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Artificial neural network model for predicting CO_2 heat pump behaviour in domestic hot water and space heating systems

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Artificial neural network model for predicting CO_2 heat pump behaviour in domestic hot water and space heating systems

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Abstract. The natural refrigerant, CO_2, possesses thermophysical properties that make it highly suitable for domestic hot water (DHW) production using heat pump technology. In this study, the development and validation of an artificial neural network (ANN) model that enables efficient design and control of a CO_2 heat pump is presented. The study employs experimental data from a CO_2 heat pump with a nominal heat capacity of 8 kW. The fully instrumented rig includes the heat pump and a pump rig designed to generate system temperatures representative of various space heat and DHW demands. A comprehensive dataset was generated through systematic variation of inlet temperatures and setpoints. The ANN provides predictions for outlet temperatures, heat production, and electricity consumption utilizing inlet flow rates, temperatures, and setpoints as inputs. These predictions are important for condition monitoring or in a smart operation management framework that determines optimal schedules for the machine.

1. Introduction

As nations and industries strive to meet global climate objectives, the adoption of efficient, standardized, and scalable solutions is vital. The ongoing global energy crisis has accelerated the need for a shift away from fossil fuels [1]. In 2022, nearly half of the energy demand in buildings was allocated to space heating and Domestic Hot Water (DHW), resulting in 2,400 Mt of direct CO_2 emissions, along with an additional 1,700 Mt of indirect emissions [2]. The transition from fossil fuels to renewable energy sources for space heating and DHW is a critical component of achieving a Net Zero Scenario. Although mature technologies such as heat pumps, bioenergy boilers, and district heating are available, their adoption needs to be accelerated [1].

While the demand for heating and cooling can vary based on numerous factors such as climate, geographic location, architectural design, building standards, and occupancy, the requirement for DHW remains relatively stable. As advancements in building design and retrofitting methods significantly reduce thermal energy needs, the demand for DHW remains unchanged [3] and in buildings without hydronic space and ventilation heating systems, there is still a DHW demand. In the US, 18% of home energy consumption is dedicated to DHW, while in the EU, it accounts for 14% [4]. Natural gas (41%), electricity (20%), district heating (13 %), renewables (13 %), petroleum products (11.5%) and solid fuels (1.5%) constitute the energy consumption for DHW in the residential sector in the EU [5]. Efficient and standardized DHW production can play a significant role in the green transition [6].

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The heat pump is a green production technology [7] that is becoming increasingly popular in heating and cooling applications [8]. An established guideline for achieving an efficient heat pump system is to minimize the temperature lift between the evaporator and the condenser [9]. Consequently, this principle poses challenges when utilizing traditional heat pumps for DHW production, considering that a safe DHW temperature typically ranges between 60 and 70°C [10], to prevent legionella bacteria growth [11].

Moreover, there are concerted efforts within a growing segment of the heat pump industry to adopt refrigerants that mitigate environmental harm [12]. While heat pumps are generally favoured over electric heaters and fossil-fuelled boilers due to their efficiency and reduction of greenhouse gas emissions [13], the evolution of refrigerants has presented challenges. Early refrigerants were phased out due to their negative impact on the ozone layer. Similarly, hydrofluorocarbons (HFCs) are now being phased out due to their significant greenhouse gas contribution if released into the atmosphere [14]. Even the contemporary "low-GWP" alternatives, like hydrofluoroolefins (HFOs), come with potential issues. Their degradation products, such as trifluoroacetic acid, can pose environmental risks [15]. Natural refrigerants on the other hand, have been found to offer comparable, if not superior, performance to HFCs and HFOs, while significantly reducing the associated environmental drawbacks [16]. Among these, ammonia, propane, and CO_2 stand out as the commercially viable options, each presenting distinct advantages and challenges [17].

Heat pumps that operate with CO_2 as refrigerant have garnered significant interest as a sustainable and efficient alternative for DHW production [18]. Unlike the conventional heat pump processes, which reject heat at a constant temperature through condensation, CO_2-based heat rejection can occur in a supercritical state, releasing heat at a variable or "gliding" temperature. Such a process can reach the necessary temperatures for DHW production while maintaining standard heat pump efficiency [19]. Optimal performance, characterized by a high Coefficient of Performance (COP), is achieved by managing gas cooler pressures to ensure a low outlet temperature for the CO_2 gas; this parameter is significantly influenced by non-linear cooling curves near the critical point [20].

