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# Optimization of HVAC Systems: Advances in Thermofluid Performance Modeling and Intelligent Control Strategies



Ebtehal S. Hussain\*<sup>®</sup>, Saja Mohammed Suhael<sup>®</sup>

Department of Mechanical Power Techniques Engineering, Al-Farahidi University, 999048 Baghdad, Iraq

\* Correspondence: Ebtehal S. Hussain (ibtihal.hussein@uoalfarahidi.edu.iq)

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Abstract: Heating, ventilation, and air-conditioning (HVAC) systems have been identified as major contributors to global energy consumption, underscoring the urgency of optimizing their performance for economic and environmental sustainability. This review presents a comprehensive examination of the thermofluid behavior, mathematical modeling techniques, and optimization strategies employed in HVAC systems. Particular emphasis is placed on the development and implementation of dynamic and steady-state models that enable predictive analysis and performance forecasting. The inherently nonlinear and time-varying nature of HVAC systems has necessitated the adoption of advanced computational approaches, including artificial intelligence (AI), machine learning (ML), genetic algorithm (GA), and simulated annealing (SA), to enhance system responsiveness and occupant comfort. AIand ML- based control strategies have been shown to improve adaptability to real-time environmental and occupancy changes, thereby increasing operational efficiency. However, these approaches are often constrained by high data requirements and computational complexity. Multi-objective optimization frameworks have been proposed to balance energy efficiency with environmental impact, yet challenges remain regarding precision, scalability, and the seamless integration of emerging technologies. The application of digital twin technology has recently gained traction as a viable solution for real-time simulation and virtual testing, offering a non-intrusive means of performance evaluation and system tuning. It is suggested that the future of HVAC optimization lies in the convergence of classical thermodynamic and fluid dynamic modeling with intelligent control architectures, enabling the development of adaptive systems capable of autonomous decision-making. This integrated modeling paradigm is anticipated to support advancements in energy-aware design, occupant-centric climate control, and sustainable building operation. Through this synthesis of traditional and data-driven methodologies, new pathways were proposed for achieving robust, scalable, and intelligent HVAC systems that respond efficiently to evolving environmental and user-specific demands.

**Keywords:** Air-conditioning systems; HVAC optimization; Energy efficiency; Mathematical modeling; Machine learning; Predictive control; Artificial intelligence; Multi-objective optimization; Sustainability

#### 1 Introduction

Such effects as those that air-conditioning systems have on indoor environmental quality and energy consumption make the refinement in those systems an essential area of research and practical application. It's no secret that air conditioning units are an essential part of a building and are responsible for almost a quarter to just over a third of the total energy use in a building, especially in commercial buildings. Given the increase of urban expansion and intensification of temperature fluctuations due to climate change, there is increasing demand for effective HVAC solutions. Thus, such optimization of these systems does not involve only bettering energy efficiency; it also greatly contributes to improving occupant comfort and indoor air quality (IAQ). A number of studies have investigated how HVAC systems can be optimized through conventional optimization techniques like linear programming (LP) and newer AI-based techniques like Model Predictive Control (MPC). Nonetheless, the area of AI and ML integration concerning dynamic, real-time optimization of HVAC systems based on changing environmental and occupancy scenarios has been poorly examined in the literature, creating a knowledge gap that needs to be filled.

Lately, there has been significant technological development in air conditioning that has resulted in the development of related advanced methods that amalgamate the functionality of cooling, heating, humidity control and purifying air. It suggests a departure from the conventional HVAC ways of operation to more integrated solutions that value system involvement instead of several one-off systems. Traditionally, conventional HVAC systems are typically run in individual modes, i.e., heating or cooling without integration to achieve effectiveness and energy conservation. Integration of modern technologies such as Building Management System (BMS) enables just-right control of HVAC functions via real-time monitoring and automation of adjustments according to occupancy patterns and environmental conditions. In addition to optimizing energy use, these innovations make an often-neglected difference, which significantly improves overall comfort within buildings by ensuring constant temperature. Air-conditioning systems are part and parcel of the indoor comfort and energy-efficiency story, but they are also responsible on a global scale for a substantial percentage of energy use. HVAC optimization, thus, is a serious issue in decreasing the operational cost as well as the environmental harm.

The significant necessity of improving IAQ is the foremost motivation for research in the air conditioning system optimization. Poor air quality is linked with certain health risks in urban areas, and therefore high pollutant levels in the urban area emphasize the need for efficient ventilation strategies in HVAC systems to alleviate poor quality of air. Continuous IAQ indicators (carbon dioxide levels, etc.) can be assessed with innovations such as smart sensors, and thus be used to fundamentally change the way the airflow rates are delivered into buildings by proactively adjusting HVAC systems. In both regards, such proactive measures help in maintaining a healthier indoor environment and improving efficiency of operations. In addition, mathematical modeling is equally important in improving the performance of HVAC. Prognostic capabilities for the system behavior under different operating conditions are provided by a variety of models extending from steady-state to dynamic simulation formulations. It is crucial to select the right model parameters to let the generated predictions accurately inform control strategies. Consistency of the data produced by models with the process to which models apply is essential and validation techniques are used for this purpose to ensure that operational tactics can continuously evolve.

Technological progress, and hence optimization strategies, is coming along. Traditional methods are still effective, but more recent heuristic as well as metaheuristic approaches are increasingly popular because of their ability to cope with complicated problems that cannot be resolved with conventional methods. The control settings can be dynamically adjusted with techniques such as GA or reinforcement learning (RL) based on historical data or real-time interactions with building occupants. Nevertheless, there are challenges in the successful application of optimization strategies in real life. Often these complexities come in the form of different building layout patterns, behaviors of the occupants, climatic factors, and operational limitations that complicate the traditional optimization process. Furthermore, difficulties with data availability, especially regarding the availability of accurate historical input data, create additional challenges in attempts to realize the complete solution for optimization.

Since the rise of more energy-efficient building practices, several new technologies have come into development for HVAC optimization. With continued promotion for sustainable construction practices, recent studies have delved into innovative methodologies such as multi-objective optimization frameworks that take into account energy saving as well as occupant comfort metrics—every balancing act. This current study attempts to answer the following major research questions: What are the ways to make HVAC energy-efficient using advanced mathematical models? How are ML and AI involved in real-time optimization of HVAC systems?

The study of optimum air conditioning intends to explore many parts, from learning basic components and operational principles to using the advanced technique that will facilitate capable choice-making so that there can be the best businesses from the outcomes. With advancing research on areas concerning AI, ML, and predictive controls such as MPC, there is immense potential to not only significantly reduce energy consumption but also to further enhance occupant experiences while operating in increasingly complex built environments [1–5]. The main aim of the review is to evaluate the recent trends in optimization methods of HVAC systems concerning the aspect of integration of predictive controls and AI-based approaches toward the better energy use and comfort of the occupants.

### 2 Fundamentals of HVAC Systems

### 2.1 Components of HVAC Systems

The indoor environments can be managed through HVAC systems in the residential, commercial and industrial premises. Improving performance and energy efficiency of these systems requires that the critical components be understood. The HVAC components can be categorized into core and ancillary. Thermal energy storage units, cooling and heating towers, boilers, chillers, heat pumps, etc. generate heating and cooling effects. Chillers extract heat from indoor air by means of evaporation and condensation processes and release it outside also by using refrigerants. However, cooling towers are an essential part of a greater chilled water system that cools the excess heat that water will re-enter chillers or air handling units (AHUs). They rely on evaporation techniques, which make use of ambient air to saturate a great amount of surface area and cool the water efficiently. Thanks to the thermal storage systems, thermal energy is captured during off-peak hours for use during peak demand in order to reduce

operational costs. They are heat pumps that use an already existing refrigeration cycle and reverse the refrigeration cycle as per the season.

Distributed conditioned air is provided to a building with the aid of ancillary components. Incoming fresh air is processed through filtration and conditioning by AHUs to be distributed via ductwork. Assuming fans are present, AHUs can change airflow rates based on occupancy sensors or thermostats monitoring indoor conditions. Heated or cooled air is moved between different zones by ducts, which are in many shapes and materials according to the design specification and the minimum airflow resistance. Conditioned airflow is managed through terminal devices such as diffusers and grilles and they distribute supply air as well as reduce return air by means of return airflow for reconditioning. The choice of these devices plays a very critical role in comfort level as well as overall energy efficiency.

Control systems are crucial in modern HVAC installations that set the temperature based upon users' preferences and improve system performance. Smart or programmable thermostats can be taught to occupants to save more energy without hurting comfort. The operation of air conditioning is based on the refrigeration cycle that includes compressors, evaporators, condensers and devices that transfer refrigerant throughout the system. Evaporators are used where refrigerant is heated to absorb latent heat, the pressure of the refrigerant being increased by compressors. Condensers are cooled and the refrigerant condenses back into the liquid form and is allowed to release heat outside. Variable Air Volume (VAV) system is a unit of an energy-efficient design strategy adopted in HVAC systems to increase energy efficiency and at the same time maintain the comfort of occupants. Controlling airflow rates in a VAV system is based on real-time thermal load fluctuations and VAV reduces total energy consumption by orders of magnitude compared with Constant Air Volume (CAV) control.

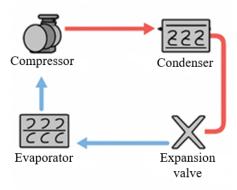


Figure 1. Refrigeration cycle diagram for the HVAC system

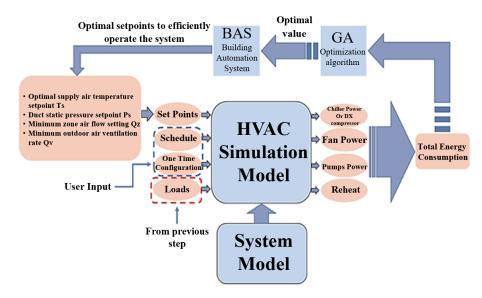


Figure 2. Schematic diagram of the optimization process [1]

Various multifunctional devices that combine the heating, cooling and purification functions have been invented due to technological improvements for the convenience of users and sustainability. Solar thermal technology,

geothermal heating solutions and related renewable energy sources also hold the potential of reducing the utilization of fossil fuels involved in conventional HVAC operation. Overall, by examining each component in an HVAC system that engineers can design, it becomes apparent that it is possible to optimize performance metrics for the best performance, which leads to a more sustainable HVAC system where more global energy and environmental requirements exist [1, 2, 5–7]. Figure 1 and Figure 2 show the refrigeration cycle and the optimization process of the HVAC system, respectively.

### 2.2 Operating Principles

Thermodynamics, fluid dynamics, and heat transfer are fundamental principles of HVAC systems, based on which these systems try to create comfortable indoor environments, in terms of regulated temperature, humidity and air quality. In the heart of these systems, the refrigeration cycle is made up of four important steps: evaporation, compression, condensation, and expansion. The refrigeration cycle starts in the evaporator where the refrigerant picks up heat from indoor air. The increasing thermal energy enters the evaporator coils, which causes the refrigerant to evaporate into a vapor-liquid state. It then flows to the compressor, where it is compressed, bringing its pressure and temperature both up while squeezing it into a smaller volume. This energy-intensive process usually involves electrical power. The second in line is the condenser unit, where the high-pressure gas divests its heat to the environment. As it cools down, it changes back to a liquid and then goes through an expansion valve or device that reduces its pressure to a very low level to be drawn into the distribution system. The pressure drop that this causes sets the refrigerant up to repeat the cycle in the evaporator to its low-pressure state.

