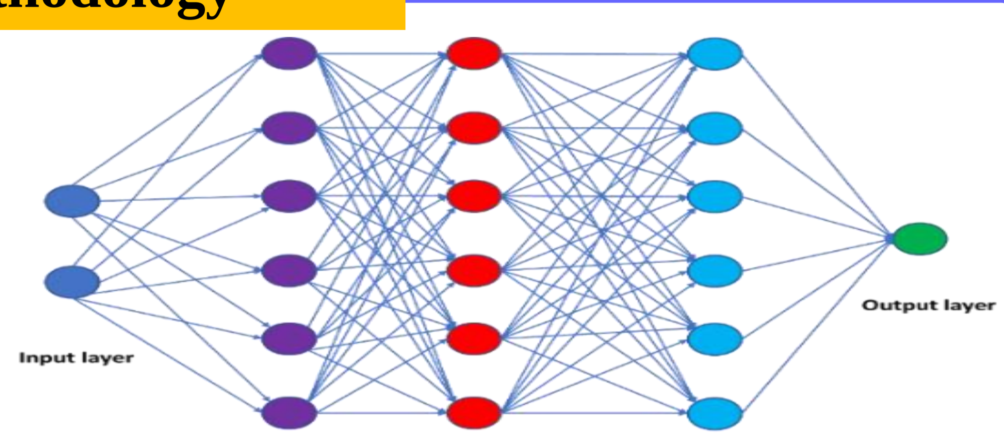


Fig. 3 A schematic of the ANN model

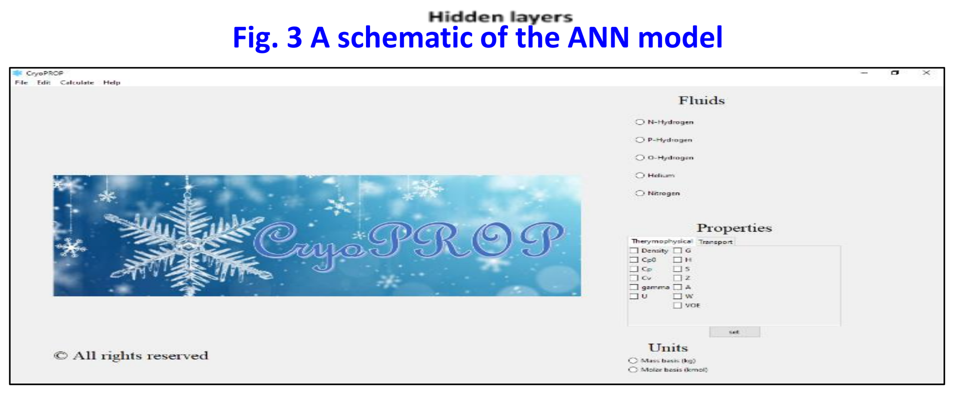


Fig. 4 GUI interface for CRYOProp

❖ Density has been chosen as an input parameter due to its small variation (76 to 80 kg/m3) in the temperature range of 15 K to 50 K, as compared to pressure variation.

❖ The collected data is normalized in Python® by dividing it by its maximum value.

