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Development of a surrogate model of a trans-critical CO_2 heat pump for use in operations optimization using an artificial neural network

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Development of a surrogate model of a trans-critical CO_2 heat pump for use in operations optimization using an artificial neural network

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Abstract. Conventional physics-based models can demand substantial computational resources when employed for operational optimization. To allow faster system simulations that can be employed for operational optimization, a surrogate model of the CO_2 heat pump has been developed using an artificial neural network (ANN). The ANN model takes in six (6) inputs: evaporator water-side mass flow, its temperature, gas cooler water-side mass flow, its temperature, set-point output temperature, and high-side heat pump pressure. The model's outputs comprise the electrical energy needed to run the heat pump, the heat from the gas coolers, the temperature of the heat pump-heated fluid, and the outlet temperature of the heat pump's evaporator. Data used for training, validating, and testing the ANN model were generated by running a calibrated Modelica model of the CO_2 heat pump for various combinations of input parameters obtained from Latin hypercube sampling. The ANN model developed includes an input layer with 6 inputs, 2 hidden dense layers, each with 30 neurons, and an output layer for 4 outputs (6-30-30-3). The ReLU activation function was implemented on each hidden layer and no regularizations were imposed. The Adam optimizer was used with a learning rate of 0.001 specified. Early stopping (patience = 2000) was implemented to ensure that the training data was not overfitted. A maximum of 30000 epochs was specified. The resulting Mean Square Error (MSE) obtained for the training, validation, and testing data sets were 1.38×10^{-5}, 2.05×10^{-5}, and 3.65×10^{-5}, respectively. When tested against one-week operational runs generated by Modelica, the Root Mean Square Errors (RMSEs) for coefficient of performance (COP)s for spring, summer, autumn, and winter operations obtained were 0.232, 0.346, 0.089 and 0.076, respectively. The resulting surrogate ANN model can be integrated into the system model as a functional mock-up unit within Modelica to facilitate faster simulations for operational optimization.

1. Introduction

Powered by low-emissions electricity, heat pumps play a key role in the global transition to sustainable heating and cooling. It is estimated to have the potential to reduce global carbon dioxide (CO_2) emissions by at least 500 million tons in 2030, which is roughly the same amount of annual CO_2 emissions of all cars in Europe today [1]. With the pace of heat pump installation growing at record levels, it is necessary that this growth is accompanied using working fluids/refrigerants that have low global warming potential (GWP). Unfortunately, some of the commonly used working fluids nowadays have very high GWP. For instance, R134a, which is widely used in domestic hot water (DHW) production, has a GWP that is 1300 times higher than that of CO_2 [2]. These high-GWP refrigerants can leak during manufacturing, installation, maintenance, and disposal, offsetting the benefits that heat pumps can bring. However, using a low-GWP refrigerant for an incompatible system can result in an inefficient heat pump system, which can lead to using more energy and emitting more CO_2. Having good operational efficiency while using low-GWP refrigerants is the ideal set up.

Carbon dioxide is possibly one of the most promising low-GWP refrigerants. It has zero ozone depletion potential and a GWP of 1. Additionally, it is non-toxic, non-flammable, easily available, and affordable[3]–[5]. The modern use of CO_2 in a trans-critical cycle was first proposed by Lorentzen [6]. Its most distinct difference from the conventional cycle is its use of a gas cooler instead of a condenser, accommodating a relatively large temperature glide in the heat rejection process [7]. So far, it has been commercially applied in combined cooling, heating, ventilation, and air conditioning in supermarkets [8], [9]; water heating [10]; and car air conditioning [11].

A Modelica [12] model of a trans-critical CO_2 heat pump, based on the 6.5 kW test rig constructed and tested by Stene [13, 14], has been developed and calibrated and was then integrated into a system model that utilizes borehole heat exchangers (BHEs), solar thermal collectors (SC), and a thermal energy storage (TES) tank for space and water heating [15]. Typically, optimization has to be performed for every energy system installation due to vastly different weather conditions, occupancy profiles, energy tariffs, government tariffs, system components, and building types [16]. Sazon et al. [17] studied the optimization of the design of this CO_2 solar-assisted ground source heat pump (SAGSHP) system for West Norway climate and demand and showed that compared to a conventional SAGSHP system, it can perform at a slightly lower seasonal efficiency, but at a comparable levelized cost of heating (LCOH). To further improve the performance of this system, it has been recommended to explore the optimization of its operations as well.

