A review on the integrated optimization techniques and machine learning approaches for modeling, prediction, and decision making on integrated energy systems

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Abstract

The optimal co-planning of the integrated energy system (IES) and machine learning (ML) application on the multivariable prediction of IES parameters have mostly been carried out separately in the literature. Meanwhile, the synergy of optimization methods and ML techniques can enhance the feasibility of a zero-emission IES, boost realistic planning, and promote accurate day-ahead scheduling. Thus, a comprehensive review of integrated optimization and ML techniques in IES is crucial and hereby presented in this study. Critical issues such as an overview of IES structure, IES modeling approaches and techniques, application of ML in IES research, and the trends of integrating ML and optimization techniques for optimal and feasible planning of IES were presented. Specifically, extant studies on the integrated approach were reviewed under ML hyperparameter tuning using optimization, combined uncertainty estimation and decision making, integrated ML and scenario generation, integrated prediction, and optimal decision-making techniques. Findings from this review show that the IES structure depends on the available technologies, the multi-energy demand patterns, the available renewable resources, and the planner's objective. It was also revealed that despite the popularity of ML models and the benefits of synergizing them with optimization models, the application of IES has not been fully explored. The main conclusion from the review is that an IES framework with the aim of a carbon neutrality target is worthy of development. Also, the application of integrated ML and optimization on IES is still at its infant stage; hence, more research exploration is required in this area.

Keywords: multi-energy system; machine learning; deep learning; mathematical programming; optimization methods; carbon neutrality.

1. Introduction

1.1 Motivation and Background

The rapid penetration of renewable energy systems (RES), the adoption of electric (EV) and hydrogen vehicles (HV), and the recent research breakthrough on energy storage have created a pathway for decarbonizing the transportation sector and actualizing the Paris climate accord [1]. This is evident in the global annual increase in renewable energy capacity installation and the surge in replacing gasoline vehicles with EV and HV [2]. Whereas, to overcome the challenges associated with operating each energy equipment separately, such as the increase in operating cost; energy loss; low efficiency; lack of optimal coordination and scheduling, an integrated energy system (IES) that deals with the co-planning and operation of energy infrastructure in one-fold have been a centre of attraction. In fact, the IES concept is described by the European Union Commission as a strategy for the deep decarbonization of the energy sector [3]. Immerse contributions have also been made in IES research either through optimization techniques or simulation approaches [4]. However, to ensure realistic optimization of IES, accurate prediction of the renewables, multi-energy demand, and other associated parameters that vary with time are criteria for optimal decision making, and machine learning (ML) techniques are recognized tools for carrying out these tasks [5]. Strictly speaking, the optimal co-planning of IES and the application of ML on multivariable prediction of IES parameters have mostly been carried out separately in the literature. Hence, only a few researchers have considered the benefits of synergizing the two approaches, and a verified framework for executing the synergized approach has not been established. To the authors' best knowledge, a comprehensive review on the current application of this integrated approach for modelling IES has not been considered. In this light, this paper seeks to address this.

1.2 Related review works

Due to the benefits associated with IES, some review studies on its state-of-the-art technologies and approaches have been conducted. Through related keywords search (i.e., integrated energy systems, multi-energy systems, integrated electricity and heat system, energy hub, multi-carrier energy systems) on the Scopus, ScienceDirect, and Web of Science, 36 review articles published between 2007 to 2021 were identified.

Table 1 presents the extant review studies on IES. It was observed that these studies focus on 1) modeling of IES, 2) planning, 3) operation, 4) flexibility, and 5) scale. For instance, Moahmmadi et al.[6] gave an overview of IES modeling components relating to energy generation, conversion equipment, transmission, distribution, IES energy storage equipment, and the multi-energy demand. Huang et al. [7] presented details on IES multi-networks. The non-linear and linear mathematical equations governing the electrical, thermal, and gas network models were analyzed, followed by the planning and operation of the network system at the district level. In ref. [8], the modeling approaches of IES optimal operation were reviewed. The identified modeling approaches included operation model with flexibility improvement, operation model with uncertainty, joint optimal dispatch of the electrical power system (EPS) and district heat system (DHS), and modeling for joint market-clearing of EPS and DHS. Similarly, optimization of IES operation under renewable energy domination was also reviewed in [9]. Chicco et al. [10] reviewed various flexibility potentials of distributed IES in terms of flexibility. The flexibility potentials were discussed with respect to input and output energy vector shifting, temporary arbitrage through virtual storage, renewable energy, energy production curtailment, and reactive power control. Also, optimal flexibility at the demand side regarding integrated demand response was extensively reviewed in [10-12]. In terms of scale, the application of IES at the building cluster level was presented in [13]. Doubleday et al. [14] presented an overview of the planning of IES for urban district applications with high renewable penetrations, while the planning and the modeling tools for IES at the national levels were described in [15, 16].

1.3 Novel contribution

While extensive reviews have been conducted on IES, especially planning, operation, modeling, and scale, the current trend and the prospect of ML application in IES have not been presented. In contrast, ML has been the primary tool for achieving smart cities [17], especially proactive measures and future events prediction. It is worth mentioning that ML is not a new tool.

Comprehensive reviews of its application regarding renewable energy forecast, energy load prediction, and building application were presented in [5]. However, surveys on its integration with renowned optimization techniques are few to the best of our knowledge. Thus, this study seeks to explore the concept of IES, identify the areas that ML has been applied to improve IES, describe the likely future trends of integrating ML and optimization techniques for optimal and feasible planning of IES, and ultimately, highlight the gaps to be addressed for zero-carbon policies actualization. In summary, the main contributions of this current study are itemized below:

1) A comprehensive overview of IES is presented, ranging from the technologies, configurations, and modeling methods;
2) A critical review of various studies that have applied optimization methods and ML techniques to IES research are compared and examined;
3) The possible application of integrated optimization and ML techniques on IES in terms of future prediction and optimal decision making are presented;
4) Potential research guidance for future studies is provided to enhance the application of integrated optimization methods and ML on IES.

Table 1. The main contributions of previous review work on Integrated Energy Systems IES

Ref.	Highlights	Area of review focus				Year
		IES Review	ML techniques review on IES	Application of optimization in IES	Integrated ML and optimization	
[19]	Analysed thermal power plants, intermittent RE and IES.	✓				2021
[20]	Developed a holistic system-of-systems approach for IES.	✓				2021
[21]	Analysis of electrical gas systems and autonomous system scheduling.	✓		✓		2021
[22]	Identified barriers in district energy-electricity system interface.	✓				2021
[23]	Extensively reviewed the sector coupling concept.	✓				2021
[24]	Analysed a cost-based function model via a hybrid optimization approach.			✓		2021
[25]	An overview of IES planning approaches and optimization methods.	✓		✓		2021
[26]	Reviewed applications and energy performance of district energy network.	✓		✓		2021
[27]	Examined the trends in the technical and economic planning of local energy systems.	✓		✓		2021
[28]	Provided an overview and study path for IES operation optimization.	✓		✓		2021
[29]	Examined the software packages needed for optimizing energy hub (EH).	✓				2021
[30]	Reviewed the modelling tools suitable for IES optimization in mixed-used districts.	✓	✓	✓		2021
[31]	Focused on the integration of renewable energies in CHP systems.	✓		✓		2020
[32]	Reviewed the research trends on integrating multi-vector energy networks.	✓		✓		2020
[33]	Review on IES modelling tools with focus on multi-criteria analysis.	✓				2020
[34]	Reviewed the demand response modelling frameworks implemented in IES.	✓				2020
[35]	Examined the combined energy modelling studies in sub-Saharan Africa.	✓				2020
[36]	Conducted a stepwise survey on customers' demand response.	✓				2019
[37]	Identified the main components of energy infrastructures (EI).	✓				2019
[38]	Presented an up-to-date overview of EH-based operational frameworks.	✓		✓		2019
[39]	Reviewed current practices in smart district planning.	✓		✓		2019
[40]	Analysed open-source tools for their maturity based on function.	✓				2019
[14]	Identified the factors influencing urban energy systems at cluster level.	✓		✓		2018

[41]	An overview on the main aspects of integrated grid based IES modelling.	✓		✓		2018
[42]	Investigated the energy flow in multi-carrier ES via a point estimate approach.	✓				2018
[43]	Reviewed the barriers on the polygeneration of integrated gasification combined cycle process.	✓				2018
[6]	Reviewed the EH concepts and applications in various energy-use sectors.	✓				2018
[44]	Presented an analytical overview on Energy Internet.	✓		✓		2018
[45]	Provided an overview of hybrid nuclear-renewable ES' operations.	✓				2018
[46]	Examined mutually dependent electricity grids and natural gas networks.	✓		✓		2018
[47]	A review on the adoption of a neighbourhood-scale distributed ES.	✓				2018
[48]	Examined the development status of power-to-gas technology.	✓		✓		2017
[49]	Investigated the main structures employed in EH models.	✓		✓		2017
[13]	Evaluated the key issues on integrated demand response (IDR) in IES.	✓		✓		2017
[50]	Critically studied the links between emerging modern energy concepts.	✓		✓		2017
[51]	Addressed issues relevant to the integration of variable RES in long-term ES models.	✓		✓		2017
[52]	An overview on the suitability and challenges of natural gas and wind power.	✓				2017
[53]	Evaluated the effects of district energy networks on multi-carrier energy systems' optimization.	✓		✓		2016
[54]	Considered the features, potentials, and barriers of future power systems.	✓	✓	✓		2016
[17]	An overview on the modelling approaches and simulation tools.	✓		✓		2015
[55]	Surveyed the strengths, and weaknesses of IES for residential ZEBs.	✓				2014
[56]	Investigated the integration concepts for CCHP and polygeneration systems.	✓				2007
[57]	Developed the energy hub concept.	✓				2007
[This review]	***An all-inclusive analysis of IES structure and modelling approach alongside the application of integrated optimization techniques and ML applications for optimal and feasible planning of IES.***	**✓**	**✓**	**✓**	**✓**	**2022**

1.4 Research Methodology

The research methodology used in this study is outlined in Figure 1. As shown, the methodology is composed of three important steps. The first step involved literature search from Scopus, Web of Science (WOS) and ScienceDirect search engines. This search was conducted by entering the following queries;

1. "Integrated energy system" OR "multi-energy system" OR "Integrated electricity and gas system") AND "Optimization”.
2. "Integrated energy system" OR "multi-energy system" OR "Integrated electricity and gas system") AND ("Machine learning" OR "deep learning".
3. "Integrated energy system" OR "multi-energy system" OR "Integrated electricity and gas system") AND ("Machine learning" OR "deep learning") AND ("Optimization").

The first, second and third bullet points are queries used in searching for documents related to optimization techniques in IES, ML models in IES, and Integrated optimization and ML approaches in IES, respectively. These three sub-topics are elaborated in sections 3, 4 and 5. The search document also covered documents published between 2007 and 2021.

Also, the results from the search queries were carefully screened, analyzed and filtered as described in step 2. Such initial screening applies to the title and abstracts. Next, a preliminary content review was done to ensure the content of each paper matches the goal of this study. Lastly, step 3 involved the detailed critical analysis of the final selected documents under sections 3, 4 and 5. The result of the critical analysis is summarized in Section 6.

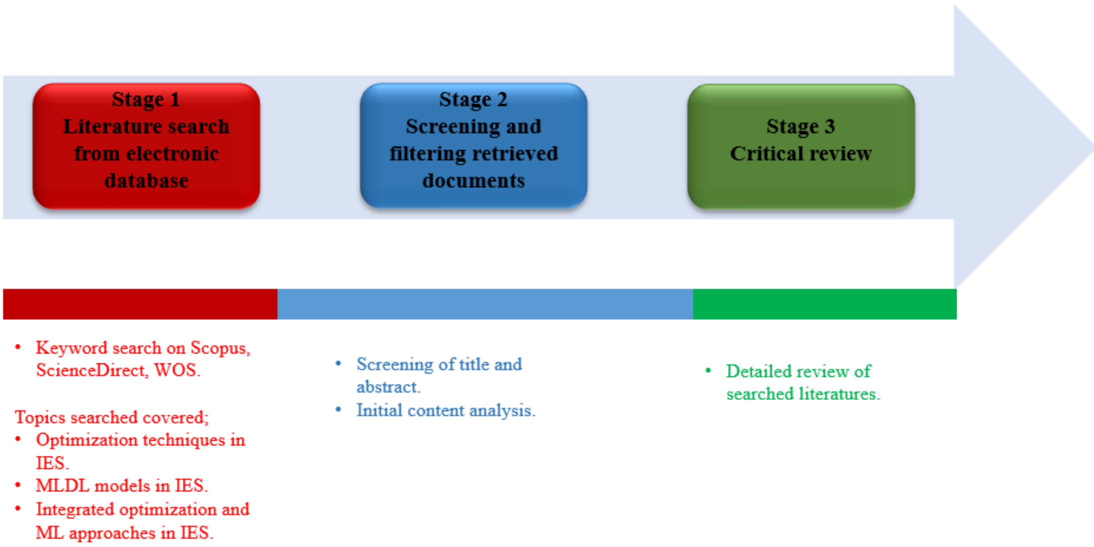

Fig 1. Survey methodology

1.5 Paper structure

The rest of the paper is structured as follows; Section 2 presents an overview of IES. Sections 3 and 4 present the various optimization and machine learning techniques used in previous IES studies. Furthermore, in Section 5, studies with information on integrated optimization and machine learning techniques in IES were reviewed. Finally, Section 6 concludes the study and proffers areas for future study. The paper's structure is graphically illustrated in Fig. 2.

