Policy Research Journal
ISSN (E): 3006-7030 ISSN (P) : 3006-7022 Volume 4, Issue 2, 2026

MULTI-SCALE THERMO-FLUID OPTIMIZATION OF HIGH-EFFICIENCY ENERGY CONVERSION SYSTEMS USING COUPLED COMPUTATIONAL AND EXPERIMENTAL FRAMEWORK

Hozaifah Shahadat Ali[*1], **Imran Hussain**[2]

[*1]*Department of Mechanical Engineering, University of Cassino*
[2]*Department of Physics Allama Iqbal Open University Islamabad*

[*1]hozaifah72@gmail.com, [2]himran873@gmail.com

DOI: https://doi.org/10.5281/zenodo.18858703

Keywords
multi-scale thermo-fluid optimization, conjugate heat transfer, topology optimization, data assimilation, digital twins, reduced-order modeling, supercritical CO_2 cycles, fuel cells (PEMFC/SOFC), low-grade waste heat recovery, micro-PIV/LIF, nuclear microreactors, physics-informed machine learning

Article History
Received: 29 December 2025
Accepted: 14 February 2026
Published: 28 February 2026

Copyright @Author

Corresponding Author: *
Hozaifah Shahadat Ali

Abstract

High-efficiency energy conversion systems operating under dynamic and off-design conditions demand integrated multi-scale thermo-fluid optimization that seamlessly bridges molecular interfacial science, pore-scale transport, continuum-level conjugate heat transfer, and full-system performance. This review presents a comprehensive coupled computational-experimental framework for the design and optimization of next-generation technologies, including low-temperature thermal energy conversion systems (LT-TECS), proton exchange membrane and solid oxide fuel cells (PEMFC/SOFC), supercritical CO_2 power cycles, and nuclear microreactors. Advanced methodologies such as topology optimization with improved Darcy-penalty formulations, physics-informed reduced-order models (ROMs), machine learning surrogates, and data assimilation techniques are shown to resolve nonlinear multi-physics interactions while significantly reducing computational cost. Experimental validation relies on high-resolution laser-based diagnostics (micro-PIV/LIF, thermographic PIV, hybrid IR/seed-gas techniques) and uncertainty-quantified measurements. The framework achieves notable performance gains: up to 15% reduction in peak temperatures and 40% lower thermal resistance in microelectronic cooling, >2% improvement in electrical output for LT-TECS, and >70% electrical efficiency potential in hybrid SOFC systems. The synthesis of high-fidelity modeling, intelligent digital twins, and real-time experimental feedback enables autonomous control, adaptive operation, and rapid design iteration, providing a transformative pathway toward resilient, decarbonized, and high-density energy conversion in the era of variable renewables and industrial waste-heat recovery.

INTRODUCTION

The transition of the global energy landscape is currently defined by a dual pressure: the escalating demand for high-density, dispatchable power and the urgent requirement for decarbonization across industrial and residential sectors (OECD Nuclear Energy Agency, 2025). As the world experiences a growing share of volatile renewable energy sources, the necessity for high-efficiency energy conversion systems that can operate under dynamic, off-design conditions has never been greater (Corigliano et al., 2022). This imperative has catalyzed the development of multi-scale thermo-fluid optimization frameworks that bridge the traditional divide between

fundamental molecular science, pore-scale transport, and macroscopic system engineering (Energies, 2025) Central to this evolution is the integration of high-fidelity computational models with sophisticated experimental feedback loops, enabling the design of systems that are not only efficient but also resilient to the stochastic nature of real-world boundary conditions (Abd Ali, 2026).

2. Macro-Scale Drivers and the Efficiency Imperative

The global energy system is undergoing a profound transformation driven by rapid digitalization, particularly the proliferation of data centers, and the growing demand for resilient power sources in both OECD nations and the Global South (Palley et al., 2025). Against this backdrop, small modular reactors (SMRs) and nuclear microreactors have emerged as critical low-carbon energy infrastructure, seeing a surge in private investment that reached approximately USD 5.4 billion by 2023 (Liu et al., 2025). However, the deployment of such advanced systems is constrained by the inherent complexity of their thermo-fluid interactions, which often involve high-temperature gradients, turbulent flows, and multi-phase dynamics (Tunkle et al., 2025).