Studies about optimizing the operation of a CO_2 heat pump system typically focus on (1) controlling the compressor operation to take advantage of the variability in electricity prices or (2) controlling the gas cooler pressure to maximize efficiency.

Heat pumps, when coupled with TES, can be operated flexibly to benefit from the variability of electricity tariffs. This is implemented by shifting electricity import from high-demand to low-demand periods, which helps in managing grid stress and averting peak plant operation [18]. By running the compressor during periods of low-electricity-price to charge the TES, stored heat can then be discharged later to meet demand when electricity prices are higher. Several studies have already investigated load shifting in conventional heat pumps [16, 18–21].

It is well known that CO_2 heat pumps exhibit an optimal gas cooler pressure due to the distinct working mode in the trans-critical region [22, 23]. Because of this, several studies have been implemented on developing empirical optimal pressure correlations or algorithms for maximizing the coefficient of performance (COP) or other performance metrics [24–32]. Typically, this is conducted offline using experiments, physics-based system modeling, and thermodynamic cycle simulations [24]. The experiment-based approach is straightforward but can be expensive and time-consuming. Correlations developed from this method can also be quite limited to the testing conditions during the conduct of the experiments. Thermodynamic cycle simulation is usually preferred over the physics-based approach because it requires fewer modeling efforts. However, simple optimal pressure correlations based on thermodynamic simulation usually ignore some parameters and cannot model complex non-linear thermal fluid behaviors [24].

The benefit of using Modelica to model the CO_2 SAGSHP system is that detailed simulation characteristics of the energy system can be obtained. This can be done by using component models of the system that are calibrated or validated. However, these tools can be computationally expensive, more importantly when used for optimization problems that involve predictive control [16, 21]. One of the ways to overcome this is to replace component models that require heavy computations with a surrogate model that uses machine learning methods such as an artificial neural network (ANN) [33]. ANN is a rapidly emerging technology that has been widely applied for system optimization and modeling in energy and process systems [34]. Conventional thermodynamic analysis involves many iterations that cause much time in calculation. In comparison, ANN can correlate complex non-linear relationships between input and output parameters more quickly, with no complicated iteration[34]. For CO_2 heat pumps, ANN has been utilized in some studies [7, 35].

In this study, a surrogate model of a trans-critical CO_2 heat pump in a SAGSHP system was developed using ANN. The model will eventually be utilized and integrated into the system model as a functional mock-up unit within Modelica to facilitate faster simulations for operations optimization studies.

2. Methods

A surrogate model of a trans-critical CO_2 heat pump, based on the 6.5 kW test rig constructed and tested by Stene [13, 14], has been developed using ANN. The surrogate model is meant to replace a calibrated model of a CO_2 heat pump in a SAGSHP system in the Modelica environment.

