

PREDICTION OF PCME'S THERMAL BEHAVIOR USING A DEEP NEURAL NETWORK

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Phase Change Material Emulsions stand out as potential latent thermal fluid in different thermal applications. This paper presents results concerning the prediction of the heat transfer behaviour of a 30 wt.% paraffin in water emulsion for a temperature range of 0-20 °C. Based on data obtained empirically, we developed a deep neural network to predict the PCME's heat transfer coefficient. The artificial neural model was developed using the most complex and new scientific and statistical tools – TensorFlow, Keras, Pandas and Python programming language. A complex statistical study was performed a priori to model's development. For comparisons, the model was first trained with 24 features (comprehensive model) and then with only 5 (lumped model), as they were the most statistically relevant. The two models have similar prediction mean squared errors (around 5% for the comprehensive model and around 6% for the lumped model), but the full model tends to converge faster (used only 30 epochs compared with 130). Both models showed very good prediction capabilities on new and unseen data: the comprehensive model predicted with only 5.0% error, while the lumped model had a mean squared error equal to 6%.

Keywords: paraffin emulsion, heat transfer, PCME, artificial neural networks

NOMENCLATURE

c_p	specific heat capacity [J kg ⁻¹ K ⁻¹]
h	local heat transfer coefficient [W m ⁻² K ⁻¹]
ρ	density [kg m ⁻³]
μ	dynamic viscosity [Pa s]
\dot{m}	mass flow rate [kg h ⁻¹]
T_i	mean mixed temperature of the PCME [°C]
T_{Ai}	plate temperature [°C]
T_{em}	inlet/outlet temperature of the PCME [°C]
u	velocity [m s ⁻¹]

Abbreviations

PCME	Phase Change Material Emulsion
PCS	Phase Change Slurry
ANN	Artificial Neural network

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1. Introduction

In a continuously developing world, the main source of the progress remains the energy. Several concerning problems such as growing energy shortage, low fossil fuel resources and climate change coupled with high oil prices have been one of the main focuses in the last century. Researchers all over the world [1] are looking for solutions to fulfill the energy demands by developing new energy sources. One of the promising solutions in the general context is the use, as previously mentioned, of latent functionally thermal fluids [2-5]. Phase Change Material emulsions (PCMEs) were found to be popular and interesting for comfort cooling applications: they perfectly fit with the required range of temperatures (0-20 °C) owing to the use of paraffin. In addition, PCMEs show significant advantages. They are safe, reliable, chemically inert, and stable, easy to produce with a high phase change enthalpy [6,7]. The paraffin/water emulsion is a system of two immiscible liquid phases in which small particles of paraffin are distributed in water and maintained in dispersion by a surfactant.

In recent years, PCMEs have been increasingly investigated. The studies have been focused especially on the preparation methods [8-10], thermal properties [11-13], reducing their supercooling degree [14-16], investigating the rheological and heat transfer behavior during phase change [17-19].

One of the biggest problems of this type of fluid is the supercooling degree. Over time, different types of paraffin emulsions with different types of surfactant have been studied. The link between the supercooling and the type of surfactant used during emulsion preparation has been scientifically demonstrated [20, 21]. An important step towards using this fluid in a practical way is to find the most suitable type of surfactant so that the degree of cooling is as low as possible.

It would be interesting to know the rheological or the heat transfer behavior of a paraffin emulsion before its preparation, since testing many types of surfactant could easily become expensive and time consuming. Therefore, this paper presents a new method of approaching the subject. Considering the high complexity of the problem, a deep artificial neural network (ANN) was trained with data obtained from an experimental stand described in paper [19]. The ANN was used due to its widely known generalization capabilities, becoming a very powerful tool when sufficient training data is available.

Even though ANN's and Machine Learning techniques, in general, are used in a wide range of domains and applications, the literature survey show very few titles [22]. Matter of fact, only three found articles were considered relevant when this paper was initially written (August 2020) and all were published recently, from January to August 2020. For example, in [23], the authors trained a multilayered perceptron using experimental data obtained from a PCM heat sink and use to predict the Nusselt number and, implicitly, the heat transfer coefficient.

