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2018

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Ziviani, Davide; Bahman, Ammar M.; James, Nelson A.; Lumpkin, Dominique; Braun, James E.; and Groll, Eckhard A., "Machine Learning Applied to Positive Displacement Compressors and Expanders Performance Mapping" (2018). *International Compressor Engineering Conference*. Paper 2533.
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Machine Learning Applied to Positive Displacement Compressors and Expanders Performance Mapping

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ABSTRACT

Positive displacement compressors are critical components in today's vapor compression refrigeration, air conditioning, and heat pumping applications and can also be applied as expanders in power generation systems, such as organic Rankine cycles (ORC). The simulation of such systems is essential to predict and optimize the performance behavior at full- and part-load conditions. To this end, comprehensive system models are built by including different sub-models corresponding to each cycle component (e.g., heat exchangers, compressor, linesets). In general, the higher the complexity of each sub-models utilized to capture the physics, the higher the computational time required to solve a simulation run.

In this work, deep learning is utilized to obtain high-accuracy performance predictions of positive displacement machines. A fixed-speed two-phase injected and vapor injected scroll compressor for air-conditioning applications and an oil-free scroll expander for low-grade waste heat recovery by means of an ORC are considered as test cases. In particular, Artificial Neural Network (ANN)-based models have been developed for each of the machines and trained using experimental data collected at the Ray W. Herrick Laboratories. The results of the training and testing of the models are presented as well as a discussion of the reliability of such models for extrapolating performance. In addition, the ANN models are compared with conventional empirical and semi-empirical modeling approaches. The models have been implemented in the Python programming language by using the open-source Keras package.

1. INTRODUCTION

In recent years, machine learning techniques and artificial intelligence methods have been utilized to accurately predict the performance of components or systems in different fields (Ledesma, Belman-Flores, & Barroso-Maldonado, 2017). With respect to positive displacement machines, Artificial Neural Network (ANN), Adaptive Neuro Fuzzy Interference System (ANFIS), and other hybrid approaches, e.g., ANN-PLS (Partial Least Squares), have been applied to characterize the performance of compressors such as reciprocating (Ledesma et al., 2017) and vapor-injected scroll (Zendehboudi, Li, & Wang, 2017), among others. The effectiveness of such artificial intelligence methods in terms of accuracy and computational efficiency have already been demonstrated for vapor compression systems. Belman-Flores et al. (2015) compared simulation results from a physical model of a reciprocating compressor with an ANN model. They concluded that the ANN model had better accuracy in representing the compressor performance because it was based directly on the measured data without any assumptions or simplifications, which are typically needed while developing a physical based model. Nonetheless, to the best of the author's knowledge, there has been a limited number of attempts to use such methodologies for ORC applications and more specifically for positive displacement expanders. For example, Massimiani et al. (2017) employed an ANN model to maximize the power output of an ORC system for WHR applications while constraining the size of the heat exchangers and, therefore, the cost of the system. The model was constructed as multi-input single-output with a single hidden layer of neurons.

In this paper, an open-drive oil-free scroll expander installed in a small-scale organic Rankine cycle (ORC) for waste heat recovery applications, and a hermetic scroll compressor with economization tested in a calorimeter are considered as test cases to explore ANN models for performance characterizations. In particular, the main contributions of the

present work with respect to the available literature are as follows:

- to develop and validate an ANN model of the scroll expander running with R245fa at different heat source inlet temperatures, pressure ratios, and rotational speeds;
- to develop and validate an ANN model of the fixed-speed hermetic scroll compressor with vapor-injection and two-phase injection utilizing R407C as working fluid;
- to compare the ANN models of the scroll expander and scroll compressor with a physical-based semi-empirical model and empirical correlations, respectively;
- to assess the extrapolability of the ANN model.