Airflow can be managed to optimize the efficiency of HVAC systems. Fans can be designed to work as split systems or centralized units that circulate air through cooling or heating coils and distribute the air through spaces that must be climate controlled. The airflow system should work based on which ducts are designed and the fans that are chosen. To achieve accurate temperature control, the balance between indoor comfort and consumption of energy must be fine-tuned. Many factors affect a balance of this, such as ambient temperature and humidity outside of buildings as well as building insulation and occupant behavior. Air-conditioning systems in use react to fluctuations in the load conditions, such as in the case of changes in the number of people using the building or in external weather. Now, real-time adjustments based on thermal demands within conditioned spaces are achievable, even using advanced monitoring technologies. These systems can be enormously more efficient by using sensors that monitor the occupancy rates or carbon dioxide levels and employing the demand-controlled ventilation strategies.

More specifically, AI is becoming a valuable tool for upgrading the air-conditioning systems, and the HVAC operations in general. AI-driven systems improve predictions of a building's cooling requirements by using ML algorithms to analyze historical data on energy consumption and environmental conditions. Additionally, computational fluid dynamics (CFD) simulation is used for predicting airflow within a climate-controlled environment with accounts taken for furnishings layout and/or architectural features that alter the airflow pathways to achieve optimum system performance during conventional operation situations. In addition to conventional refrigerants such as R-134a that is currently in widespread use, there is an important endeavor to search for alternative natural refrigerants with low global warming potential. Enhancing energy efficiency in a wide range of applications from residential to industrial is one of the transitions to sustainable refrigerants that can impose challenges and opportunities.

In the future, as industries connect their smart grids, the use of controls to adapt air conditioning outputs to available resource levels and seasonal changes will increase in proportion to adaptive HVAC design. Engineering professionals are empowered to improve the efficiency of these models and enhance existing frameworks through an understanding of these operational principles. As our changing relationship to the Earth's fluctuating climate patterns—of which we have become increasingly aware—becomes more apparent, sustainability must be prioritized in this and many other fields. It includes HVAC design engineering solutions that deal with the issues facing the contemporary world before regulations seek to eliminate those practices that are now beginning to be phased out in exchange for ecofriendly ones in the coming decades [3, 6, 8–14]. Figure 3 shows the scatter matrix of the input-output data, including the statistical data distribution.

Coefficient of performance (COP): COP is a key measure of HVAC efficiency. It can be used to compare the energy efficiency of heating and cooling systems.

$$COP_{\text{cooling}} = \frac{Q_{\text{cooling}}}{W}$$
 (1)

where,  $Q_{\text{cooling}}$  is the heat removed from the space (in watts or BTU), and W is the work input to the system (in watts or BTU).

Thermal efficiency: The concept of thermal efficiency and energy consumption can also be introduced to quantify the overall efficiency of the HVAC system.

$$\eta = \frac{\text{Useful Energy Output}}{\text{Energy Input}} \times 100 \tag{2}$$

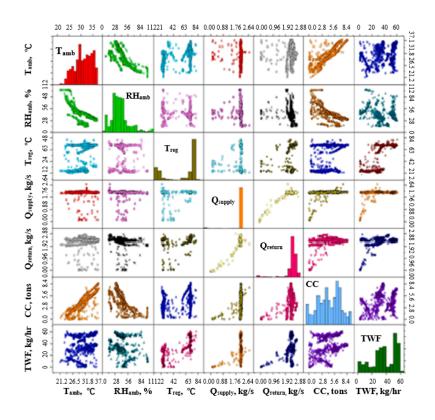


Figure 3. Scatter matrix of the input-output data, including the statistical data distribution [10]

#### 2.3 System Configurations

Depending on operational and design objectives, various configurations for HVAC systems have been designed. Energy efficiency and the comfort felt in the conditioned spaces depend on the setup chosen, as this has a major influence. Because there is a range of environments, building types, and user needs that different configurations can address, a thorough understanding of their operational principles is necessary. One of the most common configurations is VAV that varies airflow with the thermal need of different areas in a building. In VAV, AHUs provide conditioned air at the given temperature and varying flow rates. The VAV box regulating airflow in each zone is typically just one of these. The energy conservation provided by this method occurs because it eliminates the need for uninterrupted airflow in all areas and adjusts dynamically according to real-time conditions. Furthermore, some VAV boxes may have supplementary heating or reheat conventions to condition such spaces as perimeter zones with large windows.

On the other hand, CAV systems operate by supplying a constant rate of airflow in spite of the changes that might have to be made at different spaces in terms of temperature. Though CAV systems might be cheaper and simpler to install than VAV systems, they are less energy efficient, as they cannot adjust air supply with real-time thermal loads. A second important configuration is the chilled water system used in larger commercial buildings. Chilled water passes through coils in AHUs or fan coil units and cools the air prior to being passed through ducts into different rooms. This system also allows for centralized cooling and is capable of dealing with large thermal loads inherent to large commercial spaces. Split systems separate the functions of heating and cooling to the outdoor and indoor units where either the outdoor or indoor unit can be run independently for different zones in smaller buildings or rooms. Because they are easy to install, these systems are also popular in residential settings.

Besides conventional cooling systems, several innovative arrangements, such as desiccant cooling systems, are also popular for effective management of humidity and cooling. Part of these systems is equipped with desiccants; thus, materials can dry the air before more cooling takes place. With the integration of modern technologies and configuration with elements of other traditional configurations, a hybrid configuration can be seen. For instance, several modern HVAC systems have used various designs, including economizers that utilize outdoor air for cooling in instances where field exposures permit or incorporate renewable energy and non-mechanical equipment. Several recent designs have been optimized for the management of airflow within these configurations. The practice of managing stagnant pockets of warm air while maintaining continuous circulation has been enhanced through improved vent designs and the use of barriers to guide airflow.

This process relies heavily on CFD to accurately depict the indoor airflow dynamics before "taking to the field."

CFD modeling can be used to develop and visualize how different setups will influence the air distribution patterns depending on a condition, thereby allowing designers to make rational decisions based on component size and location during the design phase. In addition, advances in control strategies have added to adaptability in such HVAC arrangements via smart switching procedures that react to variable environmental conditions or occupant levels. Combining data-driven controls like AI enables system operators to continuously optimize the performance while minimizing the energy consumption without sacrificing occupant comfort. It is essential to know all options available regarding the system configuration, from traditional systems such as CAV and VAV ones to more ardent implementations utilizing desiccants and intelligent controls [13, 15–17]. Table 1 shows the comparison of the two systems based on the key factors, which will give readers a better idea about which system serves better in various requirements. Figure 4 shows the typical VAV-based HVAC distribution system.

**Table 1.** Comparison of the two systems based on the key factors

Parameter	VAV	CAV	
Energy efficiency	Higher energy efficiency due to dynamic	Less energy efficient; Fixed airflow rate,	
	adjustment of airflow based on load	leading to over- or underconditioning	
Comfort level	Offers better comfort as airflow is adjusted	Less flexible, can lead to uneven	
	to real-time needs	temperatures in some zones	
Complexity	More complex and requires more	Simpler design and operation	
	components and controls	Simpler design and operation	
Cost	Higher initial cost, but more costeffective	Lower initial cost but higher long-term	
	over time due to energy savings	operating cost due to inefficiency	
Applications	Best suited for large commercial and office	Commonly used in small to medium	
	buildings	buildings or less dynamic environments	

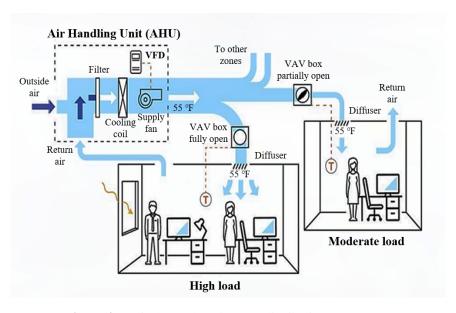


Figure 4. Typical VAV-based HVAC distribution system [17]

### 3 Mathematical Models in HVAC Systems

### 3.1 Types of Mathematical Models

### 3.1.1 Steady-state models

Under a stable condition, steady-state models are necessary for analyzing and improving the HVAC systems to understand their behavior. However, these models are based on the assumption that system variables will not change over time, making the analysis easier than that with the dynamic models. With such components, steady-state principles can be used reliably to predict performance. A major advantage of modeling in the steady state is that it is simple. Under the assumption of constant input and output conditions, i.e., temperature and pressure, engineers can propose equations describing relationships without regard for transient fluctuations. In addition, faster simulations and pertinent information on the system efficiency and capacity under typical operating conditions are obtained.

In air conditioning applications, most typical are steady-state models based on energy balances. For example, in the evaporator, energy is absorbed primarily through the refrigerant's phase transition, accompanied by changes in internal energy. This balance is important for the correct cooling load estimation as well as for validating heat exchanger efficiency. In addition, steady-state equations can be easily used to calculate performance indicators such as COP. Steady-state models of HVAC systems can be developed with various mathematical techniques. Typically, mass and energy conservation laws are combined with thermodynamic principles of refrigerants' states. Depending on the magnitude of available empirical or theoretical data and characteristics of the refrigerants in different phases, tables or equations may be used to represent the refrigerant characteristics.

Another steady-state modeling approach is based on regression analysis of actual operational data. ANNs are used in data-driven methods due to their ability to extract nonlinear relationships between historical performance metrics. With the absence of knowledge regarding physical mechanisms, ANNs are able to model HVAC components well with their knowledge of operational patterns. However, steady-state models have limitations. While not accounting for all complex behaviors like transient situations (e.g., startup and shutdown), dynamic modeling techniques are required to assess time-varying inputs and outputs at the expense of an increased computational complexity.

However, designing control strategies in HVAC systems aiming at maintaining the comfort indoors while satisfying the aforementioned conditions is nevertheless of major interest and can be supported through steady-state models. Engineers can determine the optimal thermostat settings and air flow arrangements that would result in the best possible thermal comfort under different operating scenarios, that is, controlled parameters such as the supply temperature and humidity. Models with steady-state behaviors are integrated with advanced optimization techniques to participate in the multi-objective evaluation on the energy side and occupant satisfaction. It enables researchers to study trade-offs under design constraints that are defined by the operational requirements. Advancements such as MPC frameworks coupled with steady-state modeling provide real-time optimization that is the future state guiding the current operations to meet comfort standards. Once developed, these models must be validated. Current system performance data is crucial in determining their accuracy before being used in big complexes or small buildings in the commercial or residential sector. Poor operation efficiency and unfavorable indoor climates could be caused by discrepancies.