By distributing the heat rejection over multiple gas coolers, the CO_2 heat pump can be adapted for space heating. However, the need for a low gas cooler outlet temperature to achieve high process efficiency may be a challenge when combined with the temperature levels used in traditional space heating [21], which typically range between 30-60°C [22]. The operational conditions of space heating and DHW systems are closely related to the design of gas coolers and the efficiency of a CO_2 heat pump system. For an integrated CO_2 heat pump system with fixed external conditions, there is an optimum CO_2 gas cooler pressure that will maximize the system's COP [20].

While the use of CO_2 as a refrigerant is well-established in specific sectors, including DHW heating in Japan [23] and in supermarket refrigeration [24], its widespread adoption is still limited. Any reluctance to adopt CO_2 as a refrigerant primarily stems from a lack of familiarity, limited experience, and concerns about initial costs [25]. By investigating the challenges of integrating CO_2 heat pumps into a variety of systems, simplified approaches could provide industrial designers and end-users with the tools necessary to improve both design and operational efficiency. This, in turn, could facilitate a wider implementation of CO_2-based systems.

A standard thermodynamic analysis often requires computational efforts, the use of detailed physics-based equations, and a deep understanding of the internal components of the units and systems being modelled. Gathering this specific information can be time-intensive, costly, and sometimes unattainable [26]. Furthermore, many commercial systems have internal controllers whose operations are proprietary, which can complicate the modelling process. In contrast to physics-based modelling, the Artificial Neural Network (ANN), a data-driven approach, has garnered significant attention over the past decade, emerging as a cornerstone of the ongoing Artificial Intelligence revolution [27]. The ANN methodology efficiently captures the complex non-linear relationships between input and output parameters [28].

Related works and contribution: Since Lorentzen "reintroduced" CO_2 as an efficient and sustainable refrigerant in the early 1990s [19], the CO_2 heat pump process has garnered attention from both heat pump and refrigeration engineers as well as researchers. While the application of machine learning methods to describe the CO_2 heat pump process has been explored, it remains a subject with limited extensive literature.

Wu et al. utilized ANN to predict the performance metrics of a CO_2 air-conditioning system's gas cooler [29]. Trained with inlet conditions from both the CO_2 and air-side, the network achieved predictions of heat transfer, outlet temperatures and pressure drop across the gas cooler with deviations less than ±5% from actual measurements. A limitation, however, was its dependency on flow measurements from both gas coolers sides, which due to high cost, is uncommon in real-world heat pump systems [30]. Opalic et al. [30] explored ANN's potential to predict CO_2 mass flow rate and compressor power consumption in an industrial cooling system. Using easily measurable parameters like system temperatures and pressures as inputs, they constructed a model based on compressor polynomials. When tested in a real-world setting, the model achieved a Mean Average Percentage Error (MAPE) below 5%.

Xu et al. employed an ANN to enhance calculations when optimizing the performance of an air-source CO_2 heat pump [13]. Using heat rejection pressure, gas cooler outlet temperature, and compressor displacement as inputs, the ANN predicted the CO_2 mass flow rate, the heat transfer area of the gas cooler, the pressure ratio, electricity consumption, and heat production. In another study, Yin et al. combined Particle-Swarm-Optimization with a neural network to determine the optimal discharge pressure for a CO_2 heat pump. This method achieved a relative error close to 1.5% [31].

Combined DHW and space heating systems based on CO_2 heat pumps demand careful attention to both system design and operational control. Based on experimental data from a CO_2 heat pump rig at the University of Stavanger (UiS), this paper introduces an ANN-based model that effectively predicts the heat pump's performance under various operational conditions. The heat pump features two gas coolers, one for DHW production, the other for space heating. Using inlet conditions and process targets as input, the model predicts the performance and outlet conditions of the machine, relying only on externally measured parameters. This practical approach benefits industry professionals and building owners looking to gain better control of and improve their heat pump systems.