They also found that the optimal ANN architecture is formed by 15 neurons in the hidden layer and showed fair performances with maximum difference between real and predicted values of 6.0%. S. Motahar [24] used a similar approach to estimate the melting characteristics of n-octadecane PCM. The ANN had two hidden layers with 18 and 15 neurons, respectively. The author considered as inputs three a-dimensional numbers (Fourier, Raylight and Stefan) and predicted the melted volume fraction (V/V_0) of the PCM. All the proposed ANN model's outputs fell within the range of 6.23%. A slightly different approach can be found in [25], where the authors developed an ANN to analyze a photovoltaic thermal system cooled with a nano PCM fluid. Here, the predicted values were the electricity and heat provided by the hybrid system and the accuracy parameters were: R2 - 0.8742, trend accuracy - 59.7, MSE - 0.0223, and RMSE - 0.149.

Deep Learning algorithms are a subset of a wider domain called Machine Learning [26]; they become popular due to the increased computational power of modern computers and data availability. This paper presents the results of predicting the heat transfer coefficient of PCMEs using a deep sequential neural network developed in Python and using the TensorFlow machine learning library among other scientific and computational tools.

2. Materials and methods

The experimental data used in this article for the developed model are the data recorded during the study of a 30 wt.% paraffin in water emulsion that was developed for comfort cooling applications. The previous studies focused on the experimental characterization of the thermal performances of this emulsion in laminar flow during its cooling in a rectangular plate heat exchanger. Further information on the experimental setup and experimental investigation is presented by Vasile et. al 2018 [19, 27]. Different sets of measurements were considered. These contain measured and calculated physical parameters such as density, viscosity, conductivity, specific heat capacity, flow rate, emulsion temperatures and heat exchange coefficient. The cooling section used to investigate the phase change of the PCME during its cooling, is composed of three channels. This represents to some extend a typical arrangement for plate heat exchangers. The PCME flows into the central channel. It enters the bottom and exits through the upper side. Ethanol circulates through the outer channels in counter current, thus cooling the PCME. The central channel through which circulates the PCME is composed of two stainless steel (304) plates (width = 130 mm, thickness = 4.5 mm, length = 1110 mm) [27]. This experimental setup measures different categories of data, such as: density, mass flow and velocity, 9 intermediary plate temperatures (TA_1...TA_9) and 9 mixed mean temperatures of the PCME, that will ultimately allow the calculation the

heat transfer coefficient during cooling. The positioning of the thermocouples for measuring the temperatures of PCME on the steel plate is represented in Fig. 1. The mixed mean temperature of the emulsion from the inlet to the outlet of the cooling channel was determined using the energy balance.

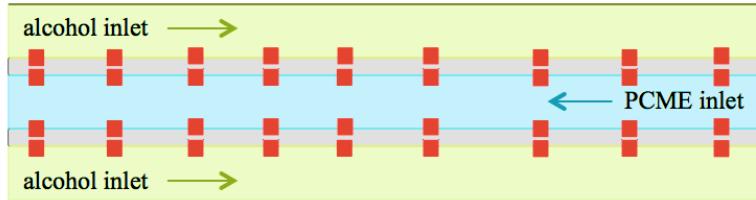


Fig. 1. Thermocouples position (red squares) on the steel plates forming the cooling channel

2.2 Data analysis and preparation

Creating accurate predictive machine learning models implies good knowledge about the data and it usually involves data preparation. The better the data ‘fed’ to the model, the better the results; thus, the data preparation process is a required and important step in developing an accurate model.

A full experiment consists in harvesting all the data for approximately 60 minutes, with a time step of 25 seconds, implying 149 timesteps; for these study data from 15 experiments was used, meaning a total of 2235 timesteps. One timestep consists of 35 values, including the heat transfer coefficient. 10 random timesteps are not used in neither training nor testing processes and will be used to test the model’s prediction accuracy over unseen-before data. Initially, the whole dataset was split into smaller training and testing datasets – 1564 (70.0%) observations for training and 661 (29.5%) observations for tests and 10 (0.05%) data points for validation (totaling 2235 datapoints); these are not used at all in neither training nor testing processes and was used to plot the results on unseen before data. The samples were split randomly so we can validate the model on wider data dispersion. Given the fact the temperatures of plate A are very similar with temperatures on plate B, only the first were considered in training the model; thus, the total number of features decreased to 25. This is a first step in getting rid of redundant features, reducing this way the possibility of model’s overfitting (when a complex model predicts a trend in ‘noisy’ and unprepared data). If the training data is full of errors, outliers, and noise (poor quality of measured features or missing values within the data, measurement errors, etc.), it will make harder for the model to find the patterns within the data; this can be caused due to an overly complex model with many inputs, redundant or constant (without variation) features [28]. The model’s overfitting can be analyzed in the scenario when the accurately predicts the values in training set, but its prediction performances decrease when fed with new, unseen data. This is a main issue in

