



AI-based prediction and optimization of energy and exergy efficiency in thermal systems

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Abstract

The integration of artificial intelligence (AI) with thermodynamic analysis is rapidly transforming the design, operation, and sustainability of modern thermal systems. This review provides a comprehensive synthesis of AI-based prediction and optimization strategies for improving energy and exergy efficiency across diverse thermal technologies, including heat exchangers, boilers, power cycles, industrial heating systems, and solar-assisted configurations. This review establishes a thermodynamically grounded perspective in which exergy is positioned not only as a diagnostic indicator but also as a structural constraint that enhances the physical credibility of AI-driven optimization. A coherent methodological framework is presented that links data acquisition, feature engineering, target definition, model development, and uncertainty treatment within multi-objective optimization environments. Comparative analysis reveals a clear transition from purely data-driven forecasting toward hybrid physics–AI models capable of maintaining conservation laws while enabling high-dimensional design exploration. Despite substantial progress, the literature exposes persistent challenges, including fragmented evaluation metrics, limited cross-domain integration, insufficient uncertainty quantification, and the absence of standardized modeling protocols. Future research is expected to prioritize interoperable data ecosystems, physics-aware learning architectures, life-cycle-oriented optimization, and system-level intelligence. These developments indicate that AI can become a critical enabler of adaptive, resilient, and low-carbon thermal energy infrastructures when supported by high-quality datasets, thermodynamic constraints, transparent validation, and uncertainty-aware evaluation.

Keywords Artificial intelligence · Energy efficiency · Exergy analysis · Thermal systems · Multi-objective optimization · Machine learning

Abbreviations

3E	Energy–exergy–economic analysis
4E	Energy–exergy–economic–environmental analysis
AGENN	Artificial neural network integrated with genetic algorithm
AI	Artificial intelligence
ANN(s)	Artificial neural network(s)
CART	Classification and regression tree
CatBoost	Categorical boosting algorithm
CCPP	Combined cycle power plant
CFD	Computational fluid dynamics
COP	Coefficient of performance
CSO	Chicken swarm optimization
DEM	Discrete element method
DL	Deep learning
ET/extra trees	Extremely randomized trees algorithm
GA	Genetic algorithm
GBM	Gradient boosting machine

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HHV	Higher heating value
HVAC	Heating, ventilation, and air-conditioning
HX	Heat exchanger
LCA	Life-cycle assessment
LCC	Life-cycle cost
LHV	Lower heating value
LSTM	Long short-term memory network
MAE	Mean absolute error
MAPE	Mean absolute percentage error
MFO	Moth flame optimization
Metrics	Statistical indicators used to evaluate predictive model performance
ML	Machine learning
MLR	Multiple linear regression
MOO	Multi-objective optimization
MSE	Mean squared error
OFC	Organic flash cycle
ORC	Organic Rankine cycle
PCM	Phase change material
PEM	Proton-exchange membrane
PDE	Partial differential equation
PINNs	Physics-informed neural networks
PV–WT	Photovoltaic–wind turbine hybrid system
PVT	Photovoltaic–thermal system
R^2	Coefficient of determination
RF	Random forest
RMSE	Root mean square error
SA	Sensitivity analysis
SCR	Selective catalytic reduction
SVM	Support vector machine
SWHS	Solar water heating systems
TE	Techno-economic analysis
TES	Thermal energy storage
UQ	Uncertainty quantification
WOA	Whale optimization algorithm

Introduction

Thermal systems are integral to modern energy infrastructure, encompassing applications such as power generation, industrial processing, heating, cooling, and transportation. Traditionally, the performance of these systems has been evaluated using first- and second-law thermodynamic principles. Beyond engineering evaluation, thermodynamic concepts have also been used to examine how energy emerges through spatial and material relations [41]. While energy analysis, based on the first law, accounts for energy conservation, it does not distinguish between different qualities of energy. Exergy analysis complements this by assessing the maximum useful work obtainable, thereby providing insights into irreversibilities and thermodynamic losses [45]. The increasing complexity of energy systems, especially with the

integration of renewable energy sources, energy storage, and low-carbon technologies, necessitates comprehensive evaluation frameworks. Recent studies highlight the importance of combining energy and exergy analyses with economic and environmental considerations to support sustainable design and operation of thermal systems [69, 151]. In parallel, the growing deployment of hybrid energy storage, microgrids, and coordinated demand-side management further reinforces the need for system-level efficiency assessment beyond conventional energy balances [24, 64, 93, 101, 154].

The advent of advanced sensors, simulation tools, and data acquisition systems has opened avenues for data-driven modeling in thermal engineering. Machine learning (ML) and deep learning (DL) techniques have emerged as powerful tools for predicting performance, detecting faults, and optimizing designs in systems like organic Rankine cycles (ORC), heat exchangers, and HVAC systems [151]. AI models can capture complex, nonlinear relationships between system parameters and performance metrics, facilitating the analysis of systems with intricate interdependencies. This capability is particularly valuable in thermal systems where multi-parameter coupling and uncertainties are prevalent. Moreover, AI is increasingly being integrated into decision support frameworks that combine diagnostics, optimization, and operational intelligence. Such integration increasingly extends to energy management and storage coordination problems in hybrid microgrids, electrified transport, and urban power systems [24, 93, 154]. Such integration enhances the interpretability, sustainability, and robustness of thermal systems, aligning with decarbonization goals. However, the application of AI introduces challenges, including the risk of generating non-physical predictions if models are not constrained by thermodynamic principles. To address this, hybrid approaches that embed physical laws into AI models are being developed. Furthermore, optimizing thermal systems often involves balancing multiple objectives, such as energy efficiency, exergy performance, cost, and environmental impact. Outside thermal engineering, Huynh et al. [75] developed a structure-preserving hybrid physics–AI framework for hydrological-flux correction and regional flood modelling. AI facilitates multi-objective optimization by efficiently navigating complex design spaces. This capability is evident in recent studies on energy storage centrifugal pumps [43], coordinated hybrid wind storage systems [101], and compressed carbon dioxide energy storage integrated with coal-fired power plants [69]. Despite these advancements, gaps remain in standardizing methodologies and ensuring the thermodynamic consistency of AI-driven models. This underscores the need for comprehensive frameworks that integrate thermodynamics with AI for sustainable thermal system design and operation [151].

A growing body of review literature has examined AI applications within specific thermal domains. Recent reviews

report systematic use of machine learning for prediction, fault detection, and optimization in ORC systems, heat exchangers, building energy systems, and other thermodynamic plants. Methodological surveys have likewise emphasized that the effectiveness of AI pipelines often depends more on data quality, feature construction, and target definition than on algorithm choice alone [108]. While these contributions have significantly advanced the field, they tend to remain fragmented along technological boundaries, focusing, for example, on heat exchangers, renewable subsystems, or individual optimization techniques, rather than developing a unified thermodynamic AI perspective. Moreover, the hierarchical role of exergy within optimization is rarely formalized, even though it can define the physically feasible design space and prevent thermodynamically inconsistent solutions [103]. This limitation is particularly important in integrated thermal energy systems, where favorable economic or operational outcomes may not necessarily correspond to improved thermodynamic performance [43, 69].

Building on this fragmentation, the present review is organized around a stepwise logic that moves from thermodynamic foundations to AI-enabled decision-making. First, it establishes a thermodynamically grounded framework in which exergy is treated not only as a diagnostic measure of irreversibility but also as a feasibility constraint for AI-enabled optimization [35, 103, 142, 151]. Second, because such a framework requires consistent learning inputs and outputs, it consolidates methodological developments in data acquisition, feature construction, target definition, validation, and uncertainty treatment across component- and system-level studies [89, 108]. Third, it evaluates hybrid physics–AI strategies, uncertainty-aware modeling, and multi-objective optimization as the computational mechanisms that translate thermodynamic consistency into scalable design and control [40, 82, 83]. Finally, it synthesizes crosscutting barriers, including dataset scarcity, interpretability, scalability, and standardization, and uses these barriers to identify research directions for adaptive, life-cycle-aware, and physically consistent thermal infrastructures [58, 114]. Thus, the review follows a logical progression from why exergy is required, to how AI models should be constructed, to where hybrid optimization can be applied, and finally to what limitations must be overcome. The manuscript is a review and synthesis of the published literature and does not present new experimental measurements, new numerical simulations, or newly trained models.

Fundamentals of energy and exergy in thermal systems

Thermal systems such as power plants, heat exchangers, refrigeration cycles, and solar energy devices are traditionally evaluated using first- and second-law metrics that

quantify the quality and quantity of energy conversion. Energy analysis, based on the first law of thermodynamics, accounts for the conservation of energy but cannot distinguish between useful and degraded forms of energy [115]. Exergy analysis augments this perspective by measuring the maximum useful work obtainable as a system comes to equilibrium with a specified environment, thereby directly linking thermodynamic irreversibilities to lost work potential and environmental impact [149]. Recent reviews emphasize that meaningful performance assessment of modern thermal systems increasingly relies on combined energy–exergy frameworks and extended 4E (energy, exergy, economic, environmental) indicators, especially in low-carbon and hybrid configurations. Deb et al., [51] experimentally developed a biomass-fueled natural convection dryer and compared operation without storage versus with paraffin wax, pebbles, and both combined. They performed a thermo-economic–environmental assessment alongside energy/exergy evaluation, and reported that combining storage materials improves heat retention, sustains higher temperatures longer, and yields superior energy and exergy efficiency; they also report an energy payback period 1 year and approximately 22.82–22.89 metric tonnes CO₂ mitigation over the system lifetime. Al-Rbaihat [11] used hourly TRNSYS simulations for a hybrid PV–wind hydrogen system (electrolyzer + fuel cell) under coastal climate conditions and conducted a full 4E assessment. The study concludes the hybrid PV–WT configuration outperforms stand-alone PV or WT for hydrogen generation and supports broader applications; it reports annual renewable electricity generation and hydrogen output under the case study climate, and frames viability using both thermodynamic and economic/environmental metrics. Although these studies examine different applications, they support a consistent conclusion: First-law (energy-only) metrics can mask efficiency losses associated with irreversibilities, whereas integrated energy–exergy assessment coupled with 4E more clearly quantifies the benefits of hybridization and makes performance trade-offs transparent.

Energy/exergy definitions, efficiency indicators, and metrics

Energy and exergy indicators are commonly used to assess thermal-system performance. In the biogas context, a review of biological upstream optimization strategies noted that predominantly laboratory-scale evidence limits commercial decision-making [138]. For AI-driven prediction/optimization, these indicators are more than “textbook equations”: They are labels/targets that must be defined consistently (system boundary, reference environment, fuel/product definition, and denominator conventions); otherwise, models learn contradictions rather than physics [82].

Recent exergy methodology and applied 4E studies [20, 47, 142] highlight that misinterpretations and inconsistent “product/fuel” definitions remain common and can materially change conclusions, especially when exergy is coupled with cost and environmental accounting (exergoeconomics/exergoenvironmental analysis) and with advanced exergy splitting (avoidable/unavoidable, endogenous/exogenous). Below, the core indicators are consolidated in Tables 1 and 2.

Recent work suggests that the practical value of energy and exergy metrics lies less in their canonical definitions than in how they influence design and operational conclusions when economic and environmental criteria are considered [142]. In a four-E study of a cryogenic carbon

dioxide purification unit with membrane integration, Costa and co-authors [47] show that operating conditions preferred under integrated energy–exergy–economic–environmental assessment can differ from those suggested by energy-only evaluation. Their optimization supports carbon dioxide recovery above 90% as competitive when thermodynamic and financial indicators are considered jointly, while demonstrating that the cost-optimal region is sensitive to carbon taxation and penalties associated with uncaptured emissions. The reported small variability around the optimum in electrical consumption, recovery, and exergy efficiency also highlights robustness, which is relevant for data-driven optimization under measurement noise and operating uncertainty.

Table 1 Core first-law (energy) performance indicators used as AI targets/constraints

Component	Indicator	Symbol	Compact definition	Common pitfalls
Any control volume [107]	Energy efficiency	η_{en}	Useful energy out/energy in	Highly boundary dependent
Power cycles/heat engines [143]	Thermal efficiency	η_{th}	$\frac{W_{\text{net}}}{Q_{\text{in}}}$	Sensitive to how Q_{in} is defined
Boilers/fired heaters [84]	Boiler/combustion efficiency	η_{boiler}	Useful heat to working fluid/fuel heat input	LHV vs HHV changes values
Refrigeration cycles [34]	Coefficient of performance (refrigerator)	COP_{R}	$\frac{Q_{\text{L}}}{W_{\text{in}}}$	A quantity metric can increase while exergy efficiency drops, due to larger irreversibilities
Heat pumps/HVAC heating [21]	Coefficient of performance (heat pump)	COP_{HP}	$\frac{Q_{\text{H}}}{W_{\text{in}}}$	Strongly climate/load dependent
Heat exchangers [85]	Effectiveness	ϵ_{HX}	$\frac{Q_{\text{actual}}}{Q_{\text{max}}}$	Good for comparing HX designs, but does not rank where irreversibilities occur
System-level benchmarking [129]	Specific energy consumption	SEC	Energy input per product	Comparable only if product definition and auxiliaries are harmonized

Table 2 Core exergy indicators and selected source-specific energy/thermal assessments

Metric family	Indicator	Symbol	Compact definition	Why it matters for AI optimization	References
Stream work potential	Physical exergy	e_{ph}	Specific physical exergy relative to a reference environment	Requires explicit T_0, p_0	[20, 47]
Component irreversibility	Exergy destruction	$\dot{E}_{\text{D}}$	Rate of exergy destroyed in a component due to internal irreversibilities	Direct thermodynamic loss map	[142, 153]
Control volume accounting	Fuel–product form	$\dot{E}_{\text{F}}$	Fuel/product/loss/destruction split	Powerful but sensitive to consistent definitions of fuel and product	[20, 142]
Second-law efficiency	Input–output exergetic efficiency	ϵ_{IO}	Ratio of product exergy to fuel exergy	A single score that can re-rank designs versus energy-only metrics	[20, 47]
Source-specific energy/thermal assessment	Energy–performance assessment and e–NTU modelling		Glass-industry energy–performance assessment and counter-flow cooling-system modelling	System-specific efficiency/heat-transfer outcomes	[107, 111]

A consistent conclusion is reached in hybridization studies that couple carbon capture with energy storage. Zhang and colleagues evaluate a cryogenic separation carbon capture system integrated with liquid–air energy storage and report reduced capture specific energy consumption, together with a higher exergy efficiency for the storage subsystem compared with a baseline configuration. They further show improved economic attractiveness under carbon pricing assumptions, reflected in shorter payback times [153]. Compared with Costa et al. [47] these results reinforce that “optimality” is governed jointly by the distribution of irreversibilities and the external valuation of emissions, making integrated four-E accounting essential for defensible comparisons. The same logic extends to end-use thermal devices. Abbasi et al. [1] report high coefficients of performance and lower energy consumption for solar/air dual-source heat pump water heating, yet their second-law assessment differentiates configurations that appear similar under first-law metrics, because exergy performance is strongly influenced by temperature lift and internal irreversibilities. This underscores a key implication for AI-based optimization: Objectives defined only on first-law indicators can yield energetically attractive but exergetically inefficient operating policies. Finally, system-level four-E studies, such as Qiao et al. [123] show that dominant loss mechanisms can shift across operating periods and subsystems depending on whether energy or exergy is used as the diagnostic lens, strengthening the case for exergy-based localization of “quality loss sinks” before techno-economic and environmental decision-making.

Loss mechanisms and exergy destruction in major thermal components

In modern thermal systems, losses are not only about how much energy leaves a device, but about how strongly useful work potential is degraded by irreversibilities. This distinction is fundamental, because energy is conserved while exergy is destroyed through irreversibilities [34,44]. Real components degrade useful work potential through mechanisms such as finite temperature heat transfer, pressure loss, mixing, chemical reaction, and non-ideal compression or expansion. First-law balances quantify total energy flows, but they often blur the physical origin of performance

degradation, whereas exergy analysis converts entropy generation into a measurable penalty in lost work potential [44]. To formalize this, compact relations are widely used to quantify and localize thermodynamic inefficiencies (Table 3). The proportionality between entropy generation and exergy destruction expresses irreversibility directly as lost useful work. Decomposing total exergy input into product, loss to the environment, and destruction helps avoid misinterpreting exergy that simply exits the boundary as internal inefficiency. Likewise, the temperature-dependent definition of heat exergy explains why heat supplied at higher temperature has inherently higher quality and produces greater destruction when degraded across finite temperature differences. Finally, definitions of physical exergy enable consistent accounting of work potential changes across compressors, turbines, throttling valves, and heat exchangers [44, 142].