The paper is organized as follows: First a description of the CO_2 process, DHW production and space heating, and the experimental rig is given, before a discussion of the dataset, including the data collection, processing, and the model's structure. Then, the prediction results and their implications are presented and discussed. The paper concludes with a discussion of potential future research and development directions and a summary of the findings.

2. Methods and materials

2.1. The experimental rig at UiS

The experimental setup at UiS is designed to closely mimic a realistic system adaptable to various real-world applications. At its core is an industrial, small-scale CO_2 heat pump, enhanced with extra instrumentation, as illustrated in Figure 1 (a).

The CO_2 heat pump has an 8-kW nominal heating capacity, aligning well with the DHW demands of a medium-sized apartment building equipped with an accumulation system. The inverter-controlled compressor, a DORIN CD300H, offers a nominal cooling capacity spanning 2.2 kW to 5.2 kW. The experimental rig is designed for both DHW and space-heating, featuring two gas coolers connected in series. The first gas cooler (GC-HT) is designed for DHW production, while the second one (GC-LT) is for conventional space heating. A temperature setpoint can be set at each gas cooler. Due to their serial connection, the temperature configuration at the first gas cooler directly impacts the available heat at the second cooler. Care in the selection of setpoints is essential to guarantee optimal performance across both gas coolers. The system can be calibrated to represent DHW production, building space heating, or a combination of the two.

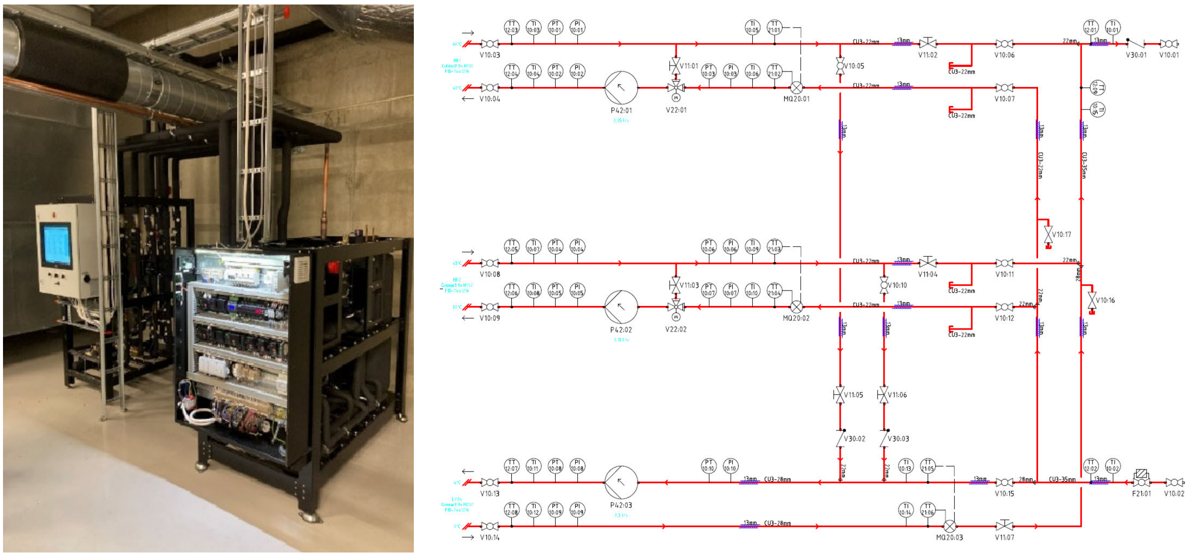

Figure 1. (a) Pump rig and CO_2 heat pump, (b) P&ID pump rig system.

The rig connects to the central cooling infrastructure at the UiS through a cold-water pipe. The temperature of the water this pipe varies between ca. +5°C and +20°C, depending on seasonal variations and the cooling requirements of the campus. The cold-water pipe serves as the heat source for the evaporator and the thermal sink for the gas coolers.