machine learning field, as the goal of a developed model is to be able to predict on future data in a specific domain. There are several techniques to reduce the overfit of an artificial neural network. For example, the mean value for the specific heat parameter is 3.62 kJ/kg/K, the mean mass flow is 846 kg/h, while the temperatures range from -2 °C to 24 °C and the target feature (heat transfer coefficient) has a min value of 131.35 W/m²/K and a max value of 9218.98 W/m²/K. Using the data in this form can lead to poor prediction capabilities or even poor generalization. Thus, the data is to be first normalized, meaning that all features are rescaled at values between 0 and 1. This can guarantee stable convergence of weight and biases and improve algorithms like linear regression-based models or neural networks.

The statistic description of the data can be analyzed in Table 1, where: count – total nonnull values, mean – mean value, std – standard deviation, min/max – minimum and maximum values, 25%, 50% and 75% - percentiles (a theoretical raw score which corresponds to a given percentile rank in a specified distribution [29]). When developing accurate models, an important step is to uniform the input features, as they present very high values dispersion.

Table 1.

Input data descriptive statistics

Thermophysical properties											
-	ρ	λ	c_p	\dot{m}	w						
count	2235	2235	2235	2235	2235						
mean	941.17	0.38	3.62	846.61	0.53						
std	0.30	0.00	1.45	254.16	0.15						
min	940.74	0.38	2.80	529.38	0.33						
25%	940.75	0.38	2.88	576.47	0.38						
50%	941.37	0.38	2.92	788.51	0.49						
75%	941.37	0.38	3.14	1081.76	0.67						
max	941.50	0.38	8.54	1404.70	0.86						
Plate A temperatures											
-	TA_1	TA_2	TA_3	TA_4	TA_5	TA_6	TA_7	TA_8	TA_9		
count	2235	2235	2235	2235	2235	2235	2235	2235	2235		
mean	2.47	2.51	2.51	2.13	2.00	1.96	1.95	1.95	1.76		
std	5.25	5.27	5.30	5.01	5.00	4.99	4.98	4.97	4.97		
min	-1.36	-1.36	-1.36	-1.49	-1.64	-1.65	-1.65	-1.65	-1.76		
25%	-0.13	-0.12	-0.15	-0.24	-0.36	-0.39	-0.39	-0.39	-0.55		
50%	0.02	0.03	0.01	-0.03	-0.18	-0.20	-0.20	-0.20	-0.37		
75%	1.24	1.33	1.36	0.54	0.37	0.29	0.24	0.19	0.04		
max	22.90	22.93	22.95	22.77	22.71	22.70	22.69	22.68	22.63		
Emulsion temperatures											
-	Tem_in	Tem_out	Tem_1	Tem_2	Tem_3	Tem_4	Tem_5	Tem_6	Tem_7	Tem_8	Tem_9
count	2235	2235	2235	2235	2235	2235	2235	2235	2235	2235	2235
mean	3.96	3.81	3.96	3.96	3.96	3.96	3.95	3.93	3.91	3.89	3.86
std	5.41	5.38	5.41	5.41	5.41	5.40	5.40	5.39	5.38	5.37	5.36
min	-0.31	-0.45	-0.31	-0.31	-0.31	-0.32	-0.32	-0.34	-0.36	-0.38	-0.40
25%	1.05	0.90	1.05	1.05	1.05	1.04	1.04	1.03	1.01	1.00	0.99
50%	1.32	1.19	1.32	1.32	1.32	1.31	1.31	1.30	1.29	1.27	1.26
75%	3.99	3.77	3.99	3.99	3.98	3.98	3.96	3.93	3.89	3.86	3.81
max	23.59	23.49	23.59	23.59	23.59	23.58	23.58	23.57	23.56	23.54	23.52

As observed from the statistic description, emulsion's thermal conductivity (λ) is a constant feature with no standard deviation (std = 0). Thus, this is a redundant feature and will not be considered for the model's training, the inputs totaling 24 features. The inputs trends are depicted in Figs. 2 to 4. Statistically, the heat transfer coefficient has the following structure: counts – 2235; mean – 1260.10; std – 840.33; min – 131.35; 25%-50%-75% - 531.87-1011.15-1809.69; max – 9218.98.