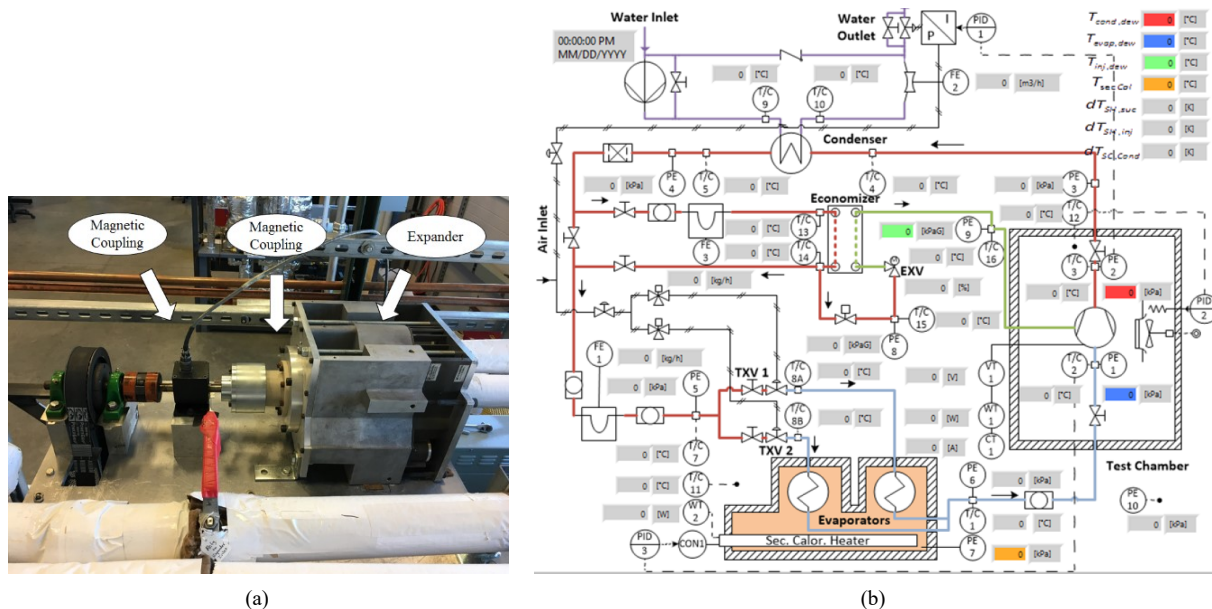


Figure 1: (a) Scroll expander installation including the magnetic coupling and the torque sensor; (b) Schematic of the injected scroll compressor installed in a calorimeter.

2. EXPERIMENTAL DATA

The scroll expander and the scroll compressor have been extensively tested in an ORC test bench and in a calorimeter, respectively. The main characteristics of each experimental campaign are provided in the following subsections. More detailed information can be found in Ziviani et al. (2018) and Lumpkin et al. (2018).

2.1 Oil-Free Scroll Expander

An open-drive scroll expander with nominal power capacity of 5 kW was used in the experimental testing. The expander has been designed for low-grade waste heat recovery by using R245fa as the working fluid. A magnetic coupling was installed in the back of the expander to limit working fluid leaks to the ambient. Thus, the expander is coupled to an electric generator by means of a torque sensor, as shown in Figure 1(a). The expander built-in volume ratio was 3.5 and it had a displacement volume of 73.6 cm³ per revolution. Due to design constraints, the operating conditions of the expander were limited as follows:

- maximum inlet pressure 1380 kPa;
- maximum temperature 175 °C;
- rotational speeds from 500 rpm to 3600 rpm.

The experimental campaign test matrix is summarized in Table 1. In particular, for each of the heat source inlet temperature conditions, four expander rotational speeds were investigated. At each expander rotational speed, the

Table 1: Test matrix of the expander experimental study.

Source Temperature (°C)	Expander Rotational Speed (rpm)				
85 °C	800	1600	2000	2500	3000
110 °C	800	1600	2000	2500	3000

pump speed was gradually increased from its minimum (between 80 rpm and 110 rpm) until one of the following three conditions occurred:

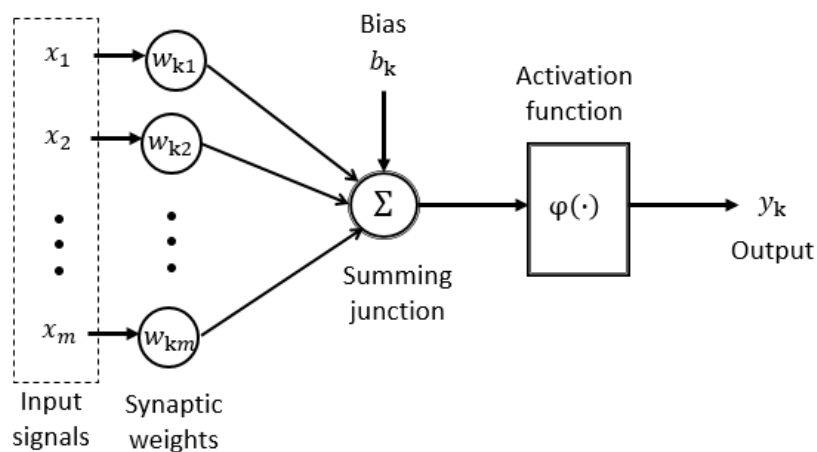
- the degree of superheat was lower than 3 °C;
- the limit of 23 Nm of the torque sensor was reached; or
- the pressure inlet of the expander was approximately 1380 kPa.

During the experimental campaign, a total of 75 steady-state data points were collected. In particular, 18 data points were obtained for the heat source temperature of 85 °C, and the remaining 57 data points for the heat source temperature of 110 °C. The data was employed to calibrate a semi-empirical model with several frictional loss terms (Ziviani et al., 2018).