On the water side of the heat pump, each gas cooler and the evaporator are connected to their own dedicated circulation pump, as shown Figure 1 (b). Currently, the mass flow rate across each heat exchanger remains approximately constant. Shunt valves on the water side of the gas coolers enable adjusting inlet temperatures by mixing in hot water produced at the same gas cooler. This feature allows the user to quickly determine the gas cooler outlet CO_2 temperature's influence on available heat and process COP. The only uncontrollable variable in the configuration is the cold-water temperature, which essentially functions as the low-temperature heat source for the heat pump.

2.2. Model structure, Data capture and Processing

The primary objective of this work was to develop a model capable of swiftly predicting the performance of the CO_2 heat pump under varied operational conditions, with a focus on controllable setpoints and changing inlet values. The model was constructed to predict heat production at both gas coolers, the electricity consumption of the heat pump, and outlet temperatures for each heat exchanger. Inputs were flow and temperature to each heat exchanger, along with the heat production setpoint at the GC-LT. DHW was always prioritized with a setpoint of +60 °C at the GC-HT, and therefore this setpoint was not selected as model input.

To gather a comprehensive dataset, a systematic variation of the input parameters was conducted by adjusting the inlet temperatures for each gas cooler and the production temperature setpoint for GC-LT. This process was carried out over a month, from May 11th to June 10th, 2023. For every parameter combination, the system operated for at least 20 minutes, ensuring that it reached and maintained steady conditions. These variations aimed to produce a dataset that mirrors potential operational conditions for a combined building heating and DHW production heat pump. The GC-HT consistently maintained a production setpoint of +60 °C for DHW production, with inlet temperatures varying between +10 °C and +55 °C at 5 K intervals. Meanwhile, the GC-LT operated at setpoints of either +40 °C or +50 °C. Its inlet temperatures started at +10°C and rose in 5 K steps, stopping 5 K below the selected setpoint. This methodology resulted in 130 unique parameter configurations. Figure 2 provides a visual representation of the inlet temperature variations over a day.

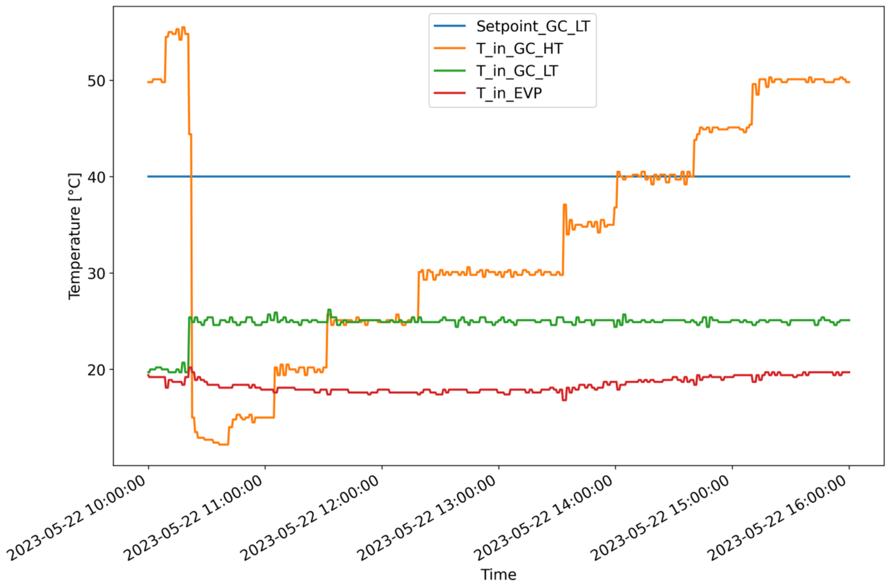

Figure 2. Example of variation of inputs to generate dataset.

In this configuration, the machine consistently prioritizes DHW production. When the GC-HT inlet temperature is low, most of the heat pump output serves DHW production, leaving only a small portion for space heating. This situation represents the heating cold mains water. With a higher GC-HT inlet temperature, less of the heat pump's capacity is available for DHW, and the rest is allocated to space heating. The amount of heat depends on the GC-LT water inlet temperature. Such a scenario can represent the heat pump heating a mix of cold mains water and higher temperature water from an accumulator tank without stratification.