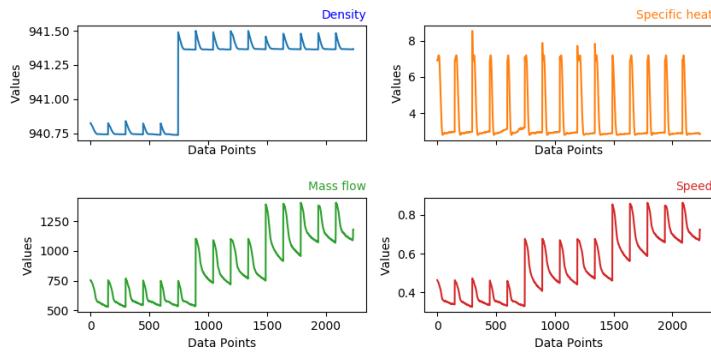


Fig. 2. Variation of the thermophysical properties

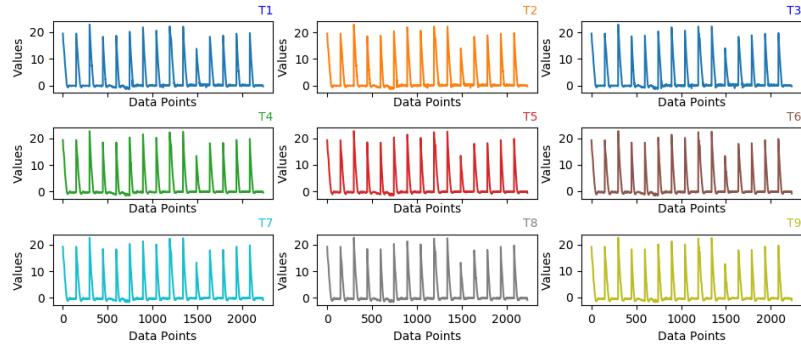


Fig. 3. Variation of temperatures along plate A

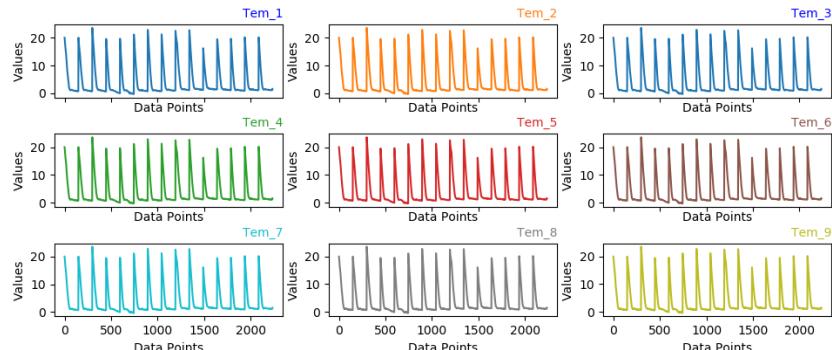


Fig. 4. Variation of the emulsion's temperature

When describing the data, it is essential to analyze the correlation between features and predictor. For the given problem, this is even more important because the input data shows high similarity as observed in the previous figures. It is worth mentioning that even if the correlation analysis provides an insight over the linear relationship, it does not provide the causality of the correlation [30]. There are several statistical approaches to determine the linear association between two continuous data, but the most used are Pearson's correlation – a parametric analysis and Spearman's rank-order correlation – nonparametric analysis [30]. The Pearson product-moment correlation coefficient is one of the most used techniques since is based on computing the covariance between data and besides the magnitude of correlation, it also indicates the direction of association (positive, zero or negative). The correlation heatmaps between temperatures and the heat transfer coefficient are shown in Fig. 5 (a and b). A positive r -coefficient indicates that the data varies in the same direction, while the negative values indicate an inverse variation trend; an r -coefficient equal to 0 shows no linear dependency between data. Moreover, a close to 0 correlation show low association between features, while values close to ± 1 indicates strong linear dependency [31]. As depicted in Fig. 5, the correlation between the temperatures and the heat transfer coefficient are positive and closer to 1, rather than 0 (indicate a strong positive linear relationship through); the r -coefficients vary from 0.708 (TA_9) to 0.751 (Tem_in and Tem_out). Additionally, all correlation coefficients computed for the emulsion temperatures are slightly higher than the ones for the plate's temperatures. The Pearson's correlation coefficients between the thermal properties and the heat transfer coefficient are shown in Table 2.