While an increasing amount of effort has shifted towards developing model development methodologies from classic, physics-based approaches to modern, data-driven ones, understanding of a whole gamut of building typologies and environmental conditions continues to be critical for application and is further needed in spite of the ongoing global sustainability challenges. Since there is continued research into integrating different fields of HVAC engineering, like CFD, to improve decision-making and intelligent design, aiming to meet future demands as efficiently and sustainably as possible [1, 2, 18–21], the next great step in the evolution of the heating and cooling field would be this.

In HVAC systems, steady-state energy balance equations are often used to analyze the heat flow within the systems. For example, the energy balance in the evaporator of an air conditioning system can be written as:

$$Q_{\rm in} = Q_{\rm out} + Q_{\rm storage} \tag{3}$$

where,  $Q_{\rm in}$  is the heat input into the systems (e.g., heat absorbed by the evaporator from the room),  $Q_{\rm out}$  is the heat output (e.g., heat rejected to the outdoor environment via the condenser), and  $Q_{\rm storage}$  is the heat stored in the systems (this could be negligible in many cases for steady-state conditions, but it's considered when dealing with thermal storage systems).

For an evaporator in steady-state conditions, the heat balance could also be simplified to:

$$Q_{\rm in} = m \cdot c_p \cdot (T_{\rm in} - T_{\rm out}) \tag{4}$$

where, m is the mass flow rate of air or refrigerant (kg/s),  $C_p$  is the specific heat capacity of the fluid (J/(kg·K)),  $T_{in}$  is the temperature of the air or refrigerant entering the evaporator (°C or K) , and  $T_{out}$  is the temperature of the air or refrigerant leaving the evaporator (°C or K).

In the air-side boundary conditions, the temperature of the incoming air is typically known or specified as a boundary condition:

$$T_{\rm in} = T_{\rm ambient}$$
 (fixed boundary condition) (5)

In the refrigerant-side boundary conditions, the properties of the refrigerant, such as its pressure or temperature, may be fixed at certain points, like at the inlet of the compressor or condenser:

$$P_{\rm in} = P_{\rm ambient}$$
 (fixed boundary condition) (6)

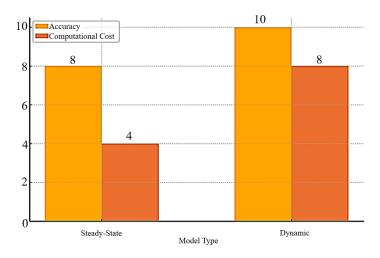


Figure 5. Comparison of steady state vs. dynamic models

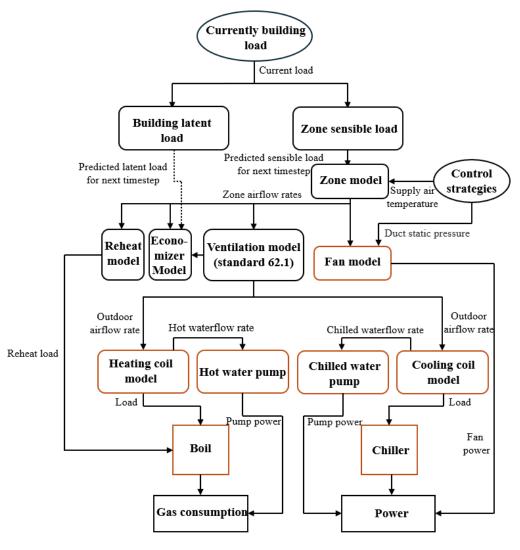


Figure 6. A schematic of the integrated optimization process [1]

Figure 5 is the so-called comparison chart of the model application scope, illustrating the trade-off between accuracy and computational cost between steady-state and dynamic models. In the steady-state model, the computational cost is relatively low, whereas the accuracy is high. The dynamic model offers higher accuracy but requires greater computational effort. This comparison in the figure is useful to explain the benefits and issues related to each

modeling technique.

Figure 6 gives an overview of how these energy balance equations are used in the different parts of an HVAC system, like the compressor, evaporator, condenser and expansion valve, in a more generalized steady-state model.

The compressor working on the refrigerant can be expressed as:

$$W_{\text{compressor}} = m \cdot h_{\text{in}} - h_{\text{out}} \tag{7}$$

where,  $h_{in}$  is the enthalpy of the refrigerant entering the compressor, and  $h_{out}$  is the enthalpy of the refrigerant exiting the compressor.

The rejection of heat to the surroundings in the condenser may be represented as:

$$Q_{\text{out}} = m \cdot (h_{\text{out}} - h_{\text{in}})$$
 (8)

### 3.1.2 Dynamic models

HVAC systems can be understood best by considering dynamic models. Unlike steady-state models, which assume that variables in the HVAC system are constant, dynamic models can effectively capture transient behaviors of the systems, which are close to real system responses under different operational cases. An increasing ability to meet these goals with energy efficiency and compliance with environmental regulations is a reason why this capability has become essential in HVAC design and operation. One important aspect of the dynamic modeling is the integration of different physical phenomena in HVAC systems. The phenomena include heat transfer, fluid dynamics, and thermodynamic processes that may exhibit an apparent change in response to changes in external ambient conditions and/or internal operational needs. For example, the dynamic models can show how the thermal storage system reacts in real time under periods of fluctuating thermal loads, such as occupancy changes in a building or changes in outdoor temperature.

In most cases, such dynamic models are developed from mathematical representations based on fundamental principles. The core conservation laws governing mass, momentum, and energy in the system are included in this approach. Such models are often presented as the state space model or the ordinary differential equation (ODE) based on relationships between different state variables. One example of such a state space model might be for heat gains due to occupants and equipment vs. heat losses through windows and walls for room temperature. Researchers have developed an air-conditioning model based on transient simulation of the automotive sector using advanced simulation tools such as SINDA/FLUINT along with vehicle analysis software such as ADVISOR. Thus, this model allows adequate prediction of system pressure and temperature and compressor power requirements in all modes of operation (e.g., from the conditions of startup to the steady-state performance under driving cycles). In the abovementioned model, manufacturers can optimize HVAC system designs that have better fuel efficiency and reduced emissions given component behavior in real-world driving scenarios.

Dynamic models are also very difficult to develop due to their nonlinear nature. Most air conditioners operate under conditions that cannot be approximated linearly. Such components give rise to nonlinear dynamics such as variable refrigerant flow (VRF) systems or multi-zone VAV controls that have many interacting inputs affecting output like temperature and humidity level. Under these challenging conditions, conventional linear control strategies may have difficulty, since they do not adequately account for time-varying component interactions. In order to confront these difficulties in dynamic modeling, sophisticated modeling procedures, especially for VAV systems in commercial buildings, have been combined with a set of novel advanced control strategies like sliding mode control (SMC). As long as the uncertainties in operational contexts are taken into account through compensation of humidity and temperature variations into adjustments of fan speeds and refrigerant flow rates, state space approaches taking into account humidity and temperature variations can lead to robust performance. It allows for energy efficiency at the cost of occupant comfort that is critical in modern HVAC applications.

Validation is an indispensable component of the development of dynamic models for HVAC systems. Validation of the modeled behavior against experimental or field data collection has been confirmed to be accurate, and the modeled behavior matches the actual performance very well. There exist many techniques for validating dynamic simulations against real-world measurements; one common technique that has been used previously is the comparison of model outputs to historical data of operational conditions. In addition, a great shift happened in using data-driven methods to build dynamic models, especially after the rise of ML algorithms that could handle complex input-output relationships took place in today's HVAC technologies. Therefore, digital twin methodologies are used for real-time monitoring and simulation of actual building performance based on empirical data gathered from smart sensors integrated into the environmental infrastructures.

These digital representations are ideal decision-making tools to evaluate system performance based on detected anomalies vs. expected system behavior and estimate maintenance needs by using detected anomalies vs. predicted behavior from operational dynamic models. Finally, the progress toward a greater degree of development of more sophisticated models of dynamics is paramount not only for helping to better understand but also constantly to

provide improvements in control capabilities in terms of energetic efficiencies of HVAC systems in a breadth of applications starting from residential buildings to industrial processes, ultimately aiding well-defined sustainability criteria established in the context of worldwide climate awareness [6, 9, 12, 22, 23].

ODE is used in dynamic modeling to explain how system variables like temperature, pressure, and flow rate change over time. Dynamic models are frequently used in HVAC systems to model temperature variations in thermal storage systems or AHUs. As an illustration of ODE in HVAC systems, the heat balance equation for a basic model that depicts how a room's temperature changes over time can be expressed as a first-order ODE:

$$\frac{dT}{dt} = \frac{1}{C} \left( Q_{\rm in} - Q_{\rm out} - Q_{\rm loss} \right) \tag{9}$$

where, T is the temperature of the room (°C or K), t is the time (seconds), C is the heat capacity of the room (J/K),  $Q_{\rm in}$  is the heat input into the room (W),  $Q_{\rm out}$  is the heat output (e.g., heat loss to the environment) (W), and  $Q_{\rm loss}$  is the heat loss to the surroundings (W). This equation is constructed based on the heat gained, lost, and transferred out of the room, and it models the variation of room temperature over time. The right side of the equation has the heat input ( $Q_{\rm in}$ ) from HVAC systems or other sources, the heat output ( $Q_{\rm out}$ ), and the heat loss to the surroundings (usually by conduction, convection or radiation). As for the annotated variables for ODE, T is the dependent variable representing the room temperature. In addition,  $Q_{\rm in}$ ,  $Q_{\rm out}$ , and  $Q_{\rm loss}$  are the terms that represent heat flow into, out of, and lost by the room, respectively, and are typically functions of external conditions, HVAC settings, or time.

The partial differential equation (PDE) is used to characterize the behavior of increasingly complicated systems, including fluid dynamics, or simulate heat transfer over multiple dimensions (e.g., within ducts or between zones). For example, as for heat transfer in an air duct, the temperature distribution varies over time along the duct's length and cross-sectional area. For this situation, the heat conduction equation (in one-dimensional form) is a frequently used PDE:

$$\frac{\partial T(x,t)}{\partial t} = \alpha \frac{\partial^2 T(x,t)}{\partial x^2} \tag{10}$$

where, T(x,t) is the temperature distribution in the duct as a function of position x and time t (°C or K),  $\alpha$  is the thermal diffusivity of the air (m²/s), x is the position along the length of the duct (m), and t is the time (s). This is a mathematical model that represents the temperature variation with time at any point x on the length of duct by taking into account the process of heat diffusion. The second derivative in x models the change in temperature in the spatial direction along the duct and the first derivative in t models the change in temperature with time.

As for the annotated variables for PDE, T(x,t) is the dependent variable representing the temperature at position x along the duct and at time t;  $\alpha$  is the thermal diffusivity of the air, a material property that determines how quickly heat spreads through the air in the duct; and x, t is the spatial position and time, respectively, indicating where and when the temperature is being evaluated.

ODE is commonly encountered when the system under consideration varies with time in one dimension (e.g., temperature in a room or pressure in a pipe). Its applications are common in models such as room temperature control or fan control in the HVAC system. PDE is more usually applied to multi-dimensional systems, e.g., the distribution of temperatures in an air duct or throughout a building zone. It is necessary in spatially distributed systems such as in heat transfer in walls or the air flow in ducts.

