Review on digital solutions for heat pump and refrigeration systems

Project: Digital twins for large-scale heat pump and refrigeration systems Work Package 1 - Deliverable 1.1

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Abstract

The project "Digital twins for large-scale heat pump and refrigeration systems" aims to develop adaptable, modular and reusable models for advanced system monitoring, fault detection and diagnosis and operation optimization. In this context, this report aims to provide a review of the state-of-the-art for digital solutions for heat pump and refrigeration systems. The focus of the review is on numerical models applied for system monitoring, fault detection and diagnosis as well as operation optimization. Three types of model-based approaches are characterized and described, namely white-box or physics-derived models, black-box or data-driven models and grey-box models, which combine the two other model types. It is distinguished that white-box models can provide detailed information about a system, which can be applied to monitor, characterize faults and optimize the operation of heat pump and refrigeration systems. Black-box models can also be used for such applications but unlike white-box models, they lack interpretability. The integration of white-box models with black-box approaches can be used to reduce data requirements compared to white-box models and increase its adaptability to different system configurations and operating conditions. From the reviewed studies, it is noted that further research is required where black-box and grey-box models for fault detection and diagnosis models are studied in operating heat pump and refrigeration systems.

Nomenclature

Abbreviations

ARMA	Autoregressive moving average
ARIMA	Autoregressive integrated moving average
ARX	Autoregressive model with exogenous variables
DBSCAN	Density-based spatial clustering of applications with noise
EWMA	Exponentially-weighted moving average
FDD	Fault detection and diagnosis
GAN	Generative adversarial networks
HVAC	Heating, ventilation and air conditioning
KNN	K-nearest neighbours
MIMO	Multiple input multiple output
MPC	Model predictive control
PCA	Principal component analysis
SCADA	Supervisory control and data acquisition
SDE	Stochastic differential equation
SISO	Single input single output
SVDD	Support vector data description
SVM	Support vector machine

1 Introduction

Incentives in sustainable energy systems can contribute to reduce greenhouse gas emissions and meet the goal of limiting global warming to not exceed 2 °C increase compared to 1990, as defined in the Paris Agreement [1]. Heat pumps can contribute to decarbonize district heating systems by recovering excess heat from industrial processes and increasing heat generation from renewable energy sources. A report from the International Energy Agency [2] stated that around 50 % of the European heating demand for buildings can be supplied by district heating. In this context, heat pumps can provide approximately 25 % to 30 % of the heat supplied in district heating networks.

The performance of heat pumps can be influenced by factors like electricity prices, operating costs, weather, operating duration and control strategies used [3]. Monitoring the operation of heat pump and refrigeration systems in real-time may contribute to increase their efficiency and reduce the need of active intervention over the system [4]. Moreover, optimizing the performance of heat pump and refrigeration systems requires selection of appropriate sets of manipulated inputs and controlled outputs [5] as well as definition of optimal control strategies [6].

The presence of faults and unexpected variations in the heating and cooling loads can have a negative impact on the system performance and availability [7]–[9]. A number of operational challenges in heat pumps may originate from the heat sources utilized. For instance, air-source heat pumps can be affected by excessive frost formation in the evaporator [10], biological fouling can be present in sewage water source heat pumps [11] and ground source heat pumps can be exposed to corrosion originating from minerals [12]. Several studies have investigated the applicability of fault detection and diagnosis (FDD) methods in chillers [13]–[22] as well as heat pumps integrated in heating, ventilation and air-conditioning (HVAC) systems [23]–[26]. However, only a limited number of studies [27]–[33] proposed FDD methods in heat pumps used for district heating and industrial applications.

Advances in communication and information technologies in the twenty-first century have enabled development of advanced control and monitoring systems based on data-driven methods. Data-driven modelling methods allow definition relationships between inputs and outputs of complex systems from observed data, providing predictions about the future behaviour of a system. Data-driven modelling can be complemented with white-box models to incorporate physics-derived relationships, so called grey-box models. Grey-box models leverage physics-based models with data-driven approaches to provide generalizable and adaptable representations of complex physical processes. Moreover, grey-box and data-driven models can be integrated with digital communication technologies to develop virtual representations of physical systems or digital twins [34]. The digital twin technology has been applied in manufacturing applications [35]–[37] and thermal energy systems [38], [39]. However, only a limited number of studies have applied digital twins for heat pumps and refrigeration systems, where the focus has been mainly on HVAC systems [40], [41].

The project "Digital twins for large-scale heat pump and refrigeration systems" aims to develop adaptable, modular and reusable models for specific services. Within this frame of reference, the purpose of the present report is to provide a review of state-of-the-art for digital solutions for heat pump and refrigeration systems regarding system monitoring, fault detection and diagnosis as well as operation optimization.

2 Methods

The state-of-the-art review presented in this report was compiled through a search in digital libraries, web search engines and journal websites, including Scopus, Web of Science, Google Scholar, Science Direct, FRIDOC database from the International Institute of Refrigeration and the database from the American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE). The strategy "reference by reference" was also applied to find relevant studies. The literature search focused on scientific publications and technical reports. However, industrial applications were also included in the review. The keywords applied were: "*heat pump*", "*refrigeration*", "*chiller*", "*fault*" or "*failure*" (standalone or in combination with "*monitoring*", "*detection*", "*identification*"), "*monitoring*" (standalone or in combination with "*system*", "*performance*"), "*optimization*" (standalone or in combination with "*operation*", "*control*", "*set point*"), "*model*" (standalone or in combination with "*numerical*", "*physical*", "*data-driven*", "*dynamic*", "*steady-state*", "*white-box*", "*black-box*", "*grey-box*").

The procedure applied throughout the review was based on four steps shown in Figure 1. First, numerical modelling methods were characterized, considering the classification white-box, black-box and grey-box models. Then, a literature search was performed to identify studies that applied digital solutions for heat pump and refrigeration systems related to FDD, system monitoring and operation optimization. Later, the frameworks used in those studies based on numerical modelling were categorized into white-box, black-box and grey-box. Finally, the frameworks applied in different case studies were described, comparing their characteristics regarding the provision of digital services for heat pump and refrigeration systems.