2.2 Scroll Compressor with Vapor injection and Two-phase injection

A single-port injection hermetic scroll compressor was considered to assess the impact of vapor-injection and two-phase injection on the overall compressor performance. The compressor was a fixed speed model and the working fluid was R407C. Calorimeter testing was conducted for a total of 43 steady-state data points: 21 data points were collected for variable injection superheat, 11 data points were obtained at a fixed injection superheat, while the last 11 data points were collected with two-phase injection. In particular, in the case of fixed injection superheat, the superheat was maintained at 5.56 K. The injection ratio, defined as $\dot{m}_{inj,comp}/\dot{m}_{suc,comp}$, ranged from 0.094 to 0.028 corresponding to an injection mass flow rate range of 7.56 – 21.17 g/s . The compressor power input ranged from 3.2 to 5.6 kW. The variable superheat conditions were achieved by keeping the opening of the electronic expansion valve (EXV) constant at 10% for different operating conditions. In the case of two-phase injection, the injection ratio ranged from 0.11 to 0.30 corresponding to an injection mass flow rate range of 8.87 – 24.84 g/s . The compressor input power ranged from 3.2 to 5.7 kW.

The experimental data points were employed to develop a new performance mapping methodology based on the Buckingham-PI (B- π) theorem and applicable to both fix and variable speed injected compressors (Lumpkin et al., 2018).

**Figure 2:** Non-linear model of the k – th neuron of an ANN.

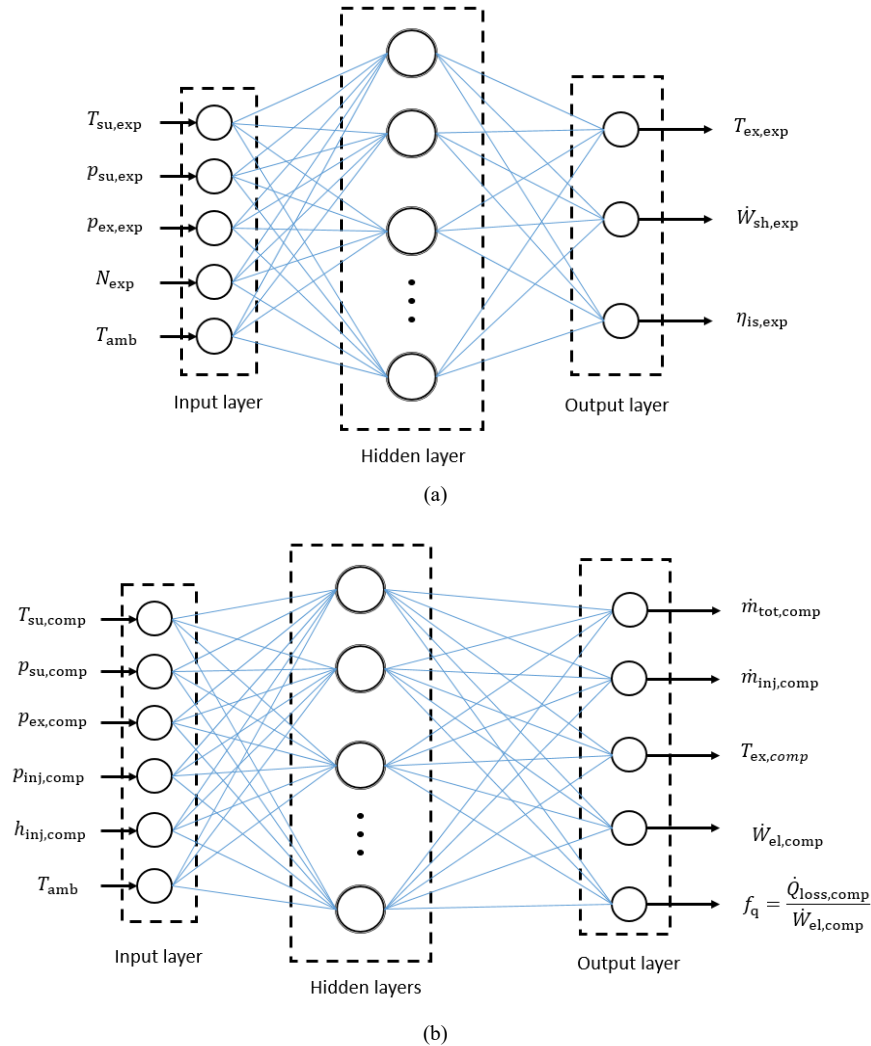


Figure 3: Schematic of the ANN model applied to: (a) oil-free open-drive scroll expander; (b) single-port injected hermetic scroll compressor (fixed speed).