The data were selected and downloaded manually from the digital control system of the rig. During preprocessing, the data were refined by removing outliers, noise cancellation, and resampling to a uniform 30-second interval to ensure consistency in later analysis and modelling.

2.3. ANN and Model Development

A data-driven model for the heat pump operation was developed using the collected data. ANNs were chosen for to their adaptability and ability to handle complex patterns and relationships in the data. Once the ANN model has been trained and set up, it offers a user-friendly tool that engineers or operators can utilize without requiring a deep understanding of its architecture. Users can enter the defined input parameters to model and instantly receive predictions of outlet temperatures and energy consumption. Within an integrated system, the ANN provides high-precision predictions, eliminating the need for potentially time-consuming recalculations. This approach facilitates real-time monitoring and adjustment of the heat pump system, potentially optimizing its performance and energy efficiency. The primary limitation of this method, within the presented framework, is the model's strong dependency on its training data. Values outside the model's training bounds may yield results with notable inaccuracies.

Figure 3 illustrates the architecture of the ANN, including inputs values and predictions. The model includes input and output layers, enhanced by three intermediate hidden layers. In each hidden layer, a designated number of artificial neurons receive input from the preceding layer. These inputs, multiplied by their associated weights, are combined, and then processed through an activation function. The training of an ANN involves the careful adjustment of these weights, which is crucial for efficiently converting system inputs into the desired outputs.

Prior to model training, determining an appropriate model configuration is essential, which includes defining hidden layers parameters such as layer count, the number of neurons per layer, and the activation functions. The training phase further involves the selection and adjustment of various parameters, such as the choice of optimizer and the calibration of the learning rate. These decisions are part of the hyperparameter tuning, which critical for the model's performance. In this work, the Bayesian optimization methodology was employed for hyperparameter tuning, resulting in the configuration shown in Figure 3 (a) that employs the Stochastic Gradient Descent optimizer at a learning rate of 0.37. The model was trained on 80% of the dataset, with the remaining 20% reserved for model validation. This reserved subset, commonly referred to as the test set in machine learning, remained untouched during training, thus facilitating an objective assessment of the model's validity.

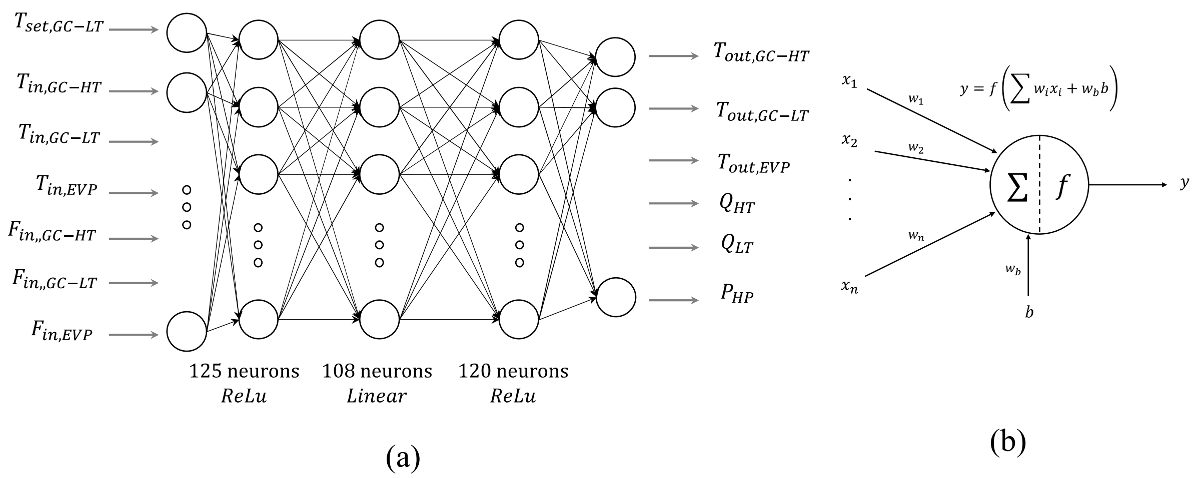

Figure 3. (a) ANN setup, (b) artificial neuron with inputs, weights, activation function, and output.