The empirical implementation of dynamic models has two examples. As for the first example, dynamic models of AHUs can be used to optimize fan speed and heating/cooling loads based on real-time conditions. The temperature or humidity that decreases/increases with time in an AHU can be modeled as an ODE, taking into consideration the heat input (external sources) and the cooling/heating process efficiency. As for the second example, dynamic models, such as ODE and PDE, are commonly used in energy management systems in buildings to forecast energy consumption given occupancy patterns, outdoor weather, and system operation. This would enable the best energy-saving measures to be implemented, particularly in commercial buildings, as shown in Table 2.

The comparison highlights the distinction between the steady state and dynamic models in the system design, performance analysis, and application. Steady-state models are more realistic when conditions are constant or near constant, e.g., an HVAC system at steady load, whereas dynamic models are more realistic in the real world where conditions are continually changing, e.g., when occupancy or the external temperature changes. Steady-state models are also computationally efficient, since they assume that there is no temporal change and can rapidly provide predictions. They are, however, computationally costly because they require solutions of the differential equations that consider the changes of the system with time. They are also quite simplified with a smaller amount of input parameters and can be solved using simple energy balance equations.

Dynamic models are sophisticated, of which time-varying changes must be dealt with, and multiple state variables and more complex numerical procedures are likely to be encountered. They are most suitable in system design and performance analysis where the operating conditions are constant or in load calculations when the system is likely

to be fairly stable. They had also better lend themselves to real-time simulations (e.g., predictive control, energy management systems, or any system that must respond to time-varying inputs). Steady-state models are applied in the system sizing and load calculations, the long-term performance estimation at constant conditions and the rapid analysis where time is not a primary concern. Dynamic models find application in simulations under varying environmental conditions, real-time control systems and insight into transient behaviors of HVAC systems, as shown in Figure 7.

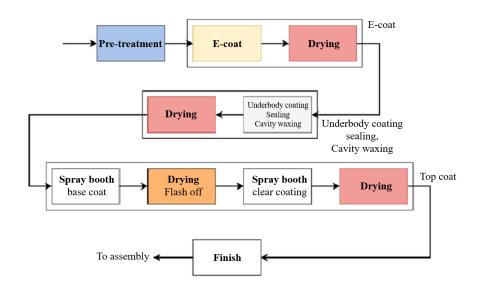


Figure 7. An adapted simplified schematic of the investigated paintshop [22]

**Table 2.** Comparison of the model application scope

Factor	Steady-State Models	Dynamic Models		
Accuracy	Provides accurate predictions under	Provides more accurate predictions		
	constant conditions.	under varying conditions.		
Computational	Low computational cost and fast to	High computational cost and requires		
cost	solve (especially for large systems).	solving time-dependent equations.		
Complexity	Simple and requires fewer parameters and simpler boundary conditions.	Complex and involves multiple variables (e.g., time and space) and complex boundary conditions.		
Time dependency	No time dependency and assumes a steady operational state.	Time-dependent and models how the system evolves over time.		
Application	Suitable for system design, steady load	Suitable for real-time simulation and		
	conditions and optimization under	transient operations and systems with		
scope	fixed parameters.	changing inputs/outputs.		
	Models only the steady-state	Models dynamic system behavior		
System behavior	performance (e.g., average temperature	under varying loads, temperatures or		
•	or pressure).	other operational changes.		
Use case example	Steady-state energy analysis, system sizing and load calculations.	Transient analysis of HVAC systems during varying occupancy or environmental conditions.		
Validation	Easier to validate due to the simplicity	More challenging to validate due to its		
	of conditions.	time-varying nature and complexity.		
	Less sensitive to small parameter	Sensitive to initial conditions and		
Model calibration	changes.	system dynamics, requiring careful		
	changes.	calibration.		

#### 3.2 Model Validation Techniques

Validation techniques of models are crucial to ensure the accuracy and reliability of mathematical frameworks used in HVAC systems. This verification is integral to the development of the model as it confirms that the physical system to be simulated is correct. Several methodologies can be used to validate whether these models meet different needs. Empirical validation method is one important way where the model prediction is compared to the existing system performance metrics with effective metrics. Typically, researchers have to conduct this process through systematic data collection during normal operation to see how well the model's results match with the real-world behavior. Such empirical datasets may be collected from HVAC systems, for example, to measure temperature, humidity, power consumption, and other relevant variables. The difference between observed and predicted values points out the limits of the process or the assumptions in the process itself.

Validation is another important one that involves sensitivity analysis. This study tries to find what changes in input parameters result in changes in output parameters. Research can analyze each of the model parameters like efficiency ratings or environmental conditions to see which are most important to the results. With this understanding, specific changes can be made, which adjust model accuracy and mark to prevent or at least highlight areas that may need better tools to measure. Cross-validation techniques are also advantageous. In particular, this approach takes models created with one dataset and tests them against independent datasets to check that predictions are robust across various conditions and operation scenarios. If a model is able to generalize findings from one dataset to another, it means that it is not particularly applied to specific instances, but rather that it is functioning as a reliable tool in any context.

To validate models, it is necessary to have qualitative evaluations by experienced professionals. In practice, these are assessments of consensus between experts on whether a listed model shows adequate representation of known phenomena associated with HVAC systems. Knowledge from an expert may make models appealing if there is scarce empirical data and can help ensure that models incorporate the right physical principles. The addition of ML has been an excellent method of validating an HVAC model. Tons of datasets are needed for algorithm training using data-driven approaches, and once trained, such models can be tested with backtesting against historical operating data or simulated scenarios meant to replicate real-world conditions. ANNs or Support Vector Machines (SVMs) have been shown in studies to have good potential in imitating the behavior of a system based on past performance records.

Furthermore, the use of hybrid or gray-box modeling strategies that integrate, among other things, physical laws along with statistical correlations based on system performance can enhance validation efficiency by combining theory and statistical correlations of system performance observed in practice. These models give flexibility while maintaining what should be the typical physical characteristics of HVAC systems with precise input adjustments based on observational inputs. Continuing monitoring of the productiveness of validated models is achieved through advanced building automation systems (BAS). Depending on the temporal nature of the model, these systems can be valuable in establishing valuable feedback loops and operational metrics that inform real-time adjustments and refinements of models based on incremental data over time.

Robust validation processes require complex calculations and simulations that are otherwise a very tiresome task to manually complete, which computational tools such as MATLAB greatly simplify. In these platforms, efficient iterated tests can be used against different conditions with parameter optimization by using integrated optimization solvers like GA or particle swarm optimizers. Validation is a continuing process that is dependent on the participation of both researchers and practitioners and is sustained in all the stages of the modeling effort directed at improving energy efficiency in HVAC systems while maintaining adequate convenience in an array of conditions.

It can be summed up by stating that appropriate model validation methods guarantee close similarities between the real-world dynamics of an HVAC system and those represented mathematically. By using empirical comparisons, experienced evaluations, and innovative ML techniques along with developer-created robust frameworks, operational efficiencies can be improved while maintaining the user expectations on the grounds of different facilities across the globe [1, 18, 20, 24].

### 4 Optimization Techniques in HVAC Systems

### 4.1 Classical Optimization Methods

Mathematical strategies employed in classical optimization techniques improve the efficiency and reduce energy expenditure in HVAC systems by optimizing performance in line with the goals such as maximum energy consumption or thermal comfort. With this regard, this study explores different classical methods that have been used in air conditioning. LP is a great technique due in part to its simplicity and the small degree to which such relations may occur to effectively deal with linear relationships among the variables. In many cases (especially applied to HVAC), variable relationships may be linear, meaning that LP can optimize aspects like airflow rates, temperature settings and energy costs. LP is extended to integer programming to cater to component selection optimization problems like the number of heating or cooling units required for a building given load profiles and constraints.

Dynamic programming (DP) is a flexible framework to break the complex problems into simpler sub-problems solved recursively. Its use is particularly relevant when decisions at one stage affect the results at the next one, i.e., for optimizing multi-stage operations in HVAC systems. For example, in some instances, thermostat settings through the day can be adjusted dynamically, based on historical usage data and predictions of those. GA is based on principles of evolutionary biology and may serve to cope with complex optimization objectives with nonlinear constraints that the traditional methods cannot deal with so efficiently. However, in the GA, this study simulates natural selection and iteratively improves the solutions based on the provided fitness value.

SA is inspired by thermodynamic principles and is designed to explore solution spaces effectively, helping to avoid local minima commonly encountered in complex optimization domains. It can help to identify optimal equipment configurations that optimize backup energy service and performance under variable operating conditions. In fuzzy logic systems, the elements of classical optimization and the existence of uncertainty and imprecision are accommodated in the real-world applications. Using fuzzy sets for the input parameters like temperature setting and occupant preference, fuzzy logic offers a more flexible approach for optimization than the binary logic. The classical techniques of these are difficult as it concerns model accuracy and computational efficiency. In order to produce meaningful results from optimization, accurate mathematical models are critical for modeling the behavior of HVAC components. As complexity of the system increases with the features, such as demand response and renewable energy integration, computational burden becomes large.

Classical methods are combined with modern ML techniques to create hybrid strategies in the name of using modern improvements in predictive capabilities while maintaining the traditional way of optimization. For instance, the integration of ANNs with LP to get more appropriate modeling for the nonlinear behavior and the reliability of LP. Classical methods that are static are complemented by real-time adjustments of occupancy patterns and environmental changes through BMS that incorporates sensor data. These large historical performance metrics can bring further calibration of optimization models by creating extensive databases.

When the system configuration complexity grows, simplistic methods prove tough, and for dealing with both discrete and continuous decision variables in HVAC design, advanced techniques like mixed-integer nonlinear programming could be required. Classical approaches have been adapted to contemporary HVAC systems that involve simultaneous optimizations which are under multiple objectives like cost reduction and emissions control, which can be modeled using high-dimensional spaces typical of HVAC applications. In particular, classical optimization methods are very important when designing and operating HVAC systems. By evolving along with the emerging technologies, their efficiency is expected to improve as these methods continue to evolve, particularly in balancing occupant comfort with increasing energy demands [1, 2, 5, 25].

LP is best used in solving linear problems in HVAC systems, including optimum component configuration under a fixed condition. It is computationally economical and can be applied to large-scale optimization. DP applies to temporal optimization, multi-stage decision-making, and problems involving nonlinearities. HVAC optimization with DP applies to time scheduling or temperature control at various times. The computational cost of DP is, however, greater than that of LP. Table 3 shows when each of the algorithms is most largely applicable and what the trade-offs are when applying them in various HVAC optimization cases.

Algorithm DP Problems with linear constraints and Problems that can be broken into Applicable scenarios objective functions. stages or sub-problems. Complex, multi-stage decision Problem type Linear objective function. problems. Computational Relatively low, especially for smaller Computationally expensive for large problems. complexity state spaces or stages. Optimizing energy consumption under Multi-stage optimization problems, fixed conditions (e.g., determining the Example use case such as HVAC scheduling under optimal operating point for HVAC time-varying conditions. system components). Highly flexible, can handle nonlinear Limited to linear relationships; cannot Flexibility systems by breaking them into smaller handle nonlinear systems. sub-problems.