Expressing losses on this common exergy basis makes it possible to identify dominant “quality loss sinks” across boilers and combustors, heat exchangers, turbomachinery, thermal storage, and network-level energy systems [20]. This is also why conventional (pre-AI) thermodynamic workflows remain essential: They generate physically consistent exergy destruction maps that become target variables, constraints, or labels in data-driven optimization, particularly when an operating point may appear efficient by first-law metrics yet perform poorly in second-law terms [142].

Recent studies show that the component identified as “dominant” can change when performance is diagnosed by energy versus exergy, and that design guidance improves when pressure drop irreversibility and environment-linked indicators are included explicitly (Table 4). In Brayton cycle gas turbine analyses, the largest useful work degradation is commonly localized in the combustor due to combustion irreversibility, a conclusion that is not evident from energy efficiency alone [56]. Heat exchanger studies further demonstrate that high thermal effectiveness does not necessarily imply low irreversibility because finite temperature heat transfer and pressure drop can compete as destruction sources and can shift environmentally preferred designs; recent exergoenvironmental frameworks quantify cases where exergy destruction impacts exceed embodied contributions and where cold-side impacts surpass hot-side impacts, which energy-only reporting cannot reveal [86]. Advanced exergy analysis of shell-and-tube

Table 3 Compact relations commonly used to quantify irreversibilities and loss locations

Relation	Purpose in diagnosing losses	References
$\dot{E}_D = T_0 \dot{S}_{\text{gen}}$	Converts irreversibility into lost useful work potential	[142]
$E_{\text{in}} = E_{\text{product}} + E_{\text{loss}} + E_D$	Distinguishes unused exergy exit from internal destruction	[44]
$E_Q = (1 - \frac{T_0}{T_b})\dot{Q}$	Shows why heat at higher temperature has higher quality	[20]
Physical exergy of a stream	Tracks exergy changes in compressors, turbines, valves, heat exchangers	[142]

Table 4 Dominant sources and localization of irreversibilities in major thermal components and their implications for performance optimization

Component type	Dominant exergy loss mechanism	Dominant exergy loss mechanism	References
Combustion-driven power cycles	Combustion irreversibility + large temperature gradients	Combustion irreversibility + large temperature gradients	[56]
Heat exchangers	Finite-temperature heat transfer + pressure drop losses	Finite-temperature heat transfer + pressure drop losses	[86]
Shell-and-tube heat exchanger optimization	Distinguishing avoidable vs. unavoidable destruction	Distinguishing avoidable vs. unavoidable destruction	[121]
ORC with thermal energy storage	Temperature-grade mismatch during charging/discharging	Temperature-grade mismatch during charging/discharging	[67]
Gas-turbine power plant	Component-level exergy-destruction localization	Combustion chamber identified as the dominant exergy-destruction source	[56]

heat exchangers shows that redesign and retuning can reduce exergy destruction by on the order of tens of percent and increase exergy efficiency by several percentage points, while decomposition indicates a substantial avoidable share, information that is directly actionable for optimization and surrogate modeling [121]. System-level evidence is consistent: ORC pilot plants with thermal storage use combined energy–exergy evaluation to separate temperature-grade mismatch from heat rate limits [67], and a gas-turbine power-plant assessment identifies the combustion chamber as the dominant exergy-destruction source [56].

AI, machine learning, and deep learning for thermal systems

The rapid growth of sensor-rich, simulation-rich, and operational data in thermal systems has made ML and DL natural complements to first- and second-law analysis. Recent reviews report systematic use of AI for performance prediction, fault detection, and design optimization in ORC systems, heat exchangers, building HVAC, and other thermodynamic plants [100]. In a standard supervised-learning formulation, the input–output relationship is estimated using a parameterized function class [37]:

$$y = f_{\theta}(x), \quad (1)$$

where the input vector x may contain geometric parameters, operating conditions, and fluid properties, and the output y includes energy and exergy efficiencies, heat transfer coefficients, pressure drops, or composite 4E indicators. Recent work explicitly trains ML regressors on model-generated or experimental datasets to predict both energy and exergy efficiencies, for example in solar panels, trilateral cycles, vapor compression refrigeration, TES units, and integrated clean energy systems [61].

AI models used in thermal systems (ML + DL)

Across recent thermal system studies, the strongest practical pattern is that “best model” is largely determined by data modality and decision use, not by model sophistication alone. In tabular, steady-state design spaces (typical of cycle simulations), gradient-boosted tree ensembles repeatedly remain hard to beat because they learn sharp nonlinearities from limited samples and provide stable variable importance screening. For example, Tao et al. [140] develop data intelligence surrogates for predicting thermo-economic performance of hybrid ORC and report that an extreme gradient boosting plus random forest stack yields the best accuracy among the tested models, with performance improving as more physically meaningful inputs are retained rather than aggressively reduced. This matters for review-level synthesis because it implies that many “deep” gains reported in the literature may actually be data regime gains: When data are sparse and structured, modern ensembles often dominate.

Simpler surrogate and metamodeling approaches should also be acknowledged in this context. Multiple linear regression, polynomial regression, and response surface methodology (RSM) models can provide transparent and computationally inexpensive alternatives when the design space is smooth, low-dimensional, or sufficiently sampled. Recent thermal and thermo-fluid studies confirm that such models remain useful as optimization surrogates: RSM has been coupled with CFD to construct objective functions for heat sink design, integrated with CFD and optimized ML models for two-phase flow prediction, and used with multi-objective optimization for thermal management fluid design [15, 97]. Although these models may not capture strong nonlinearities as effectively as ensemble learners or deep neural networks, they offer explicit equations, rapid training, easier sensitivity interpretation, and useful baseline performance for preliminary optimization. For this reason, polynomial and response surface surrogates remain valuable complements to high-capacity AI models, particularly when interpretability,

computational efficiency, and early-stage design screening are prioritized.

Deep learning becomes clearly advantageous when the system output is governed by sequence memory or spatially distributed physics. In building cooling load forecasting, a transformer-based encoder–decoder model is shown to outperform common shallow and recurrent baselines while also reporting bounded predictive uncertainty over longer horizons, which is exactly the regime where classical recurrent models tend to lose long-range dependence [98]. In component-level heat transfer problems, deep networks can exploit very large synthetic or segmented datasets to learn high-curvature response surfaces that are difficult to approximate with classical correlations. A printed circuit heat exchanger study using a microsegment dataset reports near-unity coefficients of determination for an artificial neural network trained on thousands of local segments, illustrating how dataset construction (local physics sampling) can be as decisive as architecture choice [99].

A second crosscutting insight is that optimization-oriented studies should evaluate models by “decision fidelity,” not only pointwise error. Tao and co-authors show that a neural network surrogate coupled with uncertainty propagation can enable fast robust optimization of an organic Rankine cycle, emphasizing speed and robustness of the resulting optimum rather than only prediction accuracy [140]. Similarly, experimental microchannel heat sink work demonstrates that machine learning surrogates can learn performance under non-uniform heat loads, supporting design and operating trade-offs that would be impractical to explore purely by brute-force experiments [133]. Field deployment studies reinforce the same message, as Ayoola et al., [27] highlighted the value of models that remain stable under sensor noise, occupancy variability, and control changes, because that stability determines whether an “optimal” policy survives in practice.

Hybrid AI–thermodynamic and AI–CFD approaches

A major trend is the integration of AI with first-principles thermodynamic models and CFD. In these hybrid approaches, mechanistic thermodynamic models or CFD simulations generate large datasets that are used to train ML/DL surrogates, enabling near-physics performance prediction at substantially lower computational cost [40]. Recent thermodynamic system studies also introduce ML-based predictive control that explicitly accounts for temperature delays, reporting higher modeling accuracy and improved optimization efficiency relative to conventional linear models [146]. Complementary work uses ML to discover explicit algebraic expressions for energy, exergy, and overall performance from simulator-generated data, effectively replacing iterative numerical solvers with closed-form surrogates [22].

Exergy-focused hybrids follow the same logic: Transient exergy performance in a PCM-integrated concentrated solar thermoelectric generator is learned by using exergy rates and destruction terms computed from thermodynamic balances as training labels [14]. Huang et al. used dimensionless descriptors for microchannel air-side heat-transfer prediction while Wen et al. applied ML to predict S-CO₂ heat-transfer behaviour and deterioration near the pseudo-critical region in a heated circular tube [73, 148]. Physics-informed neural networks (PINNs) further embed governing laws directly into training through a PDE residual penalty [127]:

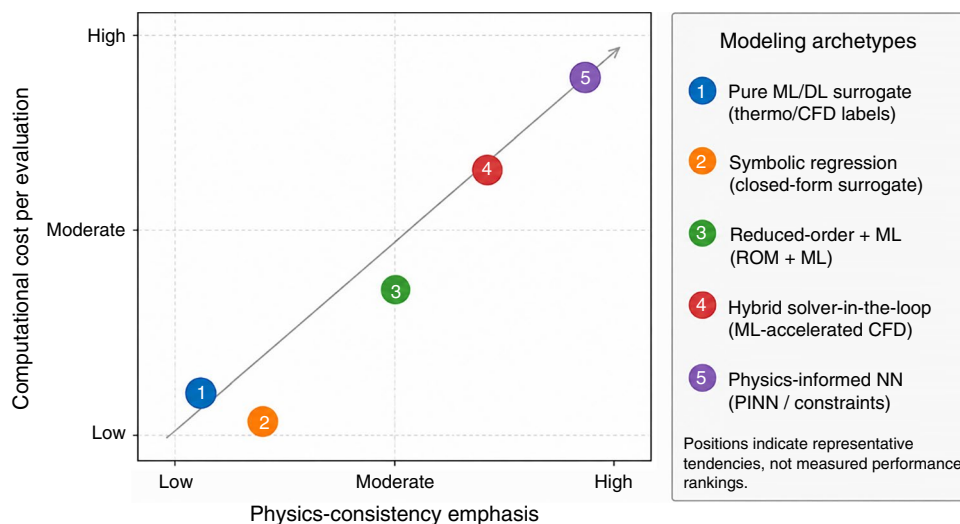
$$\mathcal{L}_{\text{PINN}}(\theta) = \mathcal{L}_{\text{data}}(\theta) + \lambda_{\text{pde}} \|\mathcal{N}(u_{\theta}(x, t))\|_2^2, \quad (2)$$

where $u_{\theta}(x, t)$ is the neural network approximation of the state variables, $\mathcal{N}$ denotes the governing equation operator (PDE residual), and the norm is typically evaluated over collocation points in the space–time domain.

Figure 1 and Table 5 explain why hybrid and data-driven thermal-system approaches can look similar in formulation yet behave very differently when used for optimization, control, or extrapolation. The key message of Fig. 1 is qualitative rather than quantitative: The figure is intended as a taxonomy of modeling archetypes, not as a performance benchmark. The methods shown were not evaluated on a single identical problem or dataset; therefore, their positions summarize representative tendencies reported in the literature regarding computational cost, physics consistency emphasis, and feasibility control. Figure 1 is the authors’ qualitative synthesis; its plotted positions are illustrative and are not measurements from a shared benchmark. ML–CFD reviews support this logic by documenting substantial speedups from surrogates and reduced-order strategies while emphasizing that physics integration is often required to avoid case-specific, fragile models under distribution shift [40]. Each point in the figure corresponds to a common archetype. Pure ML/DL surrogates trained on thermodynamic or CFD labels evaluate extremely fast, but they rely on training coverage for physical realism [146]. Symbolic regression can yield explicit closed-form expressions that remain cheap to evaluate and interpretable, though robustness outside the data domain depends on constraints. Reduced-order plus learning sits between these extremes, using compressed physics to improve extrapolation at moderate cost [73]. Solver-in-the-loop hybrids increase per-query cost by keeping mechanistic structure present during learning or inference, often improving feasibility. Physics-informed neural networks sit at the high-physics end because they directly penalize governing equation residuals, typically requiring more computation to evaluate and train [40].

Table 5 operationalizes this map for thermal-system studies by specifying what each approach replaces, the exergy or physical target/constraint used, and what is reported beyond

Fig. 1 Qualitative design space map for hybrid AI–thermodynamic and AI–CFD modeling. The numbered points identify common modeling archetypes rather than results from a shared benchmark problem: (1) pure ML/DL surrogate, (2) symbolic regression, (3) reduced order + ML, (4) hybrid solver-in-the-loop, and (5) physics-informed neural networks. The map summarizes representative trade-offs between computational cost per evaluation and physics consistency emphasis across surrogate and physics-constrained learning strategies [40, 68, 73, 146, 150]



accuracy. Based on this comparison, a broader reporting norm is proposed for future energy–exergy applications: hybrid models should be evaluated not only by prediction error but by thermodynamic credibility checks. Two inexpensive checks are particularly relevant. First, balance closure screening tests whether predicted quantities satisfy mass/energy closures within a stated tolerance. Second, irreversibility consistency screening checks that predictions do not imply non-physical behavior such as negative exergy destruction or entropy generation under the chosen reference environment. These checks are critical in optimization because small prediction errors can still mislead search algorithms if the surrogate violates feasibility or creates artificial “free lunches.”

Methodological framework in AI-based energy/exergy studies

AI-based prediction and optimization of energy and exergy efficiencies rely on a coherent methodological pipeline that links data acquisition, feature design, target definition, model training, and uncertainty treatment. Recent reviews of ML in heat exchangers, geothermal systems, and renewable energy highlight that the quality of this pipeline is often more decisive for model performance than the particular algorithm chosen [155].

Multi-objective optimization frameworks (energy, exergy, economics, environment)

Multi-objective optimization (MOO) constitutes a core methodological element of AI-based energy and exergy studies, reflecting the inadequacy of single-metric optimization for complex thermal systems. While most studies

employ similar objective sets, typically energy efficiency, exergy efficiency, economic cost, and environmental impact, comparative analysis reveals that methodological diversity arises primarily from how these objectives are structured, weighted, and hierarchically organized within AI-assisted frameworks rather than from the objectives themselves [87, 136, 155]. This distinction is particularly evident when contrasting component-level optimization with system-level and multi-energy system studies.

At the component scale, AI-based MOO frameworks generally exhibit smooth and interpretable trade-off surfaces. A study on heat recovery steam generators and ORC [125] reported well-defined Pareto fronts, where exergy efficiency improvements beyond narrow optimal regions are accompanied by increasing exergoeconomic penalties. The results indicate that irreversibility and cost are strongly colocated in the operating space, allowing exergy-based objectives to implicitly regularize the optimization problem by penalizing physically inefficient solutions.

In contrast, system-level and hybrid cycle studies display more complex and often non-convex trade-off structures. When irreversibilities are distributed across multiple subsystems, such as solar collection, thermal storage, power cycles, and fuel synthesis, objectives may conflict in non-intuitive ways. Hybrid solar and polygeneration studies show that configurations maximizing thermal efficiency frequently diverge from those minimizing emissions or maximizing exergy efficiency, particularly under changing boundary conditions or policy constraints [110]. This dispersion of losses requires system-level frameworks to accommodate shifting objective dominance. A key methodological divergence concerns the role of exergy within optimization. While some studies treat exergy efficiency as a coequal objective, others implicitly use exergy as a feasibility or screening criterion, excluding thermodynamically inconsistent configurations

Table 5 Hybrid and data-driven thermal-system approaches, exergy treatment, and validation signals

Hybrid archetype	Typical data source	What the AI replaces	Where exergy enters	What to report beyond accuracy	References
Temperature-delay identification model	Industrial-process, meteorological/ environmental, and building-energy datasets	Temperature-delay prediction	Temperature delay, not exergy, enters the model	Prediction error and stability across datasets	[146]
Robust surrogate optimization	Simulator + uncertainty model	Slow deterministic optimization loops	Net-power performance objective and chance constraints	Solve time reduction and constraint violation rate; robustness gap versus deterministic optimum	[150]
Dimensionless data-driven model	Experimentally validated CFD performance data	Microchannel air-side heat-transfer prediction	Exergy not assessed	Statistical error and input-sensitivity assessment	[73]
PINN	Governing equations, boundary conditions, and collocation points	Mesh-free prediction of velocity and temperature fields	Exergy not assessed	PDE/boundary residuals and velocity/temperature-field agreement	[68]
Delay-aware predictive control	Operational temperature data	Temperature-delay-aware prediction and control	Temperature delay included in the control model	Modelling accuracy and optimization efficiency	[146]

prior to economic or environmental optimization. Although this hierarchical use of exergy improves physical credibility and reduces search dimensionality, it remains rarely formalized in AI workflows, contributing to inconsistencies across studies while Villagran et al. identified limited long-term validation, inconsistent metrics, and weak transfer across climatic contexts in solar-assisted greenhouse and HVAC research [87, 144]. Similarly, environmental objectives influence optimal solutions primarily when formulated as explicit emission constraints or monetized costs rather than qualitative indicators [110, 144].