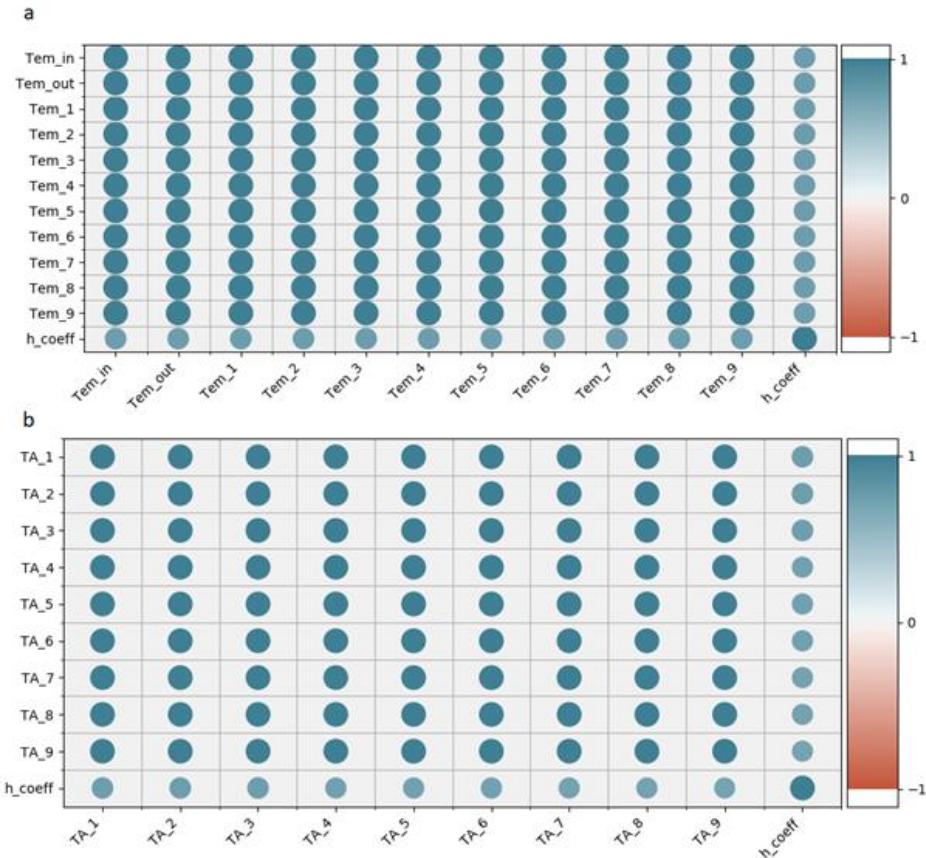


Fig. 5. Correlation heatmaps for: a – PCME's temperatures and b – plate A temperatures

Table 2.
Correlation values computed between thermal properties and heat transfer coefficient.

Property	r-coefficient value
Density (ρ)	0.281
Specific heat (c_p)	0.745
Mass flow (\dot{m})	0.419
Flow rate (w)	0.454

2.3 Model

The previous comprehensive analysis was made to select only the most important features for training the deep neural network. This data feature engineering is an essential step in avoiding overfitting the model. Consequently, we developed two models, the difference between them is consisting in the number of inputs: a *comprehensive model* containing all temperatures and thermal properties - totaling 24 features and a *lumped model* containing only statistical relevant features: specific heat, TA_1, TA_9, Tem_in, Tem_out –

totaling 5 inputs. The results will be discussed in section 3; it is worth mentioning that the computational time will be taken into consideration when comparing the two models, but its optimization is beyond the scope of this paper. Regardless the number of inputs, the models were developed using the same logic, configuration, hyperparameters and Deep Learning libraries. The final configuration of the ANN is presented in Table 3. In the presented configuration, the dropout refers to another technique used to avoid overfitting. It is a regularization technique where randomly selected neurons are ignored during training stage and ‘dropped’. The rate of ignored neurons is an important hyperparameter of the neural network [32]. At each layer, the weighted sum of inputs is computed, and the results is and feed to an activation function, which, in fact, gives the network’s nonlinearity. The rectified linear unit (ReLU) activation function has a main advantage over other activation functions: it does not activate all neurons at once. ReLU is a simple algorithmic calculation which returns the value provided as input directly (if the input is strictly greater than 0), or 0 (otherwise) [33].