Table 3. Algorithm comparison: LP vs. DP

# 4.2 Heuristic and Metaheuristic Approaches

The use of heuristic and metaheuristic strategies has become the standard way of optimizing HVAC systems because they are efficient at taking into account the complexity and multi-sided character of the problem that often

slip outside common optimization theories. These approaches are inspired by natural phenomena and behaviors that flow over vast solution spaces with ease. Because heuristic methods are not exhaustive searches, but rather based on practical rules or educated guesses, they are invaluable when time is so critical that exhaustive searches are not an option or there are so many possibilities to try. With heuristics, engineers can design pragmatic solutions that are not perfect but sufficiently effective for their use in everyday operations. Thus, GA, for just one example, makes use of principles of natural selection and genetics in an iterative refinement of solutions. It has been successfully applied to optimize the variables like the energy consumption and operational efficiency in the HVAC sector.

However, this approach has been improved using metaheuristic techniques that provide more advanced strategies than others to migrate other heuristics towards better results subject to the search space. Some notable applications of PSO, Ant Colony Optimization (ACO) and SA in HVAC optimization activities have been provided. It is based on social dynamics of nature, i.e., bird flocks or fish schools, using personal experience and collective intelligence to update potential solutions similar to PSO models. The synergy of PSO makes it an efficient convergent method to get optimal configurations. Similar to this, ACO takes inspiration from the food seeking of ants and uses pheromone trails as a guiding marker to direct the future searches to lead to better trails over time. ACO has hence demonstrated the ability to tackle system configuration modeling problems for HVAC scenarios that seek to achieve a balance between thermal comfort and energy consumption.

The combination of different algorithms in various problems is an interesting aspect of heuristic and metaheuristic methods, termed as hybrid strategies, which take advantage of the strengths of different algorithms. For instance, the integration of GA with the local search technique enhances the convergence rate while keeping the exploration ability on a large solution landscape. There are some such combinations that can greatly increase system responsiveness and operational efficiency when facing such complex HVAC environments. Being an active field of algorithmic development, there are bio-inspired methods such as the Deep Ant Colony Optimizer (DeepACO) which comprises DL manners of ACO frameworks. Improvements in these areas make it possible for algorithms to solve static problems and adapt to dynamic environments informed by real-time performance and user interest data.

Furthermore, the fusion of ML techniques with heuristic optimization has great potential to improve HVAC system performance. The contribution of ML is to bring predictive capabilities to optimize efforts enriched with the ability to anticipate critical operational parameters necessary for control strategies. For instance, a type of ML known as RL has demonstrated benefits of dynamically optimizing commercial building energy use based on observed user behavior patterns. Recent research has shown how these optimization methods work well at joint optimization of multiple objectives, including, for example, occupant comfort and energy use of complex HVAC systems. The interplay of sophisticated mathematical models and heuristic approaches allows for sufficiently comprehensive evaluation at the beginning of the design not only of individual components but also of the complete dynamics of system operation in different settings.

In addition, algorithmic design is starting to be driven appreciably by bionic-inspired design principles that are inspired by biological processes with demonstrated exceptional efficiency and adaptability, which are desirable in modern HVAC applications that are subjected to varying demands due to changes in the environment or occupancy. For example, a bionic-based multi-objective optimization methodology and other such features have been employed for air conditioning and purification with a compact unit formed by an advanced parrot optimizer algorithm prior, for example, to other algorithms like the Slime Mold Algorithm (SMA) and Beluga Whale Optimization (BWO). Making use of these innovations enables improvements in airflow, thermal efficiency, energy consumption, carbon dioxide and noise emissions while meeting strict energy constraints and outperforming traditional standalone systems in terms of the indoor environmental quality. Therefore, it can be concluded that heuristic and metaheuristic techniques indicate a transition towards extra-flexible optimization paradigms able to handle current industry difficulties related to HVAC systems. Specifically, these techniques aim to meet performance requirements without compromising environmental responsibility, offering integrated, usage-based solutions inspired by nature and grounded in adaptive problem-solving methodologies [2, 3, 26–28].

PSO is an optimization algorithm inspired by bird flocking or fish schooling, in which particles fly within a solution space and update their positions depending upon their own experience and that of their neighbors. One of the techniques of optimizing the HVAC systems is the PSO algorithm. It consists of random initialization of a swarm of particles, where each particle is a candidate solution to the optimization problem. The fitness of each particle is measured according to the objective function, and in case it leads to the improvement of fitness, the position of the particle is modified. Each particle is then moved through the velocity updating depending on the previous position, personal best position, and global best position, guiding them to move to potentially good regions of the solution space. The algorithm is repeated until it converges, and in case it does, the optimal solution is yielded.

GA is an HVAC optimization method that entails initializing a population with random solutions, assessing the fitness of these solutions with an objective function, selecting parents based on their fitness to reproduce offspring, crossing over two parents to create offspring, mutating with a given probability, and updating the generation. This is repeated through a fixed number of generations or until convergence. GA is especially profitable on complicated and

nonlinear constraints or the high-dimensional solution space. It has found utility in optimizing HVAC, especially in cases where the solution space is high-dimensional.

#### 5 Thermofluid Performance in HVAC Systems

#### 5.1 Heat Transfer Analysis

The analysis of heat transfer in HVAC systems is an essential issue for improving performance, increasing energy saving and providing good occupant wellbeing. Design and operation of HVAC units rely on conduction, convection and radiation. Thus, the knowledge of heat transfer dynamics is necessary. Heat transfer within HVAC components is mostly accomplished through conduction of thermal energy from solids like metal casings on evaporators and condensers. The thermal conductivity of materials is very important for the engineers as the material is picked up for the large change in the system. For instance, higher thermal conductivity of metal can improve heat exchange rates between refrigerant and air.

There are other main vital mechanisms affecting heat transfer in these systems, of which one is convection, which is divided into natural and forced convection. Buoyancy-driven flow from temperature differences is a natural convection process, and forced convection is from external forces like fans pushing milk over coil surfaces. The goal of an effective design is to maximize the cooling effectiveness through higher values of convective heat transfer coefficients. Designed airflow patterns around evaporators improve their ability to draw heat from indoor environments. Radiation is a minor heat transfer mechanism in HVAC systems, although it contributes to heat transfer. A key use occurs in cases in which surfaces contribute considerably to the energy content of the building, especially for large glass surfaces or reflective surfaces and solar gains in architectural designs.

Advanced techniques like CFD simulation enable the analysis of airflow patterns and temperature distribution in the ductwork and cooling coils, which in turn affects the efficiency of the HVAC system. CFD can also identify problems that relate to uneven temperature distribution or poor airflow paths that can cause suboptimal performance. Hybrid nanofluids affect current thermal performance management by providing a thermal conductivity enhancement of the conventional refrigerants being used in the HVAC systems, thus allowing for a better thermal performance. It is known that the integration of nanoparticles into traditional fluids can be highly effective in improving heat transfer rates that are beneficial to energy efficiency efforts and cost savings of operation. In addition, phase change materials (PCMs) are used with a focus on thermal energy storage during maximum loads or best conditions, releasing energy during peak loads or when less renewable energy is available. Using PCMs helps stabilize temperature fluctuations without additional energy once the initial charging phase has been completed, decreasing operational costs linked with existing cooling techniques such as the chiller.

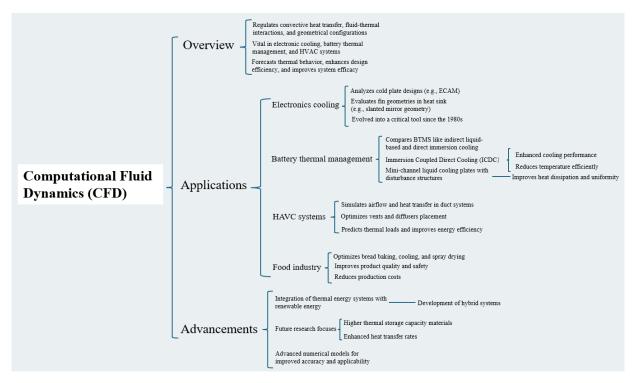


Figure 8. Key considerations related to CFD [8]

Emerging real-time monitoring technologies have been incorporated into advanced modeling like AI and ML.

They enable momentary adaptations according to present operating situations or an observed end-user behavior and offer feedback on how much the system has performed and what the future may need. Proactively managing this can reduce unneeded energy use and help steer the organization towards more sustainable operation. In addition, external environmental factors such as seasonal variations of humidity across the different climates must be considered in comprehensive analysis techniques for designing the HVAC unit size in the design phase. It guarantees achieving the best capacity that balances the capacity with actual demands, helping occupants stay comfortable all year round. Lastly, careful heat transfer analysis is the key to improving the effectiveness of HVAC systems while minimizing the inefficiencies brought about by a lack of proper modeling or maintenance practice of HVAC systems [7, 8, 29, 30]. Figure 8 shows the key considerations related to CFD. Figure 9 shows the applications of the proposed model.

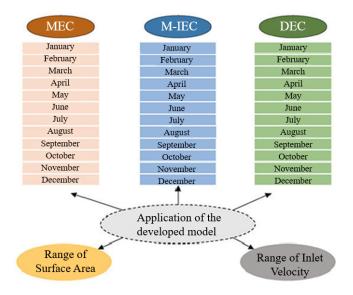


Figure 9. Applications of the proposed model [29]

The Nusselt number (Nu) is a non-dimensional parameter that is used to correlate the convective heat transfer with the conductive heat transfer of a fluid. It plays an important part in determining the capacity of fluids to transfer heat in HVAC.

$$Nu = \frac{hL}{k} \tag{11}$$

where, h is the convective heat transfer coefficient ((W/  $(m^2 \cdot K)$ ), L is the characteristic length (m), and k is the thermal conductivity of the fluid (W/  $(m \cdot K)$ ).

The Prandtl number (Pr) is another dimensionless number that helps characterize the relative thickness of the momentum and thermal boundary layers. It is defined as:

$$\Pr = \frac{v}{\alpha} \tag{12}$$

where, v is the kinematic viscosity (m<sup>2</sup>/s), and  $\alpha$  is the thermal diffusivity (m<sup>2</sup>/s).

A high Nusselt number implies the enhanced heat transfer in HVAC systems, which leads to the increased efficiency of heat exchange in such components as condensers and evaporators. The significance of convection and diffusion in heat transfer depends on the Prandtl number, and fluids with large Prandtl numbers (such as a thick thermal boundary layer) influence the rate of heat transfer. The analysis of heat transfer taking into account these relations provides a deeper insight into the influence of fluid properties on the performance of HVAC.

# 5.2 Fluid Flow Dynamics

Air conditioners are fluid flow systems since efficiency has a direct relationship with fluid flow dynamics. To achieve the best performance in HVAC applications, how the air circulates through ducts and on components needs to be understood. The dynamics also affect energy use, thermal comfort, system reliability, and exercise IAQ. The fluid flow dynamics in HVAC systems depend on effective audit control of airflow. Significantly, depending on how air travels through ducts, air has the ability to reach different areas in a building or vehicle cabin, and this alters the path that it takes in ducts. Velocity profiles and pressure losses are dependent on the duct type and these can cause a waste of energy if not optimized.