Recent evidence suggests that progress in AI-based MOO will depend less on expanding objective sets and more on restructuring optimization hierarchies. Exergy can define the physically feasible manifold, energy metrics ensure operational efficiency, economic objectives rank viable solutions, and environmental indicators re-weight decisions under external constraints. AI enables this layered formulation by making repeated objective reformulation computationally tractable [87, 155]. Figure 2 presents a reconstructed high-resolution schematic based on the multi-region integrated multi-energy system planning framework of Kim et al. [87]. To improve readability, the schematic is simplified into three interacting layers: system interaction and sector coupling concepts, regional exchange of electricity, heat, and hydrogen, and network/market/decarbonization planning considerations. The bottom row separately identifies the electricity, thermal, and hydrogen subsystems that form the decision space. This reconstruction illustrates optimization-based planning, including selected AI and data-driven methods, for coordinating coupled subsystems and regional energy flows under economic, environmental, and infrastructure constraints.

Data, feature engineering, and target definition in thermal system AI models

This subsection examines how data sources, feature construction, and target definitions operationalize multi-objective optimization in AI-based thermal system studies. Recent reviews emphasize that predictive accuracy and generalization in applications depend less on algorithm selection than on how thermodynamic behavior is embedded within data representations and learning targets [57]. Consequently, methodological choices at the data and feature level largely determine model robustness, interpretability, and transferability across thermal technologies [132]. A fundamental distinction across studies concerns data origin and resolution. Component-level investigations, such as nanofluid-enhanced PVT–PCM systems, rely on compact experimental datasets acquired under controlled conditions. These datasets preserve strong physical causality between inputs and outputs but are limited in

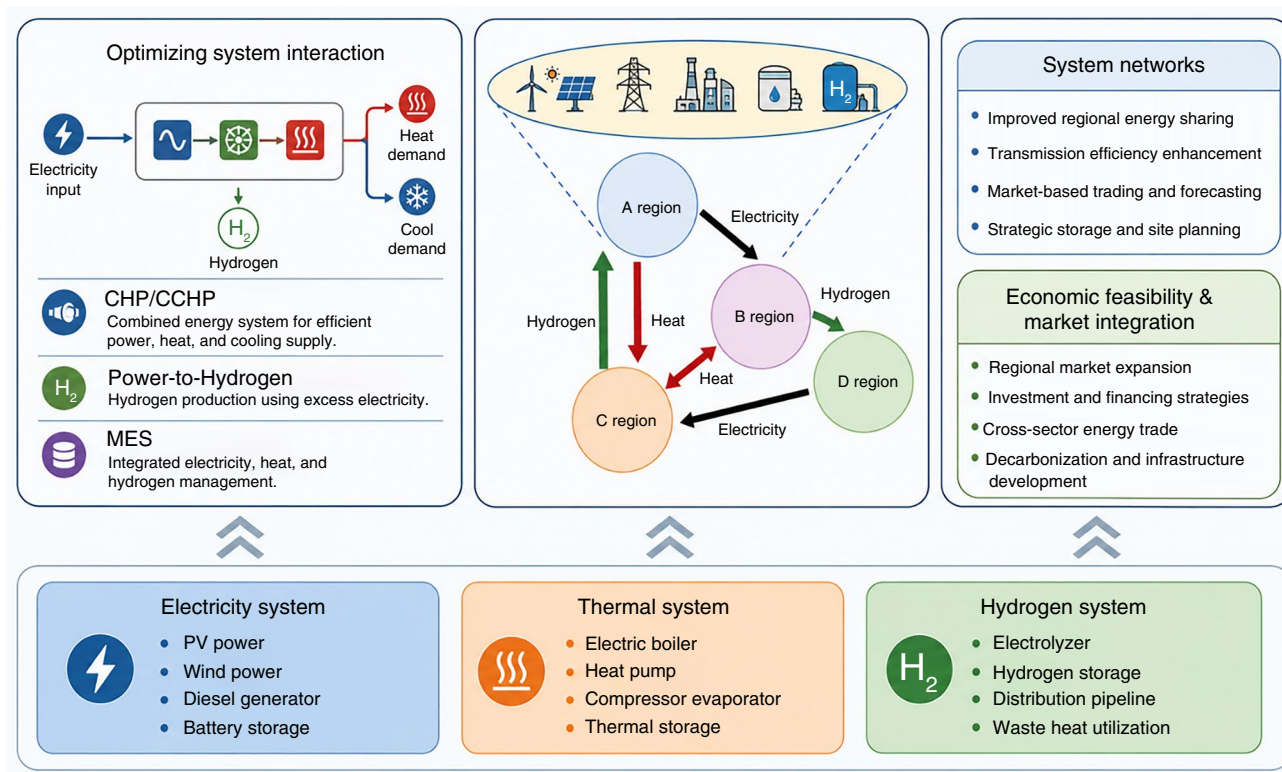


Fig. 2 Reconstructed high-resolution schematic of multi-region integrated multi-energy system planning and regional energy sharing. The simplified diagram summarizes the coupling of electricity, thermal, and hydrogen subsystems, inter-regional exchange of electricity,

heat, and hydrogen, and network/market/decarbonization considerations relevant to optimization-based planning, including selected AI and data-driven methods. Redrawn and simplified by the authors as a conceptual synthesis based on [87]

operational diversity. In contrast, system-level studies of solar water heating and absorption cooling systems integrate long-term operational and climatic data, capturing seasonal variability and user-driven fluctuations. Although such datasets introduce higher noise and heterogeneity, they enable AI models to generalize across wider operating envelopes, which is essential for deployment-oriented optimization and control [16, 114].

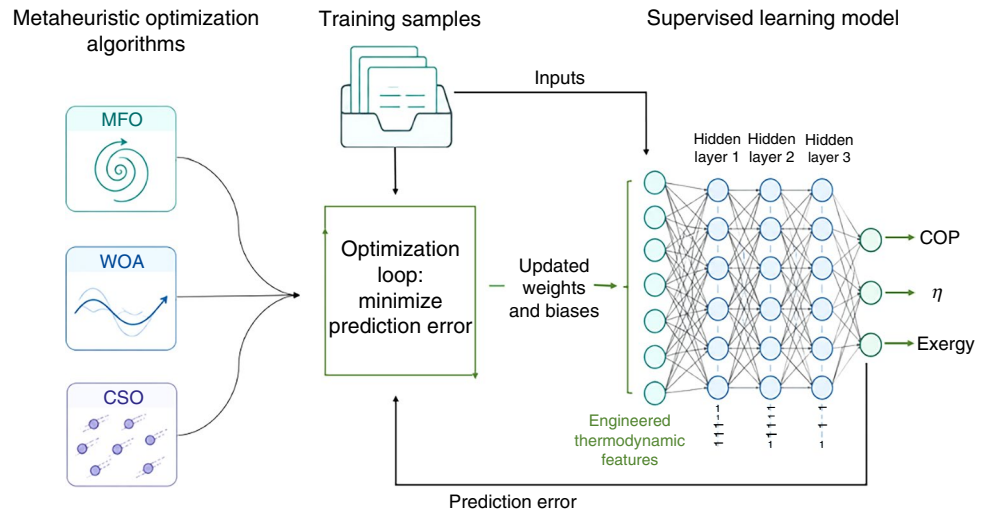
Feature engineering represents the primary mechanism through which thermodynamic knowledge is transferred into AI models. Experimental studies often employ direct control variables, such as flow rates or material properties, as inputs, allowing the model to learn smooth thermodynamic response surfaces. Conversely, large-scale thermal systems increasingly adopt derived thermodynamic features, including heat transfer rates, component efficiencies, and exchanger loads. Explainable AI analyses consistently show that these physically aggregated variables dominate model sensitivity, while raw environmental inputs become secondary once energy balances are implicitly encoded [16]. Review studies further highlight an emerging trend toward hybrid feature sets that combine sensor-level data with physically meaningful indicators, though the absence

of standardized feature definitions remains a key limitation for cross-study comparison [58, 114].

Target definition introduces an additional layer of methodological divergence. Energy-based metrics dominate system-level applications due to their operational relevance, whereas component-level studies increasingly adopt dual energy–exergy targets. These formulations reveal irreversibility trade-offs that remain invisible in first-law-only learning tasks. Although exergy is often used diagnostically, some studies use it directly in optimization; Sayed et al. [132], for example, included thermal-energy and exergy outputs in an ANFIS–PSO heat-exchanger case [58, 132].

Figure 3 synthesizes the methodological elements discussed in this section by illustrating how data construction, feature abstraction, and target selection integrate within a unified AI-based thermal system modeling framework. On the right, the supervised learning model receives engineered thermodynamic and operational features as inputs and predicts key performance indicators such as COP, efficiency, and exergy. These features embody the physical structure, enabling the network to learn relationships that extend beyond raw sensor measurements. The center of the figure highlights the optimization loop, where prediction

Fig. 3 Authors' conceptual synthesis of interaction among engineered thermodynamic features, supervised learning, and metaheuristic optimization within AI-based thermal-system modeling; the complete workflow was not evaluated as one system in the cited studies



errors computed from the model outputs are iteratively used to update weights and biases. The left side depicts the metaheuristic algorithms, namely moth flame optimization (MFO), whale optimization algorithm (WOA), and chicken swarm optimization (CSO), that drive this optimization process by searching for parameter configurations that minimize error and enhance generalization. By visually linking feature engineering, learning targets, and optimization dynamics, the figure underscores a central conclusion of recent studies: Robust thermal system AI models depend not only on algorithm choice but on how thermodynamic knowledge is encoded in data representations and exploited during training. Outside thermal engineering, an ANN surrogate was coupled with metaheuristic optimization for seismic-isolation design; this cross-domain example is not thermal-system validation [65]. This conceptual synthesis is consistent with the methodological themes reported in the cited studies [58, 132].

Model training, validation, and performance metrics

Model training strategies in AI-based thermal system research have progressed from simple regression fitting toward structured learning frameworks that address non-linearity, data heterogeneity, and multi-output coupling. A recurring distinction is observed between component-scale applications (e.g., absorption chillers, HVAC units, drying systems) and system-level studies involving polygeneration, hybrid renewable integration, or multi-energy networks. The former emphasizes rapid convergence with limited data, whereas the latter require robustness and generalization under variable environmental and operating conditions [16, 53].

Artificial neural networks (ANNs) remain widely applied due to their flexibility in representing nonlinear thermodynamic responses. However, increasing evidence indicates

that tree-based ensemble methods, including Random Forest (RF), Extra Trees (ET), Gradient Boosting, and CatBoost, often achieve superior accuracy and robustness, particularly for multi-output datasets and nonlinear thermodynamic interactions. Studies on hybrid solar–geothermal and biomass-based systems report R^2 values approaching unity with ensemble models, together with reduced sensitivity to noise and feature correlation [29, 53]. Deep learning methods tend instead to dominate in sequential or high-frequency prediction tasks, such as irradiance or microwave-based drying [60, 63].

Validation practices vary widely across the literature. While k-fold cross-validation is common in system-scale analyses, many case-specific applications still rely on single train–test splits, limiting reproducibility and inflating accuracy claims. Reviews consistently identify the absence of external or cross-climatic validation as a key weakness, especially for solar-assisted and greenhouse energy systems [114, 144]. More rigorous approaches employ stratified sampling, sensitivity-aware validation, or scenario testing under extreme boundary conditions [16, 139]. Performance appraisal relies primarily on RMSE, MAE, MAPE, and R^2 . However, high statistical accuracy alone does not guarantee thermodynamic credibility. Consequently, several studies combine statistical metrics with physics-aware indicators, such as deviations in energy/exergy efficiency or entropy generation, ensuring alignment with real system behavior. As a cross-domain structural-engineering example, Ghosh et al. coupled an ANN surrogate with metaheuristic optimization for seismic-isolation design [29, 53].

Figure 4 presents the authors' conceptual workflow for robust AI modeling in thermal systems. The redesigned schematic organizes the workflow into four stages: model training, validation, performance and physical consistency assessment, and model outcome. The training stage distinguishes component-scale and system-level applications

and summarizes representative learners. The validation stage shows a progression from basic train–test splitting to cross-validation, external checks, and scenario testing. The assessment stage combines statistical indicators with thermodynamic credibility checks and interpretability/uncertainty tools. Together, these elements clarify how statistical metrics, physics-aware criteria, and emerging explainable/uncertainty-aware tools support reliable, physically consistent, and generalizable AI models [70, 81].

An emerging direction integrates explainable AI (e.g., SHAP) and metaheuristic optimization, enabling both interpretability and adaptive performance enhancement [16, 112]. The literature indicates that robust AI frameworks should combine ensemble or hybrid learners with physically informed validation and multi-metric assessment, although the lack of standardized protocols continues to hinder cross-study comparability [114, 144].

Uncertainty quantification and sensitivity analysis

Despite major progress in AI-based prediction and optimization of thermal systems, uncertainty quantification (UQ) and sensitivity analysis (SA) remain comparatively under-developed methodological elements. The literature consistently shows that high predictive accuracy alone does not guarantee reliable decision-making, particularly in systems exposed to renewable variability, multi-energy interactions, and long-term techno-economic risks (Deveci and Yilmaz). Consequently, recent studies increasingly emphasize

uncertainty-aware approaches to enhance robustness and deployment readiness [48].

Uncertainty originates largely from variability in environmental inputs (e.g., irradiance, ambient temperature), material properties (e.g., nanofluid stability, biomass composition), and operational parameters (e.g., load fluctuations). In hybrid solar–geothermal and polygeneration systems, small perturbations may propagate nonlinearly through thermodynamic balances, significantly affecting predicted energy, exergy, and cost indicators. Deveci and Yilmaz reported very high predictive accuracy for their hybrid solar–geothermal case, while Myat et al. identified limited full-system validation in nanofluid HVAC&R research [53, 112].