3. ARTIFICIAL NEURAL NETWORK (ANN) MODELING

ANNs make use of the highly complex, non-linear, and parallel-computing aspects of the brain (Haykin, 2009). Similarly to the human brain, once a ANN model is defined, it requires a learning process in order to perform useful computations. The development of a ANN model relies upon the concept of a neuron. As described by Haykin (Haykin, 2009) and depicted in Figure 2, each neuron is characterized by a set of synapses or input signals, x_j , each of which has a certain weight, w_{kj} . All the input signals, weighted by the respective synaptic strengths of the neuron, are summed by means of a linear combiner. An activation function, $\phi(\cdot)$, is used to limit the amplitude of the output of the neuron. External bias, b_k , can be included to increase or decrease the net input of the activation function. Mathematically, the k -th neuron can be written as:

$$y_k = \phi \left(\sum_{j=1}^m w_{kj} x_j + b_k \right) \quad (1)$$

A general ANN is comprised of an input layer, an output layer, and one or more hidden layers that create the computational network. In the present work, both scroll machines are modeled with a feed-forward multi-layer ANN having multiple inputs and outputs. In particular, by considering the schematic representations of Figure 3, the input layer for

Table 2: Details of ANN network developed

Parameter	Types/Value
ANN API package	Keras
Model compiler	Theano
Number of neurons in the input layer	max 300
Number of hidden layer	max 10
Number of neurons for each hidden layer	max 300
Number of neurons in the output layer	1
Learning algorithm	AdaMax
Activation function hidden layer	hyperbolic tangent
Activation function output layer	Linear
Validation data set	0.2
Error function	MSE

the scroll expander consists of the expander inlet pressure and temperature, the discharge pressure, the rotational speed and the ambient temperature. The output layer includes the discharge temperature, the shaft power and the overall isentropic efficiency of the expander. Whereas, for the scroll compressor, the input layer includes suction temperature and pressure, injection pressure, injection specific enthalpy, and the ambient temperature. The output layer allows to predict the total mass flow rate through the compressor, the injected mass flow rate, the discharge temperature, the total power consumption, and the fraction of heat losses.

The number of hidden layers is varied in order to obtain the optimal ANN structure. Generally, the higher the number of hidden layers and neurons, the better the model captures non-linearity, but also the higher the probability of over-fitting. The modeling has been done in the Python 2.7 programming language by employing the open-source neural networks API (Application Program Interface) Keras (Chollet, 2015) in combination with the Theano's compiler (*Theano*, n.d.). A non-linear activation function, i.e. hyperbolic tangent function, has been selected for the input layer and the hidden layers. Such choice is justified by the fact that non-linear activation functions are less sensitive to noise. Whereas, linear activation functions have been selected for the output layer of neurons. Each of the ANN models require a proper training and number of data points, and their quality has a huge impact on the accuracy of the predictions. To this end, 80% of the steady-state points have been used as a training set and the remaining 20% as a testing set. Due to the fact that the inputs of the ANN have different orders of magnitude, both training and testing data sets have been normalized between 0.1 and 0.9, as outlined by (Zendehboudi et al., 2017):

$$x_n = 0.8 \frac{x - x_{\min}}{x_{\max} - x_{\min}} + 0.1 \quad (2)$$

where x is the actual data point of one of the inputs, x_n is the normalized data point, x_{\min} and x_{\max} are the minimum and maximum values defined according the input type. The optimization is carried out with the *AdaMax* algorithm developed by Kingma and Ba (Kingma & Ba, 2015) which is a variant of the stochastic gradient-based optimization algorithm *Adam* based on the infinity norm. The mean square error (MSE) was selected as the error function to be minimized for each of the output variables:

$$MSE = \frac{1}{N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} (x_{i,\text{meas}} - x_{i,\text{calc}})^2 \quad (3)$$

The details of the ANN models used in the present work are summarized in Table 2.

4. RESULTS AND DISCUSSION

4.1 Modeling accuracy

The ANN models are compared with two conventional semi-empirical and empirical models to assess their overall accuracy in predicting the performance of the scroll expander and the injected scroll compressor. In the case of the scroll expander, a semi-empirical model is considered from a previous work (Ziviani et al., 2018). Generally, semi-empirical

models are able to predict the behavior of the expanders under the identified steady-state conditions reasonably well. However, it is also known that there are a number of physical phenomena occurring inside the machine that cannot be modeled accurately because of a number of simplifications that were introduced to develop the model. The use of an ANN model can overcome most of the limitations associated with the physical modeling with a proper training over the experimental data set. The intrinsic non-linearity of the ANN model is able to better capture the behavior of the machine. The results are shown in the form of parity plots of mass flow rate, shaft power output, discharge temperature and isentropic efficiency for both models and are shown in Figure 4. The trained ANN model showed two remarkable features: (i) it was able to reduce the MAPEs considerably for all four the predicted parameters, and (ii) the spread between the predicted and measured data points was more homogeneous and less dispersed. Both features are highly desired in a model. By looking at the parity plots, the mass flow rate was predicted with a MAPE of 1.39% and 90% of the points were within 1%. The power output presented a MAPE of 2.50% without any apparent bias in the results. The discharge temperature was predicted with an error within ± 1.5 K or a MAPE of 0.2%. Lastly, the isentropic efficiency showed a MAPE of 3.0%, but with a larger dispersion in the results when compared to the other calculated parameters. This fact can be attributed to the number of factors that influences the overall isentropic efficiency of the expander such as leakage flow, friction losses, heat transfer losses and other irreversibilities.