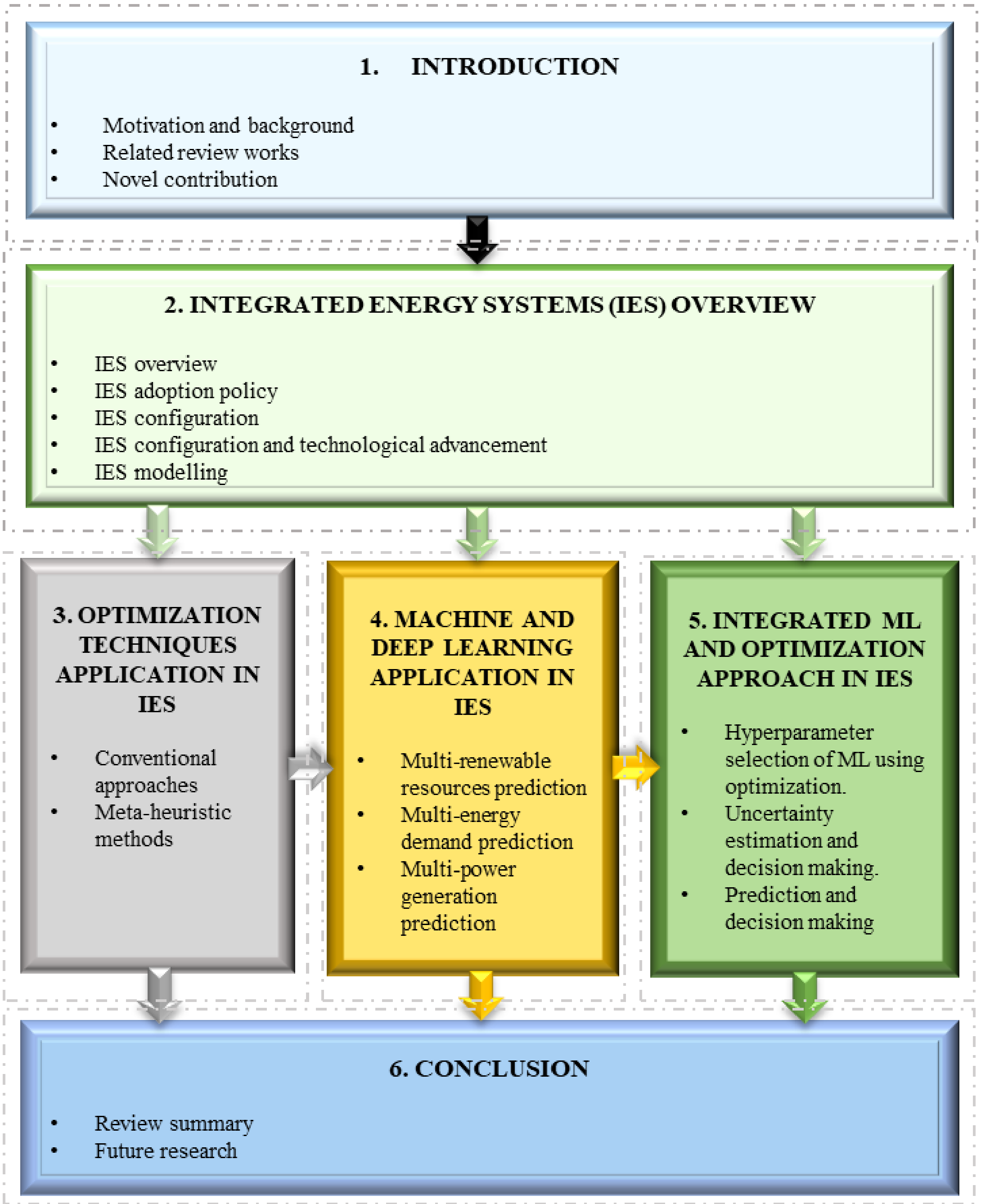

Fig 2. Structure of the paper

2. Integrated energy systems (IES) overview

Overtime challenges such as intermittency of renewable resources, huge transmission losses, energy wastage, huge capital investment, high operation cost, and the need to decarbonize the transportation and thermal production sector have been associated with standalone renewable generation. These challenges have led to a paradigm shift towards IES research and commercialization. The concept of IES was first introduced in 2005 by an ETH Zurich research team under the caption of a project called "vision of future energy networks". The goal of the project was to synergize benefits among various energy components [57]. Mancarella [58] gave a detailed account of IES benefits over operating individual energy infrastructures separately and elaborated the concept in terms of spatial, multi-service, and multi-fuel perspectives. Guelpa et al. [36] also presented an in-depth account of IES components such as power generation, energy conversion, energy storage, IES network connections, and modelling techniques. In summary, the focus of research communities has shifted towards IES exploration, and some notable contributions have been made [59]. In addition, many countries have adopted the concept of IES as a policy to drive the achievement of sustainable energy goals.

2.1 IES strategy adoption as a policy

IES has garnered numerous attention among scholars and policymakers. For instance, the International Institute for Energy Systems Integration (iiESI) was founded in 2014 to oversee the development of innovative strategies for the coordination and optimization of energy infrastructure [60]. Likewise, some countries have proposed diverse energy development strategies to fully implement IES in the different energy sectors. For example, the United States Department of Energy (DOE) established the IES development strategy in 2001 to promote renewable energy adoption and the integration of multi-energy technologies. In 2003, a research project titled “Vision of Future Energy Networks” was launched in Switzerland to consider the synergy of multiple energy sectors and their feasibility. In 2009, the Canadian government pushed the IES strategy based on the promising research output of a project entitled “Combining our Energies: Integrated Energy Systems for Canadian Communities” [61]. The German government also released an issue that detailed the technical feasibility of IES operation in Germany in 2010 [62]. In 2015, the Chinese government depicted its plan under “Energy Internet” to achieve a clean and efficient energy supply by coupling and coordinating different energy sectors [63]. The Danish government's aim to reach 100% clean energy by 2050 is also noteworthy, and implementation has begun with the development of novel CHP and central heating systems. [64].

2.2 IES configuration and technological advancement

IES integrates multiple energy carriers. To optimize these carriers and yield the benefits described in the introductory section, the configuration of this system is subdivided into four (4) components. These include the energy input, energy hub equipment (conversion and storage technologies), network configuration, and energy output. Fig. 3 illustrates the components of IES, while Fig. 4 describes the structure. The descriptions of each component are explained in the proceeding section.

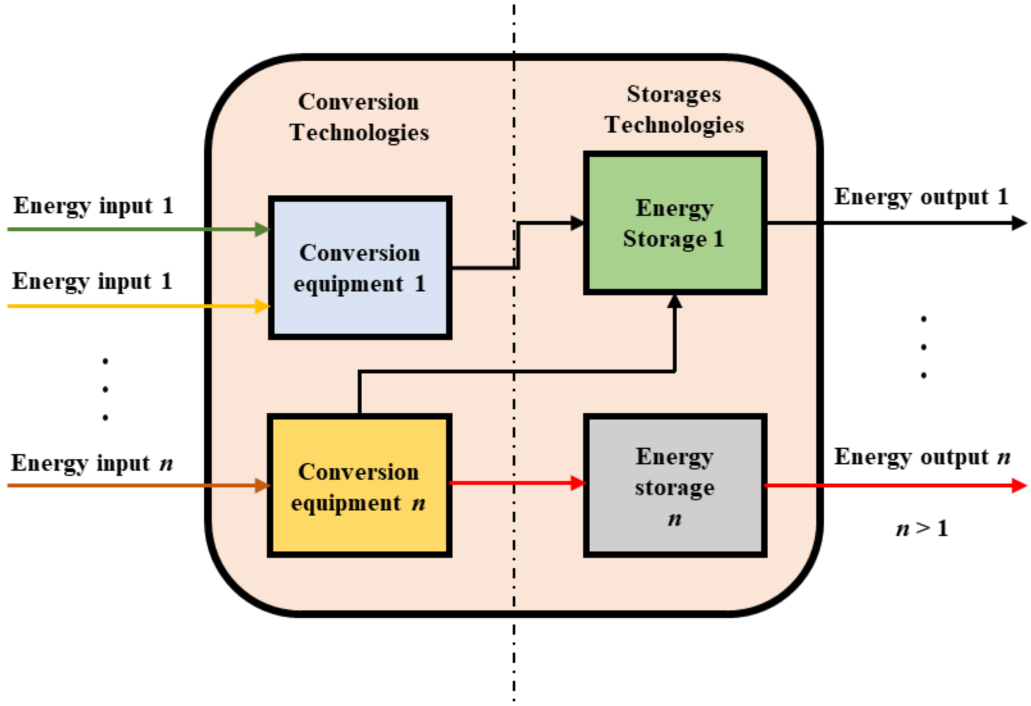

Fig 3. A typical Integrated-energy system (IES) architecture

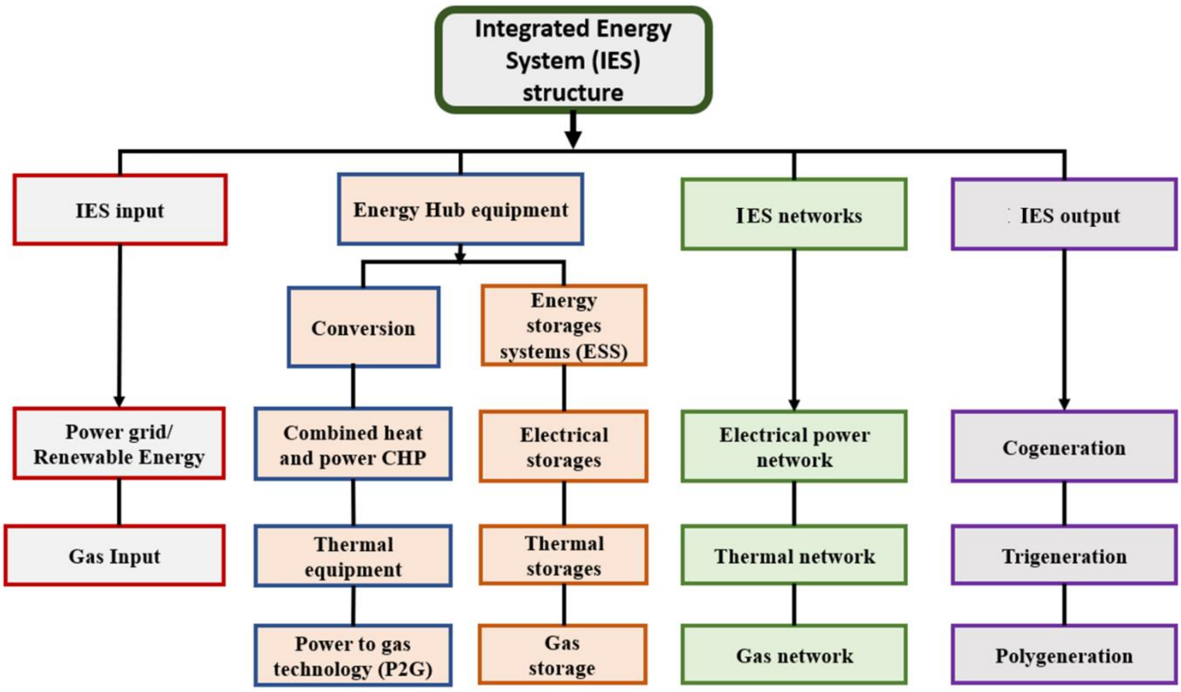

Fig 4. Integrated-energy system (IES) Structure

2.3.1 IES input structure

2.3.1.1 Electricity from Grid/ Renewable resources

IES is based on the first law of thermodynamics, which states that "energy can neither be created nor destroyed but transformed from one form to another." This principle makes IES dependent on some energy input. The electricity input to the IES is supplied from the grid or distributed renewable energy resources (DRES). The IES input port is connected to the grid distribution network via transformer and metering devices when power is imported from the grid. [65]. This procedure reduces computational stress during the planning of IES components. However, because DRES has been identified as a promising option for accomplishing GHG emission reduction targets, it has been prioritized as an electrical input in the IES configuration.

Previous studies on IES modelling have considered utility grid, renewable resources, or both as the electricity input. However, choosing between the three is based on the study's objective. For example, Ma, et al. [66] coupled the utility grid with renewable resources as the electricity input for IES when the power supply by the DRES is insufficient. The study also looked at the trade-off between grid-connected electricity and renewable energy resources. The findings showed decreased carbon penalty cost and operation cost due to renewable energy penetration. Also, Lu, et al. [67] combined municipal grid and photovoltaic as the electricity input for the

IES to increase the reliability of the input, while Cao, et al. [68] considered the photovoltaic system as the only electricity input in their model, to minimize carbon emission.

The previous studies show that the selection between utility grid or DRES depends on the predefined mode of operation of the system, which can be grid-connected or island mode. Furthermore, because renewable resources are inherently intermittent, stand-alone DRES are rarely used, which could result in a power supply mismatch. This overwhelming dependence on the utility grid in IES configuration generates two underlying questions: (1) Is IES contributing to the decarbonization of the electricity sector? (2) is IES a complete structure of the energy system as described? The typical approach in the literature is the minimization of carbon emission costs and the introduction of energy storage. Comodi, et al. [69] proposed an IES model for achieving low carbon energy communities, which involved introducing DRES, thermal storage, and district cooling. However, the model still depends on the municipal grid as part of the electricity input. A clear distinction between zero-carbon and low-carbon communities must be made in IES modeling at the planning stage to reach zero-carbon communities. This necessitates further research into making IES carbon-neutral while preserving a trade-off between investment costs., maintenance, and life cycle, which will contribute to the feasibility of achieving zero carbon communities.

2.3.1.2 Gas energy input

The distinct attribute of natural and hydrogen gas makes them the second source of energy input for IES. These gases can be converted to electricity, heat, or both by using appropriate conversion technologies at a specific temperature and pressure. Natural gas (NG) is a methane-based fossil fuel energy extracted from beneath the earth through a process called *fracking*. In contrast, Hydrogen gas (HG) is a fuel gas produced mostly using commercialized methods such as thermochemical, steam reforming, and electrolysis. [70].

NG and HG have been considered as energy gas inputs in several studies. The conversion technologies used in the energy hub usually determine the choice. For example, authors in [71-73] selected NG as their input to feed the gas turbine, while in [74-76], HG was chosen as input to meet the fuel cell demand. While HG has been identified as a clean energy source compared to NG, the latter still dominates. This is due to the high cost of hydrogen production and the additional equipment needed when using hydrogen in IES components. For instance, an electrolyser is required to split water into hydrogen and oxygen, which leads to an increment in the economic cost.

Selecting between NG and HG as an energy input requires careful analysis. According to the Energy Institute [77], methane leakages through the NG supply chain has contributed to 20% of global greenhouse gas (GHG) emissions. These environmental challenges associated with NG make HG a better alternative since it emits low carbon or zero-carbon emission if DRES is used in the electrolytic process. The benefits of HG over NG were evaluated by Ruming in [74], who concluded that the introduction of HG gas and its storage make IES a zero-carbon technology. On the other hand, the production of HG gas requires significant energy input. For example, water electrolysis requires 50-55kWh of electricity and nine (9) litres of water to produce 1kg of HG containing 33.33kWh of energy [82]. Its storage also requires high-pressure tanks of 350-700bar of ample space. Likewise, its high energy density of 120-140MJ/Kg makes it highly inflammable, posing a risk if installed in a densely populated area [78]. Therefore, in-depth analysis is required before choosing either NG or HG gas as input for IES.

2.3.2 Energy Hub equipment

IES consists of conversion and storage technologies. The conversion equipment converts the input energy, or the energy generated within the system, from one form to another, while storage equipment stores the energy for later use. This section describes the trends of conversion and storage technologies adopted in the literature for IES models.

2.3.2.1 Combined heat and power (CHP)

The research communities and the policymakers have identified the combined heat and power (CHP) plant as the prominent technology in achieving various energy policy programs. CHP refers to any equipment that produces heat and electricity simultaneously from one source of energy input, compared to other energy-generating equipment that losses part of its output as heat. CHP can recover waste heat supplied to meet the heat demand of the end-users, or it is used as an energy input for another conversion device. This distinct attribute increases the efficiency of CHP and results in primary energy consumption reduction of the system[48].

Gas turbine and fuel cell (FC) have been the most studied CHP. NG or biogas is used to power gas turbines, while most FC utilizes hydrogen. FC has high efficiency compared to other CHP, and its overall efficiency, including thermal, can be up to 90%. However, the high cost of investment and maintenance hinders its adoption in practice [79]. Different types of FC technologies have been developed in recent years. The materials used as electrolyte, operating temperatures, and efficiencies are the major parameters that differentiate them. The description of these technologies can be found in [80]. Proton Exchange Membrane PEMFC is the most adopted FC for IES due to its availability and its commercialization on a large scale. Authors in [81] considered reversible solid oxide fuel cell (RSOFC) in their model. This type of FC can function as a co-generation plant and electrolyser and eliminates the need for electrolyser in IES components. However, RSOFC is still at the research development level and is yet to be commercialized.