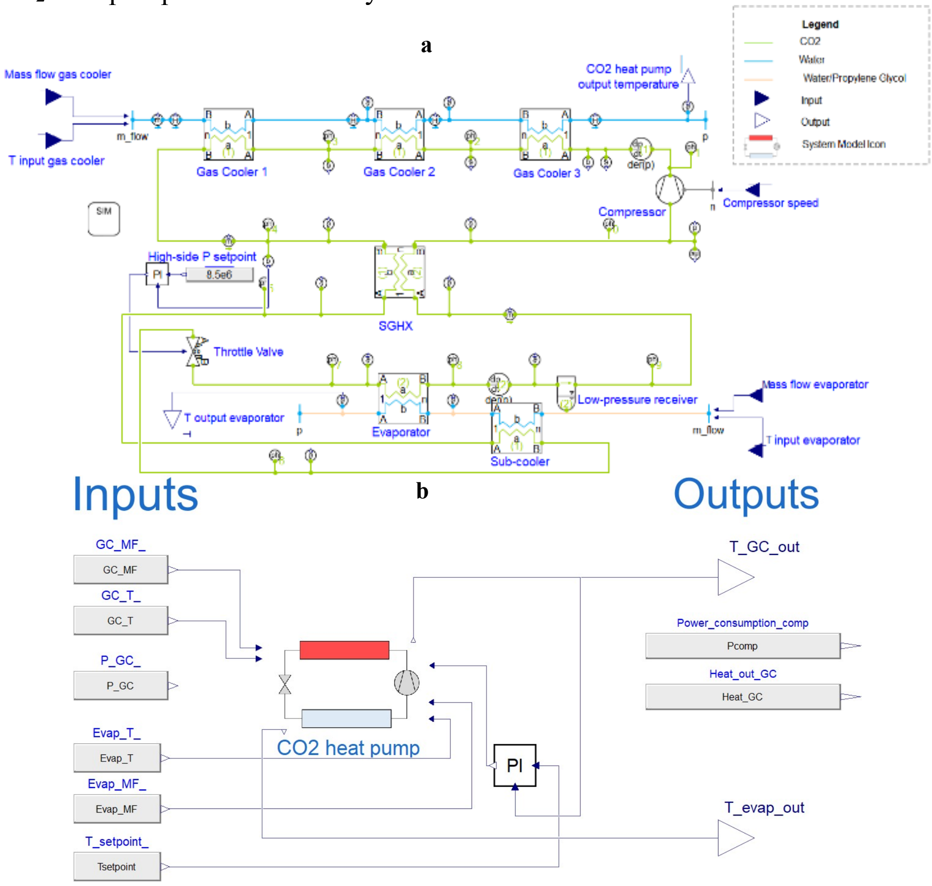

Figure 1. The Modelica Model of the trans-critical CO_2 heat pump: (a) showing the underlying components of the heat pump and (b) showing the inputs and outputs to the ANN model.

2.1. The Modelica model of the trans-critical CO_2 heat pump

The CO_2 heat pump model developed in this work was based on a 6.5 kW prototype unit. It consists of the counter-flow tripartite gas coolers, an evaporator, a compressor, a throttle valve, a suction gas heat exchanger (SGHX), a sub-cooler, and a low-pressure receiver (Figure 1a). Although the prototype can function in three modes (space heating only, domestic hot water (DHW) heating only, and simultaneous space and DHW heating), the model in this work was only calibrated for simultaneous space and DHW heating. It was developed using the Thermal Systems library [36] in the Dymola interface [37]. The Thermal Systems library, also synonymous with the TIL suite, is a commercial Modelica library for modeling thermo-fluid systems. It can be used to model various components, such as heat pump cycles, hydraulic networks, ventilation, and so on. It uses the TSMedia library to calculate the thermophysical properties of fluid and fluid mixtures. The model was calibrated against measured data at design conditions of the heat pump by adjusting the heat transfer coefficients of the heat exchangers (gas coolers, evaporator, internal heat exchanger) and the efficiency of the compressor. Details about the specifications of the CO_2 heat pump components and the calibration of the model are given in [15, 38]. In [17], this CO_2 heat pump model was integrated into a system that comprises of BHEs, SCs, and a TES and was used for space and DHW heating for climate and demand conditions in Western Norway.

2.2. Data preparation for training, validation, and testing of the ANN model

The Modelica model of the CO_2 heat pump was run for 10,000 combinations of input parameters to obtain the data needed to develop the ANN model. The inputs to the model were (1) the fluid mass flow to the water side of the evaporator (Evap_MF), (2) the temperature of this fluid (Evap_T), (3) the mass flow of the fluid to the water side of the gas coolers (GC_MF), (4) the temperature of this fluid (GC_T), (5) the set point output temperature (Tsetpoint) (controlled by adjusting the compressor speed), and (6) the gas cooler pressure set point (P_GC) (controlled by adjusting the throttle valve opening) (Figure 1b). Some of these parameters connect to the other components of the energy system while some can be controlled to optimize performance. The outputs chosen were (1) power consumption (Pcomp), (2) the total heat output (Heat_GC), (3) the output temperature of the heat pump (T_GC_out), and (4) the outlet temperature of the heat pump's evaporator (T_evap_out). The 10,000 combinations of input parameters that were simulated using the Modelica model were obtained using Latin hypercube sampling [39]. The value ranges (Table 1) for every input parameter were decided based on observed values from full-year simulations [17]. Each case was run for 15000 seconds to ensure that steady conditions of the outputs were obtained.