3. Results

Table 1 presents the error metrics for the test set. The table includes the maximum error, mean absolute error (MAE), root mean square error (RMSE), and mean absolute percentage error (MAPE) associated with the model's predictions across the dataset.

Table 1. Evaluation of model error over the unseen data in the test set.

	Max Error	MAE	RSME	MAPE [%]
$T_{out,GC-HT}$ [°C]	7.18	0.11	0.21	0.2 %
$T_{out,GC-LT}$ [°C]	4.43	0.10	0.17	0.3 %
$T_{out,EVP}$ [°C]	1.27	0.03	0.05	5.7 %
Q_{HT} [kW]	2.80	0.05	0.08	3.3 %
Q_{LT} [kW]	0.93	0.06	0.08	0.5 %
P_{HP} [kW]	1.04	0.02	0.03	2.4 %

The model consistently predicts accurately across all output parameters. The test set, derived randomly from the initial dataset during preprocessing, contains the distinct data points from training, leaving out the in-between values such as those that lie between the 5 K temperature intervals. Given the ANN's ability to interpolate, assessing the model's performance on these intermediate data points becomes essential. Furthermore, due to the random generation of the test set, presenting the model's results over a continuous period becomes challenging. To provide a more comprehensive validation, a

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secondary test was conducted. Over a 20-hour span, three months after collecting the initial dataset, the system was subjected to four distinct gas cooler inlet temperature configurations. The initial three configurations used temperatures that fell between those of the initial training, while the fourth used setpoints mirroring the temperatures from the original dataset. Details of the inlet temperature variations for this additional validation can be found in Table 2 and Figure 4.

Table 2. Inlet temperature setpoints for model evaluation.

	Inlet temperature HT GC [°C]	Inlet temperature LT GC [°C]
1	28	25
2	32	22
3	47	26
4	35	20

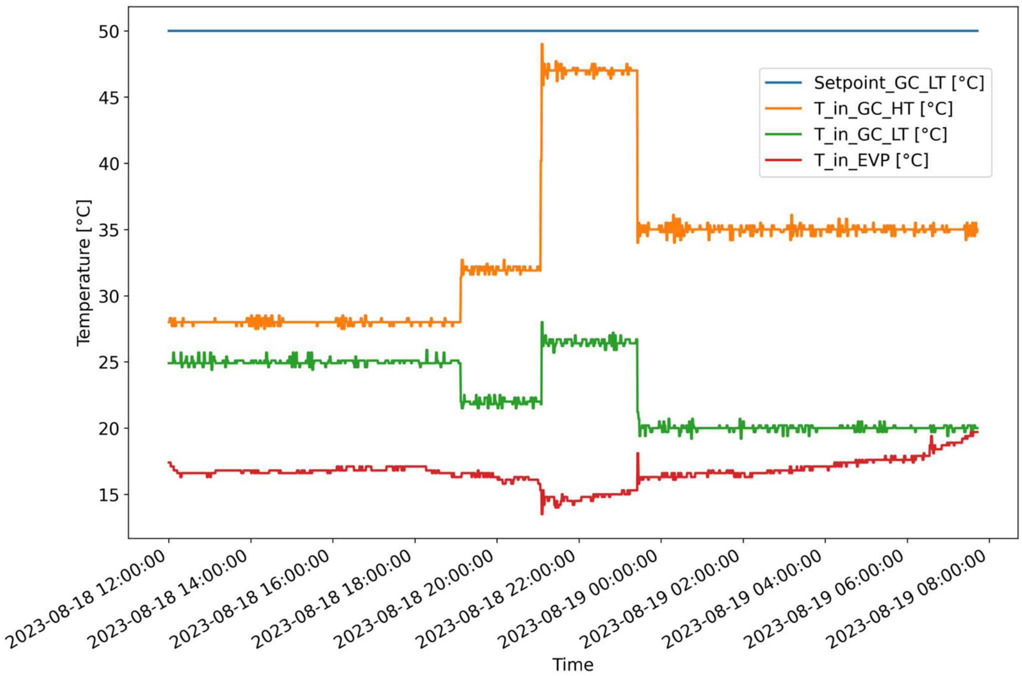

Figure 4. Visualization of inlet temperature during model evaluation.