The selection and determination of CHP capacity have been previously studied based on the energy demand priority (electricity or heat), the overall efficiencies (thermal and electricity) and the dispatch factors. Authors in [76] considered the selection of CHP among various available technologies and the determination of its capacities. CHP can be made to generate cooling in addition to its default output. This involves the integration of CHP with other equipment such as absorption or electric chiller. By doing this, the CHP changes to combine cooling, power, and heat (CCHP) equipment, and several authors used this approach as described in refs [71, 73, 82-88]. In modelling CHP or CCHP, the modellers relied on the manufacturer's data as the parameters for modelling the equipment. For instance, the coefficient of performance (COP) and the efficiencies were used directly in [84, 87, 89]. This calls for consideration since the COP and efficiencies are given based on experimental data, which may vary during the actual operation of the systems. Moreover, the computation of system COP and efficiencies is based on some measured parameters described in [90], which are subject to uncertainties since they were measured under controlled conditions.

2.3.2.2 Heating equipment

Heat has been identified as the most significant end-use energy, and it accounts for about 50% of total energy consumption [91]. While half of it is utilized in the industrial sector, 48% is used in the building sector for space heating, water heating, and cooking. Various kind of heating equipment has been considered in the literature. Heat pumps have been considered a better choice due to high efficiencies than electric heaters and boilers. These pumps help minimise the operation and maintenance cost but with a high investment cost. The use of renewable energy heat has recently received great attention. For example, the total solar thermal capacity installed as of 2017 was $472GW_{th}$, which is expected to increase by 20% in 2023 [91], while geothermal installed capacity as of 2017 was 14GW [92]. The increase in these renewable heat technologies is attributed to the need for low carbon communities. Thus, various government policies encourage its development.

The most commonly used heat equipment includes a gas boiler (GB), electric heat pump, and electric boiler. Nonetheless, GB is the most considered heat equipment because GB has a lower investment cost than ground source heat pumps, which have a higher coefficient of performance (COP). Notably, the system COP, efficiency, equipment cost, operation and maintenance cost, and carbon emission rate are the main factors in determining the selection of heating equipment in IES research. These factors require careful analysis and are affected by the main objective of the IES modelling. For instance, GB will not be considered if the objective is to achieve a zero-carbon model since it utilizes NG. Thus, selecting heat equipment from their available categories requires careful analysis, contributing to optimal selection and capacity sizing.

2.3.2.3 Cooling equipment

In the cooling dominated region, the supply of cool air into room spaces is in high demand. Similar to heating, cooling equipment is required to convert an energy input from a source to a cooling load demand for various purposes. In IES modelling, the chiller plant is the most considered cooling equipment due to its application for large space cooling and industrial application. Vapour compressors and vapour absorption are the main categories of chiller plants in terms of their processes. For vapour compression chiller, electric power is used to drive the mechanical compressor to force the refrigerant within the system. On the other hand, an absorption chiller utilizes a thermal compressor which is driven by a thermal source to move the refrigerant through the condenser within the system. The thermal energy can be supplied by a direct fire burner, low or high pressure steam, hot water, or exhaust heat recovered from the CHP plant [93]. A direct relationship has been established between the thermal source's temperature and the absorption chiller's performance (AC). For instance, an AC supplied with hot water of 500^0F has a COP of 0.7 compared an AC fed with an exhaust fire of 330^0F with a COP of 1.38 [94].

Electric chiller (EC) is the most adopted cooling equipment due to its high COP. However, considering waste heat utiliZation, the authors in [95] used a double effect AC for optimal heat recovery from the reciprocating engine (RE). Also, the optimal capacity of the AC selected is larger than the EC in [66] due to the large capacity of CHP, which will produce more thermal energy. Thus, the consideration of AC as cooling equipment depends on the quality and quantity of thermal energy available.

The use of AC in IES modelling has its setback due to low COP compared to an EC [93]. Likewise, utilizing large space for installation is another major challenge compared to EC. Moreover, AC requires two energy sources, i.e., power and heat; thus, any fluctuation in the energy supply sources will lead to inefficiency of the system during operation. In terms of sustainability, AC uses refrigerants (water or ammonia) and absorbents (lithium bromide or ammonia) which are less hazardous to the environment. Furthermore, AC is noise-free equipment compared to EC, making them the ideal equipment when occupants' physiological comforts are considered during IES modelling. Hence, modelling additional constraints into capacity sizing and real-time operations are required to model the components.

2.3.2.4 Energy storage equipment

Energy storage systems (ESS) are integral components of IES models. The main function of ESS is to capture the energy produced when they are not needed or when excess energy is produced. This stored energy is later used in the required time or fed into a nearby energy network in exchange for incentives. Some of the benefits of ESS as part of IES components are increased system reliability, resilience, and performance[48], reduced operating costs of IES and capacity sizing of IES infrastructure.

In IES models, the common ESSs considered are electrical storage (ES), thermal storage (TES), and gas storage (GS). Previously, various ES technologies have been developed. These are electrochemical, mechanical energy, and chemical storage. A detailed review of these technologies is described in [96]. TES is used to store the output of cooling or heating equipment. The design of TES depends on the storage duration, which can be short-term storage (STS) or long-term storage (LTS). The STS is designed to meet the daily thermal fluctuation needs, while the LTS is designed for long term usages, such as weeks or months. The TES can also be coupled with a district thermal network for optimal management. A comprehensive review of TES design, evaluation, and coupling with the district network was carried out by Guepla and Verda in [97]. Also, the NG or HG produced by the electrolyzer within the system is stored in the GS. Various technologies available for GS are aquifer, depleted cavern, line-pack effect, and hydrated-based technology [98]. The selection of these materials for GS depends on the storage duration, which can also be short-term or long-term. As HG gas is characterized by high energy density compared to NG, unique materials are required for its compartment. Kojima [99] reviewed HG storage alloys, carbon materials, liquid hydride, and nano-composite materials application as hydrogen storage materials. These materials were evaluated based on their gravimetric and volumetric hydrogen densities. Kojima [99] concluded that ammonia is the most suitable material for hydrogen storage due to its high HG storage density.

For modelling ESS, the key features to consider are the capacity of the ESS unit, energy and power density, storage efficiency, and life span of the units. These features also affect the system's investment, operation, and maintenance costs. Thus, a balanced approach is required in the selection of ESS. For ES, electrochemical storage is the most adopted due to its matured technology and low installation cost. They are unaffected by geographical location compared to pumped hydro storage (PHS), which requires water for functionality. Mazzoni et al. [95] studied the comparison between various electrochemical storage equipment in IES models. The authors found out that Li-ion batteries are the best options for electrical storage due to their high round trip efficiency. TES has received enormous attention in the research community due to its lower cost than ES. The rate of GS penetration in IES is low since the adoption of FC and electrolyzer usually influences it as conversion technologies in the model. Also, since the price of NG is usually constant both at the peak demand and off-peak, as in the case of [76, 88, 100], the provision of NG storage will have no economic benefit to the system.

The design of these three ESS forms in IES models is based on the system's state of charge (SOC), charging and discharging efficiency, and capacity constraints. However, most studies neglect the effect of ambient temperature and the degradation effects of the ESS model, which affects the storage efficiency over time [101]. The energy storage ageing effect also influences the system's performance, especially when it is designed for long service life [102]. This degradation effect is also applicable to all IES components. However, it is more pronounced in ESS due to the rapid depletion of the systems caused by some chemical reactions, especially in electrochemical storage. This necessitates the creation of a precise energy storage ageing model, accurate self-discharge efficiency estimation, and determining the effect of ambient temperature in ESS modelling, particularly for IES with long service life. Furthermore, for large scale and remote areas, applied electrochemical storage may not be feasible due to the high investment cost and increase in maintenance and replacement costs. As a result, a large-scale analysis of various types of ESS in IES for remote places is required.

2.3.2.5 multi-energy system networks

IES networks serve as interconnectors among various components in IES models. The networks are the edges or arcs connecting nodes in terms of graph theory. Following this description, each piece of equipment in IES models denotes nodes while the connectors between them are arcs, and these connectors can either be electric cables or pipelines, as illustrated in Fig. 5. The IES networks can be classified based on the energy type and location within the systems. Generally, IES networks are based on the energy carrier type, i.e., electrical, thermal, and gas networks. IES networks can also be classified based on their location for detailed analysis. These are the input, components, and supply network. The input networks are the energy carrier from the energy source, e.g., power grid and gas grid, into the IES models. The component networks are categorized as the interconnectors within the system components, which may be of different configurations, while the supply networks serve as energy carriers from the IES to the end-users.

To model realistic and feasible IES components, the inclusion of IES networks is important, especially for district multi-energy systems where there is a high tendency for transmission losses [103]. For the analysis of electric networks in IES models, the approach usually adopted is the maintenance of voltage magnitude regulation, reactive power, and active power, especially when it involves electric buses connection. These are achieved by formulating electrical network constraints using either direct current (DC) or alternating current (AC) power flow model [103, 104]. Similarly, a hydraulic-thermal model approach modulates thermal, and gas networks to model nodal balance, head losses, and pressure drops. Details on this approach can be found in [101]. For effective energy management, smart devices are installed, which requires optimization. These were considered by Wag et al. [105] for active distribution networks in IES models. Some of the integrated smart devices considered are capacitor banks (CB), voltage regulators (VRs), and static var compensation (SVR).

Generally, most studies on IES energy networks focus more on optimal operation and scheduling dispatch. The coupling of the approach with the capacity planning of IES is rarely explored. Furthermore, the uncertainties associated with the energy network parameters are rarely considered, while the optimal sizing of the energy networks is another area that has not been incorporated into IES modelling.

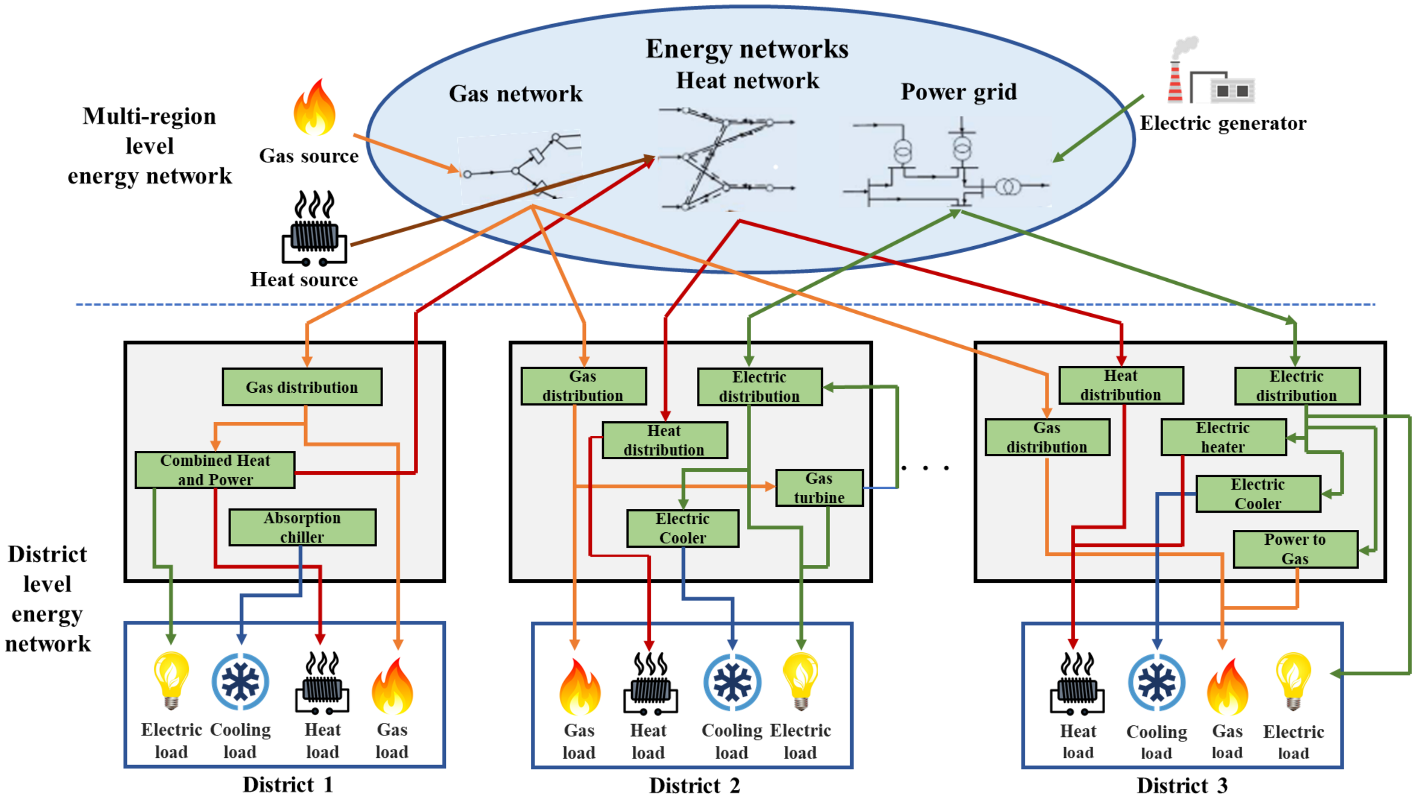

Fig 5. Integrated-energy system (IES) energy networks [7]

2.3.3 IES output structure

The output of IES depends on the energy demand of the end-users and the type of conversion technologies. These outputs are electricity, HG or NG, heat, cool air, water, and other demands. Most consumers' energy demand usually combines two or more energy vector outputs. For instance, a commercial building may demand electricity for electrical equipment, cooling of the indoor area, and a hydrogen station for fuelling the hydrogen vehicle. The terminologies adopted in describing the various combination of IES energy output are described below:

2.3.3.1 Cogeneration

Cogeneration is the production of two energy vectors simultaneously as the output of the generation system [106]. Though this terminology has been used for CHP equipment in situations where the outputs are electricity and heat, IES can be configured to produce different combinations of two energy vectors depending on the consumer's demand. For instance, an IES can be designed to generate electricity and cooling by introducing the electric chiller in the model, as illustrated in Fig. 6.