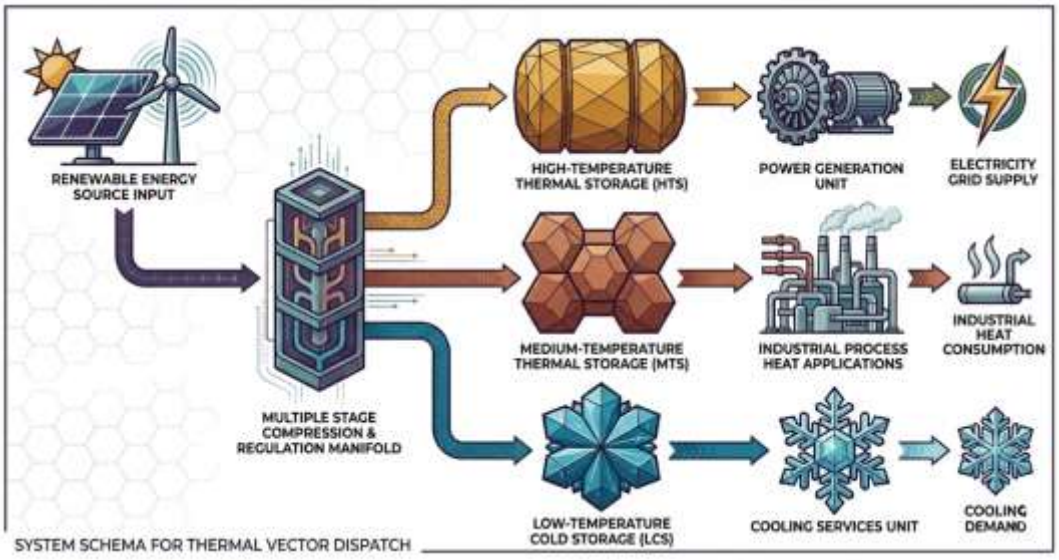


Figure 1. System Schema for Multi-Vector Thermal Dispatch and Cascade Energy Conversion

In the industrial sector, more than 50% of waste heat is dissipated at temperatures below 200 degrees C, where conventional power cycles operate with severely limited efficiency. Low-Temperature Thermal Energy Conversion Systems (LT-TECS), including thermoelectric and electrochemical hybrid configurations, offer a promising solution to recover this "low-grade" heat, yet their practical application has been historically hindered by strong nonlinear behaviors and a lack of physics-informed control strategies (Wu et al., 2025). The optimization of these systems requires a fundamental shift toward multi-energy systems (MES) that integrate electricity, heating, and cooling demands with variable energy sources (Bakircioglu et al., 2025). Traditionally, these problems were tackled using mixed-integer linear programming (MILP) or non-linear programming (MINLP) over fixed horizons, but the emergence of fluctuating weather patterns and socio-economic disruptions necessitates more robust, adaptive frameworks (Beyer, 2025).

Table 1: Overview of Energy System Types and Optimization Targets

Energy System Type	Temperature Regime	Conversion Efficiency Range	Primary Optimization Target
LT-TECS (Waste Heat Recovery)	Under 200 C	1% - 14%	Nonlinear control, adaptive physics-informed loops (ResearchGate, 2025)
PEM Fuel Cells (PEMFC)	60 C - 80 C	40% - 60% (Elec.)	Water/thermal management uniformity (MDPI, 2025)
Solid Oxide Fuel Cells (SOFC)	600 C - 1000 C	60% - 85% (Cogen)	Thermal stress, electrode microstructure (Zeng et al., 2025)
Supercritical CO2 Cycles	500 C - 800 C	40% - 56%	Fluid blends, heat exchanger compactness (Bakircioglu et al., 2025)
Nuclear Microreactors	600 C - 900 C	45% - 60%	Autonomous load-following, heat recovery

3. Fundamental Physics Across Scales: From Molecular to Continuum

The optimization of energy conversion begins at the smallest scales, where molecular interactions determine the transport properties and reaction kinetics that ultimately drive macroscopic performance. A critical challenge in current thermo-fluid modeling is the failure of continuum-scale models to accurately reflect the complexity of reactive interfaces (Chen, 2025). Traditionally, these models utilize fixed parameters derived from simple averaging across a wide physicochemical range. However, recent molecular-scale studies have revealed the stochastic nature of surface sites, where reaction mechanisms, rates, and products can vary significantly even across a single surface (Ilgen et al., 2024).