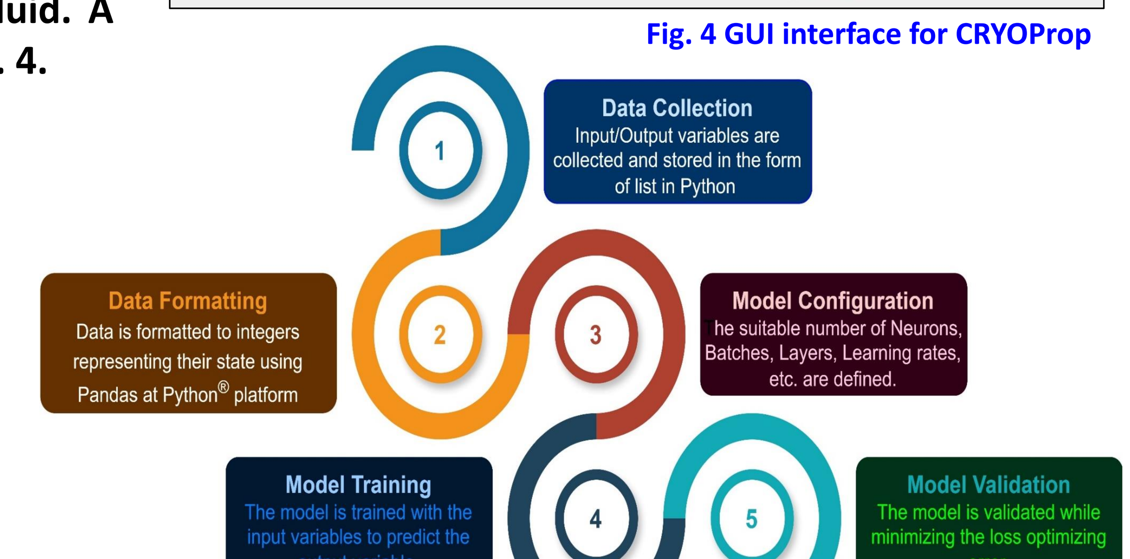


Fig. 5 Flow chart for the base model preparation using ANN

❖ To adapt this model for the domain's new range (15 K to 30 K), transfer learning by freezing the learned weights of the initial layers is employed and only the final layer is updated.

❖ The fine-tuning process involved retraining the model with new data from the experiment values, allowing the ANN to generalize and accurately predict the function's behavior beyond the initially trained range.

❖ This methodology not only demonstrated the efficacy of transfer learning in function approximation tasks but also highlighted its potential to reduce computational costs and improve model performance in extrapolation tasks.

❖ The results, visualized through a comparative plot of true and predicted values, confirmed the model's capability to accurately mimic the thermodynamic properties across the extended domain, validating transfer learning as a viable strategy for ANN-based function approximation.

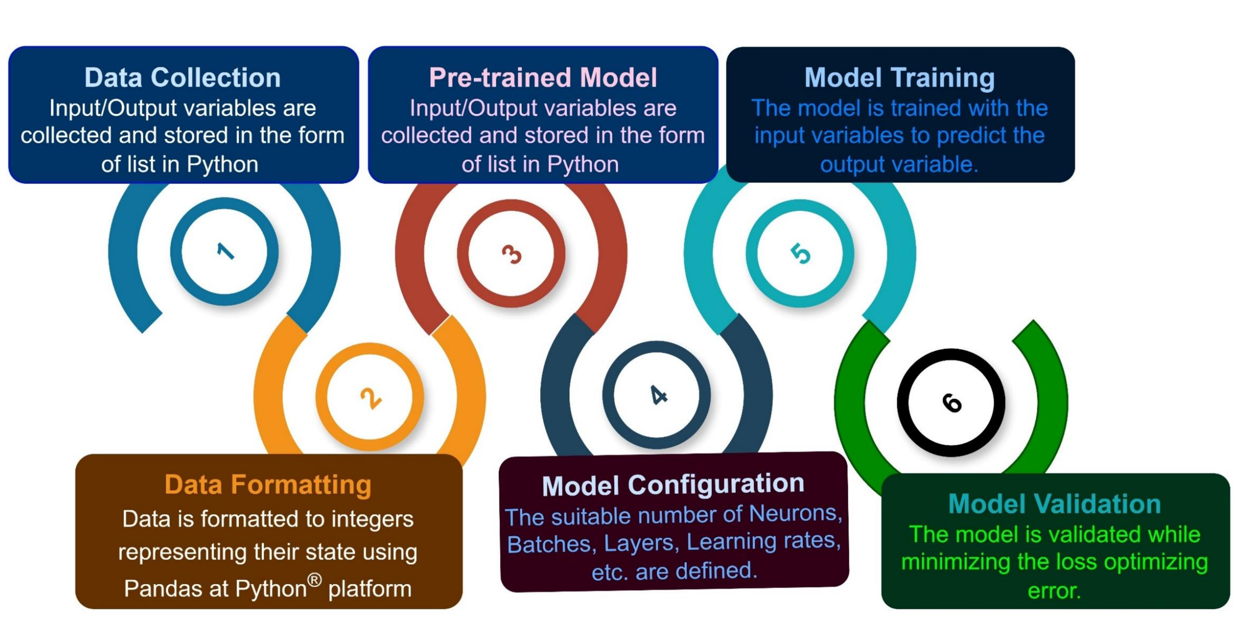


Fig. 6 Flow chart for the transfer learning process

## Results and Discussion

❖ Following the methodology explained above, the parametric analysis of the neural network has been performed for the number of neurons, layers, learning rates, loss optimizers, and batches. The outcomes are shown in the form of figures below;