Across published work, SA is more widely adopted than full probabilistic UQ. Deterministic SA methods, such as one-factor-at-a-time and variance-based screening, are commonly applied to identify dominant influences on key outputs. Biomass and gasification studies consistently rank temperature, residence time, and feedstock composition as the main drivers of hydrogen production and exergy efficiency, while HVAC and nanofluid systems highlight nanoparticle loading and flow regime as critical determinants of COP and entropy generation [29, 112]. Advanced modelling frameworks also include HDMR, which represents high-dimensional input–output relationships through individual-variable and correlated multivariable terms; Ayub applied an HDMR surrogate to biomass-gasification prediction and optimization. Shash et al. reviewed computational, AI, modelling, and simulation approaches for green-hydrogen production through water electrolysis [29, 134]. In contrast,

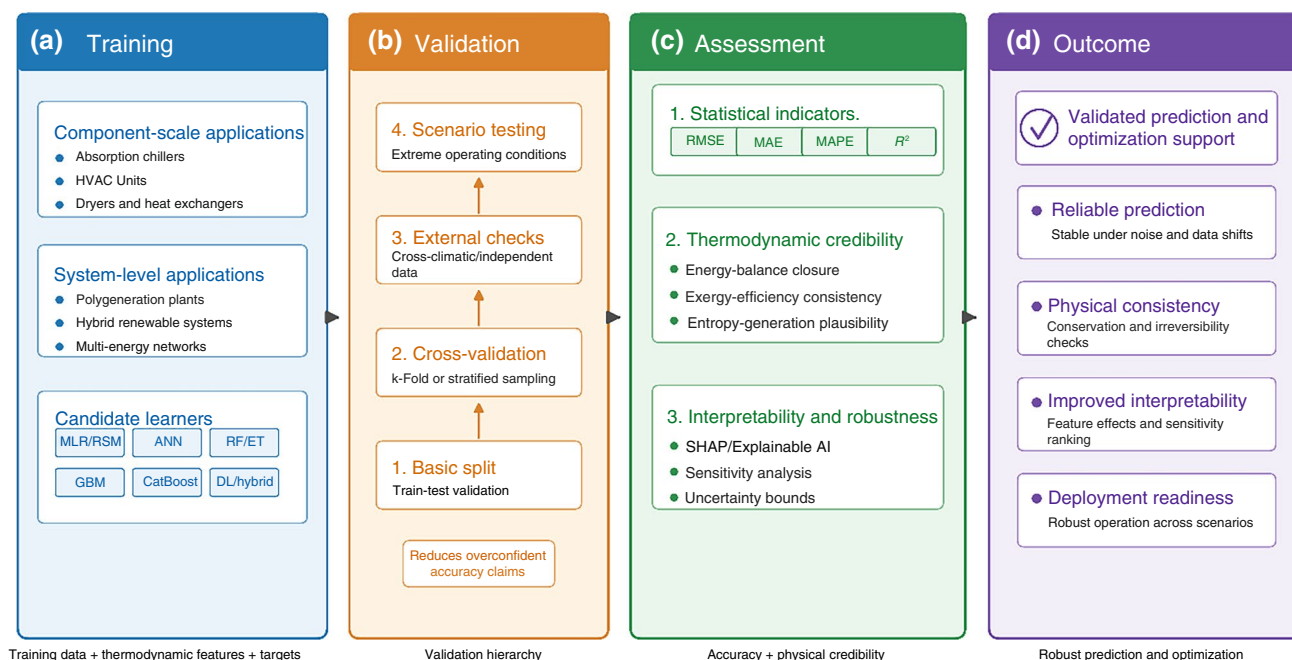


Fig. 4 Authors' conceptual workflow for robust AI modeling in thermal systems

probabilistic UQ remains rare, primarily due to computational cost and data scarcity. Most studies rely on indirect robustness indicators such as ensemble variance, cross-validation stability, or scenario-based stress testing. For integrated PV performance models, Akteruzzaman reported that linking environmental, technical, and economic layers with uncertainty propagation reduced prediction error from approximately $\pm 12\%$ to $\pm 5\%$ this is while Danish separately reviewed broader obstacles to AI adoption in energy systems [10, 48].

A key emerging direction is the integration of UQ and SA directly into validation and optimization loops, rather than applying them as post-processing diagnostics. Hybrid solar–geothermal systems involve nonlinear dynamics and

fluctuating renewable inputs (Deveci & Yilmaz), while Shash et al. reviewed computational and AI methods for green-hydrogen electrolysis. These sources motivate robustness assessment but do not quantify a nominal-performance–resilience trade-off [53, 134].

Figure 5 links uncertainty sources in thermal AI models to their nonlinear propagation through system thermodynamics, thereby affecting energy, exergy, cost, COP, and entropy outputs. It contrasts deterministic and global sensitivity analyses with probabilistic UQ and practical proxies, and shows how integrating UQ/SA into validation and robust optimization may support robustness under variability and may trade some nominal performance for

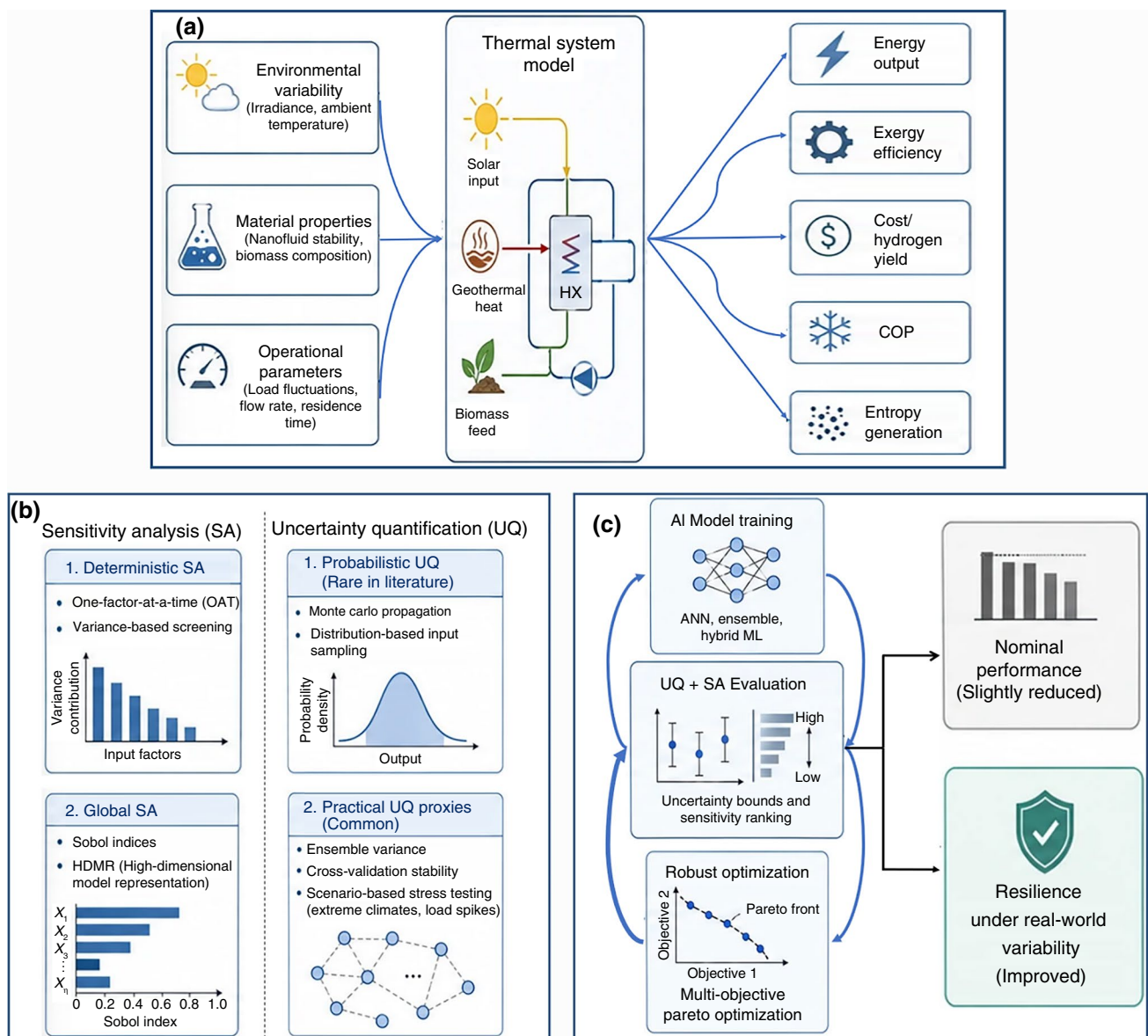


Fig. 5 Authors' conceptual UQ-SA framework for thermal AI robustness; depicted trade-offs are illustrative, not pooled quantitative results

robustness; the depicted trade-offs are illustrative rather than pooled results [10, 48, 114].

AI-based prediction and optimization in heat exchangers

Heat exchangers play a decisive role in energy, process, and building engineering by governing thermal energy exchange and irreversibility across operating domains. Their design and operation have traditionally relied on thermodynamic analysis, correlation-based methods, computational fluid dynamics, and heuristic optimization. Although powerful, these approaches are frequently constrained by the nonlinear behavior of multi-parameter systems, the influence of uncertainty, and the computational penalties of detailed simulations [102]. AI, particularly neural network-driven modeling and bio-inspired optimization, has recently emerged as a transformative complement to classical analysis. The reviewed contributions demonstrate that AI is increasingly integral not only to predictive modeling but also to multi-objective optimization, exergy-aware decision-making, and sustainability-oriented innovation in heat exchanger systems [36].

AI as a surrogate modeling and design optimization platform

AI-based surrogate modeling enables accurate representation of complex thermal phenomena while dramatically reducing computational demand. Krzywański [90] presented a generalizable hybrid AI architecture that combines artificial neural networks with genetic algorithms for the optimization of falling film evaporators used in adsorption cooling. The resulting AGENN framework accurately predicted total heat transfer rates under a wide range of geometric configurations and operating conditions, with prediction errors within $\pm 3\%$. More importantly, the approach enabled systematic exploration of design variables such as tube type and flow arrangement, providing a rigorous basis for enhanced thermal conversion. Figure 6 illustrates the role of artificial intelligence as a surrogate modeling and design-optimization platform for heat exchangers. Geometric parameters, operating conditions, and material properties are first used to represent complex thermal behavior, typically captured by computational models. An ANN-based surrogate then rapidly predicts heat-transfer performance, enabling genetic-algorithm-driven exploration of design variables to support rapid design exploration across applications; the references concern an LNG-process surrogate and a shell-and-tube heat exchanger, respectively [135, 145].

A similar AI-enabled paradigm emerges in refinery heat exchanger networks. Ayub et al. [28] applied neural network-assisted advanced exergy analysis to quantify

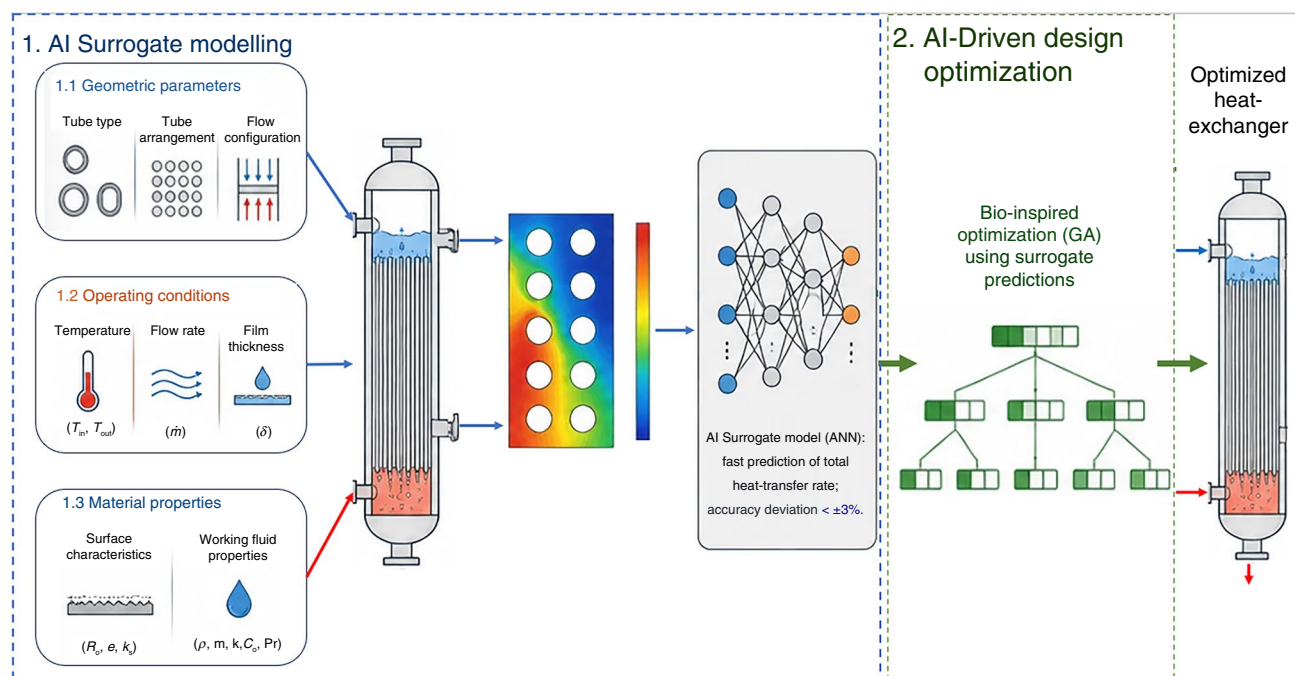


Fig. 6 AI-based surrogate modeling and genetic-algorithm optimization of a falling-film evaporator; conceptual reconstruction

avoidable and endogenous exergy destruction in preheat trains operating under uncertain refinery conditions. Their ANN models achieved correlation coefficients exceeding 0.99 across key exergy metrics, confirming the suitability of AI for supporting refinery-level decision intelligence and laying groundwork for Refinery 4.0. In both cases, AI enabled broader parametric exploration and faster assessment cycles than that would be feasible through conventional simulation alone.

Beyond process-scale exchangers, AI has also been applied to evaluate thermal enhancement strategies. Said et al. [130] developed neural network models to predict the heat transfer impact of multi-walled carbon nanotube water nanofluids in solar-assisted shell-and-tube exchangers. Their ANN surrogate achieved R^2 values approaching unity, while experiments confirmed heat transfer coefficient increases exceeding 30%. The integration of AI prediction, experimental validation, CFD analysis, and life-cycle assessment in this work demonstrates a maturing research direction in which AI is embedded within broader techno-economic evaluation routines.

AI-based energy–exergy optimization and decision support

In parallel with predictive applications, AI is increasingly employed as an optimization copilot capable of navigating thermodynamic trade-offs. Saikia et al. [131] demonstrated this capacity in sustainable air-conditioning systems through dual ANN–genetic algorithm optimization of both coefficient of performance and exergetic efficiency. Their results revealed that maximum COP and maximum exergy efficiency seldom coincide, highlighting the necessity of multi-objective modeling to avoid biased system improvements. These findings reinforce a conceptual shift from single-indicator performance targeting toward holistic AI-assisted decision support. The importance of incorporating second-law metrics is further emphasized by Ayub et al. [28], who showed that AI-assisted advanced exergy analysis can systematically distinguish avoidable from unavoidable destruction mechanisms in refinery heat exchanger networks. Such decomposition is essential for prioritizing capital investment and maintenance interventions, particularly in energy-intensive industrial contexts.

At a broader methodological scale, Ahuchogu et al. [8] discussed neural-network approaches for heat-transfer optimization in mechanical systems. This observation aligns with the hybrid modeling approaches demonstrated by Krzywański [90] and Said et al. [130], where AI is positioned not as a replacement for physics-based tools but as a complementary system that accelerates design convergence and enhances parametric coverage.

Materials, thermal storage, and hybrid system applications

The influence of AI extends beyond traditional exchanger hardware toward thermal storage-enabled envelope systems and hybrid renewable thermal configurations. Suh et al. [137] investigated luffa fiber-based phase change-enhanced gypsum composites for indoor finishing applications, demonstrating substantial improvements in thermal storage performance and reduction in temperature rise rates. Although not AI-driven, such materials represent promising candidates for integration with AI-assisted predictive frameworks for indoor environmental control, particularly in buildings seeking passive thermal buffering.

Complementary research in geothermal–solar hybrid systems underscore the importance of AI-assisted energy auditing and operational optimization, particularly under conditions of renewable variability and thermal fouling [36]. These applications illustrate the versatility of AI methodologies across energy transfer domains ranging from micro-scale material systems to industrial-scale heat exchanger networks.

Across the AI-based studies reviewed, reported benefits include enhanced predictive reliability in highly nonlinear thermal environments, improved capability for multi-objective optimization grounded in energy–exergy compatibility, and potential reductions in computational and experimental resource requirements. Nevertheless, key research challenges persist, including dataset scarcity, uncertainty quantification, interpretability of model decisions, and generalizability across operating regimes. The integration of physics-informed learning architectures and exergy-aware performance constraints represents a particularly important future direction. To consolidate the insights discussed in this section, Table 6 provides a comparative synthesis of the AI-based prediction and optimization studies and a supporting experimental thermal-characterization study across heat exchangers and related thermal systems. The table highlights the diversity of modeling approaches, objectives, and validation practices, while emphasizing the emerging trend toward hybrid AI–optimization frameworks and exergy-aware design.