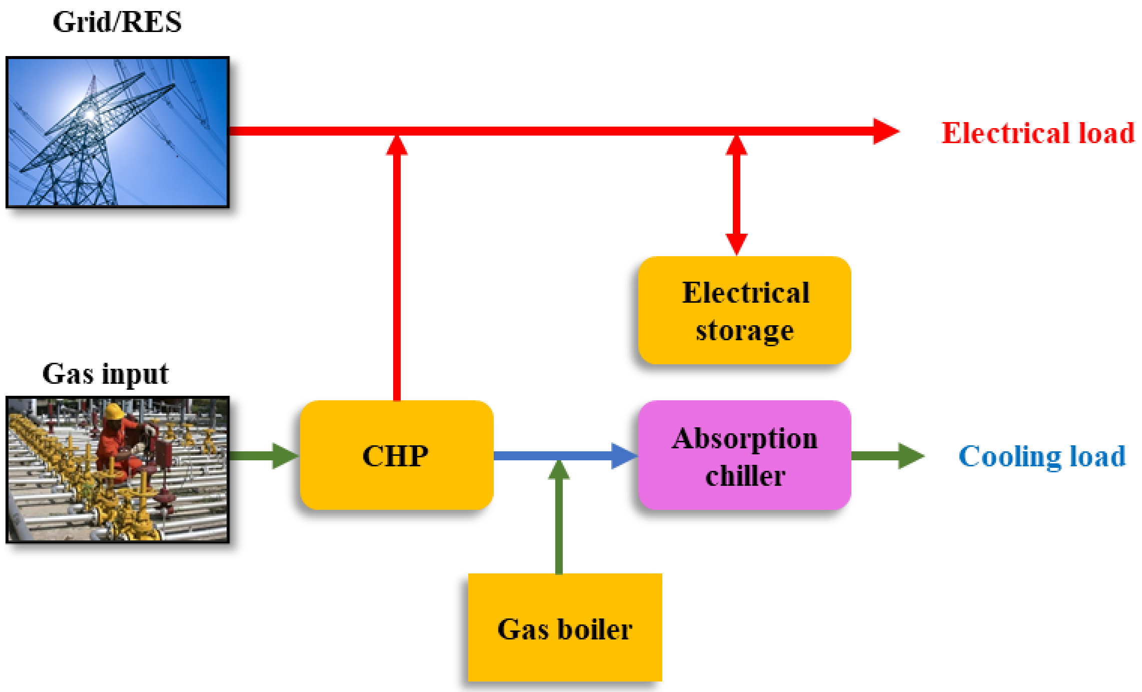

Fig 6. Cogeneration output

2.3.3.2 Trigeneration

Trigeneration is the production of three energy vectors simultaneously as output. The term is used with CCHP when electricity, heat, and cooling are produced simultaneously[66]. The system can also be configured to produce three different combinations of energy outputs, as described in Fig. 7.

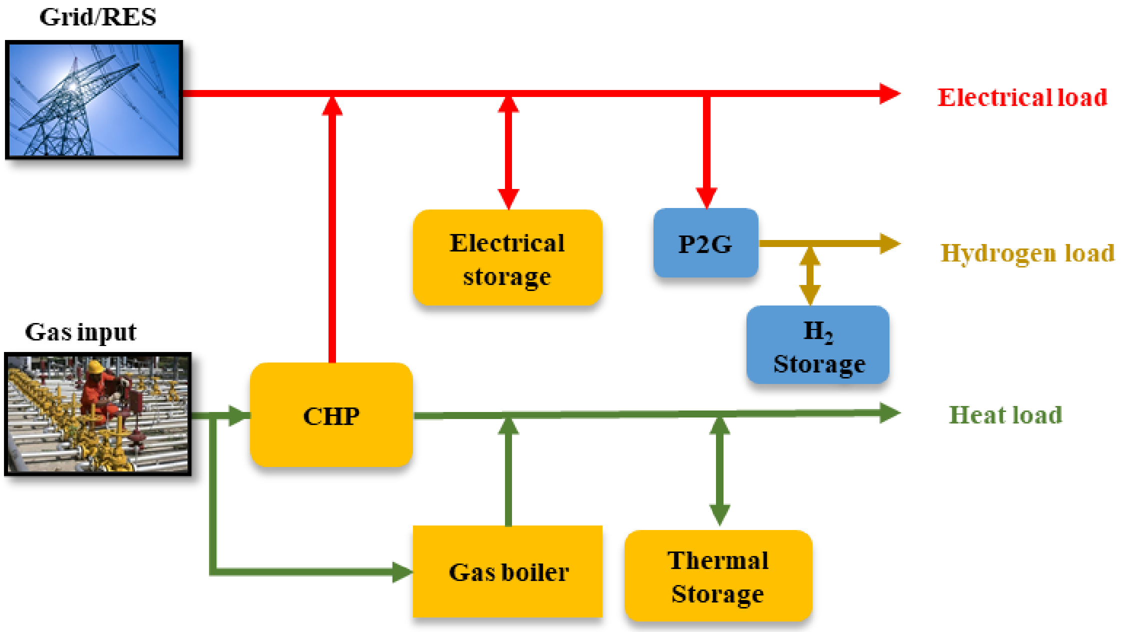

Fig 7. Trigeneration output

2.3.3.3 Polygeneration

IES is characterized as polygeneration when the energy output is more than three combinations simultaneously, as shown in Fig. 8. The concept of polygeneration originated from providing all energy-related demands of the consumer; this can involve the inclusion of electro-fuel generation or portable water production into the system[107]. In addition, the number of energy networks at the output of IES does not determine if the system is a polygeneration. For instance, a system with four (4) networks at the supply side, where two of the networks are electricity carriers, is not a polygeneration system.

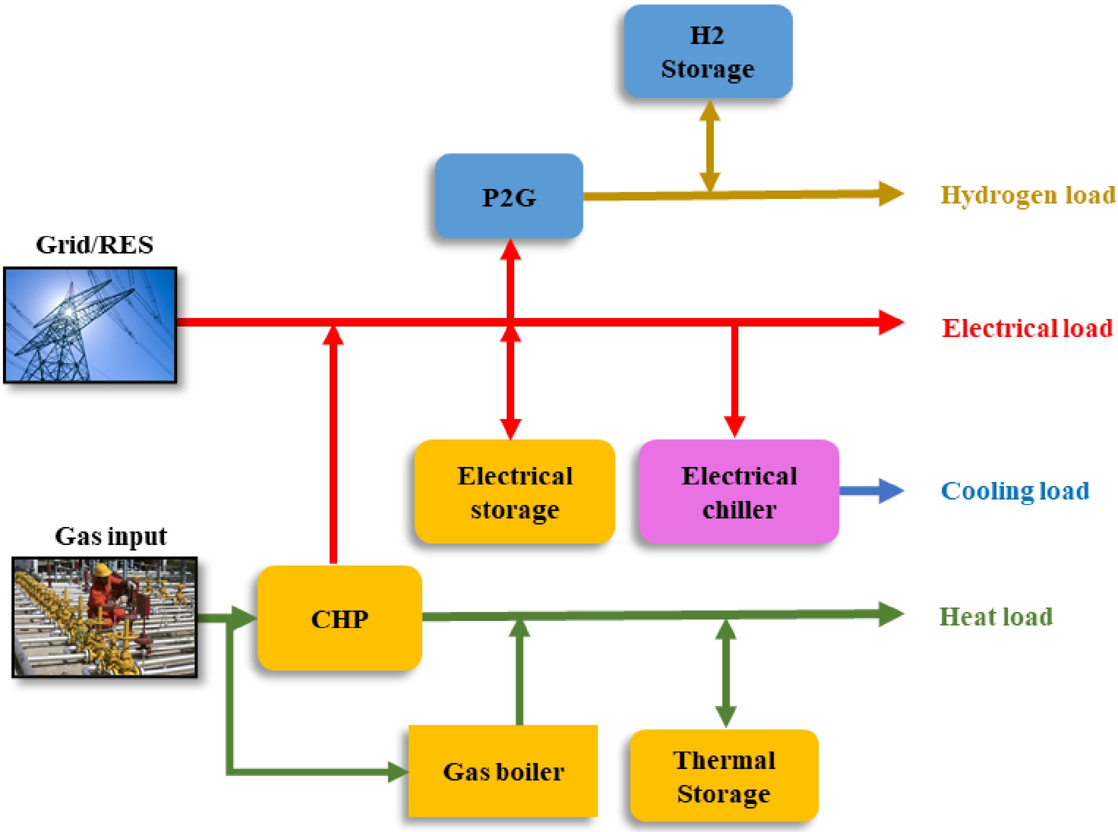

Fig 8. Polygeneration output

2.4 Modelling of IES

The modelling of IES involves the optimization of system components at the planning and operation stage. The optimal selection of available technologies, capacity sizing, and network configuration are the important factors at the planning stage, while the optimal regulation of IES dynamics behaviour is the primary consideration at the operation stage. Modelling at these two stages should be designed to be feasible and realistic while considering optimal primary energy, economics, and environmental conditions to ensure overall system stability and integrity. The modelling of IES can be classified into modelling approaches and modelling techniques, as illustrated in Fig. 9.

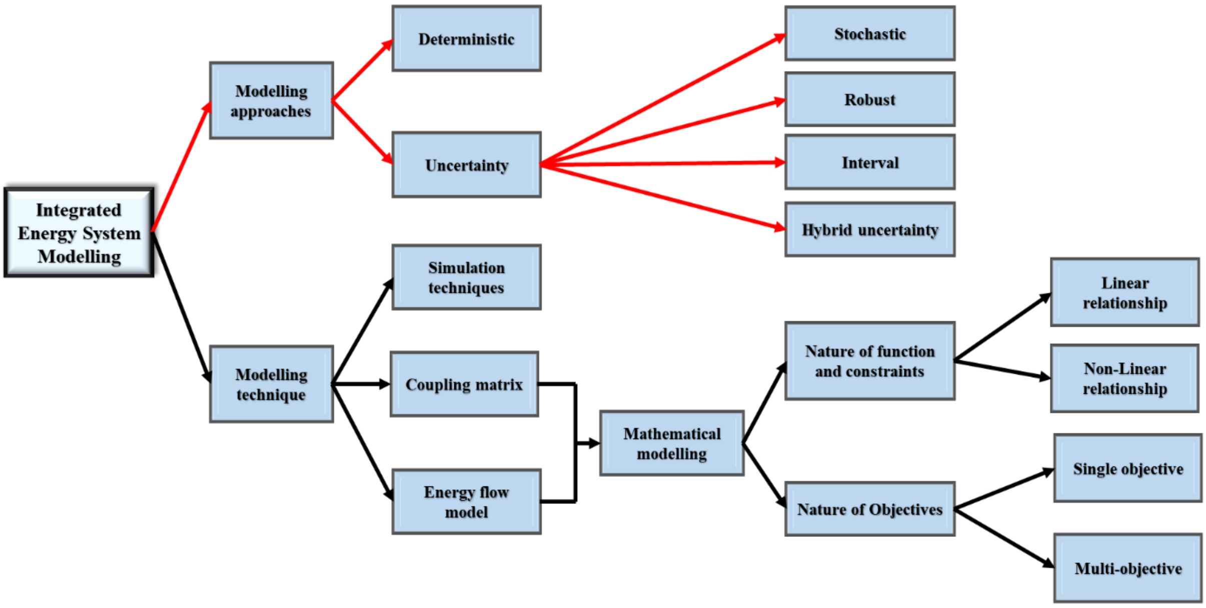

Fig 9. Integrated-energy system (IES) modelling structure

2.4.1 Modelling approach

IES requires information like energy demand data, equipment technical parameters, cost information of the available technologies, energy input data, climate data, energy price, and carbon emission details to model the system. The modelling approach is the process of considering how this information will be handled in the IES model. The most common approaches are:

- *Deterministic modelling*: This is a simplified approach with less computation time. It is based on the system's prior accurate and exact information during the modelling stage. Numerous research works have considered using this approach to prove the novelty of their techniques. Cheng et al. [108] used a deterministic approach to show the effect of thermal storage and heating network on IES performance. The study results show that the proposed method can reduce fuel costs and the capacity of the selected technologies. Also, a novel deterministic approach for modelling energy hub was proposed by Gotze et al. [109]. The authors argued that the proposed approach could simplify energy hub modelling. Furthermore, the authors in ref. [68] considered deterministic approach in modelling IES for low carbon community with electric vehicle integration (EV).
- *Uncertainty modelling*: The intermittency nature of renewable energy resources, fluctuation in energy price, non-static energy demand, and deviation from experimental

data of energy system during real-time operation have a major impact on IES behaviour. As a result, the deterministic approach is unsuitable for real-time applications. Compared to the deterministic approach, the complexity and computational time required to model a system under uncertainty will be higher, which has attracted many research efforts in recent times. The two main categories of uncertainty modelling approaches are *stochastic* and *robust* models. The stochastic model is based on developing a scenario tree by applying a probability distribution function (PDF) on known deterministic values to unveil the stochastic parameters. However, the main challenge is that the PDF may be difficult to obtain [110]. On the other hand, the robust model uses a min-max approach to explain uncertainty without using a probability function. However, the main challenge with a robust model is that it covers unlikely events that lead to conservativeness [36, 111]. Comprehensive details and comparisons between stochastic and robust optimization approaches can be found in [112].

2.4.2 Modelling techniques

The determination of IES components' optimal selection, sizing, and performance evaluation is carried out by simulation or optimization techniques. However, due to the limitation of the simulation approach in terms of optimal capacity selection and sizing, and the determination of optimal global solution [113], optimization modelling has been the main technique adopted. The optimization approach entails applying a mathematical technique to describe the complete system, which is then optimized holistically using the established objective function and constraints. In literature, modelling techniques adopted are the *coupling matrix* approach and *energy flow model*.

Geldl introduced the coupling matrix approach in 2007, and this approach involves multiple energy inflows into the energy hub model to generate multiple energy outflows in a steady state[109]. The energy hub is described as a coupling matrix representing the converter's efficiencies. The energy transition within the Energy Hub can be calculated and optimized with this concept for system planning and operation.

$$\underbrace{\begin{bmatrix} P_1 \\ P_2 \\ \vdots \\ P_g \end{bmatrix}}_{\mathbf{P}} = \underbrace{\begin{pmatrix} V_{11} & V_{21} & \cdots & V_{d1} \\ V_{12} & V_{22} & \cdots & V_{d2} \\ \vdots & \vdots & \vdots & \vdots \\ V_{1g} & V_{2g} & \cdots & V_{dg} \end{pmatrix}}_{\mathbf{V}} \times \underbrace{\begin{bmatrix} P^c{}_1 \\ P^c{}_2 \\ \vdots \\ P^c{}_d \end{bmatrix}}_{\mathbf{P^c}}$$

Fig 10. coupling matrix approach of IES[72]

Due to its simplification and effectiveness, numerous publications have adopted this approach. The authors in refs. [72, 100] used the coupling matrix approach to apply IES to responsive loads and demand response (DR) programs. The approach was also adopted in ref. [114] plug-in electric fuel cell vehicle. In addition to the systems, equipment constraints, energy balances, and variable system efficiencies are included in the model as performance constraints[109]. However, the coupling matrix approach has some limitations. It has a limited number of constraints, making it inappropriate for modelling realistic and feasible IES. Secondly, the energy storage is modelled outside the converter, leading to decreased IES performance [109].

3.0 Optimization techniques application in IES research

In a real-world application, strategically employed robust methods are vital in IES optimization whilst considering the nature of objectives (single or multi-objectives), variables, and constraints alongside technical and economic parameters of the chosen technologies. The objective function formulation depends on the objectives of the study, which can be planning optimization [111], operation optimization [115], or a combination of both. For instance, the optimization of overall investment cost applies to the planning stage while running cost and carbon emission optimization is for the operation stage [116]. Thus, this section explores the application of several optimization approaches in IES as it birthed intensified interest among researchers. Previous studies showed diverse modelling techniques developed for IES optimization, ranging from conventional to meta-heuristic methods. The conventional methods mainly include linear programming, mixed-integer linear programming, and nonlinear programming, while the meta-heuristic techniques are evolutionary techniques that mimic biology or evolutionary nature.

3.1 Conventional mathematical programming techniques

Generally, mathematical programming is an optimization method wherein the objective and constraints are sets of mathematical functions and functional relationships. The problem is formulated by describing the suitable objective function to be minimized or maximized, the application scenario constraints and decision variables bound. For IES research, the nature of the objective function may be single or multi-objective, while the constraints may be linear or non-linear. This optimization technique is, however, conventional and often referred to as *classical techniques*, which comprise linear programming (LP), mixed-integer linear programming (MILP), and mixed-integer nonlinear programming (MINLP) [117].