Maintaining an adequate airflow rate of the fluid flow in HVAC systems is a critical aspect of these systems. Therefore, the fluid flow rate must balance its heating and cooling needs with energy use. In order to prevent uncomfortable temperatures, there is not enough airflow, while too much can cause higher operational costs. Hence, there is a need to precisely calculate duct dimensions, shapes, and vent placements. CFD has greatly advanced the understanding of fluid flow in HVAC systems. Engineers can use CFD to model complicated airflow patterns under different operating scenarios and obtain information on indicators of performance such as pressure distribution and temperature uniformity. Turbulence effects on airflow characteristics near component parts such as evaporators and fans, crucial to increasing thermal efficiency, can also be tested with CFD.

Additionally, CFD can aid the visualization of temperature gradients and assess the rate of equating cool air from vents to assist in predicting any good mixture fractions in vent placements or blending ratios. Another important factor is pressure loss that occurs across different system components; pressure drops of any significance indicate increased resistance and higher energy consumption. Knowing these areas helps an engineer re-design the system or select a less resistant material part to overcome the performance without increasing resistance. To properly calculate the thermal loads, which will be subsequently used to size the HVAC equipment, the fluid dynamics behind how heat travels must be understood. Proper-sized systems do not cycle frequently: oversized units cycle too frequently, and undersized ones run constantly and are uncomfortable and inefficient.

In particular, dynamic modeling techniques are starting to be more common, given that occupancy loads in commercial buildings are dynamic (fluctuating). The second approach is a thermally driven one, considering shifting thermal loads and taking into account the real-time data of occupancy sensors in order to enable automatic adjustment so that the performance orients itself towards the users' needs instead of averaging historical values. Integration of these technologies with dynamic simulations enables responsive controls in indoor environments, which are designed to be more comfortable, conserve resources, and decrease long-term operational costs. That is in the spirit of current design philosophies seeking to be sustainable and have a lower carbon footprint. Similarly, the development of new technologies, such as hybrid renewable integration and photovoltaic-thermal (PVT) collectors, also benefits from the advances in fluid flow dynamics. Such innovations can support the achievement of net-zero energy goals in the context of growing urban populations, necessitating novel strategies for enhancing building efficiency.

Summarily, studying fluid dynamics encourages collaboration between architects, engineers, contractors and other decision-makers to design schemes that support the health and productiveness of these buildings. By building trust and mutual respect-based relationships, the industry can adjust to the changing challenges, improving the quality of life of communities as we move towards the common visions of progress [8, 9, 13, 30, 31].

The Reynolds number (Re) is a non-dimensional parameter that defines whether the flow is laminar or turbulent, which affects the pressure drop and energy losses in HVAC systems.

$$Re = \frac{\rho vL}{\mu} \tag{13}$$

where,  $\rho$  is the density of the fluid (kg/m³), v is the velocity of the fluid (m/s), L is the characteristic length (m), and  $\mu$  is the dynamic viscosity of the fluid (Pa-s). Laminar flow (low Re) is smooth, and the pressure drop is proportional to the flow rate. At high Re in turbulent flow, the flow is chaotic and pressure drop is increased. Turbulent flow in HVAC, where the Reynolds number is greater than 4,000, results in high-energy losses because of the additional pressure drop. The knowledge of this relation is important in the design of an efficient air and fluid distribution system in HVAC.

Nanofluids normally exhibit higher thermal conductivity than their base fluids. Such nanoparticles (e.g., Cu and  $Al_2O_3$ ) suspended in a base fluid (such as water or ethylene glycol) provide this enhancement in thermal conductivity. The chart quantitatively compares these improvements, which illustrate the efficiency improvement in heat transfer applications such as HVAC systems, as shown in Table 4.

Nanafuid Tema	Base Fluid	Thermal Conductivity	Improvement over Base	
Nanofluid Type	Dase Fluid	$(\mathbf{W}/(\mathbf{m}\cdot\mathbf{K}))$	Fluid	
Al <sub>2</sub> O <sub>3</sub> -water	Water	0.67	+20-30%	
CuO -water	Water	0.93	+40-50%	
SiO <sub>2</sub> -ethylene glycol	Ethylene Glycol	0.42	+15-20%	
Cu-water	Water	0.92	+60-80%	

 Table 4. Nanofluid thermal conductivity comparison

The flow velocity field distribution chart and the results of the CFD simulation show regions of high turbulence and smooth flow within a duct or pipe. They can also be used to display temperature field distribution, especially in

a heat exchanger or in a conditioned room, in order to visualize the efficiency of the heat transfer and locate hot and cold areas so that the heat exchange process can be optimized. The two charts are necessary in comprehending and maximizing the performance of the system.

#### 6 Challenges in Mathematical Modeling and Optimization

### 6.1 Complexity of Real-World Systems

Various complexities of HVAC systems in the real world result in a variety of coupled issues that present huge difficulties in deriving sound mathematical models and optimization strategies. These systems operate under a wide range of variable conditions, including ambient temperature and humidity fluctuations, changes in occupancy and any others. These systems are characterized by a very important feature, namely the Multiple-Input and Multiple-Output (MIMO) structure in which many inputs, such as the temperature and humidity of the incoming air and how much energy goes to different components, must be well and efficiently managed to achieve the desired outcomes of thermal comfort and IAQ. It is difficult to develop simple modeling techniques that faithfully give a description of actual operating scenarios because it is inherently complex.

In practice, a number of HVAC units have been integrated into complex BMSs, which subsequently influences their performance. These types of interactions would lead to unpredictable system behaviors that can be rarefied by the conventional modeling methods. For example, it may be inefficient or even lead to more energy being used to optimize a cooling system without taking into consideration the impacts of the components on heating or ventilation. The addition of operational constraints like equipment limitations and scheduled maintenance further complicates the issues. The largest problem of HVAC optimization is the gap between the theory and the practice. Most of these existing models assume phenomena that are idealized and not found in real-world situations. Simulation models may reproduce the performance accurately for the steady states but lack accuracy in using them when environmental factors or user demands change instantly. Such large discrepancies can result in large inaccuracies of projected performance metrics.

For the understanding of the complexities of real-world HVAC systems, data availability is also essential. A persistent issue encountered in the training of ML algorithms to perform in predictive modeling and optimization is insufficient quality or consistency of the data provided from the operational environment. Data inaccuracies (i.e., sensor malfunctions or inconsistent calibration standards) are factors that factor into data untrustworthiness, which in turn does not make the model reliable. Moreover, there is a lack of comprehensive datasets to enable algorithms to generalize across different operating contexts. The integration challenges involve different subsystems of the HVAC systems. An ideal HVAC system needs to have no disruptions while providing efficient performance with the humidification and filtration processes. Additionally, energy efficiency is often compromised, and crossfunctional integration between subsystems is not seamless. This is frequently due to legacy infrastructure or incompatibility between newer technologies and existing systems. Achieving energy efficiency at acceptable IAQ requires a compromise among the various objectives that can be pursued during an HVAC system's design and operation. Designers often find themselves in circumstances where improvements in one make a trade-off in another. For example, improving humidity control may require increased energy input, which can compromise overall energy efficiency.

The existing HVAC setups are more complex and even real-time adaptability further complicates the tasks; HVAC systems should respond quickly to any change in environmental parameters while keeping the occupants comfortable. It is often difficult to quickly adapt traditional optimization methods to changes that occur quickly, without substantial costs of computation. In addition, the empirical validation methods for creating reliable simulations based on real operational conditions instead of purely theoretical issues identified a research gap that indicates a continued need for the field data collection initiative to assess real performance metrics on the operational bases.

Finally, to deal with these complexities, an approach based on an integrated set of advancing mathematical modeling techniques with the capability to solve the dynamic interactions between variables is necessary. Improving collaboration across interdisciplinary teams is also important for linking HVAC operations with other building management objectives. At the same time, methodologies, both robust and integrated, to incorporate these data into traditional engineering should strive to develop robust solutions that can maintain optimal performance in the face of ever-changing environmental challenges [2, 10, 32, 33].

#### 6.2 Data Availability and Accuracy Issues

Mathematical models for predictive analytics and control based on data lie at the heart of throughput optimization of HVAC systems for which the data availability and precision are critical for the performance of the mathematical models. How effective these models are is based on the quality and diversity of the data collected from various components on a building's HVAC infrastructure. Unfortunately, a lot of obstacles arise against continuous high-quality data acquisition for effective modeling. Use of sensor data is a major hurdle, as it is seldom completed or consistent. However, integration of modern technologies like smart sensors or Internet of Things (IoT) devices in

HVAC systems causes the generated data to increase several times, making it more difficult to handle. Nevertheless, without carefully validating this data, the interpretation and understanding of the data can be impeded, resulting in suboptimal optimization strategies. Furthermore, different performance metrics reported across studies make the rightful data to prioritize at training time uncertain.

The complexity of HVAC systems exacerbates data issues. Due to the nonlinear behaviors and dynamic interactions among the components and the lack of enough empirical datasets, it is difficult to have a quantitative evaluation of these systems without incurring extensive study. Researchers have invested efforts to understand trends of energy consumption based on occupant behavior. Though it has proven difficult to capture occupant behavior through conventional modeling techniques, the trends clearly reveal how much energy is consumed with activity or without it. However, most of the existing models make such oversimplifying assumptions regarding occupancy levels or environmental conditions, while actual data that changes as per the changing of human activity in the buildings is missing. However, the promising future of ML, driven by ongoing advancements, could lead to the development of more effective models. These types of algorithms should be trained on unfair data. In general, ML algorithms typically struggle to extrapolate beyond the data on which they were trained so that models constructed from limited historical data are destined to fail when deployed against other seasons or different environmental conditions.

Data gathering overlooks such time-dependent variables as outdoor temperature and seasonal humidity that have an effect on system performance. There are many operating conditions for which datasets are needed to develop robust predictive models that can meet and change with new scenarios.

Diverse operational input streams (e.g., weather forecasts and indoor environmental quality metrics) need to be integrated in optimization algorithms while there could be a mismatch between real-time conditions and the historical averages. Such a disconnection can negatively affect energy management strategies that assume static conditions and cannot benefit from insights from the current, dynamic nature of HVAC systems. To address these limitations, novel solutions need to be developed to enhance both data collection systems and standards in reporting of performance metrics on a study-by-study basis. The sharing of high-resolution datasets that truly represent the system operation over long periods of time can be encouraged if academic institutions, industry professionals, users, and technology developers collaborate.

Advanced simulation techniques and empirical research can validate theoretical predictions on actual outcomes. That is, a digital twin allows researchers to experiment with theories of component interaction development and refinement of broader system integration informed by true usage patterns. During model development, robust parameter identification methods can improve accuracy and remain flexible enough to adjust to changes in building design or unexpected occupant behavior. Now, especially in light of the recent hybrid office environments with varying occupancy, the flexibility is particularly useful. To summarize, resolution of challenges in the availability and accuracy of the data needs includes working together with the stakeholders involved in optimizing HVAC operation, which encompasses comfort considerations and variable demand in systems designed and programmed by people [1–3, 8, 10, 14, 27, 32, 34, 35]. Figure 10 shows the HVAC optimization.