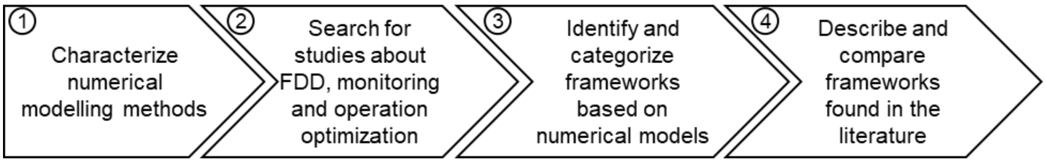

Figure 1: Four-step method applied in the literature review.

3 Results

3.1 Numerical modelling

This section provides a description of numerical modelling techniques used for the provision of digital services in heat pump and refrigeration systems. As seen in Figure 2, numerical modelling is classified into three categories, namely black-box, white-box and grey-box frameworks. The description includes numerical modelling frameworks that may be applied for system monitoring, operation optimization and fault detection and diagnosis.

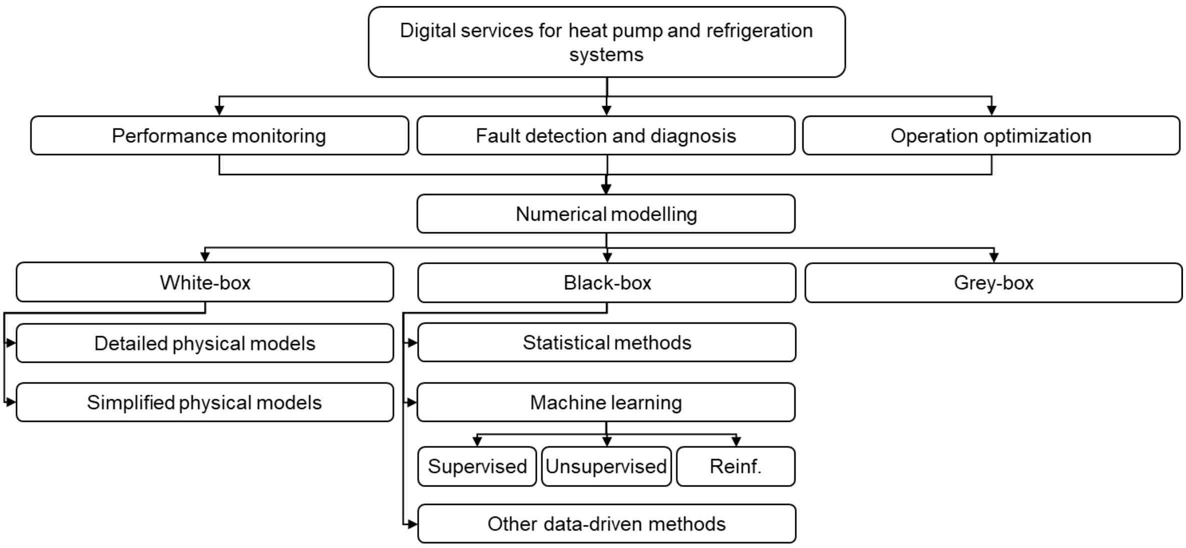

Figure 2: Scheme of the digital services using numerical modelling for heat pump and refrigeration systems based on numerical modelling.

3.1.1 White-box modelling

Physics-based or white-box models apply a comprehensive theoretical knowledge about the physical system they represent. In heat pump and refrigeration systems, physics-derived relationships include mass, momentum, energy balances, equations for describing component functionality and system equations. However, physics-based postulates can be partially or completely derived from measured data (e.g. equations of state). Bohlin and Græbe [42] suggested that the discrepancies between physics-based models and experimental data can be mainly attributed to output noise such as measurement uncertainties and modelling errors.

A number of modelling software tools have been applied to simulate the operation of heat pumps and refrigeration systems under steady state and dynamic conditions. Examples of simulation software used in such applications are Engineering Equation Solver (EES) [43], Matlab [44], Modelica [45] and Python [46]. These simulation tools may also be complemented with software libraries that include empirical and theoretical models of the thermophysical properties of working fluids. Coolprop [47] and Refprop [48] are examples of thermophysical property libraries applied to simulate refrigeration and heat pump systems. TIL Suite [49], [50] is an advanced Modelica component library for thermodynamic systems for steady-state and transient simulation of complex fluid systems such as heat pump, air conditioning, refrigeration or cooling systems. With the included substance property library TILMedia, system simulation with various mediums can be performed.

Steady-state simulation models are useful to represent systems whose behaviour can be considered fixed over time. This type of simulation is useful for the design, analysis and optimization of heat pump and refrigeration systems, characterizing their operation under different boundary conditions. However, steady-state simulations do not focus on the analysis of time-dependent processes in a system describing transient behaviour between operating points.

As opposed to steady-state models, dynamic models enable analysis of the time-dependent behaviour of heat pumps and refrigeration systems. Dynamic models can be applied to design, optimize and analyse the dynamic response of heat pump and refrigeration systems exposed to varying boundary conditions. Physics-based dynamic models are typically more complex than steady-state models, leading to larger simulation time. According to Rasmussen and Shenoy [51], the complexity of dynamic models of vapour compression systems often resides in the two-phase heat exchangers, where the thermal dynamics are generally slower than the mechanical dynamics.

A model can also combine steady-state and dynamic physical expressions simultaneously in different components. This applies when the dynamic operation of one or several components of interest in a vapour compression system is not significantly affected by the time-dependent behaviour of the remaining components. Thereby, the operation of the latter can be defined under steady-state conditions to simplify the numerical model of the system and reduce the simulation time.

3.1.2 Black-box modelling

Data-driven or black-box approaches describe a physical process or system by means of observations about its behaviour, without describing the fundamentals behind its operation. Mirnaghi and Haghighat [52] suggested that data-driven methods can provide accurate predictions about reality, adapt to different operating conditions and leverage existing sensing devices. Here, a distinction is made between statistical methods, machine learning and other data-driven methods.

3.1.2.1 Statistical methods

Statistical methods allow collection, organization, analysis and interpretation of data [53]. Methods that are based on statistics that focus on learning from data are considered within the scope of machine learning [54]. Several statistical approaches have been included in frameworks for monitoring, FDD and operation optimization of heat pump and refrigeration systems. Examples of this are principal component analysis (PCA), Kalman filtering, moving averages and autoregressive algorithms.