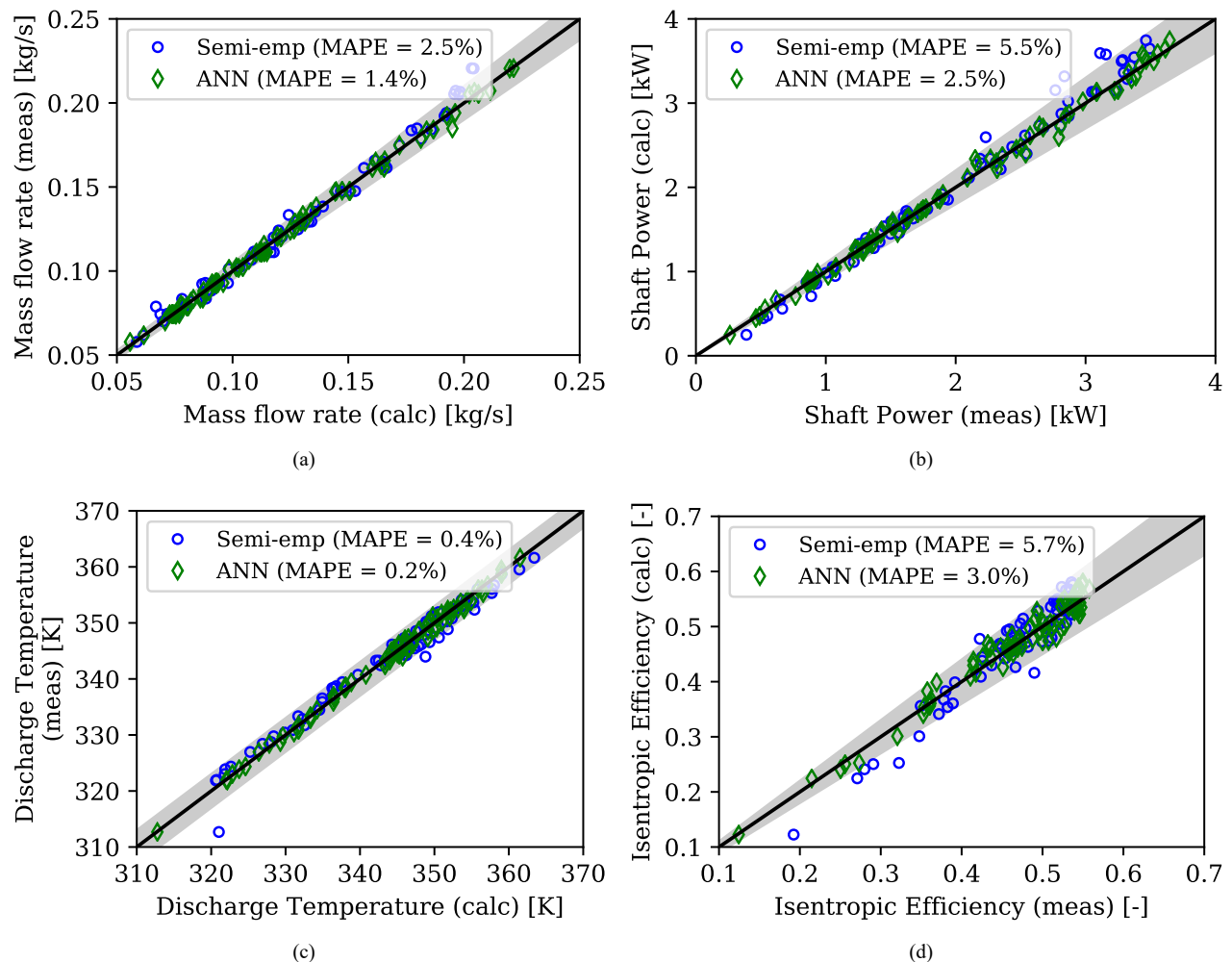


Figure 4: Comparison between measured and predicted values with ANN model and semi-empirical model for the oil-free scroll expander: (a) refrigerant mass flow rate; (b) power output; (c) discharge temperature; (d) isentropic efficiency. In the parity plots, all the steady-state points are shown.