**Figure 10.** HVAC optimization [35]

#### 7 Recent Advances and Innovations

Earned by the integration of AI in various operational aspects, the recent advancement in the optimization of an air-conditioning system has played a major role. Fundamentally, the technologies of ML and DL have profound impacts on the functions of an HVAC system and greatly improve energy efficiency, occupant comfort and the ability of the HVAC system to respond to real-time variables. The latest frameworks take advantage of abundant data from sensors and previous performance metrics with methods to make the control strategies increasingly better. Supervised learning algorithms analyzing past data are a good development in this area, setting the optimal operating

parameters. It not only helps increase the energy efficiency but also greatly cuts down on carbon emissions. RL techniques are of particular value for the use of control strategies in uncertain situations for more effective, better results for energy saving. Integrating DL models with IoT devices helps manage indoor climates efficiently while maintaining a balance between comfort and energy use.

Most of the current research is devoted to refining HVAC systems using occupant behavior and preference for thermal comfort. Researchers, however, have integrated different algorithms with real-time inputs such as occupancy rates and environmental conditions to come up with intelligent control strategies that respond responsively to the dynamics within the space. For instance, such systems using some region-based convolutional neural networks (R-CNN) for occupancy detection can use the actual usage pattern to modulate the ventilation rate and gain higher comfort while conserving energy. In addition, technology advancements of digital twins hold the potential to provide a holistic way to model HVAC systems accurately. Digital twins allow simulating the environment and the operational scenario in the real world so that faults and the opportunities for optimization could be identified before they affect the actual equipment performance. ML algorithms are added to these simulations to further create the ability to predict potential failures in time based on trends seen over time.

There is a rising niche within this landscape as the health-focused control for HVAC rises. Researchers have been exploring ways to increase IAQ as it pertains to thermal comfort, as well as creating systems that can vary ventilation rates as a function of sensor inputs regarding pollutants or pathogens in the environment. In addition to safeguarding occupant health, this comprehensive strategy also improves system efficiency as a whole. One other promising area is the development of multifunctional bionic-based units involved with combining the operations of cooling, heating, humidity regulation and air purification within a single framework. All of these innovations simulate a complex set of environmental factors simultaneously and optimize the performance of individual system components with advanced algorithmic techniques.

With increasing need for holistic optimization of multiple building operations, BMSs are gaining importance. BMSs can achieve peak performance across all areas while reducing wasteful practices typically found in traditional systems by using centralized automation platforms that integrate diverse subsystems like lighting and security. Another frontier in the use of the Graph Attention Networks (GATs) combined with ensemble learning methodologies is to further understand complex sensor interactions inside smart buildings. These advanced models analyze dependence among the several sensors dispersed in a facility to provide more precise predictive profits on exactly where to allocate resources and power burden patterns.

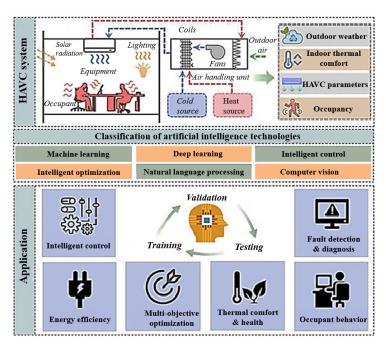


Figure 11. Application of AI technologies in the HVAC field [3]

Additionally, hierarchical DRL approaches are applied toward year-round operational optimization problems encountered by HVAC systems. The innovative structures deliver robust solutions of flexible operation modes with adjusting operations according to seasonal changes or special usage scenarios without sacrificing indoor environmental quality and overall energy efficiency. Amid the ongoing shift toward the adoption of automated smart building technologies, the industry's commitment to sustainability is evolving toward more modern goals.

The rise of automatic smart building technologies underscores the fact that the industry is keen on fast-tracking research and development to add value to HVAC functions with cutting-edge AI-derived solutions. Overall, as detailed in the recent advances, smart algorithms not only increase system performance but also, more importantly, follow responsive design principles (interacting with the occupant wellbeing of built environments through their functionality and sustainability) while pursuing their functionality and sustainability [2–5, 28, 32, 36]. Figure 11 shows the application of AI technologies in the HVAC field.

### 8 Case Studies and Applications

There has been significant progress in HVAC systems that are necessary for energy management in both commercial and residential premises. Various case studies have proved that the application of the optimization techniques can yield large energy savings and improve the operational efficiency. For example, in the optimization of combined cooling, heating, and power (CCHP) systems with a multi-objective optimization strategy, many of these key metrics were improved. Lu et al. [3] studied the optimal CCHP-linked multi-energy systems to minimize the resource scarcity in urban environments. In a commercial building in Tianjin bestowed with state-of-the-art methods such as sequential quadratic programming, a 36.2% reduction of annual operating costs was achieved.

The optimization of HVAC systems is greatly affected by AI across different contexts. In the review by Lu et al. [24], these AI technologies facilitated the development and evaluation of various methods to improve HVAC efficiency through real-time data processing. To minimize the carbon emissions and energy usage of the renovated office spaces, Gao et al. [14, 15] used nonlinear autoregressive models with PSO to optimize thermal comfort.

Air conditioning algorithms that provide intelligent solutions need to undergo development by advanced simulation tools like GT-SUITE by Gamma Technologies. A multiphysics component library with validated components has been provided on this platform to assist engineers in addressing sustainability issues while ensuring human comfort using the customized localized comfort zone modeling. The research by Sukhanov et al. [5] on data-driven cooling optimizations in commercial buildings demonstrates that data-driven control strategies improve energy efficiency of the buildings but, more importantly, increase the lifespan of their equipment by reducing wear on components across a wide range of climates. An example is the Shenzhen Qianhai Smart Community, wherein GATs enabled 15% energy savings with improved occupant satisfaction through adaptive controls of HVAC systems based on environmental data in real time.

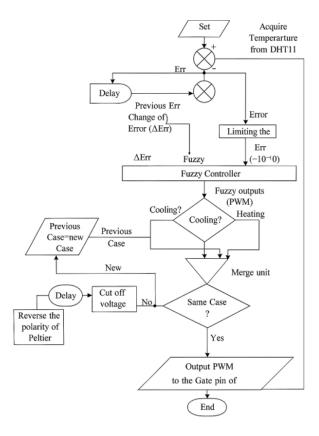


Figure 12. The flow chart of the temperature control algorithm

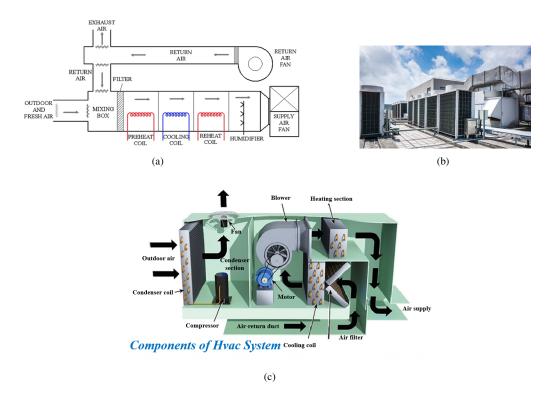
Taken collectively, these case studies illustrate creative means of further refining air conditioning systems,

lowering operational costs while supporting environmental sustainability in response to the global crises of climate change and resource depletion [3, 5, 27, 32, 37–39]. Table 5 shows the current applications of the multi-objective optimization in system operation.

The systems selected in the study were the Central Cold Water Heat Pump (CCHP) systems because they have the potential to integrate cooling, heating, and electricity generated by the same energy source that leads to high-level energy savings and system efficiency. VRF systems are efficient in terms of zone control (individual) and smaller spaces, but they are better suited to residential or light commercial structures. CCHP systems are selected when the application is larger and heating and cooling are needed in high load factors, where power generation integration is useful. They satisfy the multi-faceted energy demand of tall buildings, supplying thermal comfort and power. The economic viability of CCHP systems, especially those related to large commercial or industrial installations, is frequently more attractive because of the recovery of waste heat and onsite generation of electricity.

The CCHP systems in a large-scale commercial project were selected as the case study, where thermal energy (heating and cooling) and electricity had to be produced in an integrated fashion. The size of the building and the requirement of high-efficiency thermal and electrical systems led to the conclusion that CCHP would be the most possible system. The VRF system, in its turn, was not chosen because it could not offer integrated power generation and it was primarily suited to smaller-scale projects where the zone-level control was the most important requirement. The CCHP systems were selected based on their efficiency as well as their capacity to decrease the total amount of energy use by using waste heat to supply cooling, which is highly suitable in large buildings with complicated energy grocery lists.

Applications of the VRF systems are commonly found in buildings that require individual control of zones, e.g., hotels, offices, or (multi-story) apartment buildings. They are flexible because they enable each area to be controlled in terms of temperature and thus enhance comfort and energy savings. Where simultaneous heating and cooling is needed, however (e.g., in large industrial plants), CCHP is more efficient because it combines power generation and recovery in the same system, achieving better energy savings. Conversely, VRF systems lack this level of integration and are better suited to buildings where space heating or cooling requirements per zone may be different, but do not need to occur at the same time. The Qianhai Community HVAC System Layout entails a schematic drawing that shows the arrangement of the HVAC equipment in the community, such as the position of heat exchangers, centralized control units, piping paths, and air distribution in the ducts or ventilation system. This pictorial presentation assists in the comprehension of the management of energy distribution and makes use of optimization techniques such as predictive control in the overall design, as shown in Figure 12 and Figure 13.



**Figure 13.** Equipment arrangement for the central HVAC system: (a) Schematic diagram of a typical Air Handling Unit (AHU) in HVAC system; (b) Rooftop installation of modular HVAC units in a commercial building; (c) Schematic diagram illustrating the main components and airflow path in an HVAC system

**Table 5.** Current applications of the multi-objective optimization in system operation

Ref.	Year	Technology	Findings
[1]	2021	Demand Control Ventilation (DCV)	DCV reduces HVAC energy use by regulating airflow based on occupancy.
[2]	2025	Bionic-Based Multi-Objective Optimization	Optimizes compact HVAC systems with integrated functions using biomimetic strategies.
[3]	2025	Artificial Intelligence	Comprehensive review on AI applications for HVAC operation optimization.
[4]	2023	BMS Air Conditioning System	BMS optimizes comfort and energy by integrating building management technologies.
[5]	2024	Data-Driven Cooling Optimization	Highlights benefits and challenges in optimizing commercial building cooling using data-driven methods.
[6]	2025	Hierarchical Deep Reinforcement Learning	Optimizes HVAC operation for better air quality and energy savings throughout the year.
[7]	2018	Sliding Mode Control	Energy-efficient control design for multizone VAV systems in buildings.
[8]	2022	HVAC Sustainability Overview	Overview of sustainability practices and advancements in HVAC systems.
[9]	2025	Numerical Modeling	Surveys computational models for thermal management and environmental impact assessment.
[10]	2001	Vehicle Air Conditioning System	Model development and optimization for transient vehicle air conditioning systems.
[11]	2023	Deep Learning AI for Desiccant Systems	Optimizes water footprint in desiccant-based air conditioning using AI frameworks.
[12]	2024	Thermoelectric Wall Systems	Sustainable indoor climate regulation using thermoelectric wall system performance analysis.
[13]	2024	Thermal Exchange Modeling (TEMPO)	EU project on optimization modeling for energy and thermal exchange.  Optimization study for cooling
[14]	2018	Parametric Optimization	heat-loaded rooms using parameter adjustments.
[15]	2023	AFUCB-DQN Control Strategy	Optimizes central HVAC systems using deep Q-network-based strategy.
[16]	2024	Configuration Optimization	Review on optimization approaches for thermal system configurations.
[17]	2024	<b>HVAC Best Practices</b>	Outlines five actionable steps for improving HVAC efficiency.
[18]	2021	VAV System Maintenance	Describes operations and maintenance practices for efficient VAV HVAC
[19]	2008	Operational Strategy Optimization	systems.  Strategies for air conditioning in hot and humid climates for energy savings.
[20]	2022	Chiller System Modeling	Mathematical models used for optimizing energy use in chiller-based systems.