AI applications in boilers and steam power plants

AI in boilers and steam power plants has progressed from purely data-driven forecasting toward integrated decision support frameworks that embed thermodynamic rigor, operational diagnostics, and optimization. AI models are increasingly being used to (i) diagnose transient faults and unsafe operations in boilers, (ii) predict plant-level power

Table 6 Condensed comparison of AI-based prediction and optimization/optimization approaches and a supporting experimental thermal-characterization study for heat exchangers and related thermal systems

References	System type	AI method	Main performance	Key outcome
[90]	Falling film evaporator	Hybrid ANN + GA (AGENN)	Heat transfer enhancement, design optimization	$< \pm 3\%$ prediction error and identification of optimal tube configuration
[28]	Refinery preheat train (HEN)	ANN-assisted advanced exergy analysis	Avoidable vs. unavoidable exergy losses	$R > 0.99$ for exergy indicators; clear loss path diagnosis
[131]	Vapor compression refrigeration	ANN + multi-objective GA	COP–exergy efficiency trade-off	Demonstrated non-coincidence of COP and exergy optima
[130]	Shell-and-tube exchanger with nanofluids	ANN + CFD + experiments	Heat transfer prediction and life-cycle benefit	30% HTC improvement with $R^2 = 0.99$
[8]	Mechanical systems	Neural network approaches	Heat transfer optimization	Qualitative discussion; no quantitative or CFD-comparison outcome retained
[137]	PCM-enhanced gypsum materials	Experimental thermal characterization (no direct AI)	Thermal storage, indoor comfort	Notable peak temperature reduction and time lag effect

generation and efficiency indicators, and (iii) support energy–exergy-based operational optimization of Rankine cycle plants. Collectively, these advances demonstrate that AI is no longer limited to surrogate modeling but is becoming an enabling technology for sustainable and reliability-aware power generation [105, 152].

AI-based diagnostics and predictive monitoring of boilers

Boilers remain the dominant source of irreversibility, operational losses, and safety risk in steam power plants, which explains the strong research focus on intelligent monitoring. In a comprehensive diagnostic framework for coal-fired boiler operation, Ismail et al. [77] developed neural network-based intelligent monitoring systems to forecast multiple categories of boiler trips using thirty-two operational variables and demonstrated that both pure ANN and ANN–GA hybrids could detect trip signatures prior to conventional control system alarms, with the hybrid approach reducing RMSE marginally while improving variable selection robustness. Such early warning diagnostics illustrate how AI can supplement plant operator decision-making in high-risk environments.

Complementary work on boiler energy efficiency indicators reinforces that AI-enabled monitoring must be grounded in clear thermodynamic performance metrics. Camaraza-Medina et al. [39] developed a unified algorithm for thermal and exergy indicators for a 250 MW Cuban power plant, identifying boiler-level exergy destruction exceeding 38% of total plant exergy losses at partial loads, thereby motivating intelligent control interventions at the boiler subsystem. Similar conclusions were reported for the Montazeri power station in Iran, where exergy analysis confirmed the boiler as the principal destruction site (86% of total inflow exergy),

far exceeding condenser losses identified via first-law analysis [7]. These studies collectively underscore that AI-enabled diagnostics must remain coupled to energy–exergy awareness in order to preserve interpretability and physical meaning.

AI has also been applied directly to boiler combustion optimization. Using detailed operational datasets, neural network models combined with Nelder–Mead optimization was applied to selective catalytic reduction (SCR) operation, reducing SCR-inlet NO_x by approximately 15%, ammonia consumption by approximately 12%, and unit heat rate by approximately 0.57% in a coal-fired power-plant boiler [152]. These results illustrate the practical potential of surrogate-based optimization for balancing efficiency and emissions during plant operation.

AI for performance prediction and power cycle optimization

At the power cycle level, AI models have proven effective in predicting net electrical output and efficiency while supporting exergy-aware optimization. Asghar et al. [25] developed back-propagation neural network models for a 747 MW combined cycle power plant to forecast power generation from ambient and fuel flow inputs, achieving MSE = 0.0063 and demonstrating strong consistency between predicted, simulated, and measured efficiencies (27–28%). Similar AI-enhanced energy–exergy frameworks were proposed for steam cycle plants by Malik et al., [105] where random forest regression models were trained alongside detailed exergy modeling for a 400 MW plant. The random-forest model captured sensitivity to reheat pressure and steam quality and supported prediction of energy and exergy efficiency across operating regimes. Exergy-structured AI approaches

therefore bridge the gap between statistical accuracy and thermodynamic meaning.

Asghar et al. [25] trained a back-propagation neural network for power prediction in a 747 MW combined-cycle plant and reported $MSE = 0.0063$, with predicted efficiency close to plant and model values. Figure 7 illustrates an integrated framework for AI-driven prediction and optimization of power-cycle performance. Plant operating variables, including ambient conditions, fuel flow, and steam parameters, are used to train machine-learning models such as ANN, RF, and SVM. Predicted outputs are subsequently interpreted through energy–exergy analysis, potentially supporting thermodynamically informed; the cited studies concern related cement-plant exergy modeling and natural-gas-engine emissions control rather than validation of the complete power-cycle workflow [6, 9].

Toward sustainable AI-enabled thermal plant operation

While AI models can enhance predictive accuracy and reduce computational burden relative to CFD and first-principles simulation, their value ultimately depends on alignment with thermodynamic logic. Exergy-based benchmarking of combined cycle and Rankine cycle plants in Jordan confirms that the boiler and heat recovery steam generator

dominate both destruction and loss terms, emphasizing that AI optimization should prioritize combustion control, heat transfer intensification, and steam quality management [18]. Similarly, energy- and exergy-based planning tools reveal how performance degradation varies with load, fuel composition, and condenser operation, thereby providing physically meaningful targets for AI-enabled control.

Recent work further extends AI's role from passive prediction to proactive reliability management. Intelligent monitoring systems for trip detection [77], random-forest-assisted energy and exergy performance prediction [105], and [152] illustrate how AI can support plant monitoring, performance assessment, and emissions–efficiency optimization when integrated with expert knowledge and structured validation. At the same time, energy–exergy analysis of legacy plants [7, 18, 39] ensures that AI-driven recommendations remain consistent with thermodynamic limits and operational constraints.

Outlook and synthesis

The reviewed research highlights a convergent trend: AI is moving from stand-alone prediction toward thermodynamically grounded decision support for decarbonization. ANN, SVM, random forest, and hybrid GA models have each demonstrated value in either predicting plant performance,

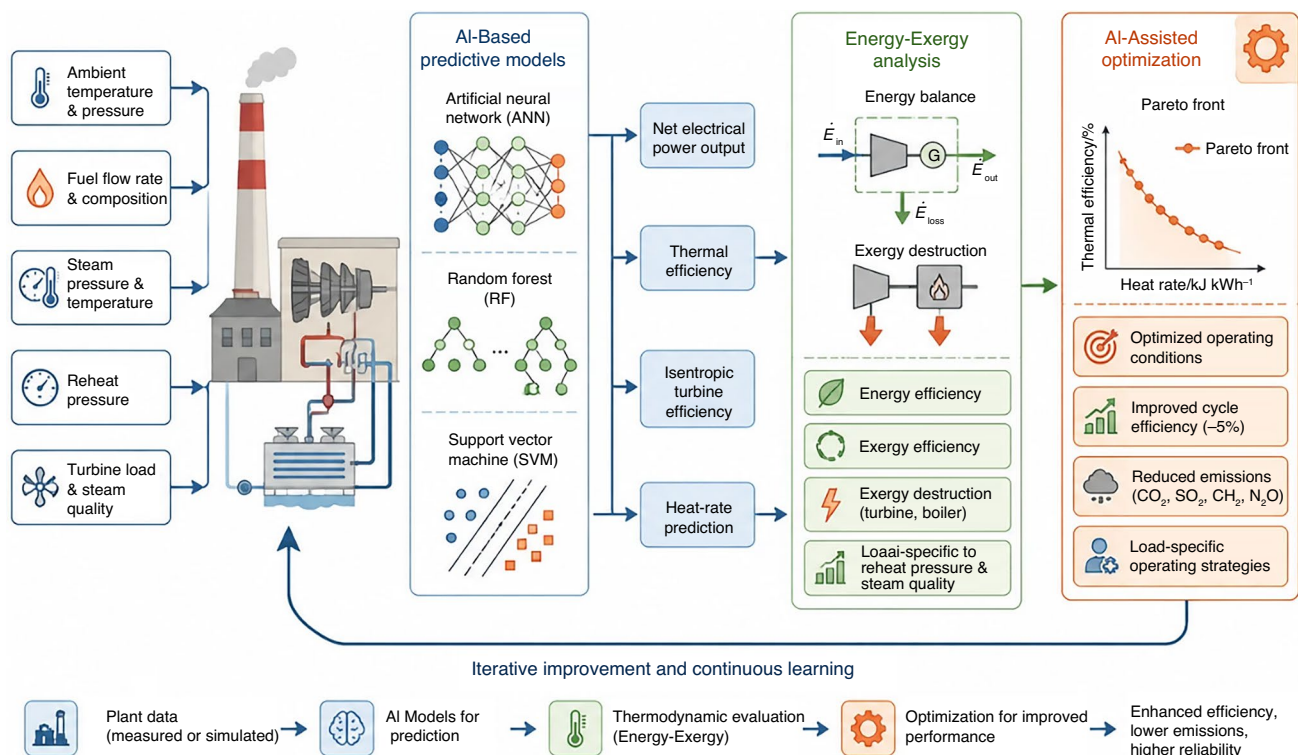


Fig. 7 AI-based prediction and optimization framework for power-cycle systems. Authors' conceptual synthesis; the outcomes shown, including the ~5% efficiency label, are illustrative

diagnosing critical events, or optimizing operational strategies. However, the most promising direction is the fusion of AI with exergy analysis and multi-objective optimization, as illustrated in Ashraf et al. [25], Malik et al. [105], and Yao et al. [152]. Such integration promotes interpretability, sustainability, and operational robustness.

Future research should prioritize (i) uncertainty-aware AI models that explicitly account for variability in fuel quality and ambient conditions, (ii) exergy-structured reinforcement learning for closed-loop control, and (iii) hybrid renewable integration where AI coordinates gas–steam cycles with solar or storage assets. As fossil fuel-based power plants continue to operate during the energy transition, AI-assisted optimization offers a pragmatic pathway to lower emissions and improved efficiency without immediate capital-intensive retrofits. Table 7 consolidates the key characteristics and outcomes of the reviewed AI applications and supporting conventional energy–exergy assessments in boilers and steam power plants, providing a comparative overview of modeling approaches, thermodynamic frameworks, and performance objectives across the examined studies.

AI-based modeling in ORC and other power cycles

The ORC and similar cycles have become key technologies for waste heat recovery from low- to medium-temperature sources such as industrial byproducts, geothermal energy, and solar heat. Recently, ML and DL have emerged as powerful tools for predicting cycle performance, reducing exergy destruction, optimizing working fluid and operating conditions, and applying them in hybrid systems. This section reviews the current state of research in this area.

AI prediction of cycle performance and exergy destruction

Many studies have applied ML/DL models to predict ORC performance, including thermal efficiency, power output, and exergy destruction, based on inputs like heat source temperature, pressure/temperature at the outlet, flow rate, and working fluid type.

A common performance measure for the cycle is thermal efficiency, defined as [147]:

$$\eta = \frac{W_{\text{net}}}{Q_{\text{in}}} \quad (3)$$

where W_{net} is the net work produced by the cycle, and Q_{in} is the heat input.

For second-law analysis, exergy efficiency is defined as [35]:

$$\epsilon_{\text{ex}} = \frac{\dot{E}_{\text{out}}}{\dot{E}_{\text{in}}} \quad (4)$$

and exergy destruction is calculated from the difference between the input and output exergy (or using the second-law balance). Some studies aim to minimize exergy destruction or improve exergy efficiency. Li et al. [100] highlighted the increasing use of ML for predicting cycle performance, exergy efficiency, and combined energy–exergy–economic indices. Peng et al. [120] used thermodynamic properties of the working fluid, heat source temperature, and flow rate as inputs to neural networks, effectively predicting thermal efficiency and power output with high accuracy.

Furthermore, Oyekale et al., [116] emphasized that ML can predict exergy destruction for various configurations and working fluids, offering a path toward rapid cycle optimization. Kumar et al. [94] examined the hybrid ORC with electrolyzer system and uses Transformer–LSTM models to predict cycle performance and hydrogen production. Thus, models are developed with mappings:

$$(\eta, \epsilon_{\text{ex}}, \dot{E}_{\text{D}}) = f_{\theta}(\mathbf{x}) \quad (5)$$

where $\mathbf{x}$ includes parameters such as heat source properties, working fluid characteristics, and operating conditions. These models act as "surrogates" in optimization or control of the cycle.

Working fluid selection and operating condition optimization

The selection of the working fluid and the associated operating conditions (evaporation and condensation temperatures, pressures, and mass flow rates) is a primary determinant of the efficiency, cost and environmental performance of ORC systems. Because these design variables are strongly coupled and the feasible design space is large, AI-based optimization offers a powerful way to explore working fluid candidates and operating ranges in a systematic, multi-objective manner rather than relying on trial-and-error or one-factor-at-a-time parametric sweeps.

Recent studies illustrate how different combinations of cycle configuration, working fluid and heat source can be evaluated using advanced optimization and AI tools. Kamfar et al. [79] analyzed eight modified Organic Flash Cycle (OFC) layouts for industrial waste heat recovery within an integrated 3E framework. By progressively introducing two-phase expanders and ejectors, the authors reduced throttling losses and enhanced expansion work. A multi-objective gray wolf optimizer was then employed to maximize thermal and exergy efficiencies while minimizing the levelized cost of electricity. Their results show that moving from a simple baseline OFC to more advanced

Table 7 Comparative synthesis of AI applications and supporting conventional energy–exergy assessments in boilers and steam power plants

References	System type	AI method	Thermodynamic framework	Primary objective	Key outcome
[95]	Steel-mill steam-power	RF + CART in an advanced boiler-combustion-control model	Combustion efficiency and gross heat rate	Real-time combustion-pattern selection and fuel minimization	Lower fuel use and gross heat rate
[25]	747 MW combined-cycle power plant	Back-propagation neural network	Thermodynamic/EES comparison	Predict net power output	Predicted power and derived efficiency close to plant and EES values
[77]	Steam boiler in a coal-fired thermal power plant	ANN and ANN-GA using 32 operating variables	Operational monitoring	Boiler-trip prediction and prevention	All six evaluated trips detected before or concurrently with plant control
[7]	Montazeri steam power plant	Conventional energy/exergy analysis; no AI	Energy–exergy	Component loss localization	Boiler identified as the dominant exergy-loss source
[105]	400 MW Rankine steam power plant	Random-forest regression + energy/exergy analysis	Energy–emissions	Plant-performance forecasting	Thermodynamically informed energy/exergy performance prediction
[152]	Coal-fired power-plant boiler with SCR	ANN surrogate + Nelder–Mead optimization	Energy–emissions and heat rate	Reduce NH ₃ use, SCR-inlet NO _x , and unit heat rate	NH ₃ ↓≈12%; SCR-inlet NO _x ↓≈15%; unit heat rate improved ≈0.57%
[39]	250 MW Cuban steam boiler	Thermal/exergy-balance calculation algorithm; no AI	Energy–exergy	Determine load-dependent efficiency indicators	Indicators calculated at 150, 180, 220, and 250 MW
[18]	Combined-cycle power plant in Jordan	Conventional energy/exergy analysis; no AI	Energy–exergy	Component performance and loss assessment	Major component-level exergy-destruction zones identified

layouts yield substantial gains in both global thermal and exergy efficiencies, together with higher net power output. Among the investigated options, the configuration with a two-phase expander and a single ejector (TPSEOF- II) emerges as the best compromise between performance and cost, highlighting how algorithm-based optimization can identify non-intuitive but high-performing working fluid–configuration combinations.

Ekanem et al. [55] considered a different application: a biomass-fired ORC with turbine bleeding for tri-generation (electricity, heating and cooling). Using a detailed exergy-based model in Engineering Equation Solver, they compared three low-GWP refrigerants (R245fa, R1234yf and R1234ze) under medium-temperature biomass conditions. Incorporating turbine bleeding and regeneration markedly increased exergy efficiency and useful power output relative to a generic non-bleeding ORC with identical boundary conditions. Among the three fluids, R245fa and R1234ze offered the most favorable balance between exergy efficiency, net power and exergy destruction, whereas R1234yf showed higher exergy losses and lower power. This work underlines the importance of matching thermophysical properties of the working fluid to the temperature level and variability of the biomass heat source, and demonstrates that appropriately configured tri-generation cycles can exploit medium-grade heat more effectively than conventional ORCs.