PCA is a multi-variate statistical analysis method in which a group of correlated variables are converted into a new group of variables, which are uncorrelated or orthogonal to each other [55]. This technique allows capturing the variability of the data using fewer variables and thereby simplifying data analysis. PCA can be used as a complement of FDD methods or for system monitoring. The dimensional reduction performed by PCA allows identification of variables that are responsible for the variability of a certain output, for example due to a fault or performance degradation [56]. Other simpler statistical techniques such as correlograms (or charts of correlation statistical indicators) can also be used to identify the degree of interconnection between input and output variables.

Discrete time dynamical models of the ARMAX type can be used to model linear time invariant (LTI) systems. Such models are actually stochastic difference equation models. The AR is the Auto-Regressive part, where the system output is a linear function of previous system output values. The MA is the Moving Average part and it is a function of the previous error values. This is the stochastic part, which enables a description of the noise entering through the system from inputs, referred to as the system noise. Finally, the X is the model part with the exogenous input, which comprises input variables driving the system output. ARMAX models are able to describe the output of a dynamic process assuming that it depends linearly on its previous values and certain stochastic terms of interest [57]. The parameters in such models are not directly interpretable from a physical point of view and thereby they are usually referred to as black-box models. However, they are excellent for performance prediction and FDD, providing to some extent interpretable results, such as stationary gains and time constants. They can be extended into being time adaptive and non-linear with non-parametric modelling techniques, e.g. basis splines.

Kalman filtering is a method that enables estimation of unknown dynamic variables from imprecise measurements observed over time by estimating a joint probability distribution [57]. ARMAX models can be implemented as a Kalman filter. As a potential application, a Kalman filter can be used for similar applications as ARMAX models, mainly prediction and parameter tracking, the latter is often used for FDD by comparing real operating data from a heat pump or refrigeration system with a physics-derived model, highlighting periods when the model does not match the measured data, as result from a fault.

3.1.2.2 Machine learning methods

Machine learning corresponds to the study of algorithms that can automatically learn about certain phenomena based on observations. According to Herlau et al. [54], machine learning can be divided into three main categories, namely supervised learning, reinforcement learning and un-supervised learning.

Supervised learning algorithms identify connections between inputs and outputs of a process based on a group of data used as example, so called training data. For instance, this type of algorithm can be applied to detect a fault or performance reduction in a refrigeration system by identifying an abnormal behaviour in one or several of its operational variables. Examples of supervised learning methods are regression algorithms, support vector machines (SVM), neural networks, Bayesian networks and decision trees.

Reinforcement learning algorithms analyse the relationship between a learning agent, the environment where it operates and the reward resulting from its interaction with the environment [54]. Unlike supervised learning, reinforcement learning methods are not provided with training data. Instead, such methods assess the consequences of every agent-environment interaction, finding the most rewarding set of decisions to reach a certain goal. Monte-Carlo and Q-learning methods are two examples of reinforcement learning algorithms. For example, a reinforcement learning algorithm could be applied to identify the optimal operation schedule of a heat pump considering constrains such as electricity price and heating demand.

Finally, unsupervised learning algorithms aim to find patterns in the data without previously defined labels [54]. Clustering algorithms are an example of unsupervised methods. For instance, such algorithms could be applied to group (or cluster) a number of faults that occurred in a refrigeration system in a year, finding associations that were not identified before. Some of the resulting clusters could include faults that are more likely to happen after the refrigeration system is serviced or when an abnormal parameter variation occurs.

3.1.2.3 Other data-driven methods

This section briefly describes other data-driven methods than those using statistics and/or machine learning that are used in numerical modelling methods for heat pump and refrigeration systems.

Fuzzy logic is a multivalued logical system adopted to express imprecise and qualitative information in mathematical terms [58]. As opposed to Boolean logic where a value can be either 1 or 0, in fuzzy logic a value can be 1, 0 or any fraction (or percentage) in between. The multivalued property of fuzzy logic allows classification of imprecise information. For instance, 60 % of the thermostats in a building are adjusted within the range that corresponds to a “cold” environment. Then, fuzzy logic can be applied to construct a rule-based scheme between imprecise and qualitative inputs with precise numerical outputs. A potential application for such a structure is to define automatic control strategies for heat pump and refrigeration systems. Considering the previous example, if 60 % of the thermostats in a building are adjusted in the category “cold”, then the heat pump is operated at a specific heating capacity (e.g. 40 % of the nominal heating capacity). Fuzzy logic can also be used for system monitoring and FDD in combination with thresholds derived from expert knowledge.

Diagnosis tables are another method used for system monitoring and FDD that can be used to formalize expert knowledge [14]. This model-free method uses heuristically acquired information to identify operational variables affected by faults. Diagnosis tables also allow definition of thresholds over which those operational variables are expected to vary under faulty operating conditions. The fundamental process behind diagnosis tables is based on a rule-based structure.

3.1.3 Grey-box modelling

A grey-box model is a physics-based model with data-driven terms to account for uncertainties regarding model formulation and measured values. Bohlin and Græbe [42] suggested that grey-box models incorporate the available knowledge about a system or a process, without requiring that such information is complete or reliable. Sohlberg and Jacobsen [59] distinguished five grey-box modelling branches shown in Figure 3.

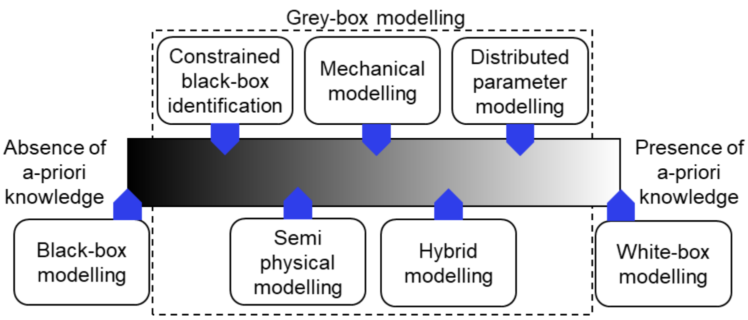

Figure 3: Scheme of the grey-box modelling branches proposed by Sohlberg and Jacobsen [59].