#### 9 Future Directions in HVAC System Optimization

Advanced technologies and strategies for energy efficiency and user comfort enhance the optimization of the HVAC system towards a great leap. With climate change and urbanism pressures increasing, future optimization will be about integrating AI, continued refining of predictive modeling, and improvements in the integration of system adaptability and sustainable practices. Just like everything else, AI will be essential to optimizing the provisions of HVAC operation. Real-time data analysis and energy demand prediction based on historical trends associated with weather, occupancy and system performance can be made possible by ML algorithms with predictive maintenance, thus giving operators the opportunity to anticipate future demand. With an adjustment of operational parameters dynamically, AI-driven systems can drastically reduce energy consumption while providing the best indoor comfort.

Future possible optimizations are exciting with the use of the digital twin technology. It generates live virtual images of HVAC systems. Therefore, building managers can test out different scenarios and see what a change might mean for the systems without influencing service. The added benefit is that it makes understanding much easier and can be used as a system design and performance decision support. Next to the emergence of the needed sophisticated mathematical models, which are able to describe the highly complex interactions in HVAC systems, an additional need for AI advancements can be seen. These traditional models fail to include nuances around the behavior of a multi-zone structure in a transient state for differing conditions. These models need to be improved in the future through more advanced computational methods such as finite element methods or CFD simulations along with AI for higher forecasting accuracy.

This can lead to adaptive demand control strategies, which are useful to optimize HVAC systems. IoT device occupancy data are used to respond to real-time variations in occupancy behavior and environmental factors in these strategies. This allows for adjusting heating and cooling outputs based on actual use patterns, preventing energy waste in case of space inoccupation and providing high comfort when the space is full. The optimization practices will be shaped by sustainability. It is no surprise that people have gotten increasingly aware of their carbon footprints. Moreover, researchers are increasingly trolling the earth for geothermal cooling solutions and energy-efficient refrigerants. In this line of work, the integration of renewable energy into HVAC applications is of importance to decrease the dependence on fossil fuels and create greener buildings.

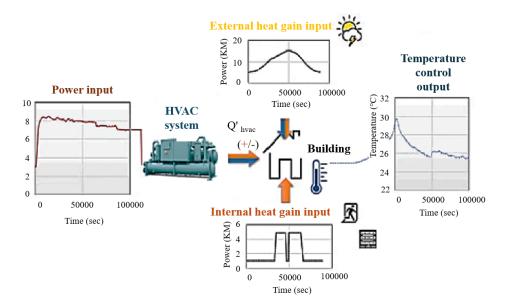
Federated learning-based collaborative methodologies are possible solutions to the privacy problem and take advantage of widely distributed datasets from multiple sources to optimize HVAC system performance. The decentralized approach gives organizations a way to share insights without losing details, which is helpful for the growth of the predictive algorithms. Modular designs will be critical to scalability, fitting into residential spaces but scalable to commercial spaces. Future innovations may choose to integrate the subsystems—an example being an existing ventilation control or humidification unit with a management platform capable of handling fluctuating demands from a single unified platform. With the advancements in technologies, HVAC systems will become more and more complex and interdisciplinary work will be needed among the engineers who specialize in analytics, material science, thermal dynamics, and building design. This will allow these teams to come up with comprehensive frameworks to deal with the multiphase problems associated with modern HVAC applications.

Time of Day	Zone 1	Zone 2	Zone 3	Zone 4	Zone 5	Assumptions
8:00-9:00	10%	10%	10%	10%	10%	Beginning of the workday, gradually
9:00-10:00	30%	30%	30%	30%	30%	Beginning of the workday, gradually
10:00-11:30	95%	95%	0%	0%	95%	Close to a full working staff
11:30-13:00	50%	50%	50%	50%	50%	Lunch break period
13:00-16:00	100%	100%	95%	95%	95%	Close to a full working staff
16:00-17:00	50%	50%	50%	50%	50%	End of workday, gradually
17:00-18:00	10%	10%	10%	10%	10%	End of workday, gradually
8:00-9:00	10%	10%	10%	10%	10%	Beginning of the workday, gradually

**Table 6.** The total savings achieved and the percentage of savings for each component [1]

However, for the design engineers who are constrained by the budget when they are deploying the technologies like AI and digital twins, open-source software platforms offer accessible alternatives at significantly lower costs than proprietary licenses, thereby fostering innovation within the engineering community. Finally, the development of education that produces professionals with the ability to work in the area of modern computational methods and traditional engineering principles will produce professionals who are ready to serve the future optimization needs in an optimal manner. In terms of these developments, it expresses a promising trajectory where HVAC is being optimized towards reduced energy consumption and better occupant experiences and becomes a vital channel in making smarter cities with sustainable solutions tailored for the specific context [1–4, 11, 20, 40–43]. Table 6 shows the total savings achieved and the percentage of savings for each component. Figure 14 shows the input-output model

of an air conditioning system.



**Figure 14.** Input-output model of an air conditioning system [3]

#### 10 Conclusions

Fueled by the improvement of HVAC systems, energy efficiency and the promotion of sustainable practices in buildings are among the key factors for the enhancement. With the increasing demand for good thermal management, new ideas can be developed to remedy the shortcomings of present HVAC systems in residential and commercial settings. Advanced technologies, including AI, ML, and RL, facilitate the integration of new opportunities for improving HVAC performance and efficiency, either simultaneously and/or independently. As in all technologies, HVAC systems have been traditionally based on well-established thermodynamics and fluid dynamics. However, the need to use dynamic modeling techniques is needed for progressively improving system responsiveness to altered environmental conditions. Modern systems are made to use real-time data coming from sensors and smart controls that help adapt exceptional efficiency to changing demands. In addition, this also offers considerable energy savings for the facility. As IoT technologies are being increasingly applied in buildings, the interconnected feature of these devices provides the complete picture with regard to energy consumption patterns to completely control HVAC systems.

Dynamic HVAC solutions are a significant advance from static solutions that are in current use in building management practice. MPC is a cutting-edge methodology that anticipates future needs based on occupancy patterns and environmental variations, making decision-making capabilities better. More accurate operation adjustments mean less energy waste and better indoor climate conditions using such predictive analytics. Additionally, the discussion concerning building design is integrating renewable energy sources into HVAC systems, which is now more prevalent. Furthermore, hybrid systems, including solar panel or geothermal heat pump technologies, decrease reliance on fossil fuels and increase redundancy in light of the unpredictability of energy markets. Recent research provides proof that such integrations increase efficiencies. For example, HVAC systems with multiple renewable energy sources have shown significant reduction in electricity and natural gas requirements compared to conventional systems. Numerous case studies show how such advanced HVAC technologies have been successfully implemented when engineers work in close collaboration with architects and environmental scientists to achieve the design goals in terms of both performance and sustainability. When frameworks can be created to enable communications between different building systems, significant enhancements in overall operational efficiency can be achieved.

While much has been achieved in developing integrated systems, especially on the pipeline and in the field, questions persist about its data availability and accuracy in these integrated systems; regular sensor calibration is essential to reach reliable results. There is also a large need for research on low-cost approaches that can broaden the use of such sophisticated optimization techniques to a larger set of economic contexts. However, in this field, it is important to have a forward-looking approach to take user experience alongside technical innovations. Users need to be informed of the advantages and functionalities of their HVAC systems to make educated decisions on how to use the systems, and encouraging proactive use of system settings can result in even more overall efficiency gains. Sustainable practice is not only a responsibility of the maintenance and repair but also of the policy; regulatory structures that

promote sustainable practices within the HVAC industry are going to provide the catalyst and obligation for the industry to innovate and for manufacturers and service providers to hold themselves accountable. The way to have widespread adoption of best practices across many different sectors is to establish clear guidelines of performance standards.

For progress to be achieved, it will require a collective effort from all stakeholders—from policymakers driving towards greener initiatives to engineers creating the most advanced technologies to increase HVAC standardization with a minimal effect on the environment. Technological advancements coupled with regulatory support point to a plausible route for developing actuating air conditioners that can deliver what contemporary society is demanding without abdicating ecological responsibility. Meaningful efforts can be made to improve indoor comfort levels while making global sustainability attempts—a worthy task in a more resource-climbed world.

Though this review gives an in-depth literature review on the HVAC optimization methods, it is notable that some gaps have not been addressed. In particular, small residential systems are outside the scope of this research and their peculiar issues and optimization methods can greatly differ compared to those that can be applied to bigger commercial or industrial systems. In addition, the review concentrates on well-known optimization techniques and does not go into the details of the investigation of newer technologies, which could be at the research or experiment stage. The next generation of HVAC optimization will be rooted in inter-disciplinary cooperation. Increasingly, the HVAC systems are being linked with smart building technologies and sustainability efforts, which means that architects, energy engineers, and computer scientists will need to work closely. The architects have expertise in building design and energy needs, whereas energy engineers have expertise on the performance and effectiveness of the systems. Instead, computer scientists offer ML, AI, and predictive control knowledge that can greatly benefit optimization of the systems. It is out of such joint efforts that HVAC solutions shall be developed, which are not just energy efficient but also capable of keeping up with the changes taking place within the environment and those that are user-driven.

In conclusion, this review has outlined the great potential that exists in the optimization of HVAC systems using mathematical models, optimization algorithms and the emerging technologies, including ML and prediction control. Although significant advances have occurred, issues relating to availability of data, computational complexity, and the requirement of adaptive and real-time systems still exist. In addition, it is necessary to note the limitations of such a review, such as the absence of small residential systems and new experimental technologies. In the future, cross-disciplinary collaboration will become more and more important in the optimization of HVAC systems. The collaboration of architects, energy engineers, and computer scientists is necessary to develop more efficient, sustainable, and flexible HVAC solutions capable of responding to the complicated and ever-changing demands of present-day buildings.

# **Data Availability**

The data used to support the research findings are available from the corresponding author upon request.

### **Conflicts of Interest**

The authors declare no conflict of interest.

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