3.1. Molecular-Scale Interfacial Science

A conceptual shift is currently underway, proposing to represent surface properties such as site acidities, charge densities, and solvation energies with probability distributions rather than discrete constants (French et al., 2010). By incorporating molecular details into larger-scale reactive transport models (RTMs), researchers can improve the predictive accuracy of systems involving solid-water or solid-gas interfaces, which are critical in fuel cell catalysts and heat exchanger surfaces (Qiu et al., 2025). This integration requires exponentially rising computational power, necessitating the use of next-generation algorithms that can bridge the molecular-to-continuum gap without resorting to brute-force increases in mesh density (Becker, 2025).

3.2. Micro- and Nanofluidic Transport Phenomena

As system dimensions shrink to the micro- and nanoscale, dominant surface forces such as surface tension, capillary forces, and fluid-solid interactions begin to deviate significantly from classical continuum predictions (Mehmani et al., 2019). In microfluidic systems, flow is typically characterized by extremely low Reynolds numbers (Re <= 1), leading to a predominance of laminar flow and precise control over sample transport (Xie & Li, 2023). However, the increased surface-area-to-volume ratio means that wall forces and wettability play a decisive role in pressure drop and heat transfer performance (Yu et al., 2025).

In nanoporous media, phenomena such as adsorption layers and steric exclusion can dominate flow mechanisms. For example, in energy storage systems based on the forcible wetting of hydrophobic pores, the hysteresis of the wetting/drying cycle results in energy dissipation (Fraux et al., 2017). Optimization in this regime involves tailoring pore diameters to minimize this hysteresis, which can simultaneously improve stored-energy density and cycling reversibility. This requires a nuanced understanding of how molecular-level interface science interacts with mesoscale transport (Nguyen et al., 2025).

Table 2: Physical Governing Physics and Modeling Focus Across Scales

Scale	Representative Length	Governing Physics	Modeling Focus
Molecular	Angstroms to Nanometers (nm)	Intermolecular collisions, adsorption, reaction kinetics	DFT, Molecular Dynamics (MD), Probabilistic distributions (Energies, 2025; Ilgen et al., 2024)
Pore	Micrometers to Millimeters (mm)	Localized phase distribution, capillary forces, surface tension	Lattice Boltzmann Method (LBM), Pore-network models (Energies, 2025)
Continuum (REV)	Millimeters to Meters	Navier-Stokes equations, Darcy's law, effective properties	CFD, Finite Volume Method (FVM), Finite Element Method (FEM) (Energies, 2025; Smith et al., 2025)
System	Meters to Kilometers	Integrated energy balance, load-following, economic dispatch	System codes, Digital Twins, MILP optimization (Energies, 2025; Preprints.org, 2025)

4. Advanced Computational Optimization Frameworks

High-efficiency energy conversion systems demand sophisticated computational frameworks that can resolve the complex interactions between solid and fluid phases, particularly in high-power-density applications such as microelectronic cooling and advanced heat exchangers (Thermal-Fluid Topology Optimization, 2025).

4.1. Coupled Thermo-Fluid Modeling and Conjugate Heat Transfer

Unified thermo-fluid modeling platforms are increasingly incorporating incompressible Navier-Stokes equations with transient heat conduction and transfer equations. Using hybrid FEM/FVM numerical schemes allows for the effective treatment of complex geometries and nonlinear interactions at solid-fluid interfaces (Ranjbarzadeh et al., 2025). In representative microelectronic cooling systems including microchannel heat sinks, nanofluid-imbued channels, and phase-change-aided hybrid systems coupled modeling has proven to be over 12% more effective in predicting temperatures compared to decoupled models (Wali et al., 2025). Multi-objective optimization schemes targeting the reduction of maximum device temperature, thermal resistance, and temperature non-uniformity have achieved peak temperature decreases of up to 15% (Smith et al., 2025).

4.2. Topology Optimization and the Darcy Penalty Challenge

Topology optimization (TO) provides an expansive design freedom by allowing the complete distribution of cooling channels to be optimized simultaneously, rather than being restricted to sizing or shape parameters. This methodology is particularly relevant for the design of liquid-cooled heat sinks manufactured through modern additive techniques (ResearchGate, 2025). However, TO for conjugate heat transfer systems is fraught with accuracy issues, specifically within the widely used Darcy penalty model (Ahmad et al., 2025).