LP is a broad and vast decision-making tool wherein the objective is a linear function, the nature of the variables is linear, and the constraints on the decision problem have a linear relationship. Its result is achieved by finding the minimum or maximum value of the objective function [118]. A typical LP problem can be expressed in the standard matrix form [119]:

$$\min_{x} f_x^T$$

Such that:

$$\begin{cases} A.x \ \leq b \\ A_{eq}.x = \ b_{eq} \\ l_b \leq x \leq u_b \end{cases}$$

where, f, x, b, b_{eq}, l_b, u_b are vectors and A and A_{eq} are matrices.

As regards IES setting, researchers have applied LP models to propose hybrid off-grid energy systems [120], analyse characteristic regional energy systems with varying renewables [121, 122], optimize energy storage and hybrid power systems and capacities [123, 124], evaluate future energy-financial plans and incentive policies [125], improve energy schedule [126], and so forth. To achieve the model results, most objectives tend to minimize cost, maximize profit, address DR issues or meet energy demands, while some focus on integrating different objective functions such as import energy, export energy and storage as considered in [126]. Positively, LP has been a forthright optimization tool in IES applications since it is easy to code and allows for optimal scheduling. Nevertheless, it is limited to cases where linear functions can be used to describe the relations among the integrated systems.

In contrast to LP, MILP combines continuous and discrete mathematical modelling techniques used to detect likely trade-offs between competing objectives. It is also used to address intricate optimization problems [127]. It is usually applied in IES when describing binary decision variables, integers values, and continuous variables in an optimization problem. For instance, the ON and OFF status of energy equipment, selection, sizing, and location of energy infrastructure [128]. Authors in [129] optimized the total energy cost and system reliability of DES via a MILP model to provide an ideal integrated plan which reduced the total cost, CO_2 emissions and primary energy use. Omu et al. [130] applied the MILP model to analytically compare the economic and environmental effects between distributed energy resource systems (DERS) and centralised ones. The model reduced the annual cost and CO_2 emissions and provided an optimal design for DERS. MILP approach was used in [131] to transform the optimal scheduling model of an IES whilst considering unit commitment (UC) to coordinate the energy supply systems and energy storage operation. Similarly, the UC problems of hybrid power systems (HPS) were solved in [132] through an improved MILP approach based on hierarchical constraints to promote a higher efficiency of the HPS.

Generally, several computation complexities, chiefly those with large decision variables, have been tackled via the MILP approach, with cost minimization being the most common objective function. Thus, it assures global optimality and few iterations since its decision variables are constrained to be integer values. It is also effective for demand-side management due to its simple usage and platform support [23]. Nonetheless, the drawbacks of MILP include low execution time [14], risk of problem high dimensionality [12], non-feasibility for large scale integrations [25], among others. However, decomposition algorithms like Benders decomposition [133] and Dantwig-Wolfe algorithm [134] can be applied to enhance MILP, especially for large scale problems.

The MINLP is a versatile optimization method that integrates the MILP and NLP capabilities and applies it to objective functions and/or constraints having nonlinear problems alongside continuous and integer variables [135, 136]. This modelling approach often considers the feasibility, reliability, flexibility, and optimality of constraints in the design, sizing, and operation of IES. Previous methods introduced the MINLP solver in a generic algebraic modelling system (GAMS) software to find out the optimum operation strategies for CHP units [137], CCHP systems [138], polygeneration systems [139], energy storage systems [140], and energy hub [141]. It is worth mentioning that these MINLP solvers can operate in both convex and nonconvex regions. Meanwhile, in the absence of MINLP solvers, linearization and relaxation techniques are applied to reformulate the model before applying available commercial solvers [142].

3.2 Meta-heuristic methods

Due to the growing diversities and complexities in energy generation, conventional techniques are gradually fizzling out owing to their inability to deliver optimal solutions within finite time [143, 144]. Hence, *meta-heuristic algorithms* have been applied to tackle the challenges of continuous and nonlinear problems since they are quick and effective for obtaining the global optimum. Scientifically, these methods can be biology-based, physics-based, sociology-based and mathematics-based [145], as shown in Fig. 11. Meanwhile, genetic algorithm, particle swarm optimization, evolutionary algorithm and simulated annealing are the most implemented meta-heuristics for solving optimization and design problems in IES.

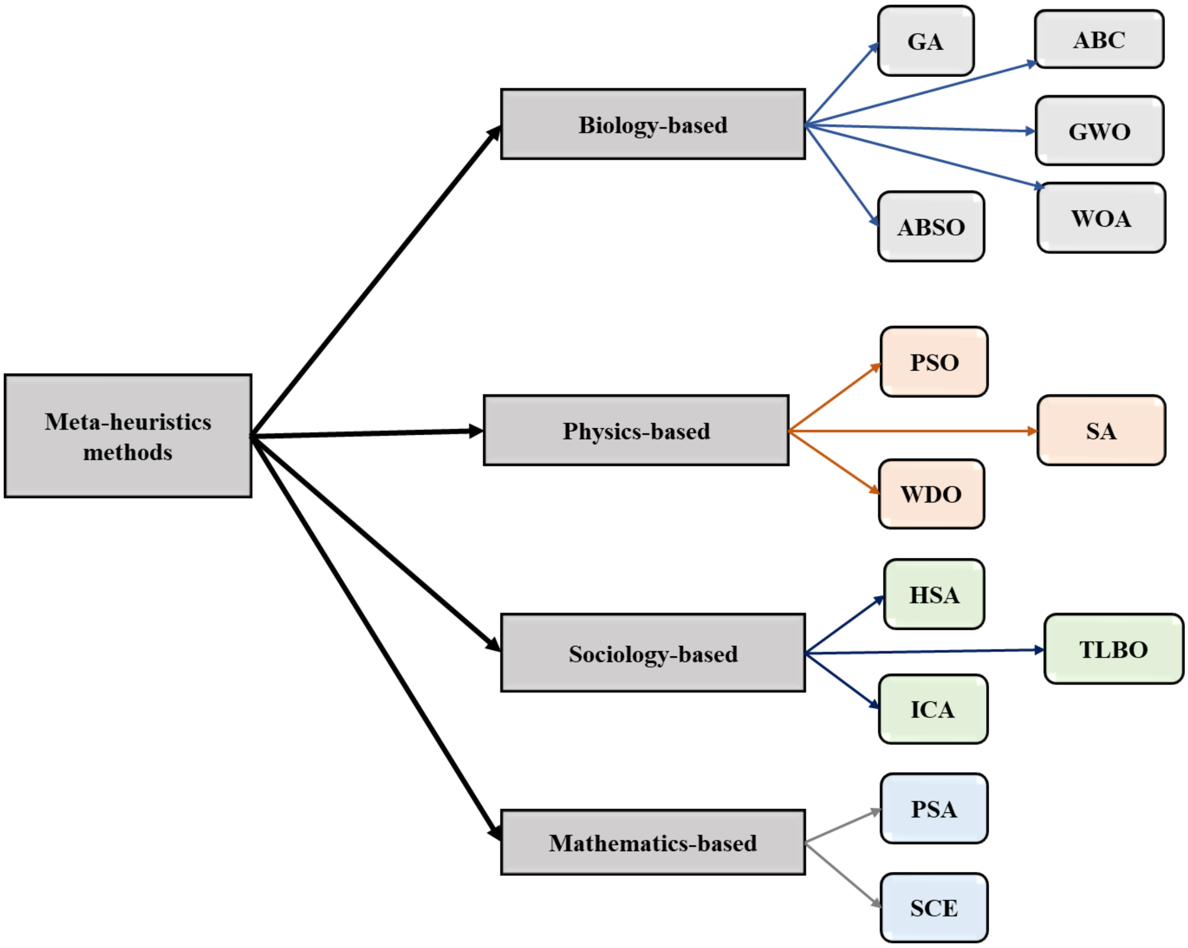

Fig 11. Meta-Heuristic methods**;** **GA**: Genetic algorithm; **ABC:** Artificial bee colony; **GWO:** Grey wolf optimization; **ABSO**: Artificial bee swarm optimization; **WOA**: Whale optimization algorithm; **PSO**: Particle swarm optimization; **SA**: Simulated annealing; **WDO**: Wind-driven optimization; **HSA**: Harmony search algorithm; **TLBO**: Teaching learning-based optimization; **ICA**: Imperialist competitive algorithm; **PSA**: Particle search algorithm; **SCE**: Shuffled complex evolution

4.0 Machine learning and Deep learning (MLDL) applications in IES research

ML is a computer algorithm that learns from previous data to predict future outcomes [146]. Overtime, ML has become one of the artificial intelligence (AI) techniques explored in the architecture, engineering and construction (AEC) industry [147]. Generally, the chief ML tool is an artificial neural network (ANN) [148]. Nonetheless, other ML tools like support vector machines (SVM) and Gaussian process regressors (GPR) have been used in building energy studies [149, 150]. Studies show that ML models have been used to predict building energy consumption [148]. ANN and clustering have proven to be alternative energy analysis tools for determining energy performance. [151, 152]. GPR has also been used in determining heat, ventilation and air conditioning (HVAC) loads [148]. A summary of some established ML models for building energy research is outlined in Figure 12, while further reading on these models can also be found in [153].

Furthermore, ML algorithms can identify objects in images, transcribe speech into text, match items with users' interests, and select useful search results. These applications use a class of techniques called deep learning (DL) [154]. DL is an ML concept based on ANN. The main distinction between ML and DL lies in the latter's ability to recognise images [155]. Also, unlike ML, DL consists of more than one hidden layer organised in a deeply nested network [155]. In a broad sense, the convolutional neural network (CNN) and recurrent neural network (RNN) are the major DL models. However, other DL models like deep belief networks (DBNs), autoencoders (AEs), and long short-term memory (LSTM) networks also exist [156]. Previously, DL has been used for estimating building energy use and photovoltaic (PV) power [146, 157, 158]. Also, DL has been implemented in solar, wind, biomass, and hydro energy research [159-161]. Figure 13 summarises DL models in renewable energy research, while further details on DL for solar and wind forecasting are provided in [162].

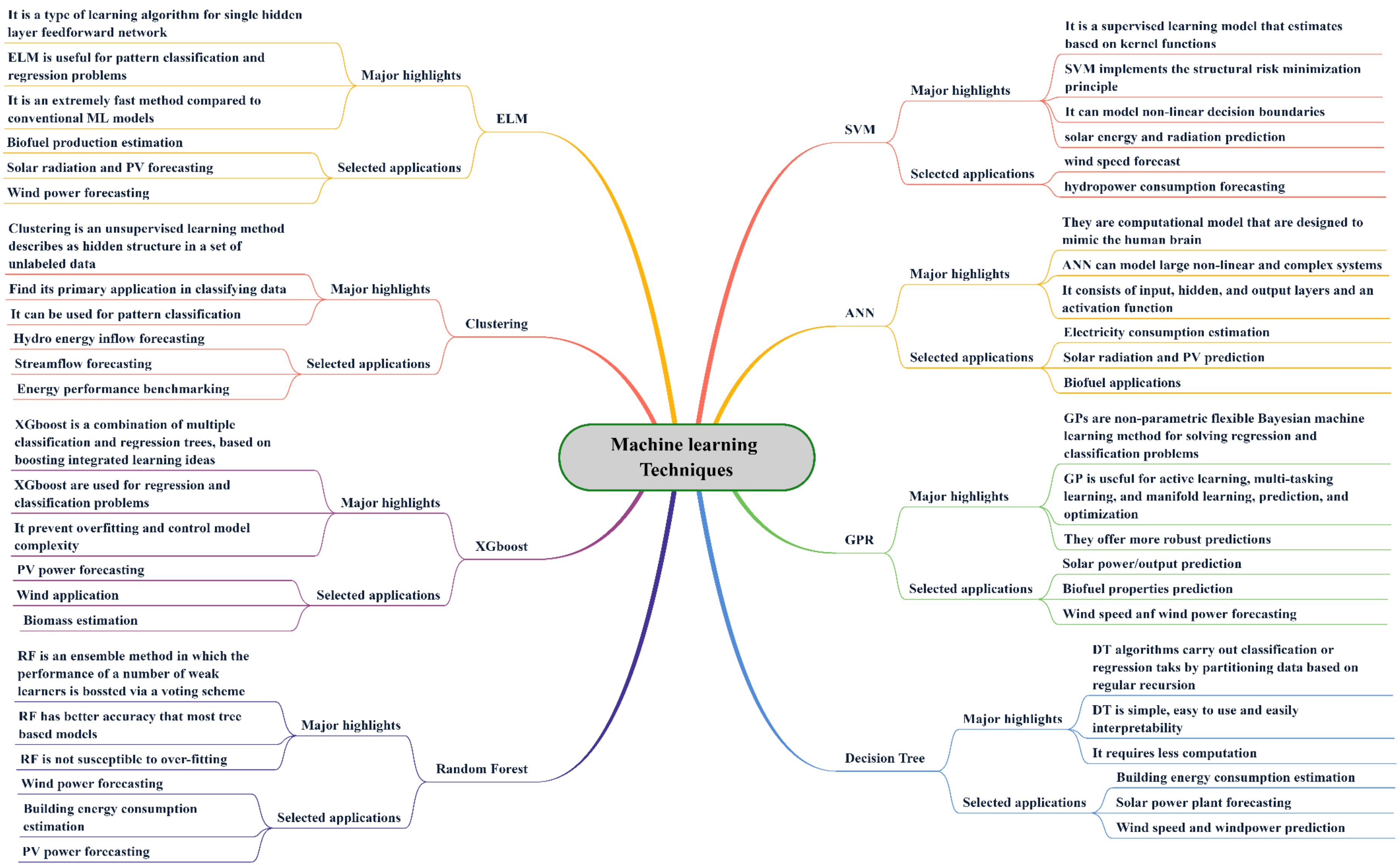

Fig. 12. ML models for renewable energy applications.