The structure of the grey-box branches depends on how the physical information known a-priori is applied in the model, which is described as follows:

- *Constrained black-box identification:* uses data-driven models that include parameters constrained by physical relations. For instance, this could be applied to detect fouling in a heat exchanger. A data-driven model could identify abnormal variations of the mass flow rate of the heat exchanger over time that can be attributed to fouling. Here, previously known variations of the mass flow rate associated to the operation of a pump can be included in the model as constrain.
- *Semi physical modelling:* applies physical relationships to represent the non-linear behaviour of measured data, which are complemented with linear data-driven models. Considering the previous example, the heat transfer performance of a heat exchanger can be represented by a physics-derived parameter such as the UA-value. This indicator could be used as an input for a data-driven model to identify when its variability may be associated to fouling.
- *Mechanical modelling:* applies a model that was initially described using physical derivations but its structure was refined based on measured data. For example, a model of the pressure loss across a heat exchanger could have been initially defined using a physics-derived friction factor model (e.g. Blasius correlation). However, overtime this model may not provide an accurate description of the pressure drop in a heat exchanger due to corrosion or other fault mechanisms affecting its surface. In this context, a data-driven model could be developed to describe the friction factor under the current operating conditions.
- *Hybrid modelling:* uses physics-based and data-driven models as two separated components that complement each other in series or in parallel. As an example of this approach, a physics-based model of a vapour compression system can be used to represent the overall performance of the system and the relationship between components. This could be complemented with an independent data-driven model that allows identifying the performance degradation of the isentropic efficiency of the compressor over time.
- *Distributed parameter modelling:* enables identification of the optimal spatial discretization of a physical element by using data-driven methods to find the integration of a physics-derived discretization that minimizes modelling errors. For instance, this approach could allow developing an optimal discretized model of a heat exchanger. Discrete components may include thermodynamic and fluid dynamic expressions to represent the heat transfer and pressure loss across the heat exchanger. The optimal number of discrete elements to minimize modelling errors may be found by using a data-driven model based on measured data.

Grey-box models based on stochastic differential equations (SDEs) allow describing the dynamic behaviour of real systems, using a combination of physical and statistical modelling [57]. SDEs integrate deterministic expressions derived from physics with stochastic models to account for the disturbances entering a real system. For example, a physical model can represent the structure of a system and statistical methods can be applied for validation and parameter estimation (e.g. heat transfer and pressure loss coefficients). Bohlin and Graebe [42] suggested that stochastic grey-box models rely on the person designing the model to adjust its structure. The authors indicated that this model adjustment is often performed as an iterative process where the model designer proposes and tests different tentative model structures. As an alternative to this human-dependant process, a number of model adjustment methods were developed [60], which can automatically identify model structures based on prediction performances.

3.2 System monitoring

This section summarizes digital solutions applied to monitor the operation of heat pump and refrigeration systems. Monitoring is regarded as the process of obtaining information about the operation of a system, verifying whether its performance is within expected values. For the given system, the heating or cooling rate provided and the power consumed are relevant examples of quantitities to monitor. These are further connected into coefficient of performance (COP) which shows the ratio between the energy service provided and the cost of providing it. Tsutsui and Kamimura [61] suggested that model-based monitoring approaches provide a better description of the operation of the system than only determining the COP, since the latter is highly sensitive to weather conditions. Model-based approaches enable monitoring of the relationships between input and output system variables as well as predicting their future behaviour. Model-based approaches can be physics-derived (white-box), data-driven (black-box) or a combination of the latter (grey-box). This review included model-based frameworks for real-time monitoring considering steady-state and/or dynamic operating conditions.

3.2.1 White-box frameworks

The operation of heat pump and refrigeration systems can be monitored by using thermodynamic simulation models validated with measurement data to identify daily and seasonal performance indices. Naicker and Rees [62] monitored the performance of a geothermal heat pump system with an installed heating capacity of 440 kW by means of measured data and a steady state thermodynamic model. The real system was monitored over a period of three years of operation using temperature and flow rate sensors independent from those of the existing control system. Other control-related variables such as valve positions and compressor speed were obtained from the central control system of the heat pump. The framework from Naicker and Rees was capable of calculating the COP and the seasonal performance of the heat pump, identifying how the existing control approaches affect the overall performance of the system. Gordon et al. [63] developed steady-state thermodynamic models to monitor the performance of two centrifugal chillers with 352 kW of cooling capacity each. The data to adjust the numerical models was obtained on a 30-minute interval from both chillers. Their model-based framework was used to monitor the COP of the system under full- and part-load conditions, characterizing its operation before and after maintenance was provided. Noel et al. [64] proposed a non-invasive method to assess the performance of heat pumps based on defining an energy balance of the compressor. This method was validated on a residential air source heat pump, in which the COP was calculated under steady-state conditions.

System monitoring methods for heat pumps based on thermodynamic models are included in services available in the market. The Energy Machines Verification Tool (EMV) [65] provides performance monitoring and predictive maintenance by means of smart sensors and thermodynamic simulation models of heat pumps. This tool uses temperature and pressure measurements from different points in the refrigerant loop as well as the compressor power uptake to determine performance indicators such as COP, compressor efficiency and heating/cooling capacities.

3.2.2 Black-box frameworks

One of the simplest data-driven system monitoring approaches apply regression algorithms that relate the COP or power uptake from a heat pump with temperatures from the sink and/or source streams. The method from Okuno et al. [66] included a relationship between the COP of a sewage water source heat pump with the heat source water inlet temperature. This approach was applied to monitor the performance of the system and its variation resulting from the presence of fouling in the evaporator. Other studies [67], [68] proposed polynomial regressions to estimate the power uptake from ground source heat pumps based on the temperatures of the source and sink streams and/or the heating capacity of the heat pump unit. Zou et al. [69] used linear and polynomial regressions to model the dynamic behaviour of the COP of a lake water source heat pump with a heating capacity of 1244 kW. The proposed COP model was defined as a function of the daily average temperature of the lake water. This model was able to predict the daily and seasonal var9iations of the real COP of the system.