Table 1. The lower and upper bounds of the input parameters.

Input Parameters	Lower bound	Upper bound
Evaporator water side mass flow, kg/s	0.2	0.8
Evaporator water side temperature, °C	-5	25
Gas cooler water side mass flow, kg/s	0.0085	0.048
Gas cooler water side temperature, °C	15	55
Output temperature, °C	60	70
Gas cooler pressure, MPa	8.5	10

Some combinations of input parameters that are known to produce unfavorable heat pump performance, i.e., it both fails to reach the target output temperature and produces very low COPs, were filtered out from use in the development of the ANN model. This occurrence can happen when combinations of the following are met: the temperature of the fluid to the gas cooler is too high, the mass flow to the gas cooler is too low, or the evaporation temperature is too high. Only 6604 data points remained after doing this.

These data were then divided into training, testing, and validation sets. Twenty percent (20%) of the whole set was set for testing the ANN model. Afterward, 20% of the remainder was used for validation. All that remained were used for training the model. Given this, the training set, testing set, and validation set got 4226, 1321, and 1057 input/output combinations.

Since the different inputs and outputs have different magnitudes and units, it is necessary to subject all of them to normalization to remove the bias to parameters with high magnitudes. Here, min-max scaling was done. Min-max normalization is done by subtracting the minimum value from the data and then dividing this by the difference between and minimum and maximum values in the parameter set. This shifted and rescaled the values of every parameter, so they all ended up ranging from 0 to 1. Histograms of the normalized outputs in the training, testing, and validation sets for every input and output are given in Figures 2 and 3, respectively. It can be seen that the different values of the inputs and outputs seem to be equivalently represented in the data splits.

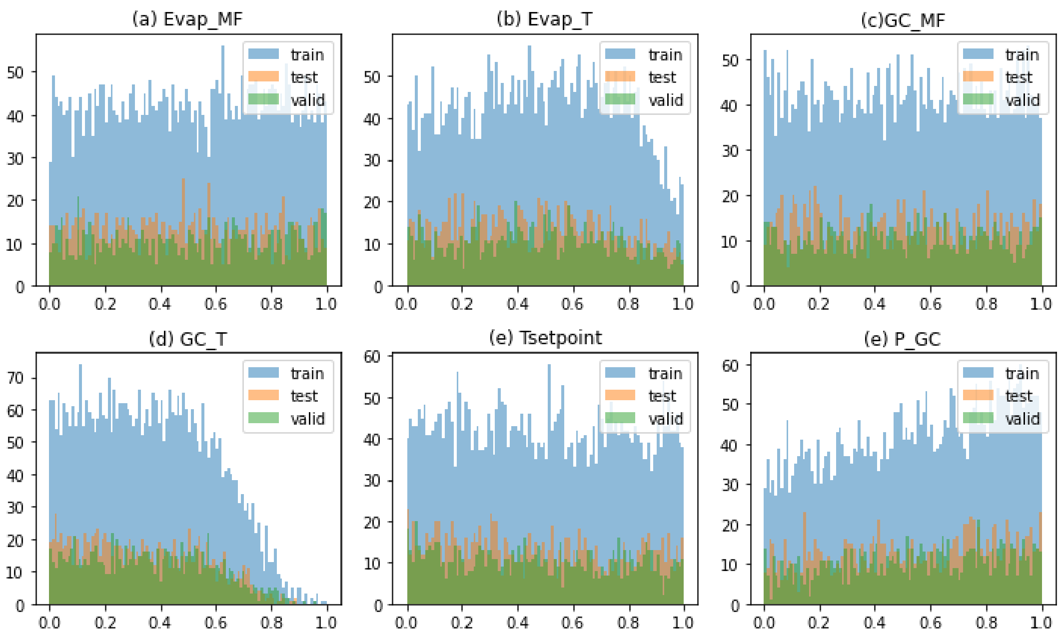

Figure 2. The histograms showing the splits of the inputs for training, testing, and validation: (a) mass flow of waterside evaporator fluid, (b) fluid temperature water side evaporator, (c) mass flow of waterside gas cooler fluid, (d) fluid temperature waterside gas cooler, (e) set point output temperature, and (f) set point gas cooler pressure.