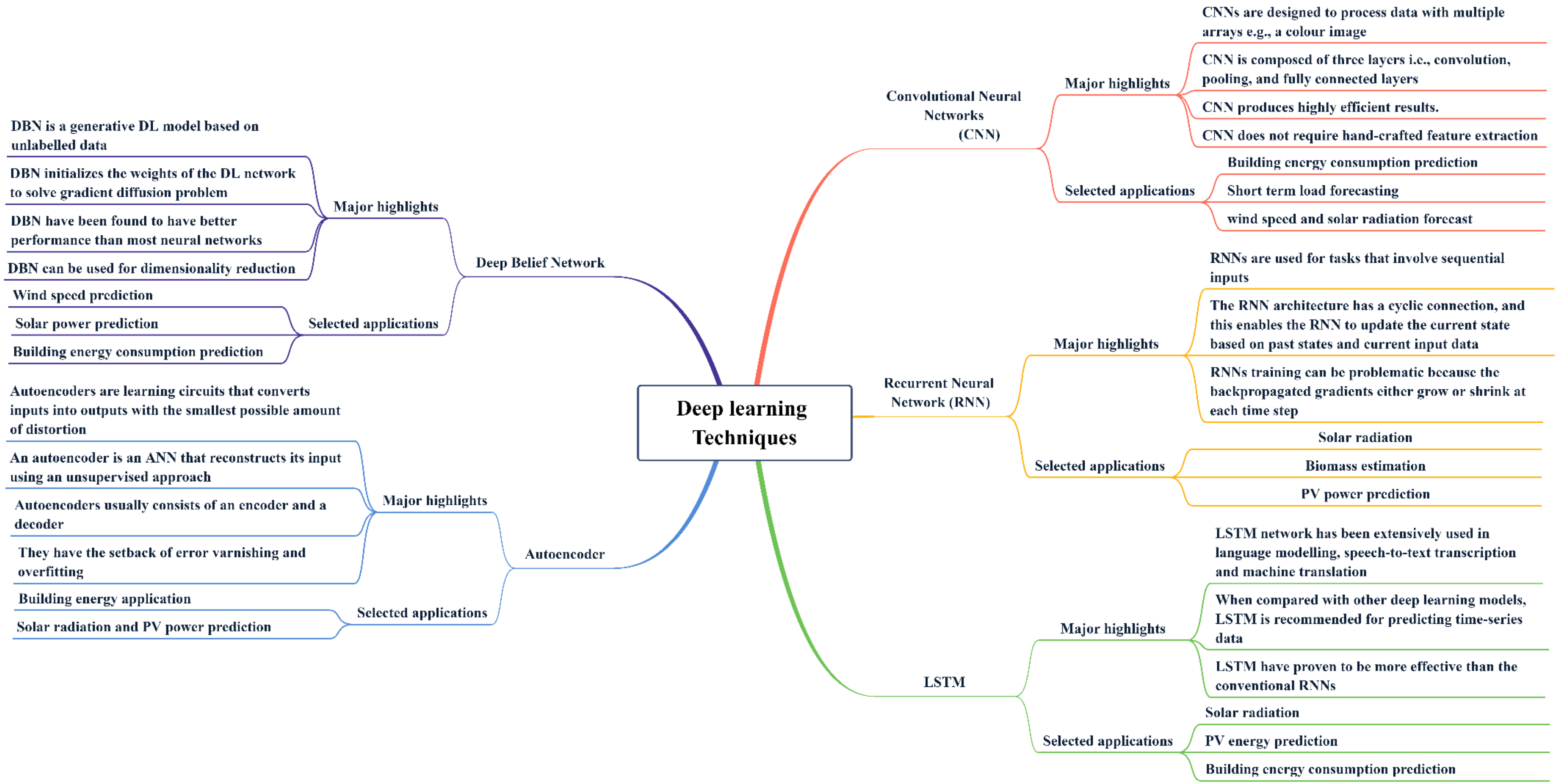

Fig. 13. Deep learning models for renewable energy application

Generally, a model's accuracy is known by determining its errors, and the smaller the error, the better its' performance [163]. Some of these metrics include the coefficient of determination (R^2), root mean square error (*RMSE*), mean bias error (*MBE*), mean absolute error (*MAE*), among others. A comprehensive review of statistical metrics can be found in Despotovic et al. [177].

Following the success of ML and DL (MLDL) models in building energy research, the remaining part of this section reviewed studies where MLDL have been applied in IES research. As a reminder, IES is made of multi-input and multi-output generation. Thus, we consider extant studies where MLDL have been applied for multi-energy demand prediction, multi-power generation prediction and multi renewable resources data prediction. The statistical accuracies of some of these extant models were also presented. Before a review of the relevant literature (i.e., Section 4.5 to 4.7), we briefly provide an overview of the ML models used in the identified IES studies;

4.1 Artificial neural networks (ANN)

ANN are computational models designed to mimic the human brain [164]. This model consists of input, hidden, and output layers and an activation function [165], and the data processing is performed within the hidden layer [166]. Commonly used ANN are feed-forward network multi-layer perceptron and radial basis function networks. Importantly, since DL models also stem from neural networks, other forms of ANN are CNN, LSTM and RNN, among others. While CNN is designed to process data with multiple arrays, RNN is used for tasks with sequential inputs [167]. Eqn. (1) shows the general mathematical expression of a neural network, while Figure 14 shows an overview of an ANN structure, RNN architecture, and CNN architecture.

$$\hat{y} = v_0 + \sum_{j=1}^{NH} v_j g(w_j^T x^i) \tag{1}$$

where x^i is the input vector x, w_j is the weight vector for jth hidden node, v_0, v_1, …, vNH are the weights for the output node and $\hat{y}$ is the network output. Also, the function g represents the hidden node output given in terms of a function.

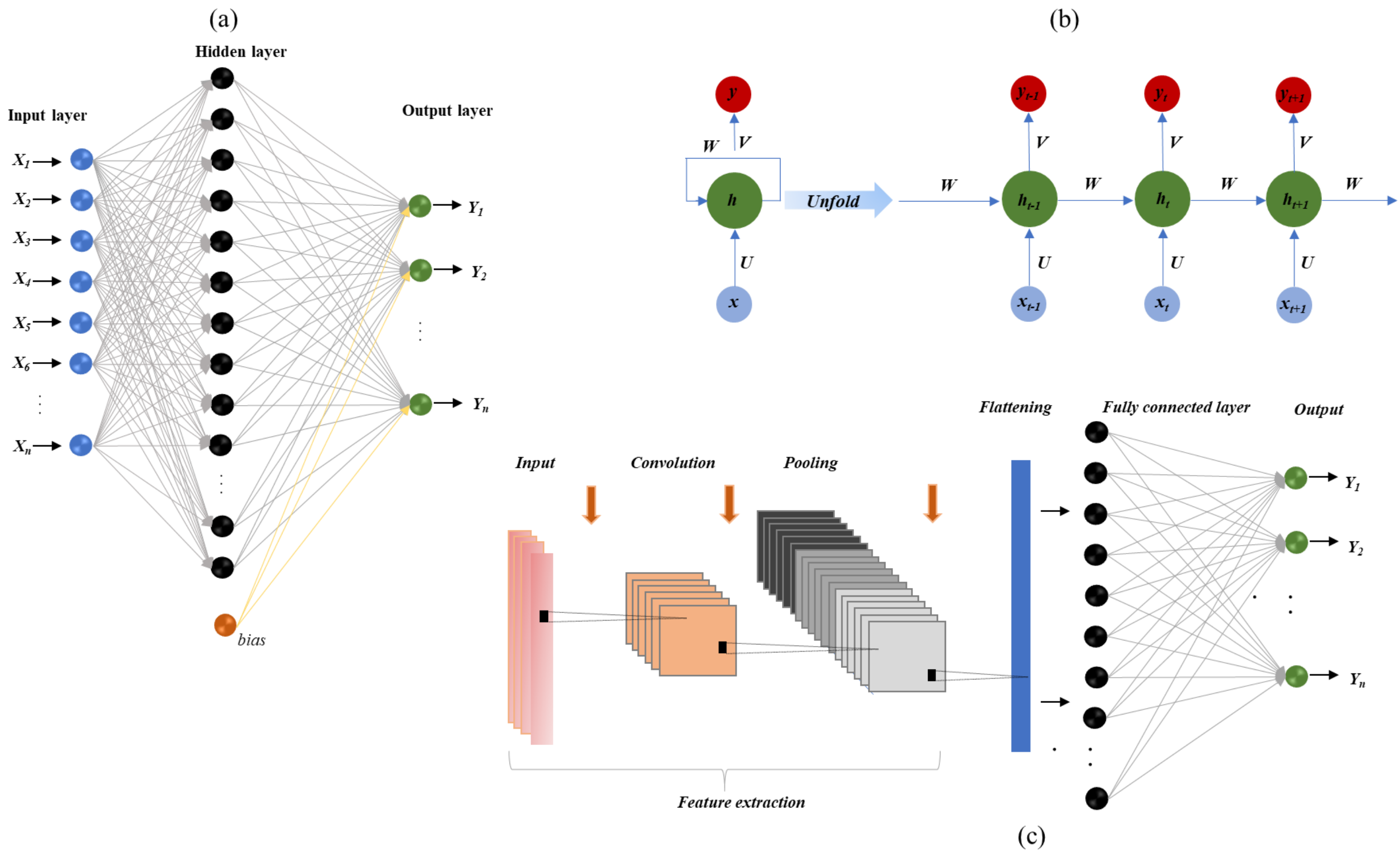

Fig 14. (a) artificial neural network (ANN); (b) Recurrent neural network (RNN); (c) Convolutional neural network (CNN)

Generally, ANN can model large, non-linear, and complex systems. They are fault-tolerant, robust, and immune to noise [165] and can be used to reduce data dimensionality (Bermejo et al., 2019). Similarly, DL networks like CNN and RNN produce highly efficient results during image and speech processing [168]. The drawback of using ANN is that large data is required, and determining the optimum number of hidden neurons can be challenging [169]. Additionally, the DL models can be computationally complex and prone to overfitting [170]. Some renewable applications of ANN are solar radiation forecasting [171], electricity consumption estimation [152], PV energy prediction [172], wind energy forecasting [173], hydraulic energy prediction [174] and biofuel applications [165, 175].

4.2 Support vector machines

The SVM algorithm was developed by Vapnik [176]. Figure 15 presents the structure of a SVM. For a regression problem, the support vector output (y_{svm}) is expressed as;

$$y_{svm} = w^T.\theta(\chi)+\text{b} \quad (2)$$

where *w* is the weight vector, *b* is the bias term, and $\Theta(\chi)$ represents the non-linear mapping function that maps δ into higher dimensional feature space.

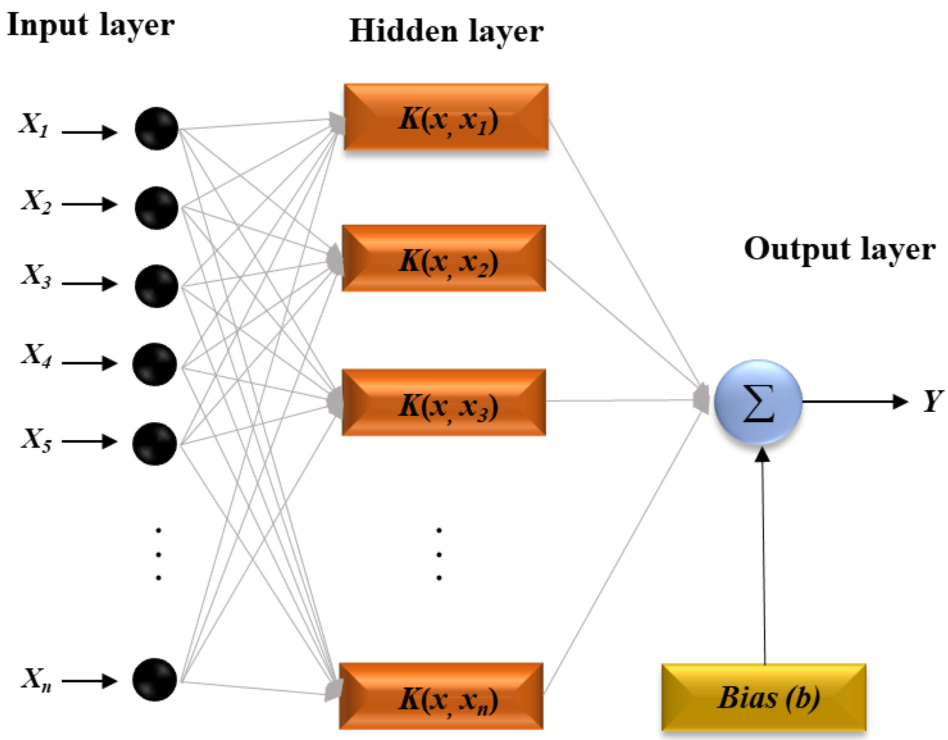

Fig 15. Support Vector Machine (SVM)

The SVM is a supervised ML model that estimates based on kernel functions. Different kernel functions form different SVMs, and this influences its prediction accuracy. The commonly used kernel functions are linear, polynomial, radial basis and sigmoid. However, the RBF expressed in Eqn. 3 is the most used in many applications [177].

$$K(x_i, x_j) = e^{\frac{-\|x_i - x_j\|^2}{2\sigma^2}} \quad (3)$$

where σ defines the width of the kernel.

For a support vector, the optimum result is derived when a hybrid approach is used [178]. Such hybrid SVM is derived using optimization algorithms like Bayesian optimization, grid search algorithm, firefly algorithm, genetic algorithm (GA), particle swarm optimization (PSO), among others. In general, SVM is generally implemented using the structural risk minimization principle [179]. It has less likelihood of overfitting, and local optimal solution can be easily obtained. SVM is robust and has high accuracy [166, 178]. Despite its advantages, SVM implementation requires much computational time and selecting the appropriate kernel can be challenging.

Furthermore, SVM has been applied in energy research involving solar radiation and energy prediction [167], wind speed and power estimation [180], biofuel classification [181], hydropower consumption forecasting [182] among others.

4.3 Random forest (RF)

RF was proposed by Breiman et al [183]. It is a tree ensemble method that simultaneously grows several decision trees (DT) to reduce the model's bias and variance [184]. Also, in RF, the performance of a number of weak learners is boosted via a voting scheme [185]. Bootstrap resampling, random feature selection, out-of-bag error estimation, and full-depth decision tree (DT) growing are the main features of RF [186]. Strictly speaking, RF has better accuracy than most tree-based models [187]. Also, it is invulnerable to over-fitting and has a high tolerance for noisy data [187]. Interestingly, RF is particularly useful in determining variable importance in a model [188]. Eqn (4) shows the mathematical expression of RF;

$$\hat{f}^{C}_{RF}(x) = \frac{1}{c}\sum_{i=1}^{C} T_i(x) \tag{4}$$

where x is the vectored input parameter, c is the number of trees, and $Ti(x)$ is a single regression tree based on a subset of inputs and the bootstrapped samples.

In renewable energy applications, RF has been used for wind power forecasting [189], building energy consumption estimation [190], solar radiation prediction [166], biofuel applications [191] among others. Figure 16 shows the structure of a typical RF.