Complementary to these studies, Kumar et al. [91] examined a small-scale solar ORC (SORC) employing a dual enhancement strategy that combines a hybrid nanofluid in the solar collector with nanorefrigerants in the ORC loop. Experimentally, a MWCNT + SiC/water hybrid nanofluid in the evacuated tube solar collector increased the useful heat gain and collector thermal efficiency compared with the base fluid, thereby improving the quality and stability of the thermal input to the power cycle. This measured input was then used in an ORC model (implemented in EES) to evaluate two oxide-based nanorefrigerants, $\text{SnO}_2/\text{R141b}$ and $\text{Co}_3\text{O}_4/\text{R141b}$, over different particle loadings. Both nanorefrigerants enhanced energy and exergy efficiencies relative to pure R141b, with $\text{SnO}_2/\text{R141b}$ delivering slightly superior performance. The study shows that nanoenhanced working fluids can provide performance benefits without fundamentally changing the basic ORC layout, but their advantages must still be assessed in terms of exergy and overall system irreversibilities.

Based on the selected studies [55, 79, 91], Figs. 8 and 9 present source-verified efficiencies grouped by study. Figure 8 reports 13.24% for Kamfar et al.'s optimized TPSEOF- II/i-pentane organic flash cycle and 16.76% for A. Kumar et al.'s $\text{SnO}_2/\text{R141b}$ solar ORC at the reported optimum. Because system boundaries and operating conditions differ, the values are descriptive rather than a controlled cross-study comparison.

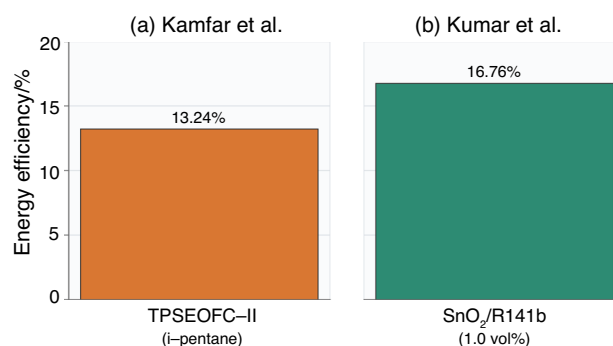


Fig. 8 Source-reported energy efficiencies for (a) Kamfar et al.'s TPSEOF- II/i-pentane OFC and (b) A. Kumar et al.'s $\text{SnO}_2/\text{R141b}$ solar ORC. Values are not directly comparable across studies

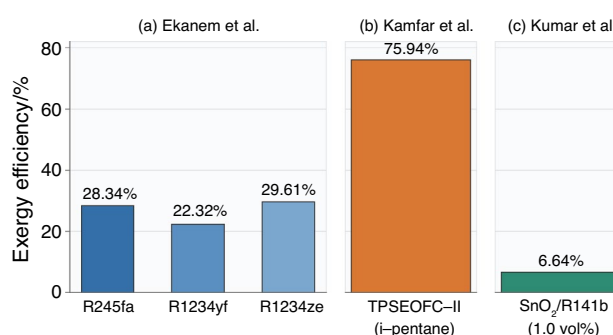


Fig. 9 Source-reported exergy efficiencies for (a) Ekanem et al.'s with-cooling ORC, (b) Kamfar et al.'s TPSEOF- II/i-pentane OFC, and (c) A. Kumar et al.'s $\text{SnO}_2/\text{R141b}$ solar ORC. Values are not directly comparable across studies

Figure 9 reports exergy efficiencies of 28.34%, 22.32%, and 29.61% for R245fa, R1234yf, and R1234ze, respectively, in Ekanem et al.'s with-cooling case; 75.94% for Kamfar et al.'s optimized TPSEOF- II/i-pentane OFC; and 6.64% for A. Kumar et al.'s $\text{SnO}_2/\text{R141b}$ solar ORC at the reported optimum. These configuration-specific values are not a universal working-fluid ranking [55, 79, 91].

Integration with waste heat recovery and hybrid systems

ORC units are increasingly embedded in hybrid energy systems rather than operated as stand-alone cycles. Typical configurations couple ORCs with solar collectors, biomass furnaces, gas turbines, heat pumps, electrolyzers, or desalination units, and often exploit multiple temperature levels of waste heat. In these complex layouts, AI models are used not only at the design stage but also for coordination and supervisory control under variable operating conditions [94].

For hybrid renewable systems, Kumar et al. [94] combined ORC technology with hydrogen production and

electrolysis. They proposed a hybrid solar–biogas ORC integrated with a proton-exchange membrane (PEM) electrolyzer and auxiliary components, and developed an ensemble machine learning framework to predict global performance and optimize green hydrogen production. The trained models simultaneously account for variations in solar irradiance, biogas flow, and electrical demand, enabling multi-objective optimization in terms of energy efficiency, exergy efficiency, and specific hydrogen yield with far fewer full thermodynamic simulations. Similarly, several multi-generation concepts integrate ORCs into larger sets of power, cooling and desalination units. Mehrenjani et al. [106] studied two geothermal-driven multi-generation systems that combine ORC, absorption refrigeration, reverse osmosis desalination, thermoelectric generators and LNG regasification. A data-driven optimization strategy was used to improve net power, freshwater production and cooling capacity while reducing total cost and exergy destruction, demonstrating that surrogate models can efficiently explore large design spaces involving many coupled subsystems. In another line of work, Alvi et al. [19] carried out a 4E assessment of hybrid solar–biomass ORC systems and highlighted their potential for greenhouse gas reduction. Subsequent studies suggest that coupling such thermodynamic frameworks with ML-based optimizers can further refine sizing and operating strategies under seasonal and resource variability.

The integration of ORC technology with fluctuating industrial and waste heat sources also benefits from AI-assisted modeling. Gu et al. [66] showed that an ORC recovering waste heat from a hydraulic system can operate stably despite strong fluctuations in oil flow rate, but the dynamic response and control requirements are non-trivial. Building on this, Feng et al. [62] performed an experimental investigation of a small-scale ORC and used machine learning models to optimize operating conditions, showing that data-driven surrogates can capture nonlinear dependencies between heat source conditions, expander performance and net power more accurately than simple correlations. At the control level, Hernandez et al., [72] used ML and deep reinforcement learning for tasks such as superheat control and performance prediction in coupled systems, thereby enabling more robust operation under transient and uncertain conditions. These studies show that AI significantly facilitates the integration of ORCs into hybrid and waste heat recovery systems by providing fast, accurate predictors and optimizers that can handle multi-source, multi-component layouts and highly variable boundary conditions, capabilities that are difficult to achieve with classical, purely equation-based approaches alone.

Integration of AI-assisted and conventional optimization approaches

Conventional optimization of ORC systems has traditionally used first-principles thermodynamic models, parametric studies, gradient-based methods, evolutionary algorithms, and, increasingly, data-driven surrogate models. Therefore, the distinction is not between “physics-based classical methods” and “data-driven AI methods” in a strict sense; rather, the main methodological difference lies in how optimization algorithms are coupled with physical models, empirical correlations, or learned surrogate representations. These approaches remain indispensable for understanding physical behavior and for ensuring thermodynamic consistency [124], but they become computationally expensive and hard to scale when the number of decision variables is large (e.g., multiple fluids, pressures, temperatures, component choices) or when multiple objectives such as efficiency, cost, environmental impact, and reliability must be optimized simultaneously [71].

Recent reviews have systematically compared classical and AI-based approaches in this context. Oyekale and Oreko [116] reviewed machine learning applications for the design and optimization of ORC plants and concluded that data-driven models can act as accurate surrogates for detailed cycle simulations, drastically reducing computational cost in multi-objective optimization and enabling more exhaustive exploration of the design space. Dumka et al. [54] developed a Python-based classical-ML surrogate for Rankine-cycle performance prediction and optimization.

As a separate low-temperature thermal application, Pandey et al. [119] reviewed mathematical modelling and energy-storage approaches for sustainable solar drying. Feng et al. [62] showed experimentally that ML-assisted optimization of a small-scale ORC can outperform simple design-of-experiments strategies, especially when nonlinear interactions between mass flow rate, superheat and expander efficiency are present. By contrast, Oliveira et al., [50] studied a complex ORC layouts such as dual-loop systems integrated into existing power plants still rely heavily on classical methods, illustrating the growing opportunity to couple these frameworks with ML surrogates to reduce computation time and broaden the explored design space.

Nonetheless, ML is not a drop-in replacement for physics-based optimization. High-quality, representative datasets; careful feature selection; and rigorous validation (cross-validation, uncertainty analysis, extrapolation checks) are required to avoid overfitting and non-physical predictions. Moreover, purely data-driven models can lack interpretability and may violate thermodynamic constraints if used without safeguards. Emerging hybrid approaches, such as physics-informed neural networks, constraint-aware optimization, or deep reinforcement learning controllers trained

on validated dynamic ORC models, aim to combine the strengths of both worlds by embedding physical knowledge into AI frameworks [72]. For ORC systems operating under uncertain and fluctuating conditions, the most promising strategy is not to replace classical methods with AI, but to integrate them. Thermodynamic models provide the physical backbone and generate reliable training data, while ML and DL serve as accelerators for multi-objective optimization, fast performance prediction and real-time control. This hybrid paradigm offers higher flexibility, better scalability and improved robustness than either purely classical or purely data-driven optimization on its own.

AI for solar-thermal collectors and solar-assisted systems

AI has recently become a key enabling technology in the design, optimization, and operation of solar-thermal collectors and solar-assisted energy systems. Across water heating, hybrid building energy systems, heat pumps, solar desalination, and solar-assisted biomass conversion, AI techniques, including neural networks, random forests, support vector machines, and hybrid metaheuristic frameworks, provide enhanced predictive accuracy, reduced computational burden, and improved real-time control compared with fully physics-based models. There are three common drivers for the integration of AI into solar-thermal research: (i) the inherent dynamism of climatic conditions, (ii) the need for multi-objective performance trade-off evaluation, and (iii) the complexity of hybrid system architectures that combine thermal and electrical subsystems [59, 114].

AI-enabled modeling and performance prediction in solar collectors and solar-assisted systems

Recent advances in AI have had a significant effect on the modeling of solar collectors and their integration into heating systems. In solar water heating systems (SWHS), machine learning models, particularly ANNs and LSTM structures, have been shown to accurately predict heat collection rates, exergy indicators, and overall system efficiency while accounting for environmental variability [76]. This predictive capability enables data-driven optimization, fault detection, and intelligent control beyond what traditional regression-based or steady-state models provide.

A parallel development occurs in solar-assisted heat pumps (SAHPs), where multilayered perceptron networks, support vector machines, and random forests have been benchmarked for COP prediction. Among these, random forests produced the most accurate and computationally efficient predictions, confirming the suitability of ensemble learners for nonlinear thermo-fluid processes [104]. The

advantage of these AI approaches lies in their ability to capture coupled dependencies among operating variables, mass flow, irradiation, ambient temperature, and compressor state, without explicit physical parameterization.

Solar collectors themselves are increasingly modeled through hybrid data-driven approaches. Modern collector configurations, particularly those including tracking systems, nanofluids, or photovoltaic–thermal (PV/T) coupling, exhibit performance characteristics that are highly sensitive to dynamic climatic fluctuations. Studies therefore emphasize hybrid AI–CFD or AI–thermodynamic frameworks as a path toward improved design flexibility and adaptive real-time operation [114]. A related trend is found in solar-assisted thermochemical conversion of agro-waste, where process and solar inputs can be evaluated for biofuel production and performance improvement [92].

AI for hybrid solar-thermal integration and multi-objective optimization

The need to integrate thermal collectors with broader energy systems has driven AI research beyond single-device modeling. Hybrid solar-drying systems provide a related example. Barzigar et al. [31] conceptually highlighted AI-enhanced supervisory integration for hybrid solar-dryer subsystems.

At a system scale, AI further supports supervisory control, particularly in environments characterized by high intermittency or storage coupling. For instance, AI-supported solar water heating enables learning-based demand prediction and energy scheduling, making SWHS both more efficient and more user-adapted [76]. Solar-assisted heat pumps benefit similarly from AI-enabled COP monitoring to support adaptive operating strategies [104].

Beyond buildings, parabolic solar collectors are also applied in sustainable water-treatment systems, where optical, material, and operational advances support performance under variable irradiance [118]. Collectively, these studies illustrate that AI is most powerful when embedded in hybrid frameworks, accelerating computation, enabling stochastic control, and revealing high-dimensional relationships. Figure 10 schematically shows the hybrid solar-assisted building energy system, combining photovoltaic panels, solar-thermal collectors, storage, and auxiliary units. It also reflects the AI workflow in the section: TRNSYS simulation data feed an ANN surrogate, while a genetic algorithm optimizes cost, emissions, reliability, and efficiency for adaptive system operation [59].

Comparative insights and emerging research directions

When results across the reviewed studies are compared, three notable patterns emerge. First, the reviewed literature

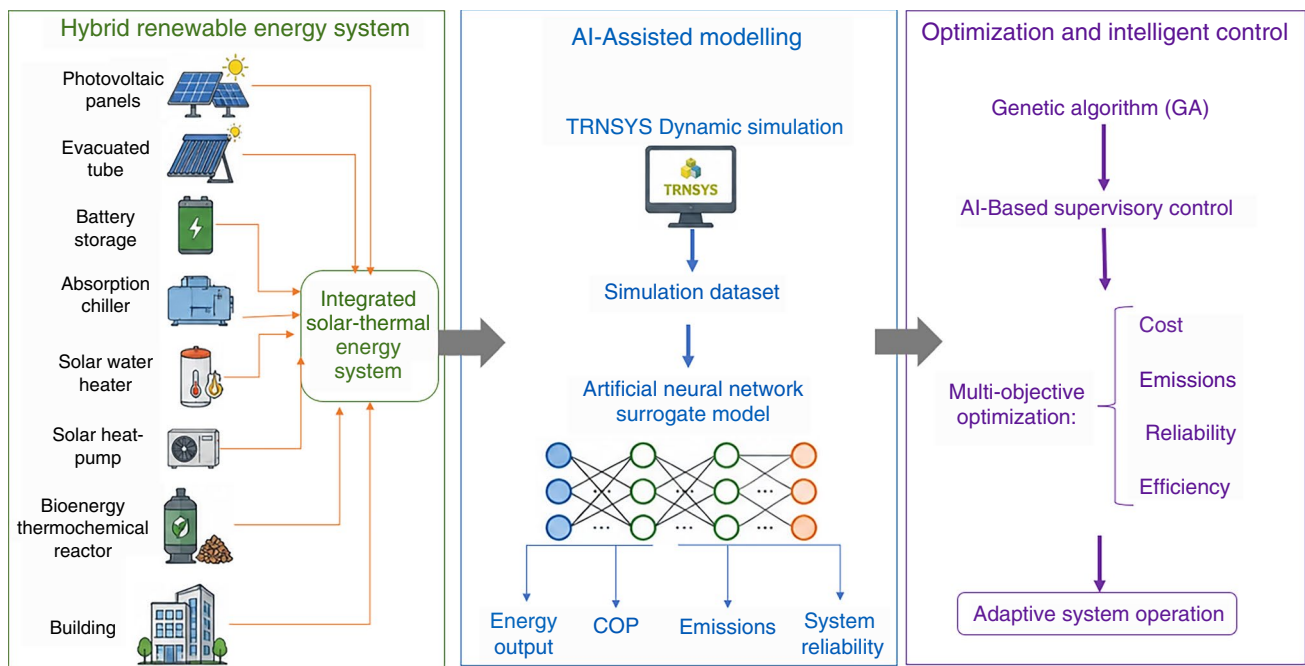


Fig. 10 Hybrid solar-thermal energy system with AI-assisted modeling and optimization

indicates that AI techniques can support nonlinear modelling and optimization, particularly in hybrid systems. Examples of AI application and proposed integration include SAHP COP prediction [104], SWHS optimization [76], and AI-enhanced hybrid solar-dryer integration proposed by [31]. Second, AI is most effective where sufficient high-quality training data exist. Studies emphasize the continued challenge of dataset availability, especially for emerging collector designs and developing region installations [76]. Third, the literature reveals a methodological shift toward hybridization: AI is not replacing physics-based models but rather augmenting them by acting as a surrogate, optimizer, or supervisory layer [31, 59, 92].