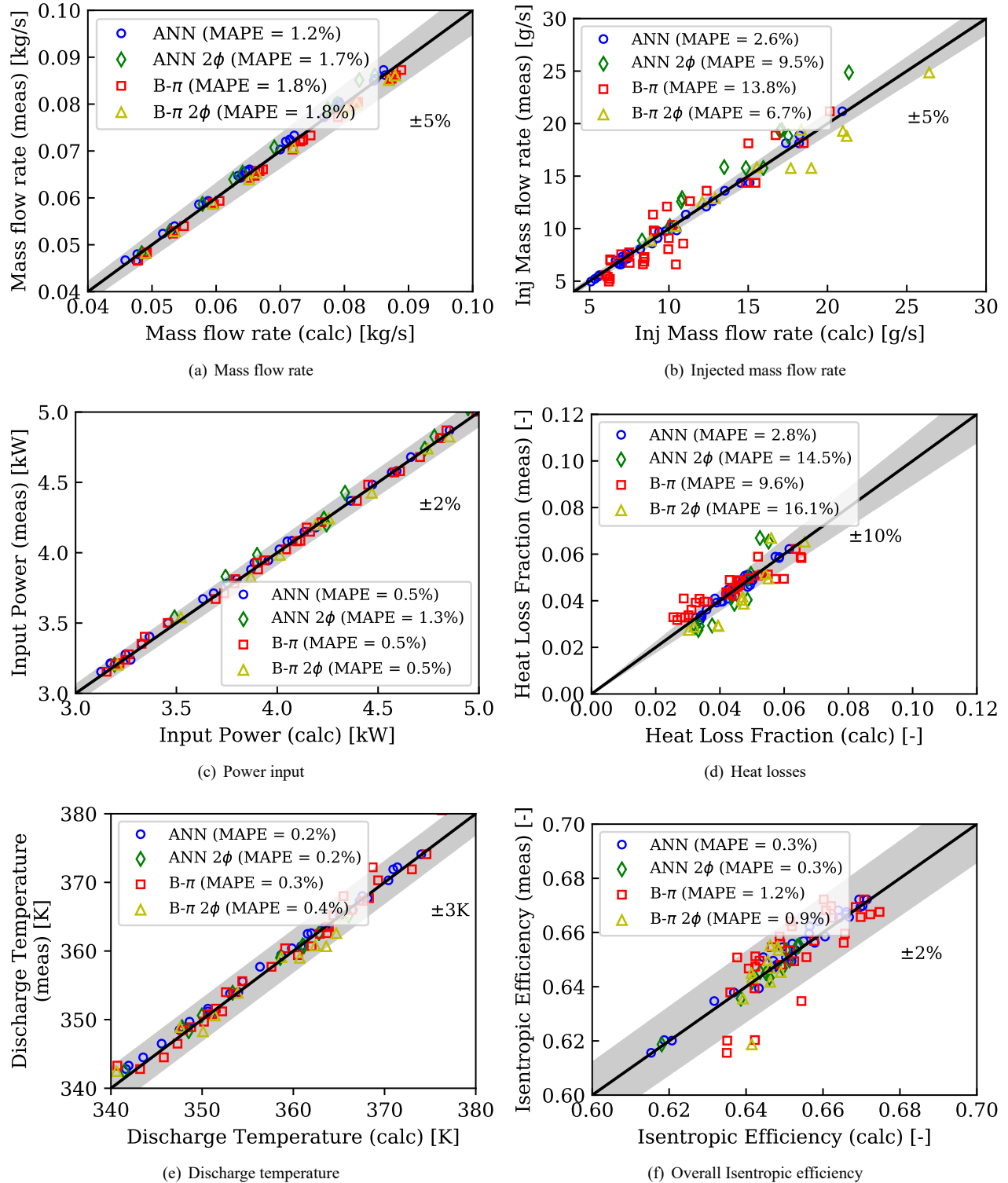


Figure 5: Comparison between measured and predicted values with ANN model and Buckingham-PI (B- π) dimensionless correlation for the injected scroll compressor. In the parity plots, all the steady-state points are shown. Vapor-injected and two-phase (2 ϕ) injected conditions are shown separately.

In the published literature of ANN applied to positive displacement machines (Belman-Flores et al., 2015; Ledesma et al., 2017; Zendejboudi et al., 2017), the isentropic efficiency has not been included as one of the neurons of the output layer. It is possible that more complex neural network models (Haykin, 2009) could be more suitable to fully capture the behavior of the isentropic efficiency.