More advanced data-driven frameworks for system monitoring included machine learning techniques. The framework proposed by Yan et al. [70] applied several machine learning algorithms to monitor the performance of a ground source heat pump system with 670 kW of heating capacity. The algorithms included neural networks, classification and regression trees as well as support vector machines. Those algorithms were trained with real-time measured data from the system, which did not include state point measurements of the refrigerant cycle. This framework was capable of estimating the short-term and long-term performance indicators of a system operating under dynamic conditions. Cirera et al. [71] applied a data-driven method using a self-organizing map (a type of artificial neural network) and PCA to monitor the COP of chillers. This approach was able to recognize the implications of different control strategies and at the same time identify anomalies in the operation of the system. The proposed framework integrated online and offline modules. In the offline part, the method was trained based on historical data, which was then updated in the online module using real-time measured data.

3.2.3 Grey-box frameworks

A number of studies [72], [73] have combined physics-derived models with data-driven methods to monitor the performance of heat pumps and refrigeration systems. Tardif et al. [72] applied Functional Muck-up Units (FMU) to combine the dynamic model of a heat pump and a building made in TRNSYS with the electricity grid domain developed in Python. The aim of their study was to analyse the interaction between the electricity grid and the power load represented by the heat pump, evaluating the flexibility potential of such system configuration. Green et al. [73] investigated how to operate supermarket refrigeration systems optimally based on an accurate monitoring of a variable cooling load. The authors focused on the problem of adjusting the operation of refrigeration systems with multiple compressors with different capacities considering that the cooling load could be directly estimated. They proposed a monitoring approach based on measured data and thermodynamic simulation models to indirectly calculate cooling loads and to estimate the COP of the system in real-time. The calibration of a thermodynamic model is often performed manually by adjusting parameters of the model so that its output matches measured variables of interest. Data-driven methods can be used for the calibration of physics-derived models, increasing the level of automation in the modelling process. Mehrfeld et al. [74] developed a framework to calibrate the dynamic physical simulation model of an air-source heat pump. Their framework included a thermodynamic model developed in Modelica with an optimization algorithm implemented in Python, where the minimization of a scalar objective function was performed. The optimization applied the heating circuit flow temperature and electrical power uptake of the heat pump as target variables, achieving a root mean square error of approximately 1.6 % between simulated and measured values.

3.3 Fault detection and diagnosis

This section provides a review of fault detection and diagnosis (FDD) methods applied to large-scale vapour compression systems. Large-scale systems are considered as those with heating or cooling capacities equal or above 200 kW. This classification was also used in a related study [75] to categorize large-scale heat pump systems. Previous studies also investigated the performance and application of FDD techniques for HVAC systems and small-scale heat pump applications, as summarized in [9], [52], [76]. However, the scope of the present section was limited to large-scale systems.

In this report, the term *fault* is regarded as the state of an item characterised by its inability to perform an expected function, which can be total or partial [77]. FDD are procedures that aim to determine whether a fault has occurred and identify the characteristics of a fault (e.g. type of fault, location, magnitude and time of occurrence) [56]. The faults presented in Table 1 were investigated in previous studies that applied FDD methods in large-scale vapour compression systems. The FDD methods used in such studies are summarized in Table 2. Among all the 26 studies found in the literature, seven studies focused on large-scale heat pump systems, all of which applied physical models for FDD. The other studies focused on FDD for chillers, where the largest fraction of them applied experimental data developed by ASHRAE RP-1043 [13]. Katipamula and Brambley [78] proposed that FDD methods can be categorized based on their structure, namely model-based methods and process history based, as shown in Figure 4. The authors defined model-based methods as those that apply information of the system known a-priori, which is in agreement with the definition of white-box frameworks used in the present report. Process history based models correspond to those that use observations rather than a fundamental insights about the system, analogous to black-box frameworks. Grey-box frameworks were also regarded as process history based methods since they are partially defined based on observations. Quantitative model-based methods apply detailed or simplified physical models (e.g. thermodynamic model of a heat pump system or hydrodynamic model of the pressure drop across a pipeline) to identify and characterize faults. Physics-based models may also be applied in qualitative model-based methods, but here the output is nonnumeric. In this type of methods it is possible to identify the presence of a fault and its potential causes but not the mathematical expressions that allow characterizing them. Moreover, qualitative model-based FDD comprise rule-based methods, which can use knowledge based on experience, first principles and specific thresholds. Model-based and process history based methods may analyse the inconsistencies between measured and expected outputs, referred to as residuals. This type of FDD methods take measurements from the system as inputs and produces a residual as output, where a residual signal equal to zero refers to a non-faulty operation.

Table 1: Faults targeted in FDD methods for large-scale vapour compression systems

Fault	Abbreviation
Condensation in the suction line	CS
Condenser fouling	CO
Defective expansion valve	DE
Defective sensors (temperature, mass flow and power uptake)	DS
Evaporator fouling	EF
Excessive oil	EO
Low mass flow in the sink stream	LMC
Low mass flow in the source stream	LME
Oil leakage	OL
Non-condensables in the refrigerant	NC
Reduced compressor efficiency	CE
Refrigerant leakage	RL
Refrigerant overcharge	RO
Rotor wear	RW

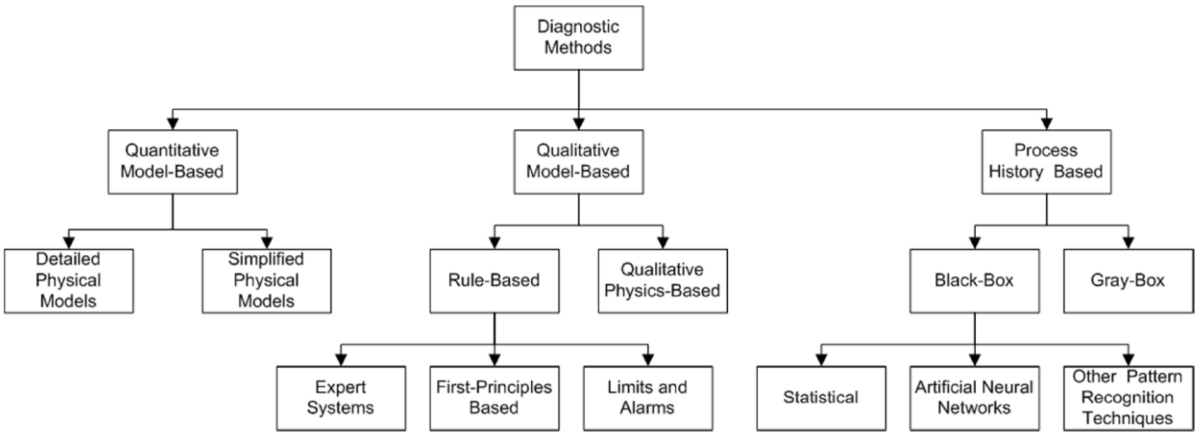

Figure 4: Classification of fault detection and diagnosis methods according to Katipamula and Brambley [78].