The Darcy penalty model often fails to satisfy the no-slip condition at the solid-fluid interface, leading to "leakage flow" in the solid region. This leakage induces artificial advection cooling, which is especially problematic in thermal-fluid problems where accurate boundary layer resolution is essential (John et al, 2019). Improved hydraulic models, where the viscosity in the Darcy penalty term is a function of porosity, have shown promise in achieving grid-independent temperatures and more reliable optimized designs (Delpishehet al., 2024). Furthermore, continuous adjoint approaches combined with monolithic solvers have allowed for the optimization of conjugate heat transfer systems with significantly lower thermal compliance up to 6.7% lower while using 44%

less volume compared to traditional finned heatsinks (Bhattacharyya et al., 2025).

4.3. Machine Learning and Model Reduction Strategies

The high computational cost of high-fidelity CFD simulations limits their use in real-time monitoring and rapid design iteration. To address this, researchers are turning to Reduced-Order Models (ROMs) and machine learning surrogates (Bertram et al., 2018). Proper Orthogonal Decomposition (POD) is a common technique used to create scalable ROM libraries from CFD data, capturing the essential thermal dynamics of a system with minimal degrees of freedom (Mao et al., 2025).

Supervised machine learning models including Neural Networks, Decision Trees, and Support Vector Regression are then trained to predict optimal ROM configurations for given operating conditions. In applications such as headlamp heatsink thermal management, Neural Networks have achieved high predictive accuracy, enabling rapid digital twin updates (Na'im Abdullah, 2026). Beyond simple surrogates, hybrid computational approaches that combine low- and high-fidelity fluid models can reduce core-hour costs by 59% to 86% while retaining the majority of performance gains (Rajashekaraiah et al., 2025).

5. Integrated Experimental Frameworks and Diagnostics

The validation of multi-scale models requires experimental frameworks capable of high-resolution, non-intrusive measurements across diverse flow and temperature regimes (Kim & Kihm, 2025).

5.1. High-Resolution Laser-Based Techniques

Particle Image Velocimetry (PIV) and Laser-Induced Fluorescence (LIF) remain the cornerstone of experimental thermo-fluids. PIV uses precisely timed pulsed light sources to track fluorescent particles, providing whole-field velocity information (Alwafi et al., 2022). In micro-particle image velocimetry (micro-PIV), the entire test section is illuminated volumetrically, which poses challenges for the signal-to-noise ratio but allows for sub-millimeter diagnostics (Voulgaropoulos et al., 2022).

The combination of PIV with two-color LIF enables the simultaneous measurement of instantaneous temperature and velocity fields. This is critical for investigating the hydrodynamic properties of micro-scale flows, such as the buoyancy-driven fields in heated channels or the flow surrounding migrating bubbles in capillaries (Hiromasa et al., 2023). Recent developments in thermographic PIV, which uses seeded phosphor particles to simultaneously capture temperature and velocity, have demonstrated 3 K accuracy in heated air jets (Naumann et al., 2026). This direct visualization of heat and mass transfer is indispensable for understanding turbulent heat fluxes in stagnation and self-similar regions (Carlomagno & Cardone, 2013).

5.2. Hybrid Measurements and Uncertainty Quantification

Advanced measurement frameworks are increasingly adopting hybrid approaches to overcome individual technique limitations. A notable example is the combination of Infrared (IR) thermography with the seed gas concentration technique for film cooling measurement (Shi et al., 2025). While IR thermography provides high-spatial-resolution surface temperature maps, it can be sensitive to thermal disturbances and facility-induced errors (He et al., 2025). The seed gas concentration technique serves as an in-situ calibration ground truth, correcting for imperfect insulation and viscous dissipation effects, thereby yielding results that are both highly accurate and spatially resolved (Ali et al., 2025).

Uncertainty quantification (UQ) is equally critical, especially when experimental data is used to validate CFD codes. Facilities like the MIR (Matched Index of Refraction) permit non-intrusive measurements through complex models, but they require robust UQ methods to account for particle motion, image distortion, and data processing errors (Avramova et al., 2021). Techniques such as the Uncertainty Surface Method and the Signal-to-Noise Ratio

method are being developed to quantify the uncertainty of every vector in space and time, providing a reliable basis for code-to-code comparison and validation (Furlong et al., 2025).