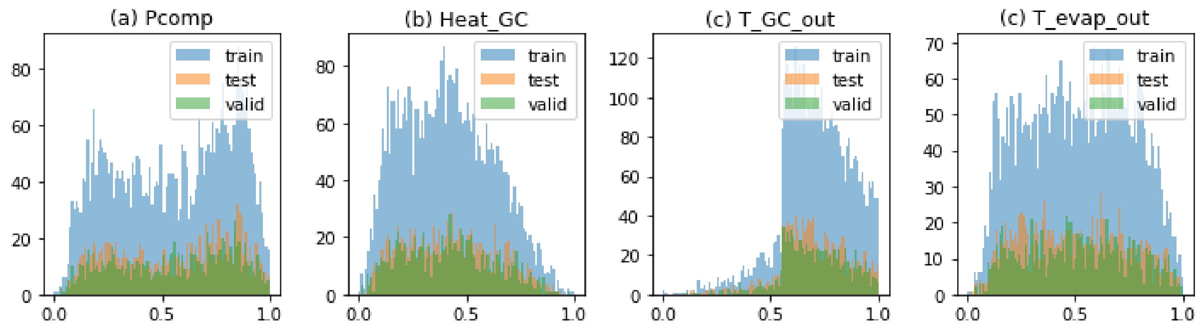

Figure 3. Histograms showing the splits of the labels for training, testing, and validation: (a) power consumption, (b) thermal energy generated, (c) output temperature of the heat pump, and (d) outlet temperature of the heat pump's evaporator.

2.3. Hyperparameter tuning and ANN model evaluation

The three (3) output parameters from the Modelica model were used as labels in the training of the ANN model. This was treated as a batch supervised regression problem and was implemented using Keras [40] in Python. The ANN was trained through backpropagation [41].

The hyperparameters tuned in this study include (1) the number of neurons, (2) the number of dense layers, (3) the optimizer, (4) the learning rate, (5) activation functions, and (6) the number of epochs. Early stopping was implemented as a callback to ensure that overfitting the training set was avoided.

The model was trained using mean square error (MSE) as the loss function.

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \widehat{Y}_i\right)^2 \tag{1}$$

The metrics used to evaluate the model's performance after training and during model evaluation is the root mean square error (RMSE)

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$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \widehat{Y_\iota}\right)^2} \quad (2)$$

Where n is the number of data points, Y_i are the observed values, and Y_i are the predicted values.

3. Results and discussions

The iterations involved in solving physics-based models make them computationally heavy. Comparably, ANN can correlate complex non-linear relationships between the inputs and outputs (labels) in a quicker way, without complicated iterations. When compared to statistical models, it has also been seen to perform at a higher accuracy [42]. After data generation and filtering, the ANN model was trained using backpropagation while considering six (6) input parameters (Evap_MF, Evap_T, GC_MF, GC_T, Tsetpoint, P_GC) and 3 outputs (Pcomp, Heat_GC, T_GC_out).

3.1. ANN model hyperparameter specifications

The training set, testing set, and validation set containing 4226, 1321, and 1057 input/output combinations, respectively were inputted to data frames in Python and used to develop the ANN model. The performance of an ANN significantly depends on its structure and hyper parameter settings. Here, the ANN performance was developed using trial and error approach. The loss function and metrics used were the MSE and the RMSE, respectively.

In developing an ANN model, there is no one-size-fits all approach. Often, it involves a combination of experimentation and best practices. Here, we started with the simplest model with 1 layer and 5 neurons while setting reasonable defaults for other hyper parameters. The number of neurons were increased until no significant improvement to the loss function was observed. By then, another hidden layer was added. The number of neurons investigated ranged from 5 to 50. The number of hidden layers from 1 to 3 were tested. Normalization of the inputs and outputs must be done to remove the biases to parameters with significant magnitudes. The min-max normalization was seen to give lower MSEs compared to standard scaling. The Adam optimizer outperformed other solvers, like SGD and RMSprop. Initially, SGD was giving better MSEs, but when the learning rate was reduced from 0.1 to 0.001, Adam performed better in terms of speed and accuracy. Among the activation functions tested (tanh, rectified linear unit (ReLU), sigmoid, scaled exponential linear unit (SELU)), ReLU gave the lowest MSEs. These observations underscore the iterative and dynamic nature of ANN model development, where a blend of experimentation and informed choices is essential to fine-tune the architecture and hyperparameters for optimal results.