### ❖ Impact of no. of neurons

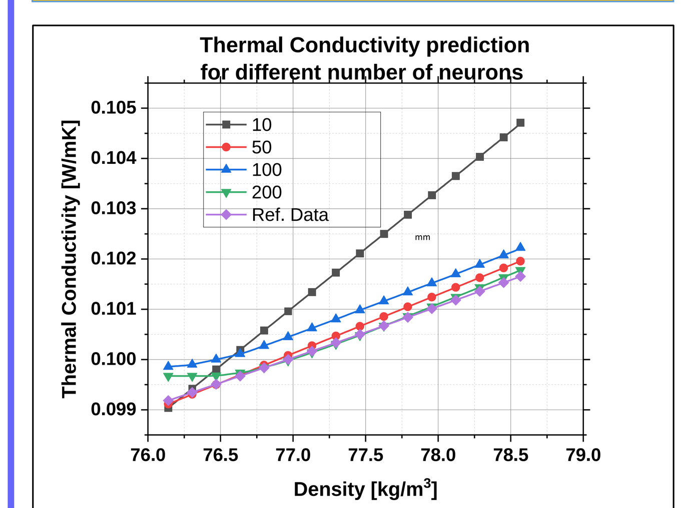


Fig. 7 Thermal conductivity predictions for different number of neurons

### ❖ Impact of no. of layers

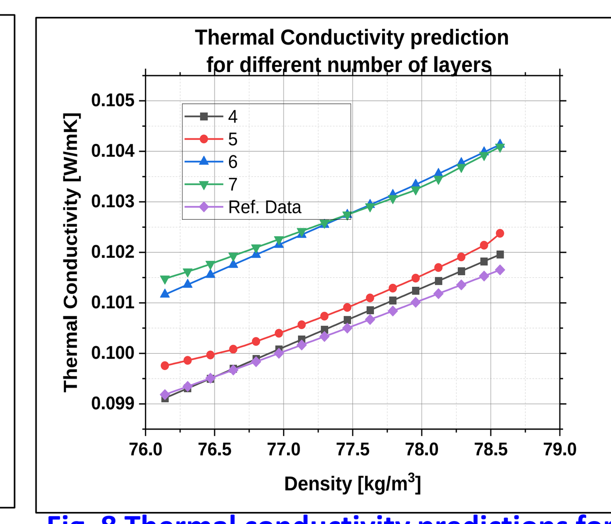


Fig. 8 Thermal conductivity predictions for different number of layers

After a certain number of neurons, overfitting of the data takes place, and predicted values deviate from the reference data. Similarly, number of the layers in the neural network has been optimized and 4 layers have been chosen in the present work.

❖ Learning rates determine how fast the neural network model has been learning the input data.

❖ In the present work, a learning rate of 0.001 has been chosen. Different loss optimizers are also tried as shown in Figure and in the present study, the mean absolute error loss optimizer has been adopted.