3.3.1 White-box frameworks

The white-box FDD methods presented in Table 2 used quantitative rule-based approaches based on first principles, considering the classification scheme shown in Figure 4. Pelet and Favrat [31] identified a dynamic increase of the pinch-point temperature difference in the evaporator of a heat pump, which was attributed to the presence of fouling. The existence of fouling was also detected in [29], [32], [33], by observing an increase of the thermal resistance of the evaporator and/or a COP and capacity reduction. Meesenburg et al. [30] identified condensation in the suction line of an ammonia heat pump by using a dynamic simulation model and physical principles. They observed that the wall temperature of the suction pipeline was below the saturation temperature of ammonia during fast ramp-down operation. This may lead to refrigerant condensation that can have a negative impact over the compressor. Chamoun et al. [27] used a dynamic simulation model to evaluate the effect of an air-purge during the start-up of a large-scale heat pump using water as refrigerant. Here, the existence of non-condensables was observed from the differences between the dynamic behaviour of measured and simulated operational variables (e.g. condensation and evaporation temperatures and pressures).

A number of companies have proposed products and/or services for FDD in heat pumps and refrigeration systems based on physics-based models. Wronski and Jonsson [79] developed a remote FDD system for container refrigeration units applied in shipping applications. Their framework applied a generic steady-state simulation model to evaluate simultaneously the operation of multiple refrigeration units using measured data that was obtained remotely. This approach was able to improve the energy efficiency of the refrigeration units by optimizing maintenance actions.

3.3.2 Black-box frameworks

All the studies found in the literature that used black-box methods for FDD in large-scale vapour compression systems focused on chillers (see Table 2). Moreover, in all those studies experimental data was obtained under steady-state conditions. The only exceptions for this were the studies from Bailey and Kreider [88] and Yan et al. [97] that developed FDD methods for a dynamic system operation. The black-box FDD methods found in the literature were the following:

- Supervised machine learning methods: neural networks, Bayesian networks, support vector machines (SVM), associative classifier, k-nearest neighbours (KNN), linear discriminant analysis, as well as linear and polynomial regressions.
- Unsupervised or semi-supervised machine learning methods: support vector data description (SVDD), Density-based spatial clustering of applications with noise (DBSCAN), and principal component analysis (PCA).
- Learning methods based on fuzzy logic
- Time series models: autoregressive model with exogenous inputs (ARX)
- Discretization algorithms: decision table, entropy-based discretization, equal-width discretization, and equal-frequency discretization [100].

Principal component analysis (PCA) was the most frequently used black-box FDD approach in the reviewed studies, as shown in Table 2. According to Russel et al. [56], the dimensional reduction of a dataset performed by PCA allows identification of the variables responsible for a fault and/or the variables that are most affected by a fault. Other machine learning methods such as Bayesian networks and support vector machines (SVM) were also commonly used in the literature as stand-alone methods or together with PCA.

Table 2: FDD methods applied in large-scale vapour compression systems.

Ref. Source	FDD Method	Type of FDD	Faults	System type / Compressor / Refrigerant / Nominal capacity [MW]	Type of Data
[18]	ARX; ARMAX; Box-Jenkins + Correlogram + Decision table + Simplified physical model	Grey-box	LME; LMC; RL; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[80]	Associative classifier	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[17]	Bayesian networks	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[16]	Bayesian networks	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[81]	Bayesian networks + Discretization algorithms	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[82]	Bayesian networks + PCA	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[83]	DBSCAN + Simplified physical model	Grey-box	LME; LMC; RL	Chiller / Screw / R-22 / 0.4	Experimental
[84]	Decision tree + Simplified physical model	Grey-box	LME; LMC; RL	Chiller / Screw / R-22 / 0.4	Experimental
[27]	Detailed physical model	White-box	NC	HP / Screw / R-718 / 0.4	Experimental / Simulated
[29]	Detailed physical model	White-box	EF	HP / Screw / R-134a / 0.8	Observational
[30]	Detailed physical model	White-box	CS	HP / Reciprocating / R-717 / 0.8	Observational / Simulated
[31]	Detailed physical model	White-box	RW; EF	HP / Screw / R-717 / 3.9	Observational
[32]	Detailed physical model	White-box	EF	HP / Screw / NS / 0.7	Simulated
[33]	Detailed physical model	White-box	EF	HP / NS / R-717 / 2.4	Observational
[85]	EWMA + Simplified physical model	Grey-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[21]	GAN	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[86]	Linear discriminant analysis	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[63]	Linear regression + Detailed physical model	Grey-box	EF	Chiller / Centrifugal / R-11 / 0.7	Observational
[87]	Linear regression + Fuzzy logic + Expert knowledge	Black-box	LME; LMC; DE; CE	Chiller / Reciprocating / R-22 / 0.3	Experimental
[28]	Linear regression + Simplified physical model	Grey-box	LME; EF	HP / NS / R-134a / 0.4	Observational
[88]	Neural networks	Black-box	RL; RO; OL; EO; LMC; CF	Chiller / Screw / R-22 / 0.2	Experimental
[89]	Neural networks + Fuzzy logic	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[90]	Neural networks	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[91]	PCA	Black-box	LME; RL; LMC; CE	Chiller / Centrifugal and Screw / R-134a / 0.2	Experimental
[92]	PCA	Black-box	DS	Chiller / Screw / NS / 1.4	Experimental
[19]	PCA	Black-box	RO; EO; NC; CF; EF	*Chiller / Centrifugal / R-134a / 0.3 and 5.0	Experimental / Observational
[93]	PCA + SVM + KNN	Black-box	RL; RO	Chiller / Screw / R-134a / 0.4 and 0.7	Experimental
[14]	PCA; FDD Table; Multiple Linear regression; Linear discriminant analysis + Simplified physical model	Grey-box	LME; LMC; RL; RO; EO; NC; CF; EF	*Chiller / Centrifugal / R-134a / 0.3	Experimental / Simulated
[94]	PCA; SVDD	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[95]	Polynomial regression + Relative sensitivity	Black-box	LME; LMC; RL; RO; EO	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[22]	Polynomial regression + Simplified physical model	Grey-box	LME; RL; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3 and 5.0	Experimental / Observational
[96]	SVDD	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[97]	SVM + ARX	Black-box	LME; LMC; RL; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[98]	SVM	Black-box	LME; LMC; RL; RO; EO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental
[99]	SVM + EWMA + Simplified physical model	Grey-box	LME; LMC; RL; RO; NC; CF	*Chiller / Centrifugal / R-134a / 0.3	Experimental