At the same time, significant gaps remain. Few studies fully integrate AI with digital-twin architectures for collectors or hybrid systems. Long-term field validation is limited. Reliability and interpretability remain open issues, particularly where AI decisions directly impact thermal safety or user comfort. Finally, the research landscape shows strong geographic imbalance, with data generation concentrated in a few regions, potentially limiting model generalizability [76]. Nevertheless, the convergence of AI, thermal storage, hybridization, and smart energy management represents a decisive step toward adaptive solar-thermal infrastructures. These developments position AI not as an auxiliary analytical tool but as a structural component of future solar-assisted energy systems. To consolidate these comparative insights, Table 8 synthesizes AI applications together with review-level and proposed approaches across solar thermal

collectors and solar-assisted energy systems, highlighting their modelling roles, optimization functions, and reported or proposed benefits. By juxtaposing studies ranging from solar water heating and heat pumps to hybrid building energy systems and solar-driven desalination, the table clarifies the breadth of AI-related work and its differing levels of maturity across sectors. The comparison distinguishes demonstrated, review-level, and proposed benefits, including improved prediction accuracy, potential reduction of experimental burden, and proposed supervisory control, while emphasizing that progress remains uneven due to data limitations and system-specific constraints.

AI applications in thermal end-use systems

Refrigeration, heat pumps, and chillers

Artificial intelligence has emerged as a decisive enabler for enhancing the performance, operational flexibility, and sustainability of refrigeration systems, heat pumps, and chillers, which collectively account for a dominant share of thermal end-use electricity consumption in buildings and district-scale energy systems. Recent sector-coupling work highlights how heat pumps and thermal storage can exploit part-load operation, thermal inertia, and multi-component interactions [2]. Related integrated control architectures transform real-time operational data into short-term forecasts and optimal control actions through

Table 8 Comparative overview of AI-related studies in solar thermal collectors and solar-assisted systems, highlighting application domains, modelling approaches, optimization roles, and reported or proposed benefits

Application domain	Primary solar component	AI method(s) used	Key objective	Performance benefit reported	Source
Hybrid hotel-building energy system with storage and absorption chiller	PV + evacuated-tube collectors	TRNSYS + ANN surrogate + GA	Cost-emissions–reliability trade-off optimization	Efficient best-compromise system design across climatic conditions	[59]
Solar water heating systems	SWHS collectors	ANN, LSTM, swarm-based optimization	System-level optimization and scheduling	Higher thermal efficiency and reliability	[114]
Solar water treatment	Parabolic solar collectors	Technology review including AI-driven automation; not an AI performance experiment	Review treatment applications, technology advances, and future directions	Reported efficiency, scalability, and reliability advances; no empirical AI gain	[118]
Solar-assisted heat pump	Solar collectors + heat-pump loop	RF, MLP, and SVM/SVR	COP prediction	RF reported the lowest error and shortest modelling time	[104]
Solar-assisted agro-waste-to-bio-fuel conversion	Solar-assisted thermochemical reactors	Performance assessment + AI/ML application review	Yield/emissions prediction and process optimization	Review-level potential to reduce experimental burden and improve prediction/control	[92]
Solar-collector modelling under changing climatic conditions	Solar collectors and tracking systems	Review of thermodynamic, CFD, NN/LSTM, and AI-assisted methods	Climate-aware collector-performance modelling	Comparative modelling insights and future research needs	[76]
Hybrid solar drying	PV/T, solar collectors, TES, biomass, and desalination	Neural networks and reinforcement learning discussed conceptually	Proposed supervisory coordination and optimization	Proposed real-time adaptive control; no demonstrated performance gain	[31]

machine learning models and metaheuristic optimization [88].

Chan et al. [42] and Kin et al. [88] demonstrated the most mature and operationally validated AI applications. Both works implement hybrid ANN–PSO frameworks trained on real operational data to predict cooling demand and equipment power consumption, subsequently optimizing chiller sequencing, chilled water supply temperature, and pump speeds in real time. Despite differences in scale and context, their results converge: System-level COP improvements of approximately 5–9% and energy savings near 5–10% are achieved without hardware retrofits. A key insight emerging from their comparison is that AI-derived benefits arise less from algorithmic novelty than from the ability to continuously reconfigure plant operation around variable-speed equipment and shifting load profiles, capabilities that static, design-based control cannot exploit.

In contrast, heat pump-oriented studies [17, 26, 30] emphasize AI as a coordination and integration layer rather than a component-level optimizer. AI is used to harmonize heat pumps with geothermal sources, wastewater heat recovery, district networks, and thermal energy storage. These works collectively show that AI-enhanced heat pump systems achieve value primarily through multi-objective optimization, simultaneously reducing cost, emissions, and peak electrical demand, rather than through COP maximization alone. Notably, AI-enabled control frameworks integrating storage and demand-side flexibility [23, 38] reveal that heat pumps act as controllable thermal batteries, where predictive control and learning-based optimization unlock load shifting and grid support services that are invisible to first-law efficiency metrics.

Ayalew and Andrzejczyk [26] reviewed PCM-based latent thermal storage for HVAC and reported case-study energy savings of approximately 10–30% and peak-load reductions

of 20–50%; these ranges concern thermal-storage integration and were not attributed specifically to AI control.

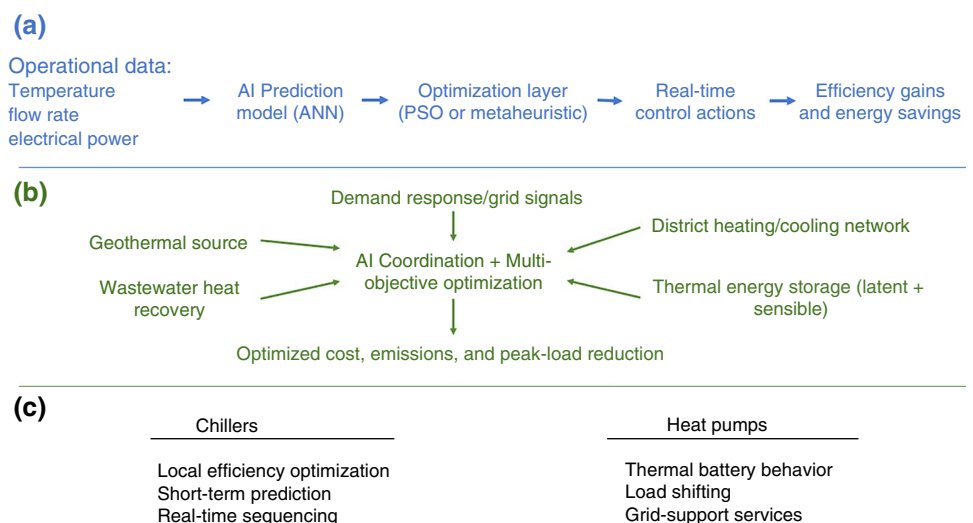
The comparative synthesis of studies indicates that the most impactful AI applications in refrigeration, heat pumps, and chillers are those that integrate predictive modeling with optimization across multiple timescales and energy vectors. Incremental efficiency gains at the component level are now well established; future innovation lies in AI frameworks that unify thermodynamic performance, storage dynamics, and grid interaction into a single, learning-enabled control paradigm. Figure 11 synthesizes the role of artificial intelligence across refrigeration systems, chillers, and heat pumps by contrasting local predictive optimization with system-level coordination. This visualization emphasizes on how AI simultaneously enhances component efficiency, integrates multiple thermal resources, and enables multi-objective control across diverse timescales.

Furnaces, dryers, and process heaters

Industrial furnaces, dryers, and process heaters represent some of the most energy-intensive thermal units across manufacturing sectors, particularly in food processing, pulp and paper, biomass conversion, and building-integrated thermal systems. Unlike power cycles, these systems operate over wide temperature ranges and are strongly influenced by transient load behavior, fuel flexibility, and process-specific constraints. The efficiency enhancement in such equipment increasingly depends on system-level integration, waste heat valorization, and data-driven operational strategies rather than isolated component upgrades.

Among the analyzed articles, the most explicit treatment of furnaces and dryers is presented through biomass-based thermal substitution. Dasappa et al., [49] demonstrated that gasifier-coupled furnaces can reliably meet both

Fig. 11 Conceptual overview of AI-enabled control in thermal end-use systems: **a** component-level AI prediction, optimization, and real-time control, **b** system-level coordination of thermal resources, and **c** comparative outcomes for chillers and heat pumps



low-temperature drying demands and high-temperature heat treatment requirements, replacing fossil fuels entirely while maintaining operational stability over extended runtimes. This study showed that a single gasification unit can supply multiple furnaces with heterogeneous temperature demands. In contrast to conventional furnace retrofits that focus primarily on burner efficiency, this system-level approach reveals that fuel switching combined with centralized thermal control yields larger economic and environmental benefits. Figure 12 synthesizes the main themes discussed in this section by illustrating how biomass gasifier-based fuel switching (Panel A), process-level efficiency improvements in steam dryer systems (Panel B), and AI-enabled monitoring with thermal energy storage (Panel C) are presented as complementary pathways toward next-generation industrial heating systems that integrate alternative fuels, waste heat recovery, and data-driven control [52].

Drying processes, especially in agro-industrial and pulp-based industries, emerge as critical energy bottlenecks. Batouta et al. [33] investigated on steam systems in a recycling pulp and paper mill. They showed that drying alone can account for the dominant share of thermal demand, with measurable reductions in energy use achievable through relatively simple interventions such as insulation, combustion optimization, and blowdown management. Steam-based dryers benefit primarily from loss minimization within existing infrastructures, whereas gasifier-driven dryers benefit from fundamental changes in fuel quality and heat delivery architecture [49]. This comparison underscores that the marginal

gains from optimization depend strongly on whether the system boundary is defined at the equipment level or the energy supply level.

Ragoowansi et al., [126] introduced a different set of constraints, notably compactness, intermittency, and low- to medium-temperature waste heat availability. The building-scale analysis of thermal energy recovery from furnaces and appliances demonstrated that a significant fraction of rejected heat lies below 300 °C and can be economically stored using phase change materials, yielding substantial primary energy savings. While this study does not directly target industrial furnaces, its implications are transferable to process heaters operating under fluctuating demand. When juxtaposed with industrial furnace studies, it becomes clear that the integration of thermal storage is more impactful in systems subject to demand–supply mismatch than in continuously operated furnaces. A recurring limitation across furnace and dryer systems is the lack of high-resolution operational data to support advanced control strategies. High-frequency end-use electrical data, although originating from residential systems, illustrate how temporal resolution fundamentally alters the perceived load profiles of thermal auxiliaries such as furnace fans and heaters [78]. Translating this insight to industrial furnaces suggests that many reported efficiencies may be overestimated when based on coarse time-averaged data. This creates an opportunity for artificial intelligence and data-driven models to bridge the gap between design efficiency and actual performance. Although several of

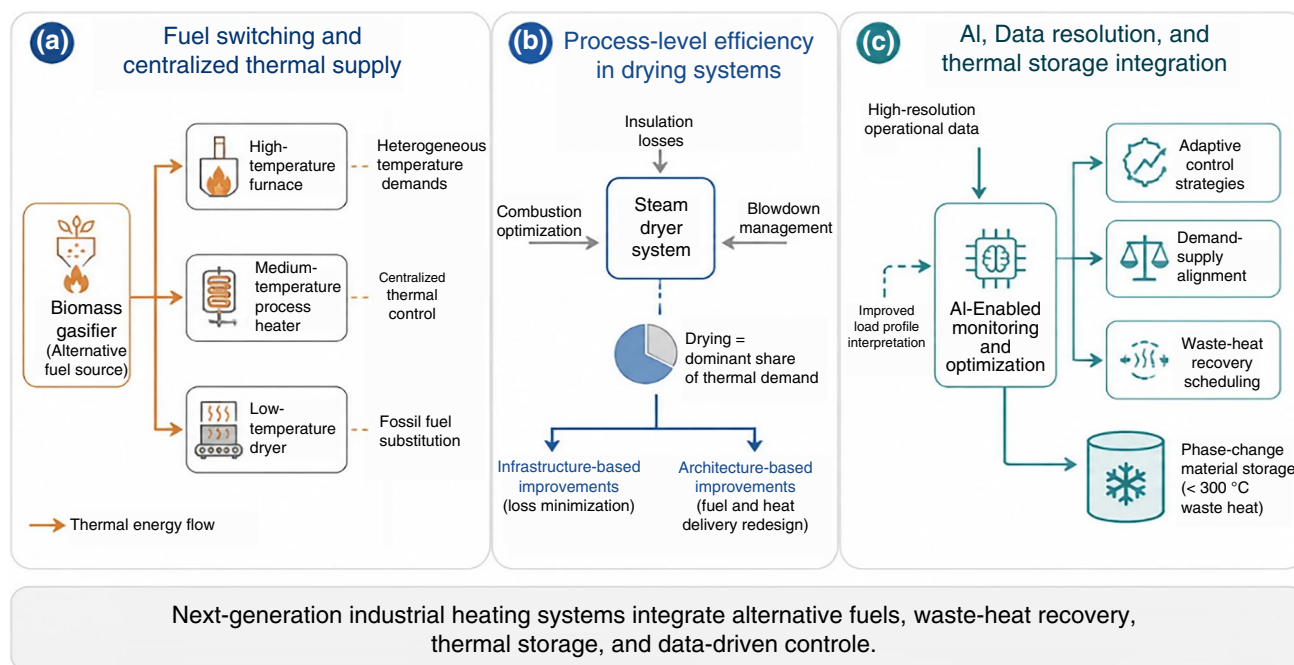


Fig. 12 Next-generation industrial heating systems integrate alternative fuels, waste heat recovery, thermal storage, and data-driven control

the provided articles are not directly focused on thermal equipment, they contribute conceptually to the emerging methodological landscape. Studies employing data-driven modeling, statistical pattern recognition, and nonlinear regression demonstrate how complex systems with multivariate dependencies can be accurately represented using limited but well-structured datasets. Table 9 summarizes the key operational characteristics, energy strategies, and reported outcomes or review-level optimization potential of furnace, dryer, and process heating technologies.

Synthesizing these findings, future development of furnaces, dryers, and process heaters is likely to combine alternative fuels, waste-heat recovery, thermal storage, and data-driven control. For solar-assisted agro-waste conversion, the reviewed literature identifies AI-based yield/emissions prediction and process optimization as potential directions rather than demonstrated system gains [92]. Consequently, research that combines thermodynamic rigor with AI-enabled monitoring and optimization is likely to define the next generation of high-performance industrial heating systems.

Crosscutting challenges, advanced AI topics, and methodological gaps

The rapid convergence of AI, sustainable fuels, digitalization, and advanced thermochemical conversion technologies is redefining the operational and strategic boundaries of modern energy systems. Despite substantial progress across biomass valorization, smart microgrids, AI-driven manufacturing, and renewable fuel pathways, the literature reveals persistent fragmentation in methodological frameworks, inconsistent evaluation metrics, and limited cross-domain integration. Addressing these challenges

is essential for transitioning from isolated optimization toward holistic, resilient, and low-carbon thermal infrastructures.

System-level integration and energy transition complexity

One of the most prominent crosscutting challenges is the need to redesign energy systems beyond simple fuel substitution. Biomass gasification, for example, has emerged as a strategic pathway for decarbonization due to its ability to produce hydrogen-rich syngas while supporting dispatchable heat and power generation [4]. However, current research remains largely fragmented, frequently addressing efficiency improvements, emissions, or reactor performance in isolation rather than evaluating their collective role within the broader energy transition.

Similarly, Alcocer et al. [13] emphasized that biomass must be embedded within multi-product biorefineries supported by process intensification, heat integration, and supply chain coordination to unlock its full systemic value. This perspective aligns with circular bioeconomy frameworks, which advocate for closing material loops through digital tools such as AI, IoT, and blockchain to enhance traceability and resource efficiency [46]. Yet, the transition toward circular and digitally enabled energy systems introduces new technological and regulatory barriers, including infrastructure constraints and the need for coordinated policy support.

Comparatively, methanol-based fuels illustrate how alternative pathways can achieve substantial greenhouse gas reductions—up to 95% relative to gasoline when produced from renewable sources, while remaining compatible with existing infrastructure [12]. Nevertheless, high production costs and toxicity concerns highlight the persistent tension between environmental performance and economic feasibility.