Table **3** and Figure 5 document the error calculations and predictions when the trained model was applied to the data series from August 2023. The model's predictions for this secondary test set are more than acceptable, closely matching the results observed with the original test set. The most pronounced discrepancies occur when the gas cooler inlet temperatures change rapidly, leading the inlet temperature to oscillate before stabilizing in a new state.

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Table 3. Evaluation of model error over the unseen data, August 2023.

	Max Error	MAE	RSME	MAPE [%]
$T_{out,GC-HT}$ [°C]	5.90	0.50	0.61	0.8 %
$T_{out,GC-LT}$ [°C]	2.62	0.29	0.42	0.7 %
$T_{out,EVP}$ [°C]	0.17	0.02	0.03	0.9 %
Q_{HT} [kW]	2.36	0.06	0.10	1.4 %
Q_{LT} [kW]	1.97	0.14	0.18	1.1 %
P_{HP} [kW]	0.17	0.02	0.03	0.9 %

Towards the end of the data series, a noticeable rise in error is evident in both the gas coolers' outlet temperatures and the heat production predictions. This variation can be attributed to the single unpredictable model input: the evaporator's inlet temperature. As illustrated in Figure 4, this temperature, labeled as T_in_EVP [°C], increases rapidly from +16 - 17 °C to around +20 °C, exceeding the temperature range used in the initial training. Figure 6 showcases conditions from the training stage with gas cooler inlet temperatures like those from August 2023. Within the red rectangle, the inlet temperature to the evaporator during training is documented. The temperature was relatively stable, within a range between 15-17 °C, and thus below the values used in the practical evaluation.

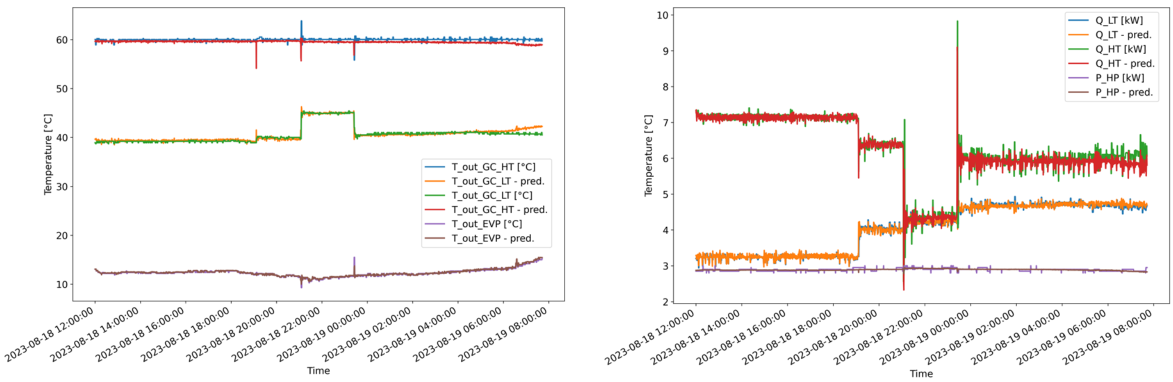

Figure 5. (a) Temperature predictions and, (b) heat and energy predictions, using the final model.

The visual validation emphasizes both the strengths and limitations of the ANN. It demonstrates its effective interpolation capabilities, while also revealing challenges encountered during extrapolation. From a design and operation standpoint, the model offers consistent accuracy for design evaluations and control operations, ensuring the training data aligns with realistic operational parameters. The model's occasional deviations, especially when inlet values are outside its familiar range, suggest caution in less-known conditions. However, these deviations might also underscore the model's potential in pinpointing operational anomalies, indicating its applicability in system malfunction detection.

Figure 6. ANN training inputs corresponding to August 2023 data.