* Experimental data from ASHRAE RP-1043

3.3.3 Grey-box frameworks

The study from Gordon et al. [63] was the only one shown in Table 2 that applied a detailed physical model and a data-driven method for FDD. This framework was based on a thermodynamic model of a chiller complemented with a linear regression to identify the existence of fouling in the evaporator. The other grey-box FDD frameworks for large-scale systems found in the literature were based on simplified physical models. As shown in Table 2, several studies using the ASHRAE RP-1043 database [14], [18], [85], [99], [101] applied grey-box models as a combination of data-driven methods and simplified physical models. The simplified physical models in such studies corresponded to a combination of direct measurements, calculated variables and control variables, defined as characteristic variables and parameters in ASHRAE RP-1043 [13]. Examples of characteristic variables and parameters are the UA-value of heat exchangers, the super heating and the COP of the system. Previous studies [13], [14], [102] suggested that using characteristic variables and parameters for FDD provide more robust and sensitive estimations than using direct measurements.

3.4 Optimization of system operation

Control strategies for heat pump and refrigeration systems often relies on conventional control techniques such as ON/OFF controllers, proportional-integral (PI) controllers and proportional–integral–derivative (PID) controllers [103]. The operation of heat pumps and refrigeration systems depends on the non-linear thermal and mechanical behaviour of the system and its interaction with source and sink streams. Conventional control strategies can only operate reactively to that behaviour. To overcome this limitation, advanced control strategies such as model predictive control are applied in different thermal energy systems [104]. Model predictive control is a framework that relies on dynamic models of a system and its forecasted behaviour to provide real-time control optimization. Such a control strategy enables optimizing the operation of complex systems considering multiple constrains from inputs (sensors) and outputs (actuators) [105]. Data-driven modelling methods may also be included in model predictive control strategies to optimize the operation of heat pumps and refrigeration systems by adapting their structure using measured data [106].

Control strategies for vapour compression systems include SISO (Single Input Single Output) control, MIMO (Multiple Input Multiple Output) control. Karjalainen [6] performed a simulation-based study to compare different capacity control strategies for heat pumps, evaluating their potential use in online set point optimization frameworks. This study suggested that a MIMO control strategy to adjust the expansion valve and compressor speed could reach a higher COP than the other strategies like SISO, considering superheat control and heat exchanger pump operation. However, using MIMO increased the complexity to define optimal operation points of the system compared to the other control strategies analysed.

3.4.1 White-box frameworks

Model predictive control frameworks based on physics-derived models to optimize heat pump operation were studied in [107]–[109]. Kajgaard et al. [107] integrated a simplified physics-based model of a house and a heat pump into an MPC framework. Similarly, Weeratunge et al. [108] included physics-derived models in an MPC to optimize the operation of a solar assisted ground-source heat pump with thermal energy storage for space heating. The MPC proposed by Antonov et al. [109] also focused on the optimization of a ground-source heat pump, which was coupled with auxiliary boilers and passive heating systems. The three MPC frameworks [107]–[109] aimed to minimize costs related to space heating by optimizing the operation schedule of the heat pumps subject to electricity price variations and capacity constraints. The physical derivations used in those frameworks were limited to a static COP model of a heat pump without considering the thermal or mechanical dynamics present in real systems.

A number of studies proposed self-optimizing set point frameworks for heat pumps considering steady-state operating conditions [5], [110] and dynamic conditions [111]–[113]. Hu et al. [111] and Wang et al. [112], [113] applied extremum seeking control algorithms to solve real-time set point optimization problems on Modelica-based simulation models. As defined in [114], extremum seeking control is a real-time adaptive control method that can adjust to the unknown dynamics of a system. In general terms, this control strategy adjusts the function being optimized (i.e. objective function) according to artificially induced perturbations in the system. Extremum seeking control has been applied to optimize the operation of dynamic heat pump models since it can search for an optimal input in real-time considering non-linear relationships between variables.

3.4.2 Black-box frameworks

The MPC framework proposed by Burns et al. [115] was able to optimize the operation of vapour compression systems with different configurations by using an adaptable data-driven structure. The proposed MPC could activate or deactivate individual evaporators, where a single control algorithm could be used for different system configurations. According to Burns et al, such a MPC may lead to a lower computational complexity and computational storage requirement compared to other system-specific MPC approaches.

3.4.3 Grey-box frameworks

Peirelinck et al. [116] developed a set point optimization algorithm based on reinforcement learning to adjust the operation of a simulated heat pump for building space heating supply. In their study, the heat pump, building components and HVAC systems were simulated with Modelica under dynamic operational conditions. The reinforcement learning framework was implemented using the Keras Python library [117]. Another grey-box set point optimization method was proposed by Green et al. [118], who studied the optimization of supermarket refrigeration systems with a compressor rack. In this study, a simplified thermodynamic model was complemented with an optimization method named invasive weed optimization. The proposed framework was capable of searching for optimal set points for local controllers in the refrigeration system under steady state and dynamic operating conditions.

Laferriere and Cimmino [119] developed an MPC to optimize the operation of a ground-source residential heat pump. The case study heat pump was provided with an electrical heating device in the source stream outlet to increase the temperature of the injection and thereby assisting the heat pump when required. The operation of a physics-derived model of the heat pump and the electric heating device implemented in Modelica was adjusted based on measured data from the case study using a Kalman filter.