### ❖ Impact of learning rates

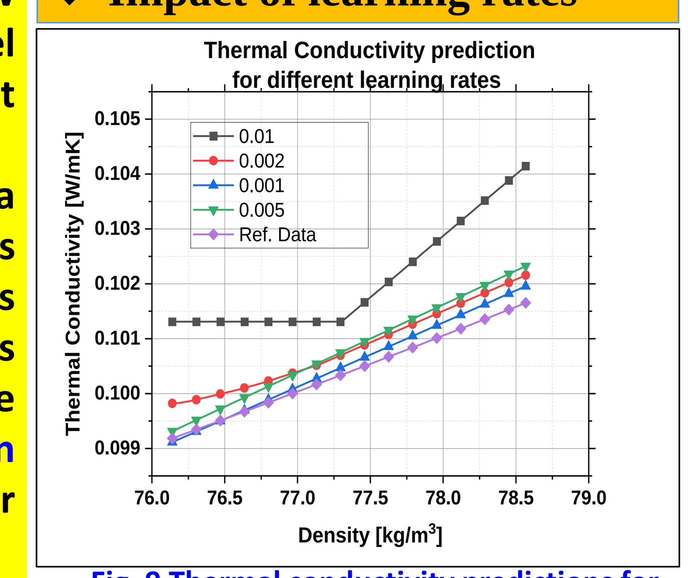


Fig. 9 Thermal conductivity predictions for different learning rates

### ❖ Impact of loss optimizers

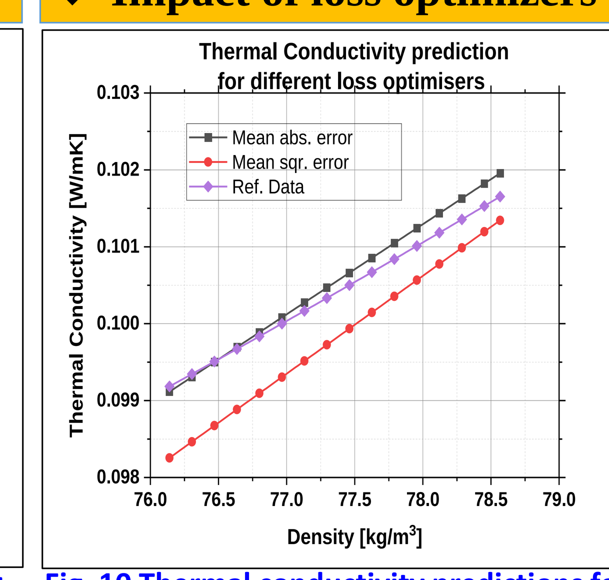


Fig. 10 Thermal conductivity predictions for different loss optimizers

### ❖ Impact of batch sizes

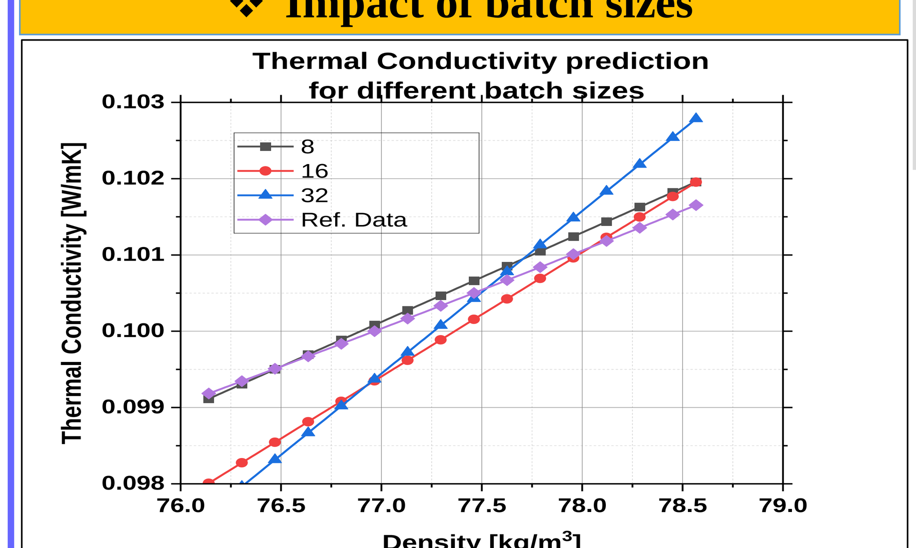


Fig. 11 Thermal conductivity predictions for different number of batch sizes

Parametric analysis has also been performed for the different batch sizes, and it was observed that 8 batch size predicts more accurate values than higher batch sizes as shown in Figure 11.

❖ After the parametric analysis, 50 neurons, 4 layers, 0.001 learning rate, batch size of 8, and mean absolute error as a loss optimizer have been adopted.

❖ The predicted values show very good agreement with the reference data with an error < 1 % as shown in Figure 12.