The resulting model after tuning the hyperparameters contains an input layer with 6 inputs, 2 hidden dense layers, each with 30 neurons, and an output layer for 4 outputs (6-30-30-4 structure). The ReLU activation function [43] was implemented on each hidden layer and no regularizations were imposed. The optimizer used was Adam [44] and a learning rate of 0.001 was seen to produce the best results for training. Early stopping, with a patience equal to 2000, and a maximum epoch of 30000 were specified.

3.2. Training, testing, and validation results

The training of the ANN model terminated after 17627 epochs. Figure 4a below shows that the training and validation MSE decreased quickly at the start of the runs and remained almost constant until it satisfied the conditions for early stopping (patience = 2000). Figure 4b zooms into the last 500 epochs, showing the differences between the training and validation MSEs. Although a bit lower, the training losses obtained were comparable to the validation losses.

Figure 4. The MSE performance plot of the ANN during the training: (a) for the whole training period and (b) for the last 500 epochs.

The resulting values of the MSE and RMSE for training, testing, and validation at the end of the training process are given in Table 2. All of them seem to be sufficiently small, inferring a good match between the data and the simulation. Additionally, the MSE and RMSE for the testing data set are very close to that of the train set. This implies the capability of the developed ANN model for generalization. Figure 5 illustrates the ANN model-generated values of the outputs compared to those generated by the Modelica model. Most data points have been matched.

Table 2. MSE and RMSE for the training, validation, and testing sets.

	Training	Validation	Testing
MSE	1.38×10^{-5}	2.05×10^{-5}	3.65×10^{-5}
RMSE	0.0037	0.0045	0.0060