A notable limitation of this method is its dependency on large datasets for model development. The extent of data in this study is relatively limited. Up until now, the heat pump has operated only at its peak output, maintaining constant power consumption throughout the training phase. Additionally, only DHW production has been prioritized and the setpoint at GC-LT has been evaluated at two temperatures: +40 °C and +50°C. In different scenarios, the machine could operate without any heat extraction from GC-LT, adopt lower temperature setpoints for both gas coolers, and reduce the compressor frequency to operate at part-load conditions.

4. Further research and development activities

This research serves as a foundation for future developments by presenting a demo case. The model equips both users and designers with a robust tool for swift and precise analysis and control capabilities of the CO_2-heat pump. These are essential for achieving objectives like condition monitoring and the identification of optimum operation by set-point selection.

Fast et al. developed a Graphical User Interface (GUI) for an Artificial Neural Network (ANN) model for an industrial gas turbine [32]. Their Excel-based GUI allowed the plant operators, even those unfamiliar with ANNs, to evaluate the degradation of their gas turbine by comparing the predicted and the real-time data. Their aim was to automate this GUI for real-time condition monitoring. Inspired by Fast et al.'s work, Figure 7 showcases an initial GUI for the CO_2 heat pump investigated in this study. The GUI uses color coding to differentiate between inlet conditions (blue), controllable set-points (yellow), actual measurements (green), and predictions (red). The Coefficient of Performance (COP) is then estimated based on heat production and electricity consumption and compared against actual measurements.

This research may lead to numerous advancements. These range from data-driven demand predictions to system operation optimization influenced by dynamic elements, such as heat demand and electricity pricing. Additionally, there is potential for integration with energy storage, geothermal boreholes, and solar heating systems.

A CO_2 heat pump connected to a stratified storage system can play a significant role in a hybrid microgrid [33], which integrates electric and thermal loads and productions systems [34]. Managing

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decentralized energy systems like microgrids is becoming increasingly complex, given that energy supply is only partially controllable due to the variable nature of renewable sources [35].

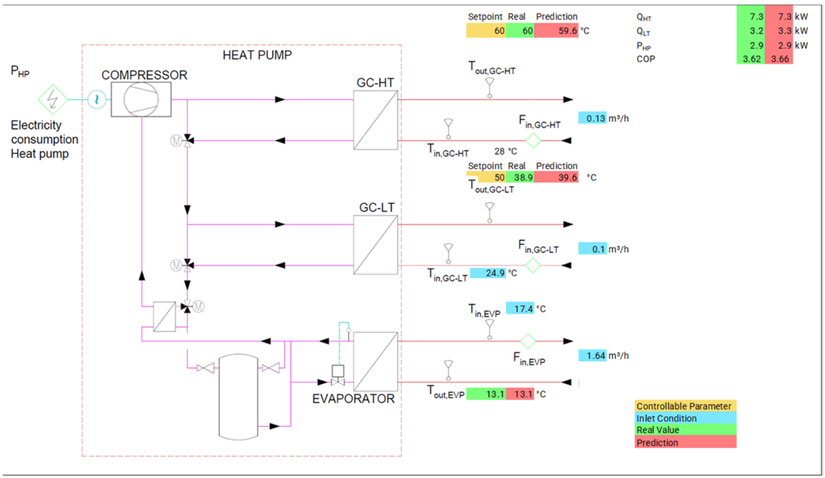

Figure 7. Example of GUI in Excel of the ANN model.

These systems often consist of multiple production units that need to be managed and optimized in a holistic manner. Therefore, the model and methodology presented in this study serve as an initial step toward developing a comprehensive sub-model for a CO_2 heat pump within a microgrid environment.

5. Conclusions

This paper has introduced the development of an ANN model tailored for a small-scale CO_2 heat pump. A profound understanding of the heat pump's behavior under variable inlet conditions provides designers and operators with insights essential for effectively managing these variations and building a robust energy system using the CO_2 heat pump. Employing a set of easy-to-measure parameters, the model predicts the heat pump operations, achieving a MAPE below 6% across all outputs in the test set, with the same or superior accuracy during the practical evaluation. The limitation of the methodology was documented when inlet parameters outside the bounds of the training set were used as input to the model, with predictions deviating from the real operation.

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