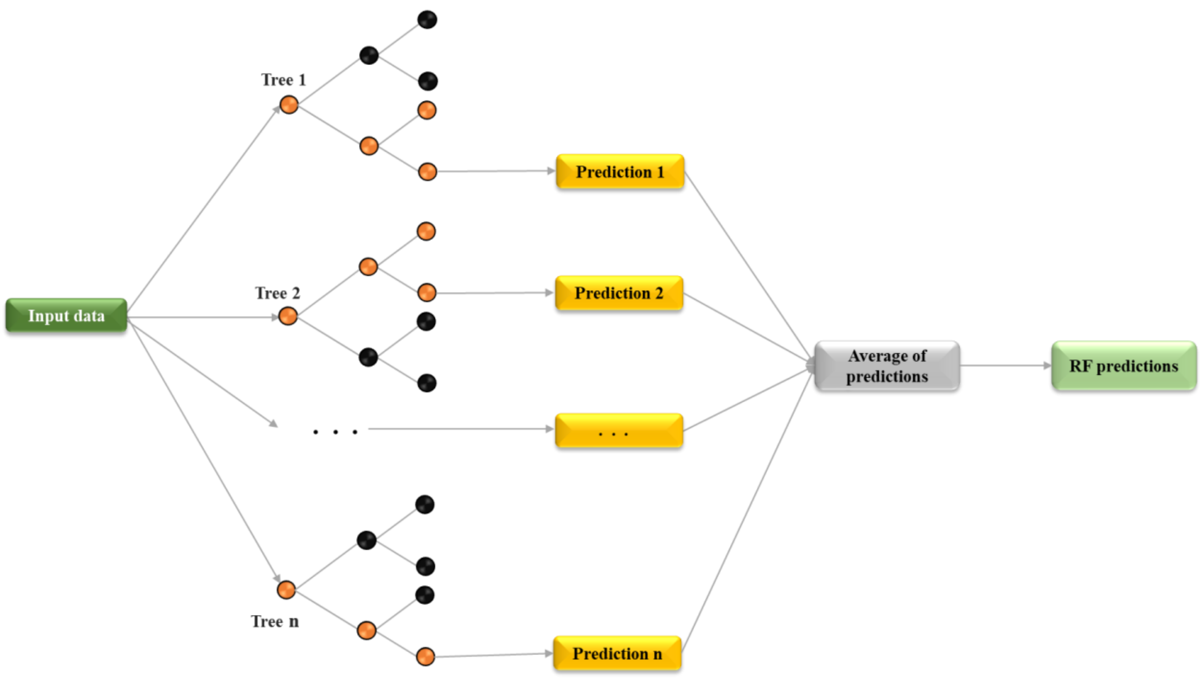

Fig 16. Random forest

4.4 Linear regression (LR)

Linear regression is one of the most often utilized mathematical methods in supervised ML. [192]. It is considered the easiest ML algorithm for data mining beginners because there is no requirement for parameter modification. [193]. LR investigates the linear relationship between a continuous dependent variable and one or more independent variables [194]. The mathematical expression of the most common LR is;

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \dots \beta_p x_{ip} + \varepsilon \tag{4}$$

where *i* represents n observations, y_i is the dependent variable, x_i is the independent variable, β_0 is the constant term, β_p is the slope coefficients of each independent variable, and ε is the error term.

However, other regression models can be found in Fahrmeir et al. [195]. Generally, LR requires fewer computing resources and offers a fast prediction speed [193]. It is simple and minimizes the amount of input data [196]. Nonetheless, LR models can barely meet high-precision prediction, especially for HVAC loads, influenced by non-linear and uncertain factors. Also, they cannot accurately predict weather-sensitive loads [193]. Despite its shortcomings, LR is useful in building energy performance load prediction, solar radiation forecasting [194], wind forecasting [195], and whatnot.

4.5 ML in multi renewable resources data prediction

One of the most important components of building energy studies is gathering data for renewable energy applications. Previously, Shboul *et al*. [197] used ANN to estimate global, direct and diffuse solar radiation alongside wind speed and direction in the Arabian Peninsula. The input variables were used for solar radiation, clock time, day, month, solar azimuth, solar altitude, and cloud identification quality. Likewise, clock time, day, month, air temperature, relative humidity, atmospheric pressure and precipitable water were input parameters for predicting wind speed. It was observed that the model could efficiently predict the output variables with correlation coefficient (*R)* values of over 0.96 and a mean absolute percentage error (*MAPE*) that does not exceed 3%. The study also concluded that the Levenberg–Marquardt (LM) ANN function gives a better prediction when compared with the predictions of the scaled conjugate gradient (SCG) ANN learning functions. Alhussein *et al*. [198] estimated short term global solar radiation and wind speed in the United States of America (USA) using a multi-headed convolutional neural network (MH-CNN). The MH-CNN was compared to the conventional smart persistent model. The study concluded that the MH-CNN outperformed the conventional ML models used for comparative analysis. In reality, the predicted wind and solar data RMSE were reduced by 44.94% and 7.68%, respectively. Also, [199] used the multilayer perceptron, generalized feedforward, radial basis function and RNN models to predict wind speed and six other meteorological variables. The other meteorological variables predicted were relative humidity, sunshine hours, evaporation, maximum, minimum and dew point temperature, while the input variables were latitude, longitude, solar altitude, months, temperature, relative humidity, sunshine duration maximum, and minimum pressures. The study deduced that the DL model (i.e., RNN) outperformed the other ML models. Bamisele *et al*.[200] predicted the global and diffuse component of solar radiation using an array of MLDL models in Nigeria. The precise models used were ANN, CNN, RNN, polynomial regression, SVM and random forest. The input data for the models were the year, month, day, hour, ambient temperature, wind, speed, and sun altitude. Apart from SVM, all MLDL models proved effective for predicting global and diffuse irradiance. However, the best performing model was RNN, and it had *R*, *RMSE* and *MAE* values of 0.954, 82.22W/m^2, and 36.52 W/m^2, respectively. Moreso, an ANN model for predicting the luminous efficacies of direct, diffuse and global radiation, was developed in [201, 202]. Luminous efficacies have been previously used to derive irradiance or illuminance data [176]. The input data used were direct transmittance, atmospheric pressure, solar zenith angle and diffuse fraction. Findings from the study showed that ANN can replace conventional empirical modelling techniques for modelling luminous efficacies. Also, the *RMSE* for the complex ANN was < 2% for each of the predicted luminous efficacies. A general finding from the reviewed studies shows that DL are better for predicting multi-energy demand data. Nonetheless, before using DL, careful consideration should be made since they can be computationally intensive [200].

4.6 ML in multi-energy demand prediction

The short-term and multi-energy prediction of energy loads is highly desirable for building energy management. [203] incorporated wavelength transforms (WT) with fixed and adaptive ML models such as MLP, radial basis functions (RBF), linear regression (LR), and generalised autoregressive conditional hetero-schedastic (GARCH) to forecast electricity demand and gas prices in the United Kingdom (UK). The proposed models used electricity demand and supply alongside gas prices as inputs. It was concluded that combining the WT and adaptive model improved forecasting accuracy. Moreover, the MF combined with adaptive MLP and GARCH proved to be the best model for predicting electricity demand and gas price forecast, and these had normalised *RMSEs* of 0.02314 and 0.15384, respectively. Zhu et al. [204] proposed a new hybrid neural network model made of LSTM and CNN to predict heating, gas, and electrical loads in combined cooling, heating, and power (CCHP) systems in Beijing, China. The model input data were environmental factors (i.e., moisture content, humidifying capacity, dry bulb temperature, and total radiation) and historical heating, gas, and electrical load values. These data were used to test and train the proposed model in a comparative analysis with backpropagation (BP) network, ARIMA, SVM, LSTM, and CNN models. The MAPE result showed that the BP network and SVM's performance is relatively poor compared to CNN and LSTM. Overall, in comparison with other models, CNN-LSTM has the highest forecasting accuracy. Precisely, the *%MAPE* of CNN-LSTM was 0.056, 0.055, and 0.082 for heating, gas, and electric load, respectively. In a recent and further study, Zhang *et al*. [157] proposed a hybrid multi-task learning model, which consisted of a CNN and a sequence-to-sequence model (CNN-Seq2Seq) to forecast short-time multi-energy load for Zhejiang, China. Electricity load, day type and meteorological variables were used as input, while the multi-energy load consisted of heating, cooling and electricity demand. According to the comparison findings with CNN-LSTM, CNN, and LSTM models, the proposed model had the best overall forecasting accuracy. The results confirmed the feasibility, efficiency, and superiority of CNN-Seq2Seq models in multi-output prediction. Zheng et al. [205] proposed a bi-directional gated recurrent unit multi-task neural network (BiGRU-MTL) to forecast multi-energy load in an

IES. The forecasting effect of the proposed model was verified using cooling, heating, and electricity loads, dry bulb temperature, relative humidity, charging of thermal energy storage and discharging of thermal energy storage data from the University of Texas at Austin. The advantage of the proposed model was probed against GRU, BiGRU,LSTM-RNN and DBN. Findings show the proposed model had the lowest *MAPE* (i.e., heating 3.253; cooling 1.744; electricity 1.420) and *RMSE* values for heating, cooling and electricity loads. It was also deduced that BiGRU has the second least errors as compared to other models. However, its accuracy is further increased by the addition of MTL, thereby reducing its *MAPE* for forecasting cooling, heating and electricity loads by 9.29%, 26.54% and 10.30%, respectively. Luo *et al*. [157] created single and multiple objective models to predict heating, cooling, lighting load, and BIPV power. The multi-objective models were based on ANN, SVM, and LSTM. The inputs were hourly weather data, building energy data and building operating schedules, while the study location was London, UK. A comparative analysis of the single and multi-objective models showed that although the *MAPE* of both multi-objective and single models were quite similar, the multi-objective model reduced the computational time by over 87%. It concluded that the multi-objective ANN model is the best when considering both prediction accuracy and computational time. In a bid to forecast the net load of the integrated local energy system, Zhou *et al*. [206] proposed a multi-energy forecasting framework using a deep belief network (DBN) with multi-energy coupling in China. The input parameters for the study were electrical, thermal, and gas loads. For performance comparison, the DBN model was compared with a DBN model without using multi-energy coupling. The result showed that DBN with multi-energy coupling reduced the *MAPE*, *RMSE*, and coefficient of variation of root-mean squared error (CV-RMSE) by 3.74%, 8.1% and 4.46%, respectively. Also, the model outperformed other MLDL models like BP neural network, autoregressive integrated moving average (ARIMA) and SVM. From the studies reviewed, it can be inferred that predictions of MLDL models can be improved when made into hybrid models. Furthermore, hybrid models can further be improved by adding boosters such Seq2Seq.

4.7 ML in multi-power generation prediction

Studies have shown that ML can be applied in multi-energy power generation of hybrid systems. Qadir *et al*. [207] enhanced the prediction accuracy of a hybrid PV- wind energy system using ANN. Weather parameters like solar irradiation, wind speed, ambient temperature, humidity, precipitation, atmospheric pressure, and wind direction were used for the analysis. Aside from using ANN for prediction, other ML algorithms were used for feature selection

(FS). FS exercises have been found to help improve the accuracy of ML models by removing redundant variables, and this agrees with Quadri *et al*. [207] findings. Specifically, the linear regressor was the best model for FS, and it gave a *MSE* of 0.0000001, *MAE* of 0.00083, R^2 of 99.6% and computational time of 0.02 seconds. Furthermore, Chandrasekaran [208] used ANN as a decision-making tool for a proposed hybrid renewable energy system composed of PV, battery and wind turbine. All components of the system were connected to an electrical grid with the aid of an inverter. The study concluded that ML algorithms could serve as an optimization tool for planning and designing power plants to meet energy demand and supply. Generally, just like the aforementioned applications of MLDL in multi-energy studies, MLDL is an emerging tool in multi-power generation leading to a scarcity of studies. Such scarcity is understandable since, more recently, Rahman *et al*. [209] recommended using ANN and other DL models in hybrid renewable energy forecasting. The recommendation by Rahman *et al*. also shows limited use of MLDL in IES studies.

5. Integrated machine learning and optimization approach in IES.

As described in the preceding section, ML has garnered strong research attention in the energy field, both in industrial application and academic research exploration. Specifically, ML is used as a data-driven model in energy-related research and application to predict future expectations in time series scenarios, regression analysis, or classification purposes. On the other hand, optimal capacity planning [210], unit commitment scheduling [211], energy network planning [212], operation scheduling [213], energy market trading [214], active and reactive power regularization [115] are solved by describing the problems using mathematical modelling formulations. The problem is formulated by describing the objective function to be minimized or maximized and the application scenario constraints and decision variables bound. Next, an appropriate commercial solver (GUROBI or CPLEX) or an improved solver is applied to obtain the optimal decision variables at the feasible region. Optimization techniques have been a versatile tool used by engineers and decision-makers for many decades. Compared to the simulation approach, an optimization formulation can achieve global optimal solution and provide flexibility in modelling uncertainty parameters randomness [113]. In contrast, the main drawback of optimization techniques is the computational period and the hardware requirement, which may affect the overall economic cost [8]. Generally, the computational period of the optimization algorithm is affected by the hardware properties of the computer, such as the RAM, processor speed, operation systems, and the number of cores [215]. In addition, the nature of the optimization problem also contributes to the number of iterations of the problem before converging. For instance, an integer problem (IP) is an NP-hard problem that is difficult to solve by most solvers [216]. In addition to the nature of the problem (either convex or non-convex), the linearity of the problem (linear or non-linear), number of constraints and number of decision variables [215] are other influencing factors. Hence, for real-time decision making that is dynamic and requires an ultra-fast response, the application of optimization techniques become a perplexing task. Whereas, with the availability and accessibility to enriched historical data, a data driven MLDL model that is suitable for rapid future forecast or output expectation can be developed using any of the suitable ML techniques illustrated in section 4.

Meanwhile, MLDL also have some shortcomings, which are 1) MLDL is a black-box model which is usually trained using the trial and error method by tuning the associated parameters until the desired result is achieved; hence, the global optimality cannot be guaranteed, 2) MLDL is only suitable for prediction or forecasting, not applicable for decision making or optimal planning, and 3) while the accuracy of MLDL is determined by achieving the lowest discrepancy, i.e., the error between the predicted and test data. During practical application, the accuracy may deviate from the observed value in real-time. Hence, considering the strength and weaknesses of these two approaches, few studies have considered their integration to complement each other. The following section describes works on the integration of ML and optimization techniques and extends the analysis to its application for IES.

5.1. Machine learning hyperparameter selection using optimization.

The accuracy and reliability of ML models are evaluated by achieving the lowest error. The value of these errors is affected by the ML hyperparameters such as the number of hidden layers, number of neurons, selected training algorithm, number of batches, etc. To ensure a global optimal solution, researchers have adopted the formulation of ML algorithm as an optimization problem. This is done by defining the selected evaluation metric as the objective function, formulation of the ML algorithm as constraints, and the definition of the hyperparameters as a decision variable. A typical example is a simplified ReLU optimization problem described in eq(5)-eq(9). Where the loss function to be minimised is *MSE* described in eq(5) for a feedforward neural network (NN). ReLU activation function is described as $y = \max(0, w^T x + b)$ where $x \in \mathbb{R}^n$ and $y \in [0, \infty)$ denote the input and output of a node, respectively, while $w^T x + b$ is the preactivation. Parameters $w \in \mathbb{R}^n$ and $b \in \mathbb{R}$ represents the weight and bias of the node, respectively. A big-M linearization method is introduced to properly encode the NN problem as a mixed-integer problem (MILP) where LB and UB denote the lower and upper bound of the output node to tight the formulation. This approach is adopted in [217-219]. However, the evolution algorithm (EA) has been the most applied for ML hyperparameters tuning [220]. A genetic algorithm (GA) was integrated with the ANN model to optimize the short-term photovoltaic power forecasting [221]. This was carried out by formulating the overall ANN as a mathematical problem. Then a GA was used as an optimizer to select an appropriate combination of ANN hyperparameters. Joaquim et al. [222] developed an integrated GA-ANN model for short-term electricity load forecasting using Portugal, New York, and Rio de Janeiro. The proposed method achieved an average percentage error lower than 2%. Particle Swarm Optimization (PSO) is another inspired nature global optimization algorithm applied as a hyperparameter tuning optimizer in [223]. PSO was used to optimize an integrated convolution neural network (CNN) and LSTM energy forecasting model. The proposed model achieved nearly perfect prediction and the lowest mean squared error. Wang et al.[224] further proposed an integrated optimizer of simulated annealing (SA) and PSO for the tuning of SVM hyperparameter in forecasting electricity load.