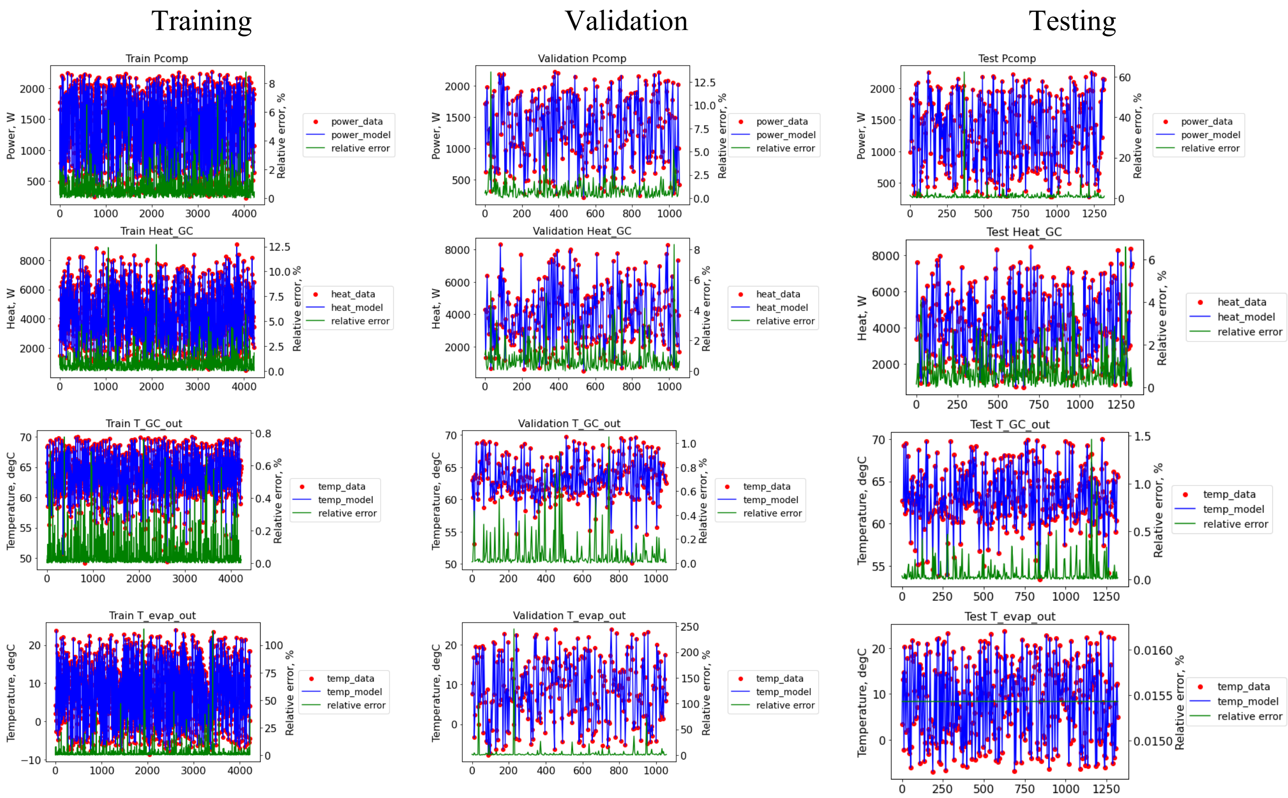

Figure 5. Match between the data and the ANN model-generated results for the training, validation, and testing sets.

3.3. Testing the ANN model for operational runs

To see if the training implemented is sufficient for the intended purpose, the ANN model was also tested against one-week operational runs generated in Modelica for different representative seasons (spring, summer, autumn, and winter). It can be seen that the model can follow the expected trends of output parameters of the CO_2 heat pump (Figure 6). This is slightly more evident for autumn and winter operations than for spring and summer. The RMSEs for each output for every season are summarized in Table 3. It shows that the average error the ANN model generates seems to be within reasonable levels. In particular, the COPs it generated differ from the Modelica-generated COPs only by 0.076 to 0.346.