In the case of the injected scroll compressor, a more comprehensive comparison between the ANN model and the dimensionless correlations obtained by employing the Buckingham-PI theorem is proposed. The correlations and associated coefficients have been previously published by (Lumpkin et al., 2018). As already mentioned in Section 2.1, experimental data points were obtained for both vapor-injected and two-phase injected conditions. Therefore, the ANN model and the dimensionless correlation are compared by considering both conditions. The comparison of the numerical predictions includes the following parameters: refrigerant mass flow rate at the compressor suction, refrigerant injected mass flow rate, electrical power input, compressor discharge temperature, heat loss fraction, and overall isentropic efficiency. Furthermore, to better visualize the different operating conditions, the results for vapor-injected and two-phase injected conditions are separated. The parity plots are shown in Figure 5. By looking at the results, the ANN model and the dimensionless correlations present similar MAPEs when predicting the suction mass flow rate, input power, and discharge temperature and the ANN model performs only slightly better. One possible explanation is that these parameters are less affected by uncertainties associated with measurements and thermodynamic effects. However, the usefulness of the ANN model can be proven when the injected mass flow rate, the heat loss fraction, and the overall isentropic efficiency are considered. In particular, the injection mass flow rate, especially under two-phase conditions, is challenging to be accurately predict. Both models struggled with the two-phase conditions, but the ANN model yields better overall predictions. The heat loss fraction is affected by both measurement uncertainties and physical phenomena that are difficult to predict with a simple correlation. The ANN model does a better job in predicting the heat losses in the case of vapor-injected conditions due to the larger data set available. Nevertheless, it is also able to outperform the dimensionless correlation in the case of two-phase injected conditions. With respect to the overall isentropic efficiency, the ANN model shows a remarkable consistency between the two data sets with a MAPE of 0.3%. The dimensionless correlation performs reasonably well, but the spread of the predictions is larger for some data points.

4.2 Extrapolation capabilities

It has been shown that the ANN models lead to a generally higher accuracy in mapping the performance of the two scroll machines. However, it is important to assess the extrapolation capabilities of such model (Dumont, Dickes, & Lemort, 2017) and its usefulness in performing parametric analyses. To this end, the ANN model of the scroll expander is compared to the semi-empirical model which contains physical aspects to some extent. A parametric study has been set as follows: inlet temperature of the expander fixed at 110 °C, discharge pressure equal to 150 kPa, pressure ratio between 3 and 10, and five rotational speeds of the expander, as investigated experimentally (800 rpm, 1600 rpm, 2000 rpm, 2500 rpm and 3000 rpm). The aim is to compare quantitatively the results of the mapping in terms of power output and isentropic efficiency. The results are shown in Figures 6, and 7. With respect to the expander shaft power output reported in Figures 6(a), and 7(a), all the models predicted a linear increase of the power with the pressure ratio, with the exception of the ANN model at 800 rpm. The reasoning for this fact will be addressed later. The semi-empirical model was the most conservative in terms of maximum power output and it is related to the emphasis of the model on the diversification of the mechanical losses. At 3000 rpm, all the models predicted the lowest power output for a pressure ratio of 3 and the highest for a pressure ratio of 10. Additional considerations on the quality of the predictions can be done by analyzing the trends of the isentropic efficiency in Figures 6(b), and 7(b). At the lowest rotational speed of 800 rpm, the ANN model was not able to capture the decay in over-expansion when the applied pressure ratio was lower than the internal volume ratio. In fact, the power output showed a non-linear behavior. The reason is likely that there were limited data points collected at that rotational speed and located at pressure ratios between 6 and 8. However, the ANN model captured the maximum isentropic efficiency measured at 1600 rpm for a pressure ratio of 5.95 very accurately. Furthermore, both the modified semi-empirical model and ANN model were able to predict the decay of the isentropic efficiency at higher pressure ratios. From the present analysis, it can be concluded that the ANN model showed very good results in predicting the actual behavior of the expander and did so in a computationally efficient way. However, the training of the model could likely be improved through additional data and possibly through modifying the layered network of neurons. Nonetheless, ANN can be regarded a very useful tool for mapping the performance of positive displacement machines for integration in a system simulation model.