### ❖ % error prediction against the Ref. data

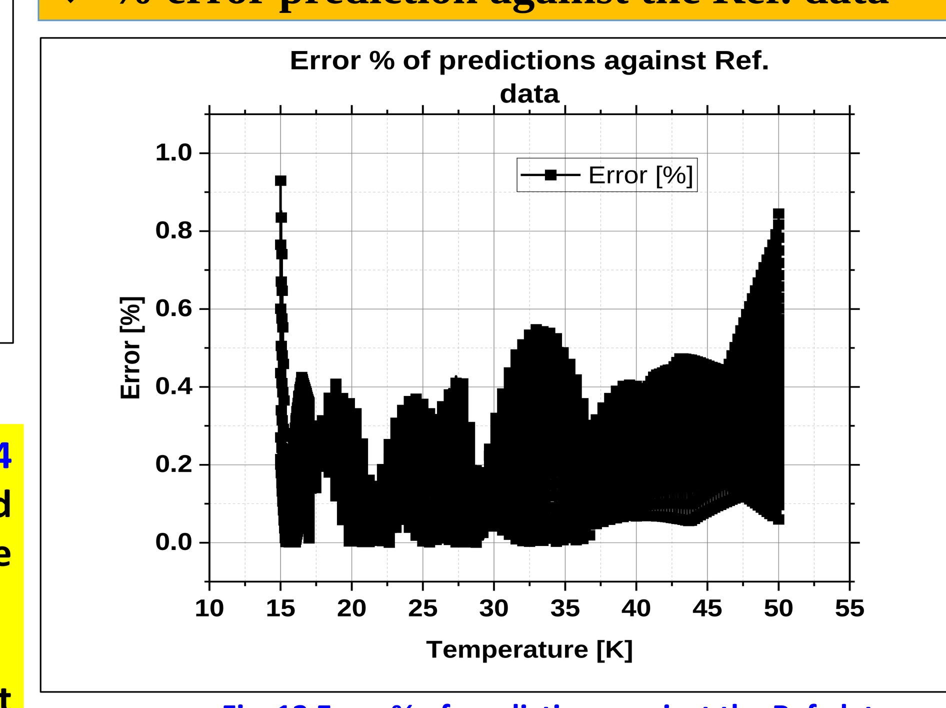


Fig. 12 Error % of predictions against the Ref. data

❖ There are three methods, which have been tried to re-train the base model with the new experimental values.

❖ In method 1, the weights and biases of the base model are modified with new data points.

❖ In method 2, the weights and biases of the base model are frozen and then one additional layer is added for the training of a new model with new data points.

❖ In method 3, the weights and biases for all the layers (except the last one) are frozen and then new data points are provided to get the weights and biases for the last layer only.

### ❖ Comparison of the Th. Cond. Data with exp. data

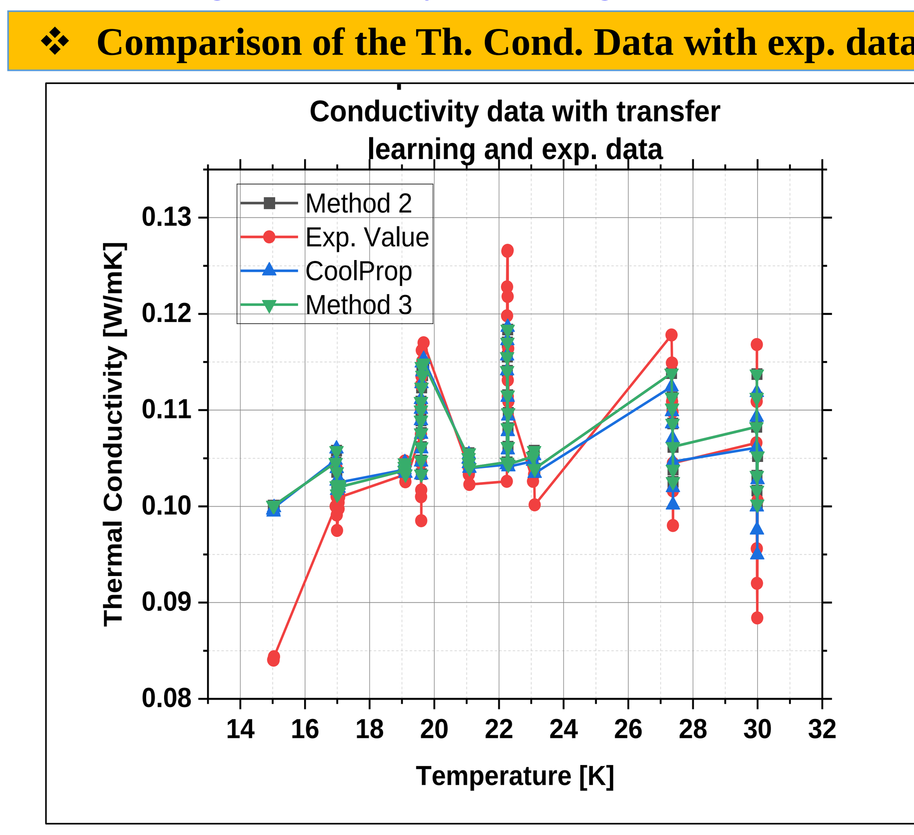


Fig. 13 Comparison of the Th. Cond. Data with transfer learning and exp. data

## Conclusions

❖ The ANN base model was trained with the simulation data for the thermal conductivity of n-hydrogen and the predictions were accurate with < 1% error.

❖ In the temperature range of 15 K to 30 K, experimental data has been used to re-train the base model to improve the predictions. Results show minor improvements.

❖ The ANN models can be used to predict the thermo-physical properties, however, sources of more experimental data in the open domain are required to achieve better accuracy of the model.

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