Table 3.

ANN’s layer configuration and activation functions

Layer type	Neurons	Activation function	Dropout rate
Input	128	Rectified Linear Unit - (ReLU)	yes – 20%
Hidden 1	64	Rectified Linear Unit - (ReLU)	yes – 20%
Hidden 2	64	Rectified Linear Unit – (ReLU)	yes – 20%
Output	1	Linear	no

After choosing the right architecture, the model is to be compiled (or configured) to be further used. This essentially defines the model’s training configuration: optimizer, loss function and metrics to be analyzed. For this model, the following training metrics were chosen:

- optimizer: Adam – learning rate: 0.002 [details about Adam opt. in Ref. 26].
- loss (objective) function – mean squared logarithmic error.
- metrics – mean squared error and mean absolute error.

All these are used in the training process, where additional information is required – the batch size and the number of epochs, as well as the data used for training and validation. Essentially, training a neural network means finding the optimal weights that links the inputs and the output using the backpropagation of errors (as the data flows from inputs to outputs, the error flow backwards modifying the weight accordingly). The Backpropagation algorithm is the most used training technique in machine learning problems, regarding their kind (classification or regression). For this paper, it was chosen a batch size of 64 timesteps and 200 epochs. This was obtained experimentally (trial and error).

3. Results and discussions

The first model, *comprehensive model*, uses all 24 input features and predicts the heat transfer coefficient. The errors between the real and predicted values are the interest point in this study and were computed for both training and testing datasets. The ‘unseen’ values were fed to the network after the testing process and the results were plotted (Fig. 6). The computed mean squared error for each step in the prediction was around 5% regardless the configuration. Moreover, even if the number of epochs was set initially at 1000, we implemented an ‘early stopping’ feature, which automatically halts the model training if a monitored metric (validation loss reduction was selected) has stopped improving over a specified number of iterations. Thus, the model only trained for 30 epochs at most. The mean squared errors are: for train data - 5.2% and for test data - 5.8 %, validation data - 5.0%. The errors variation can be analyzed in Fig. 7. Besides numerical meaning, the loss variation indicates that, indeed, all the anti-underfitting measures worked, and the model performs well even for new, unseen before data.

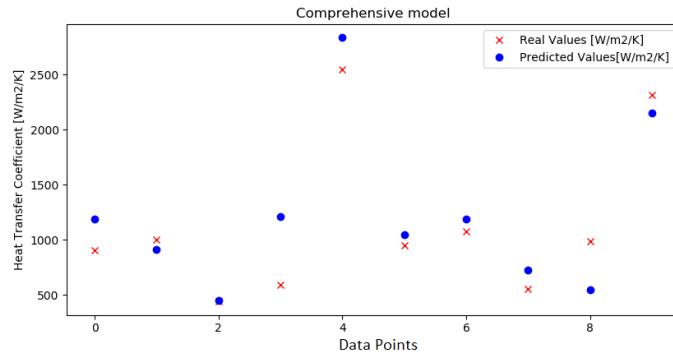


Fig. 6. Comparison between 10 ‘unseen’ values and the *comprehensive model*’s predictions

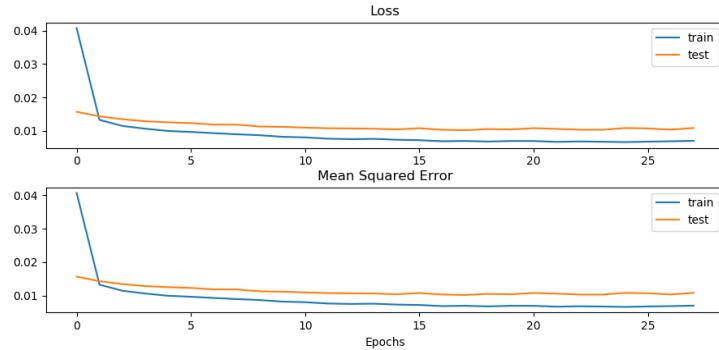


Fig. 7. Comparison between training and testing loss and mean squared error values for the *comprehensive model*

For comparison, a simplified model was developed – ‘lumped model’ for which only statistical relevant features were considered i.e. the emulsion’s specific heat and inputs and outputs temperature for both plate A and emulsion. Thus, the model will only have 5 input features and will predict the heat transfer coefficient. The model’s architecture and hyperparameters were the same as used for the comprehensive model. For this, the computed mean squared errors were 5.5 % for the training dataset, 6.2% for the testing dataset and 6.0% for validation. Even if the errors are similar, the early stop occurred after 130 epochs, increasing this way the computational time. The errors variation and the analyze of the model’s performances on new data are shown in Figs. 8 and 9.