4 Discussion

Physics-derived simulation models allow simulation for analysis of design and operation of heat pump and refrigeration systems under different system configurations and boundary conditions. Several white-box frameworks for monitoring, FDD and operation optimization presented in the review required the development of thermodynamic models of the real system. Thermodynamic models can provide comprehensive information about the operation of the system and they may provide insights about the root cause of faults. However, the development of thermodynamic models requires enough operational data for the validation process. These measured data can be obtained using portable sensing devices and/or existing sensors, actuators and software parameters incorporated in the plant supervisory control and data acquisition system (or SCADA system). As suggested by Venkatasubramanian et al. [120], historical data from a system is not always available from its SCADA interface since only a few data patterns may be present, covering only fractions of the period of interest. Rasmussen and Shenoy [121], described challenges faced when developing dynamic models of vapour compression systems. The highlighted challenges included using different time scales within the same dynamic model, reducing the simulation time of complex systems to perform real-time analysis, performing a detailed validation of dynamic models and the simulation of hard transients (e.g. system start-up or shutdown).

Grey-box models leverage the advantages of physics-based and black-box modelling approaches. Complementing physics-based dynamic models with data-driven methods has the potential to reduce the required data for modelling, improve model reproducibility and improve its ability to adapt to different system configurations and operating conditions. As proposed by Sohlberg and Jacobsen [59], the combination between a physics-derived models and black-box models can be achieved with different model structures. The grey-box monitoring frameworks proposed by [72], [73] applied physical models to describe the components of vapour compression systems, whereas black-box models were applied to represent systems that can be directly described by deterministic expressions (e.g. electricity prices and cooling loads). The share of the black-box component in a grey-box model depends on the availability of a priori knowledge about the system and the discrepancies between the model and the real system.

MIMO control strategies for vapour compression systems may reach higher COP values than SISO [6]. However, optimizing such control strategies may lead to more complex optimization problems and thereby longer calculation times compared to simpler control methods like SISO. The optimal control strategy for vapour compression systems often depends on the specific characteristics of the system and its boundary conditions. In several studies [28], [62], [91], either a physics-based, black-box models or a combination of both was used to evaluate the system behaviour resulting from different control strategies. This approach allows estimating which control strategies and set points achieve the highest performance indicators. As indicated in [7], a period of several months is often required to adjust the control system of large-scale heat pumps after they were installed. A method to evaluate potential adjustments in the control system with model-based methods could be implemented to reduce the fine-tuning period of heat pump control systems during the start-up phase.

Model-based FDD methods, whether white-box, black-box or grey-box, can reduce the requirement for redundant sensors to identify and characterize faults. Numerical models implemented in digital platforms enable assessment of analytical redundancies between the real system and the model, e.g. by using residual analysis. Thereby, the abnormal operation of a system can be identified without the need to install additional sensing devices, which is associated with extra cost and space requirements. However, model-based approaches often simplify uncertainties associated with data collection (e.g. measurement uncertainty, state estimations) [120]. According to Willsky [122], the more complex the real system is, the more the FDD method depends on the model and the more important the robustness of the FDD method becomes. Here, robustness is interpreted as the capacity of the FDD method to provide accurate results regardless of the noise and uncertainties involved in the data collection process. Another challenge to consider in FDD is to model the nonlinear relationships between system variables, which is the case for heat pumps and refrigeration systems. Therefore, simple FDD methods such as linear regressions, may not reach the expected prediction performance. In particular, this may apply when attempting to identify multiple faults occurring simultaneously. Several studies [15], [123], [124] have developed FDD methods for multiple-simultaneous faults in vapour compression systems by using virtual sensors. Virtual sensors combine physics-based models with data analysis methods using measurements from low-cost sensors, to isolate specific variable behaviour associated with a certain fault.

The outcome from FDD methods often changes with varying conditions of a process, as described in a number of studies [92], [120], [125]. The performance of a heat pump and refrigeration systems may degrade over time due to component wear or changes in its boundary conditions (e.g. weather, electricity prices, heating/cooling load). Detecting performance degradation besides identifying particular faults may prevent the occurrence of severe failures. Therefore, system monitoring frameworks could be coupled with FDD methods to alert about potential failures in the system, e.g. due to aging of the components. For instance, Staino et al. [126] analysed experimentally the performance degradation of a refrigeration compressor. The information obtained experimentally was used to develop a framework for system monitoring and FDD that was later applied continuously in a real refrigeration system. This study relied on a thermodynamic model of the system validated with experimental data to define the admissible limits of operation in which faults were not expected. Other approaches that characterised performance degradation focused on the detection and diagnosis of fouling in heat exchangers [127]–[129], which used empirical models of material deposition.

A number of studies applied black-box and grey-box approaches for FDD in experimental setups (see Table 2). However, only a fraction of those studies was based on observational data from case studies. Moreover, there is a lack of standardized criteria for further implementation of data-driven frameworks in heat pumps and refrigeration systems. For example, no standardized document provides guidelines about which machine learning methods are better suited for FDD or for system monitoring, or how such methods should be implemented in real applications. Defining standardized criteria for data-driven frameworks may allow improving their description and prediction performance, accelerating their integration in existing monitoring and control systems, as well as enabling the interoperability across different services they provide.

5 Conclusions

The present report provided a review of digital solutions for heat pump and refrigeration systems. The review focused on services such as system monitoring, fault detection and diagnosis as well as operation optimization, considering numerical models integrated in digital platforms. Physics-based or white-box models were described to provide comprehensive insights related to the operation of real systems in real-time, which can be used to analyse potential unexpected operation of a system. Integrating physics-derived models with data-driven methods may reduce the requirement for measured data, increase the reproducibility of the model and improve its ability to adapt to different system configurations and operating conditions. It was noted that system monitoring could be integrated with fault detection and diagnosis methods to distinguish performance degradation that may later lead to severe faults. Moreover, the selection of suitable model-based fault detection and diagnosis methods should consider aspects such as model adaptability, robustness and prediction performance. From the reviewed studies, it was identified that further research is needed regarding the analysis of black-box and grey-box fault detection and diagnosis models for heat pump and refrigeration in operation.

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