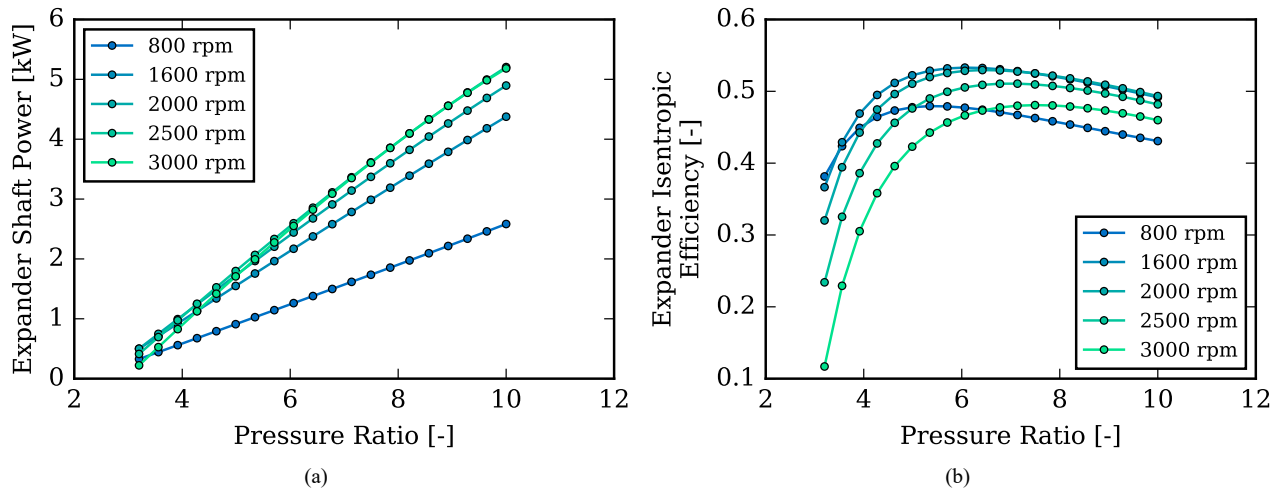


Figure 6: Performance mapping by using the modified semi-empirical model: (a) shaft power output; (b) isentropic efficiency.

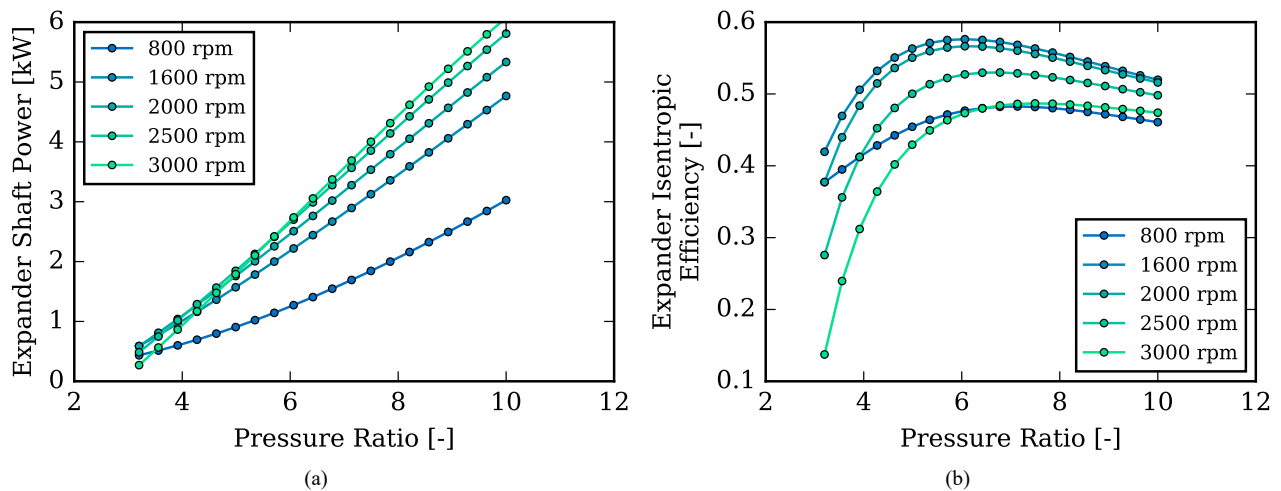


Figure 7: Performance mapping by using the ANN model: (a) shaft power output; (b) isentropic efficiency.

5. CONCLUSIONS

In this paper, artificial neural network (ANN) models have been compared with conventional semi-empirical and empirical models in order to predict the performance of a scroll expander and an injected scroll compressor. The following conclusions can be drawn:

- ANN model achieved the highest accuracy in modeling predictions because it was trained directly on the experimental data without the need of modeling assumptions. However, the usefulness of the ANN is limited to performance mapping with limited extrapolation capabilities. Different deep learning techniques could be explored to improve the ability of the model to perform parametric studies.
- The accuracy of the ANN model relies on the training data set. A more in-depth analysis is required to understand the minimum number of data points needed to train an ANN model for a specific problem and which neural structure could be most effective.
- Further research efforts should be pursued to optimize the activation functions, number of neurons per layer, and training algorithm in the case of thermodynamic problems.

NOMENCLATURE

b_k	k-th bias	(-)	Subscript	
f_q	heat loss fraction	(-)	amb	ambient
h	specific enthalpy	(kJ/kg)	comp	compressor
\dot{m}	mass flow rate	(kg/s)	el	electrical
p	pressure	(kPa)	ex	exit
\dot{Q}	Heat rate	(W)	exp	expander
T	temperature	(K)	inj	injection
w_{kj}	k-th and j-th weight	(-)	is	isentropic
\dot{W}	Power	(W)	max	maximum
x_k	k-th synapses	(-)	min	minimum
y_k	k-th neuron	(-)	su	supply
η	efficiency	(-)	2ϕ	two-phase

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