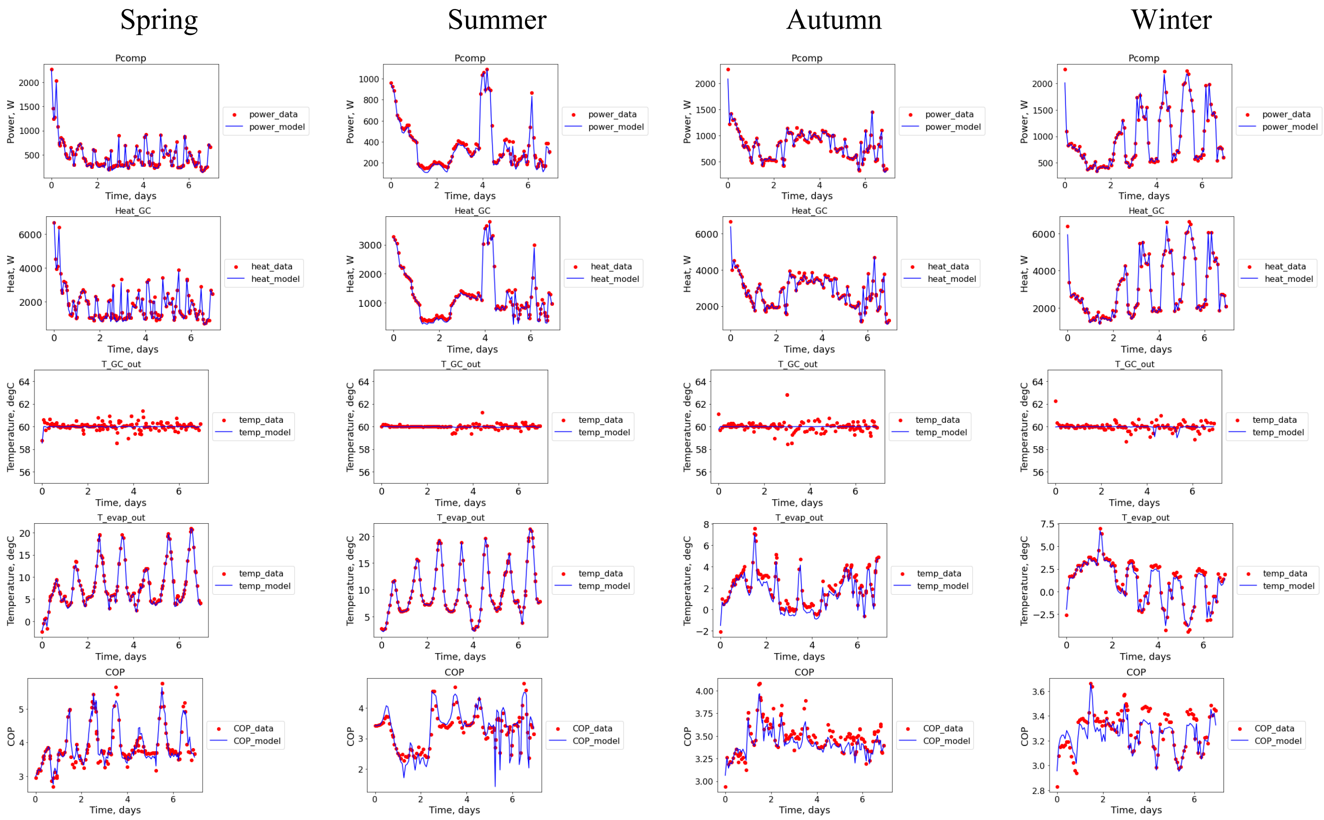

Figure 6. Match between the data and the ANN model-generated results for 1-week operational runs for different seasons

Table 3. RMSE for the model outputs for 1-week operation runs different seasons.

	RMSE				
	Pcomp, W	Heat_GC, W	T_GC_out, °C	T_evap_out, °C	COP
Spring	34.314	125.252	0.356	0.252	0.232
Summer	32.410	123.414	0.204	0.145	0.346
Autumn	31.990	95.921	0.489	0.346	0.089
Winter	31.859	79.933	0.413	0.293	0.076

4. Conclusion

Physics-based models of the trans-critical CO_2 heat pump can entail significant computational resources, particularly when used for operational optimization and predictive control. One way to bypass this is to replace them with a surrogate model developed using ANN. In this study, we successfully developed an

ANN-based surrogate model for a trans-critical CO_2 heat pump in a SAGSHP system. The key takeaways from this work can be summarized as follows:

- The selection of input parameters for the ANN model was based on three criteria: (1) controllability during operations, (2) strong correlation with the chosen outputs, and (3) dependence on inputs from other system components. In this work, the inputs considered include (1) the fluid mass flow to the water side of the evaporator (Evap_MF), (2) the temperature of this fluid (Evap_T), (3) the mass flow of the fluid to the water side of the gas coolers (GC_MF), (4) the temperature of this fluid (GC_T), (5) the set point output temperature (Tsetpoint), and (6) the gas cooler pressure set point (P_GC).
- The selected outputs should represent the CO_2 heat pump's performance and supply the necessary input data for interconnected system components. In this work, the outputs chosen were (1) power consumption (Pcomp), (2) the total heat output (Heat_GC), (3) the output temperature of the heat pump (T_GC_out), and (4) the outlet temperature of the heat pump's evaporator.
- Normalization is essential for both inputs and outputs to eliminate biases resulting from parameters with significant magnitudes. In this work, it was seen that min-max normalization generated lower MSEs and RMSEs.
- For the CO_2 heat pump considered in this work, an ANN architecture comprising an input layer with 6 inputs, 2 hidden dense layers, each with 30 neurons, and an output layer with 4 outputs (6-30-30-4) yielded satisfactory results with reasonable MSEs and RMSEs. The ReLU activation function was implemented on each hidden layer and no regularizations were imposed. The Adam optimizer was used with a learning rate of 0.001. Early stopping (patience = 2000) was implemented to ensure that the training data was not overfitted. A maximum of 30000 epochs was specified.
- The resulting MSE for the training, validation, and testing data sets were 1.38×10^{-5}, 2.05×10^{-5}, and 3.65×10^{-5}, respectively. Correspondingly, the RMSE for the training, validation, and testing data sets were 0.0037, 0.0045, and 0.0060, respectively. These results demonstrate a reasonable alignment between the model and the data.
- The ANN model was also tested against the Modelica model for one-week operational runs for different seasons. The results indicate favourable performance, with RMSEs for the COP to be 0.232, 0.346, 0.089, and 0.076, for spring, summer, autumn, and winter, respectively. This demonstrates its suitability for operational simulations.

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