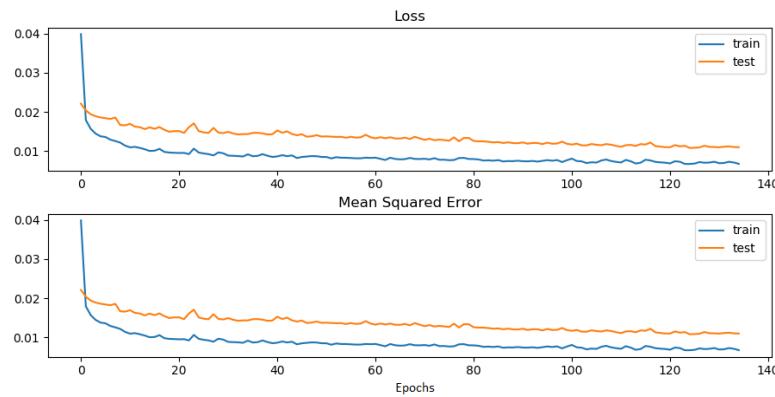


Fig. 8. Comparison between training and testing loss and mean squared error values for the *lumped model*

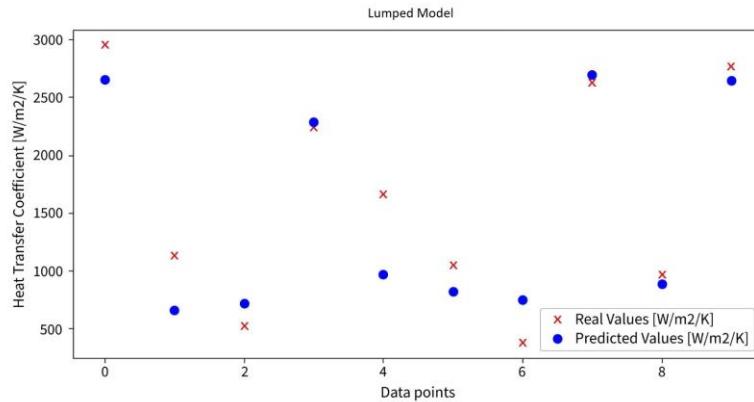


Fig. 9. Comparison between 10 ‘unseen’ values and the *lumped model*’s predictions

This study indicates that the two models have similar accuracies and even if the first model converges faster, the fact that there are just 4 temperature sensors used (instead of 20) increases its practical usage. Therefore, this study allows the improvement of experimental facilities for testing these types of fluids. For the

feature, a smaller and cheaper experimental stand can be developed and exploited. Moreover, different configurations and sensor positioning will be tested.

4. Conclusions

This paper presents the steps in creating a deep neural network used to predict the heat transfer coefficient for PCME material. The dataset was obtained during one of the author's Ph.D. research period and comprises information about emulsion's thermophysical properties and temperatures and intermediary temperatures of the plate. Moreover, a detailed statistical analysis was performed to better understand how the features affects the predicted value and two deep neural networks were developed and compared: one using all inputs and one using only the relevant features found. The results did not differ much, as the errors were relatively equal (around 5% for the *comprehensive model* and 6% for the *lumped model*), but when using all 24 inputs, the model converged faster – 30 epochs compared with 130 epochs. The models were both trained with around 70% of the dataset, validated with the rest of the data and 10 timesteps were used as new data to verify the models' prediction accuracy on unseen features.

The research is ongoing, and several detailed feature importance algorithms will be implemented. This will help to accurately establish which parameters influence most the heat transfer coefficients, thus reducing the overall complexity of the current model. Moreover, another ANN architecture is in development and will be used to analyze the dynamic changes in different PCMEs thermo-physical properties. This recurrent Long Short-Term Memory network is appropriate for this kind of study as it is generally used to analyze sequential data. The study will be focused on reducing the pumping energy consumption of the PCMEs infrastructure by analyzing the thermal properties of several types of emulsions at different distances and temperatures. Additionally, an experimental PCME experimental will be designed and used in research and teaching activities.

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