Remarkably, optimization techniques have been applied extensively to select the best hyperparameters combination and to achieve the global optimal loss function of ML model, especially for single load prediction. However, since IES multi-energy demand forecasting or renewable energy prediction require special attention due to the coupling relationship between the system, the application of optimization techniques to aid the selection of optimal hyperparameter settings has not been explored. Although, some studies have proposed some innovative approaches considering the correlation between multi-energy demand forecasting in the ML architecture. Another example is Xuan et al. [225] which considered the introduction of multi-task learning and homoscedastic uncertainty for multi-load energy prediction for regional IES. The proposed method outperformed CNN and conventional LSTM. However, the hyperparameter selection was based on the rule of thumb selection which may lead to a sub-optimal solution.

5.2 Uncertainty estimation and decision making

The intermittency of renewable resources and unpredicted demand fluctuation during real-time operation cannot be neglected during operation scheduling and planning of IES [111]. In fact, using the deterministic approach is an obsolete method for IES unless for model verification. In the literature, these uncertainties are mostly quantified using statistical methods. Then the output serves as input parameters for the formulated optimization problem [102]. Recently, few researchers have applied a generative adversarial network (GAN), and some novel MLDL approaches for uncertainty quantification in IES.

5.2.1 Generative adversarial network (GAN)

A generative adversarial network (GAN) is a promising DL architecture for data generation while considering the randomness of the data during real operation. The model has been mostly applied for image restoration and generation and numerical data scenes generation. It was introduced by Goodfellow et al. [226] in 2014. The model is made of a generative network (GN) and a discriminating network (DN). The main idea of the model is a game-theoretic approach within a deep learning context between GN and DN. The GN acts like a counterfeiter by generating samples similar to the original data using a random vector as input. On the other hand, the DN acts like a judge to determine if the data generated by GN is real or fake compared to the original data. The training continues until the GN can fool DN by generating data that cannot be identified by DN as fake. Then the trained GN can generate multiple data scenarios that can serve as input for other analyses. Figure 17 illustrates GAN architecture, while a comprehensive review of the GAN was conducted by Navidan et al. in [227]. Considering the advantage of GAN, the approach has been applied in energy-related research. Wang et al. [228] utilized the Wasserstein GAN approach for photovoltaic and wind power multi-scenario generation. A time-series GAN was proposed as a controller for smart control of microgrids in [229], while a realistic building electrical load profiles with uncertainties were generated through GAN by Zhang et al. in [229]. Similarly, the optimal operation of the hydro-wind-solar hybrid system in the short term was improved using GAN in [230]. The application of GAN has also been extended to IES in a few studies. Liao et al. [231] proposed an improved GAN for multi-energy load stochastic scenario generation. This was combined with an autoencoder-decoder to transform the load curves from high-dimensional to low-dimensional variables. GAN was developed as IES operating scenario generator in [232]. Similarly, Kong et al. [233] applied an improved WGN integrated with a gaussian process (GP) for the scenario generation of IES multi-load. Despite the uncertainty nature that GAN considers compared to other DL architecture, the approach has rarely been applied on time-series sequential prediction. Also, considering the limited number of studies that adopted GAN, its application on IES is still open for more studies

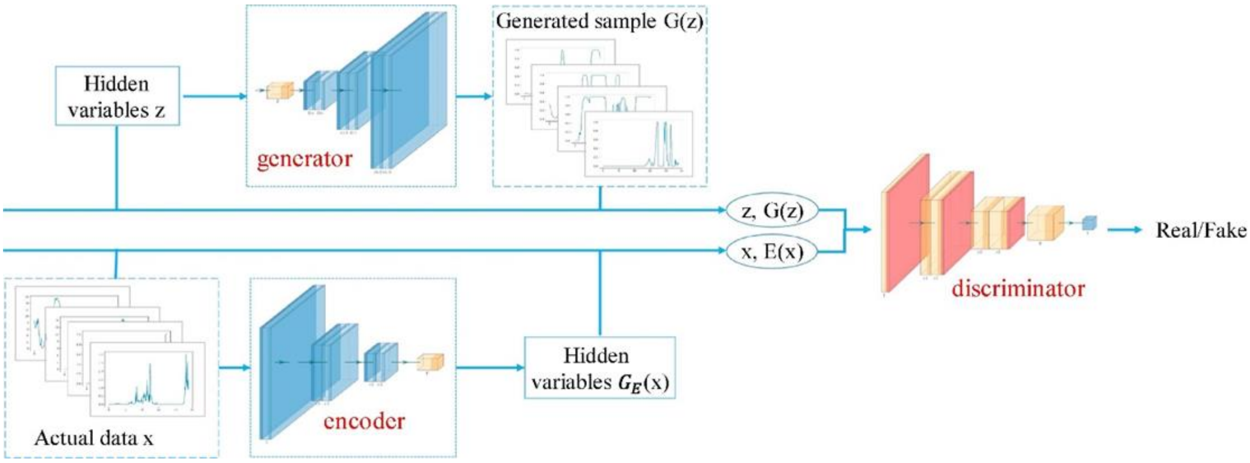

Fig 17. Generative adversarial Network architecture [230]

5.2.2 Integrated MLDL and statistical scene generation

Aside from using optimization as hyperparameter tuning, few studies have also considered the integration of ML and optimization techniques for uncertainties estimation instead of using statistical methods such as Monte-Carlo sampling [234], Latin-hypercube sampling [235], and non-parametric estimation. An example of such integration is the use of kernel density estimation during decision making. The approach has mostly been used for time-series forecasting of renewable power, electricity price, and energy demand. The methodology adopted for this process is illustrated in Fig. 18. As described, a historical model is used to build ML time series, forecasting models. The standard deviation (also the mean squared error) obtained by the model is then used for multiple scenario generation using the normal distribution function. The aim is that the error series have low autocorrelation with zero mean. Then the generated scenario is used to update the predicted values, followed by a scenario reduction approach. The advantage of this approach is that the algorithm considers the non-linear relationship and autocorrelation of the time series and variables compared to pure statistical methods. In addition, the introduction of stochastic sampling further increases the reliability of the time-series forecasting by lowering the deviation during real-time. Zeynali et al. [236] proposed ANN-stochastic based scenario generation model to generate a set of input for IES home energy management. The ANN was used for time-series forecasting, which is updated by stochastic scenario generation. Then the energy management was formulated as an optimization problem for the operation scheduling process. In [237], a first order autoregressive model is used for wind speed forecasting followed by multiple scenario generation by Monte-Carlo sampling, while the whole wind prediction scenarios is transformed by using aggregated power curve model.

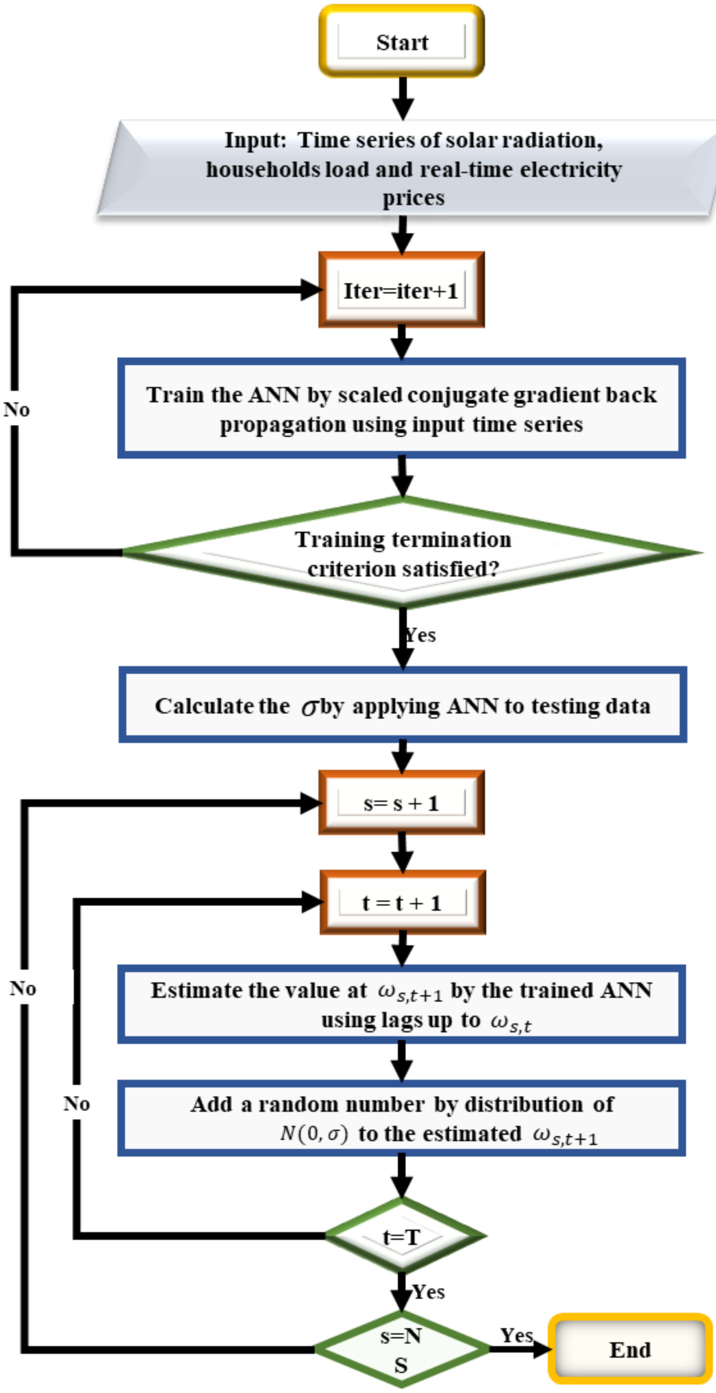

Fig. 18. Integrated ANN and Monte-Carlo Scene generation[236]

In summary, numerous studies have been conducted on integrating uncertainty estimation using statistical methods and optimal decision making. Hasan et al. [238] presented a comprehensive review on uncertainty modelling for power systems . However, most of the highlighted methods in their reviews are statistical approaches that neglect autocorrelation between variables and sequential influence. Furthermore, the few studies that considered integrated ML, stochastic, and optimization models for realistic forecasting and decision making focused on conventional time series models (ARIMA, autoregressive model) affected by gradient vanishing and explosion, especially for long-term series model [239], compared to LSTM. In addition, their model cannot be guaranteed to achieve a global optimal solution since the hyperparameters were selected based on trial and error. Notably, to the best of the authors' knowledge, the approach described in this section has rarely been applied to IES and considering its judicious advantage, the approach is worthy of exploration in IES research and implementation.

5.3. Prediction and optimal decision making

Considering the strength of ML for prediction and forecasting and the possibility of achieving global optimal decision-making on energy systems using a suitable optimization method, the integration of these two approaches becomes a viable mechanism for the optimal planning and operation of IES in the island or coupling mode. Without hesitation, numerous contributions have been made to improve MLDL models' accuracy and computational efficiency. Also, the utilization of optimization techniques in providing solutions to IES decision making has been well established. Nonetheless, only a few studies have considered the application of the integrated approach, especially for IES. Although an integrated predict and decide approach has been presented in [240], a typical innovative example was demonstrated in [241], where a combination of the autoregressive model and Cholesky decomposition was applied for prediction purposes. This was followed by optimal decision-making considering consumers' psychological preferences. However, ML, especially the DL techniques, supersedes the statistical approach for time-series prediction.

Taheri et al. [242] used a deep RNN for the long-term planning of IES. The DRNN, based on LSTM with three (3) layers, was proposed for heat and electricity demand prediction. While a co-optimization and operation planning was formulated as a MILP problem, the day-ahead energy prediction is fed into the step-by-step optimization problem that GPR facilitates. Interestingly, the proposed integrated deep learning and optimization algorithm predicted the energy demand and scheduled the energy hub (EH) for day-ahead operation with a less computational period. Kong et al. [233] applied GAN for multi-load generation. Then a two-stage robust stochastic optimization was proposed to solve the scheduling problem undertaken by a multi-energy virtual power plant (MEVPP). Alabi et al. [243] also applied an integrated approach of deep learning and optimization methods for the optimal prediction and scheduling of IES. Notably, throughout our literature consultation, we observed that the application of integrated ML and OP for prediction and optimal decision making on IES is still at its infant stage, which indicates a huge research gap that requires further exploration.

6. Conclusion and future research trends

In this section, we presented the summary of our review under each concept for clarification purposes, and the possible future research directions were identified.

6.1 Review summary

IES has been identified as the substantial approach to achieving deep decarbonization of the energy sector and the right strategy toward carbon neutrality. Thus, a comprehensive review spanning its energy components, structure, its modelling approach, and the application of optimization and MLDL are presented in this study. The review summary is presented below:

1) IES structure is categorised into energy input, energy hub equipment which comprises conversion technologies, storage technologies and IES networks. The last part is the IES output structure that is subdivided into cogeneration, trigeneration, and polygeneration. Specifically, the contributions of various studies on each IES structure were identified, and the main submission is that the structure depends on the available technologies, the prosumers or consumers' multi-energy demand patterns, the available renewable resources, and the objective of the planner, either to minimize carbon emission or to achieve zero-emission.
2) In this study, the IES modelling is also classified into the modelling approach and modelling techniques. The modelling approach is the first level when deciding either to consider the uncertainty or fluctuation associated with IES parameters or deterministic. Simulation techniques and optimization are categorised under the modelling techniques. The optimization technique is the most adopted technique due to its flexibility and ability to achieve global optimal decisions compared to simulation. The optimization technique is classified into conventional mathematical and meta-heuristics methods, while a succinct description of their applications was also described.
3) The application of ML and DL in IES research was also presented in this study. The MLDL applications were reviewed under three categories: multi-power generation prediction, multi-energy demand prediction, and multi-renewable resources prediction. The submission was that despite the popularity of MLDL, its application on IES has not been fully explored, and there is no verified universal framework for executing the task.

4) The final part of the review was the application of integrated optimization techniques and ML approach in IES. This part was reviewed under three subheadings i.e., ML hyperparameter selection using optimization, uncertainty estimation and decision making, and prediction and optimization decision making on IES using the integrated approach.

6.2 future research trend

In respect to the review presented, some noticeable areas for possible future research exploration are summarized below:

1) A framework that will enable in-depth analysis of IES structure, components selection and configuration is worthy of development, as this will clearly illustrate the pros and cons of the approach in terms of feasibility, economic implication, environmental impact, and the suitability of the approach in terms of carbon neutrality target.
2) Numerous modelling techniques with the consideration of uncertainties influence have been proposed in the literature. However, a robust model that considers the uncertainties associated with IES energy network parameters, consideration of IES degradation (especially storage technologies, real-time COP and efficiency of the equipment instead of constant parameter), and the consideration of flexibility potentials will create a pathway towards the feasibility of carbon neutrality.
3) Generally, MLDL has not been extensively applied in IES and the few studies that have implemented it either for multi-renewable resources or multi-energy prediction only select the hyperparameters using a trial and error approach. Thus, extensive research on the suitable MLDL for IES time-series forecasting is still required.
4) Despite the benefits of synergizing optimization and MLDL in IES research, the application is still at the infant stage. Thus, a universal approach for the integrated optimization and MLDL while considering the correlation among IES variables, uncertainty influence on the predicted variables, the optimality of overall process, especially in terms of convergence speed and optimal decision making, is a promising future direction.

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