Table 9 Comparative overview of furnace, dryer, and process heating technologies

References	Thermal equipment type	Energy carrier	Temperature range	Optimization strategy	Primary outcome
[49]	Furnaces and dryers	Biomass producer gas	Low to high	Fuel substitution and centralized gasification	Complete fossil fuel replacement with stable operation
[33]	Pulp-and-paper mill steam system	Steam	Medium	Steam Loss reduction and combustion optimization	Thermal energy reduction
[126]	Building-scale process heaters	Waste heat	Low to medium	Thermal energy storage integration	Primary energy savings
[78]	Furnace auxiliaries	Electricity	Indirect	High-resolution load characterization	Improved realism of performance assessment
[5, 92, 109]	Solar-assisted thermochemical agro-waste conversion	Solar thermal energy and agro-waste	Process-specific	Performance assessment and review of AI applications	Yield/emissions prediction and optimization potential

From a macro-energy perspective, stationary fuel cells further demonstrate the complexity of system transformation. However, stationary fuel-cell deployment remains constrained by commercialization barriers [3]. These studies suggest that the energy transition is less a technological substitution problem than a multilayered integration challenge requiring synchronized advances in fuels, infrastructure, digitalization, and governance.

Advanced AI paradigms and digitalization of thermal energy systems

AI is increasingly positioned as a foundational enabler of adaptive, data-driven energy management. In smart buildings and local microgrids, reinforcement learning, hybrid model predictive control, federated AI, and digital twins are enabling predictive coordination of distributed resources while extending optimization toward life-cycle environmental and economic objectives [117]. However, a substantial portion of existing research still prioritizes short-term operational gains over long-term resilience.

In addition Villagran et al. [144] revealed that AI-based predictive control, deep reinforcement learning, and energy management platforms can significantly enhance microclimate regulation, solar forecasting, and thermal storage performance. Yet, persistent gaps remain in long-term validation and metric standardization, limiting cross-context comparability. Figure 13 conceptualizes the digital architecture underlying advanced AI-enabled thermal energy systems. It illustrates how physical domains, buildings, microgrids, industrial plants, and combustion systems, generate data that feed an integrated AI layer (MPC, federated learning, digital twins, regression models), potentially supporting adaptive management, efficiency gains, emission control, and long-term resilience and decarbonization [32, 122].

Industrial analytics provide complementary insights. Machine learning regression applied to compressed air systems has demonstrated measurable energy improvements of approximately 8% while achieving high predictive accuracy ($R^2 \approx 0.846$) [80]. Although seemingly localized, such plant-level intelligence illustrates the broader potential of AI to translate operational data into quantifiable decarbonization outcomes.

Notably, syngas combustion research underscores the need for adaptive modeling frameworks capable of addressing fuel variability, ignition dynamics, and emission behavior [128]. Integrating these physics-based insights with AI-driven predictive models represents a critical frontier for next-generation thermal systems. Across these domains, a consistent pattern emerges: AI technologies are advancing rapidly, yet their deployment often occurs within disciplinary silos. Bridging thermodynamic modeling, life-cycle assessment, and autonomous control remains a central methodological challenge.

Methodological gaps and emerging research directions

Beyond technological barriers, methodological inconsistencies pose a significant limitation to scientific progress. Adeoye et al. [4] indicated that research on biomass gasification has progressed through distinct developmental phases but still lacks comprehensive evaluation frameworks capable of capturing its systemic contribution to the energy transition. Similarly, sustainability assessments increasingly rely on multi-objective optimization and integrated modeling, yet these tools are rarely harmonized across studies [13]. Table 10 synthesizes the principal crosscutting challenges, digital enablers, and strategic research priorities identified across the reviewed literature.

Fig. 13 AI-driven digital architecture for resilient thermal energy systems

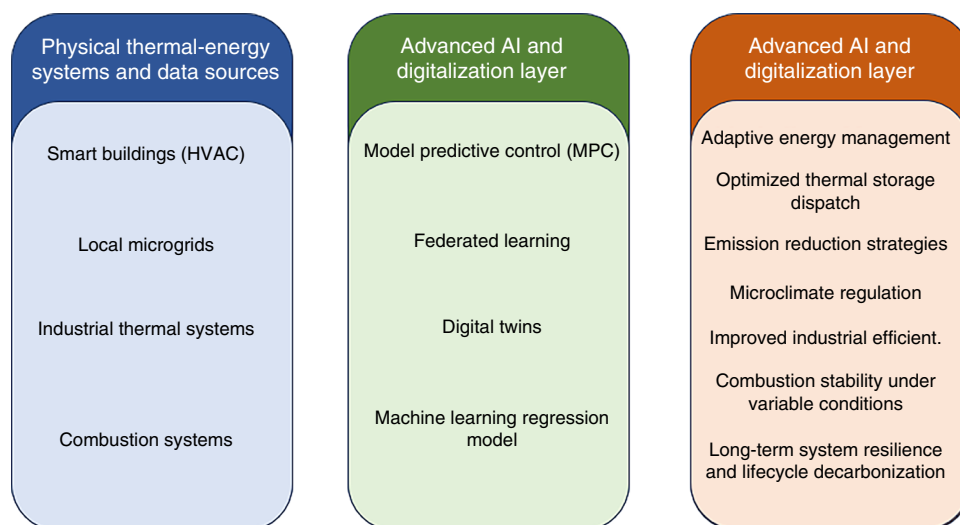


Table 10 Crosscutting challenges and methodological priorities in AI-enabled sustainable thermal energy systems

Domain	Key challenge	Digital role	Limitation identified	Strategic research direction	References
Biomass gasification	Fragmented evaluation of transition impact	Data-driven optimization	Lack of systemic frameworks	Integrated transition modeling	[4, 128]
Circular bioeconomy and energy communities	Resource-loop closure and distributed-resource coordination	IoT, blockchain, AI, transactive energy, and digital twins	Regulatory and infrastructure, and lifecycle-integration barriers	Digitalized biorefineries and lifecycle-aware energy management	[46, 117]
Biomass process design and intensification	Multi-product biorefinery integration	Process-design modeling and heat integration	Scale-up and supply-chain coordination	Sustainable integrated biorefineries	[13]
Industrial systems	Hidden efficiency losses	ML prediction	Limited scalability	Plant-to-grid analytics	[80]
Renewable fuels	Economic viability	AI process optimization	Cost and logistics constraints	Policy–technology coupling	[12]
Fuel cells	Deployment barriers	Market assessment	Commercialization constraints	Strategic deployment roadmap	[3]
Solar-assisted systems	Fragmented AI adoption	Deep learning	Lack of long-term validation	Unified AI frameworks	[144]

Digitalization offers a pathway to overcome this fragmentation. Autonomous smart biorefineries supported by open data platforms and biotechnology–nanotechnology convergence is projected as future research directions within circular bioeconomy models [46]. Meanwhile, AI-driven transactive energy frameworks propose multilayered architectures that align operational intelligence with life-cycle sustainability, highlighting the importance of integrating carbon footprint and cost metrics into optimization routines [117]. However, methodological maturity must also address socio-technical dimensions. Fuel transitions such as methanol adoption require multi-stakeholder cooperation, regulatory support, and innovation ecosystems to fully realize their sustainability potential [12]. Likewise, stationary fuel cell deployment continues to face commercialization barriers [3].

Taken together, the reviewed literature suggests that the next phase of AI-enabled thermal energy research will likely prioritize interoperable modeling environments, standardized performance indicators, hybrid physics–AI frameworks, and system-level resilience metrics. Moving beyond incremental efficiency improvements toward integrated, adaptive infrastructures will define the trajectory of sustainable thermal systems.

Future research directions

The convergence of AI with thermodynamic analysis is rapidly reshaping the design, operation, and sustainability of thermal systems. Although significant progress has been achieved in AI-based prediction and optimization of energy and exergy performance, the reviewed literature indicates

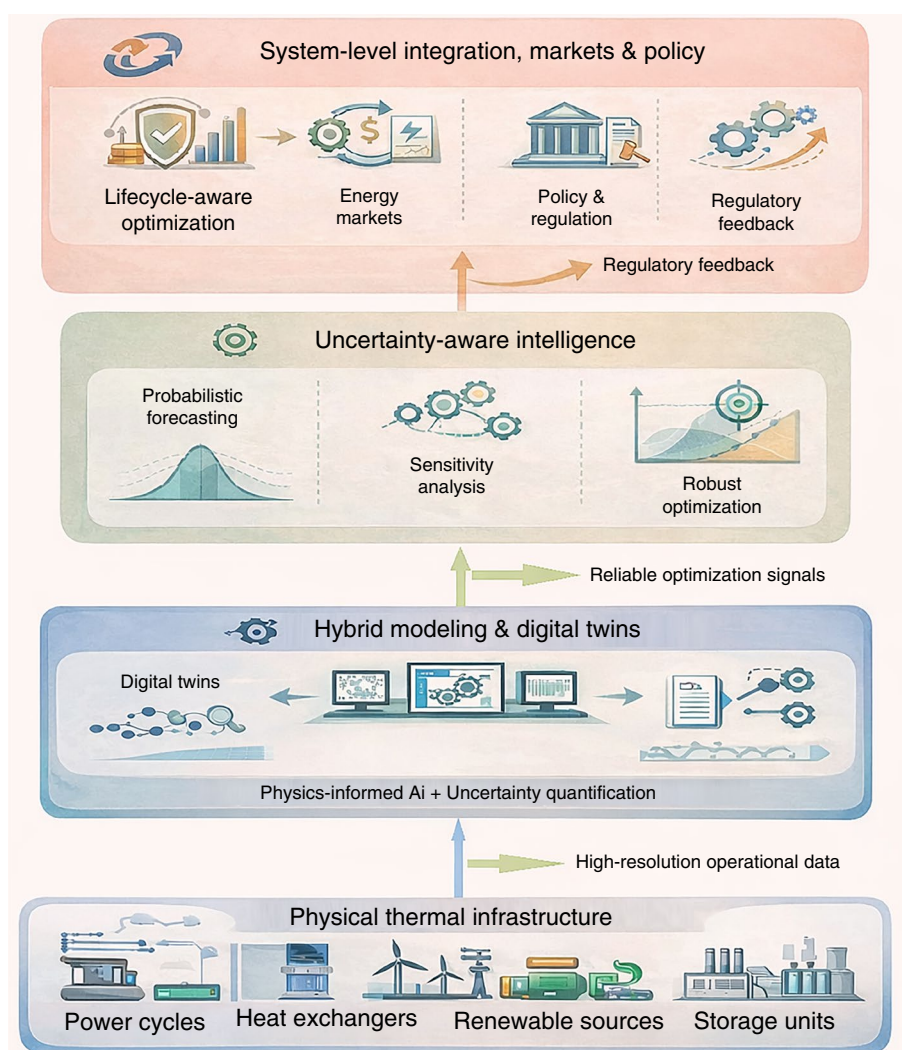
that future research must move beyond incremental efficiency improvements toward integrated, adaptive, and physically consistent energy infrastructures [68]. The emerging research landscape can be conceptualized as a multilayered architecture integrating physics-aware AI, uncertainty-resilient intelligence, and system-level governance. To synthesize the crosscutting research priorities identified in the literature, Fig. 14 presents an integrated physics–AI framework that connects physical infrastructure, hybrid modeling, uncertainty-aware intelligence, and system-level integration.

Toward physics-grounded and hybrid AI frameworks

A primary research priority is the development of hybrid modeling architectures that tightly couple machine learning with first-principles thermodynamics. Current studies increasingly employ physics-informed neural networks, solver-in-the-loop strategies, and CFD-labeled surrogates to enhance extrapolation capability and maintain thermodynamic feasibility [40]. Huang et al. [74] compared energy-storage configurations for renewable combined cooling, heating, and power systems using techno-economic indicators. Independently, future predictive models should satisfy conservation laws and avoid nonphysical outcomes such as negative entropy generation or exergy destruction.

Future frameworks must therefore incorporate systematic thermodynamic credibility checks, including mass/energy balance closure and irreversibility consistency, within training and validation pipelines. Such integration is essential because small prediction errors can still mislead optimization algorithms if physical constraints are violated [58]. An applied example is provided by Sayed et al. [132], who used ANFIS–PSO with thermal-energy and exergy outputs in a

Fig. 14 Integrated physics–AI framework for next-generation, multi-energy thermal systems



nanofluid PV/T–PCM system. Fully integrated pipelines linking feature abstraction, hierarchical targets, and optimization remain an open challenge in the present review. Advancing these pipelines will enable AI models to function not merely as predictive tools but as reliable decision support systems embedded within operational workflows.

Standardization, data ecosystems, and uncertainty-aware intelligence

Another critical direction concerns methodological standardization. The absence of unified feature definitions and evaluation protocols continues to hinder cross-study comparability and transferability across technologies [114]. Future research should prioritize interoperable modeling environments and standardized performance indicators to support reproducible AI-driven thermodynamic analysis (Deveci and Yilmaz). UQ represents an equally important frontier. Despite high predictive accuracy reported in many AI studies, uncertainty-aware modeling remains comparatively

underdeveloped, even though renewable variability, material heterogeneity, and load fluctuations can propagate nonlinearly through thermodynamic balances [48].

Emerging evidence suggests that integrating UQ and SA directly into optimization loops can produce solutions that are slightly less optimal in nominal terms but substantially more resilient under real-world conditions. In parallel, the creation of open, high-resolution datasets and digital infrastructures will be essential for training robust AI models capable of generalizing across broader operating envelopes. Autonomous smart biorefineries supported by open data platforms have already been proposed as a pathway toward digitally enabled circular bioeconomy systems [46].

System-level integration and life-cycle-aware optimization

Future research must also address the growing complexity of multi-energy systems. Stationary fuel-cell deployment faces commercialization barriers [3]. More broadly, AI-driven

optimization should expand from component-level improvements toward plant-to-grid analytics and lifecycle-aware control strategies.

Digital twins, reinforcement learning, and transactive energy frameworks are expected to enable predictive coordination of distributed resources while embedding environmental and economic metrics within operational decision-making [117]. Integrating carbon footprint, cost, and resilience indicators into optimization routines will further support the transition toward adaptive thermal infrastructures. Renewable-methanol pathways require life-cycle and techno-economic assessment of production and system-integration options [12]. These considerations highlight the need for interdisciplinary research that bridges engineering, policy, and industrial ecosystems.

The next generation of AI-enabled thermal systems will likely be defined by physics-aware learning, uncertainty-resilient optimization, standardized methodologies, and deep system-level integration. Moving toward interoperable, hybrid, and life-cycle-oriented frameworks will allow AI not only to enhance thermodynamic efficiency but also to guide the development of sustainable, intelligent energy infrastructures capable of supporting long-term decarbonization goals.

Conclusions

This review examined the rapidly evolving intersection of artificial intelligence and thermodynamic analysis, highlighting how AI-based prediction and optimization are redefining performance assessment in thermal systems. Evidence across the literature demonstrates a shift from conventional energy-only evaluation toward integrated energy–exergy frameworks that more accurately diagnose irreversibilities and guide meaningful efficiency improvements. At the same time, AI has progressed beyond surrogate modeling to become an enabling technology for diagnostics, operational control, and reliability-aware optimization. A central insight emerging from this synthesis is the growing importance of thermodynamic consistency in AI workflows. Hybrid physics–AI approaches increasingly ensure that predictive models respect conservation laws and avoid non-physical outcomes, thereby strengthening their suitability for real-world deployment. Equally important is the recognition that optimization in modern thermal infrastructures must balance multiple objectives, including efficiency, cost, environmental impact, and resilience, rather than pursuing single-metric gains.

However, the review also identifies several structural gaps that continue to limit methodological maturity. Fragmented modeling practices, inconsistent feature definitions, and the lack of standardized evaluation protocols hinder reproducibility and cross-study comparability. Moreover,

uncertainty-aware intelligence remains underdeveloped despite the nonlinear propagation of renewable variability, material heterogeneity, and operational fluctuations through thermodynamic balances. Addressing these limitations will require open, high-resolution datasets, interoperable modeling environments, and integrated validation pipelines.

Looking forward, the next generation of AI-enabled thermal systems will likely be characterized by physics-aware learning, life-cycle-oriented optimization, and deep system-level integration spanning plant-to-grid architectures. Digital twins, reinforcement learning, and transactive energy frameworks are poised to support predictive coordination of distributed resources while embedding environmental and economic indicators into operational decision-making. Ultimately, moving beyond incremental efficiency improvements toward adaptive and physically consistent infrastructures will be essential for supporting long-term decarbonization and sustainable energy transitions.

At the same time, the conclusions of this review are limited by the heterogeneity of published datasets, inconsistent reporting of model validation procedures, and the limited availability of external validation across technologies. Therefore, the performance gains reported in individual studies should be interpreted as application-specific rather than universal until benchmark datasets and standardized thermodynamic validation protocols become available.

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Data availability No datasets were generated or analyzed during the current study.

Declarations

Conflict of interest The authors declare no conflict of interest.

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