Table 3: Summary of Experimental Methods and Resolution

Experimental Method	Primary Data	Spatial Resolution	Key Error Sources
micro-PIV / LIF	Velocity + Temperature	75 um x 67 um	Brownian motion, particle accumulation (MDPI, 2025; Kihm et al., 2025)
Thermographic PIV	Flow + Temp Imaging	Sub-millimeter	Multiple scattering, non-uniform laser profile (Carlomagno & Cardone, 2013)
High-Speed IR	Surface h (2D)	Full 2D Map	Lateral conduction, thermal inertia (Carlomagno & Cardone, 2013)
Hybrid IR/Seed Gas	Film Cooling Effectiveness	Full Surface	Facility disturbances, ingress/egress (Carlomagno & Cardone, 2013)

6. Data Assimilation and State Estimation

Data assimilation (DA) represents the synthesis of physical knowledge with experimental data. By merging governing equations the physical constraints with sparse, noisy measurements and statistical error models, DA transforms predictive solvers into adaptive estimators (Cheng et al., 2023).

6.1. DA Mechanisms in Thermo-Fluid Systems

Unlike purely data-driven machine learning, DA relies on a predictive physical model, allowing for the determination of initial fields or unmeasured states using limited time-series measurements (Succetti et al., 2025). Deterministic DA methods, such as the Kalman filter (KF) and three-dimensional variational (3D-VAR) methods, have shown robustness against varied noise types in natural circulation loops (Shu, 2024). These frameworks are capable of significant uncertainty reduction in state variables and parameter estimation, even under challenging oceanic conditions for nuclear system analysis (Adumene et al., 2022).

In experimental fluid dynamics, DA is being used for multi-physical-field reconstruction, data analysis, and measurement data augmentation. By blending partial observations with governing equations, high-fidelity trajectories can be produced that are anchored to real data (Luo et al., 2024). This is particularly useful for state estimation in complex thermo-fluid systems where full optical access or dense sensor placement is impossible (Hu et al., 2025).

6.2. ROM-Based Data Assimilation

To alleviate the high computational cost of high-fidelity solvers in the DA loop, Reduced-Order Models are often employed. These models preserve the underlying physics while drastically reducing the number of degrees of freedom, enabling near-real-time state estimation and control (Kadeethum et al., 2022). This is a fundamental requirement for physics-aware digital twins that must operate at or faster than real-time to provide useful diagnostic feedback or adaptive control signals (Faraji et al., 2025).

7. High-Efficiency Energy Conversion Technologies

The multi-scale optimization framework is being applied across a spectrum of advanced energy conversion technologies, each with unique thermo-fluid challenges (Sarkar, 2024).

7.1. Low-Temperature Thermal Energy Conversion (LT-TECS)

LT-TECS are critical for recovering low-grade waste heat from industrial and geothermal sources. Optimization in this regime often utilizes surrogate-assisted, physics-based strategies to construct control maps (Šturek et al., 2025). Time-domain simulations have shown that adaptive control loops can increase average electrical power output by up to 2.2% and

conversion efficiency by 0.7 percentage points compared to conventional control, while reducing load and heat-flux fluctuations by up to 40% (Bergström et al., 2025). These gains are achieved without hardware modifications, highlighting the efficacy of simulation-driven optimization. Experimental investigations into sand-fluidized reactors have further demonstrated that inlet design is crucial for performance, with Ring configurations increasing electrical output by 25% (Vargas-Salgado et al., 2021).

7.2. Advanced Fuel Cell Systems (PEMFC and SOFC)

In Proton Exchange Membrane Fuel Cells (PEMFCs), thermal and water management are intricately linked. Excessive temperatures can accelerate degradation, while improper hydration leads to either membrane dehydration or electrode flooding (Veza, 2025). Optimized multi-fin channel configurations on bipolar plates have demonstrated a 13 K reduction in cathode temperature and a 40% increase in power density. Experimental validation of these designs shows a deviation of less than 3% from CFD predictions (Saeed et al., 2025).

Solid Oxide Fuel Cells (SOFCs) operate at significantly higher temperatures (600-1000 C), offering higher efficiency up to 85% in cogeneration applications but posing severe thermal stress challenges (Haider et al., 2021). Multiscale modeling for SOFCs involves a top-down approach integrating stack configurations with electrode microstructure. Techniques like Generative Adversarial Networks (GANs) are being used for the fast, low-cost construction of 3D heterogeneous models to optimize mesoscopic electrode behavior (Jang et al., 2025). Furthermore, hybrid SOFC configurations with gas turbines have the potential to achieve electrical efficiencies exceeding 70% (Alfaifi et al., 2025).

7.3. Supercritical CO2 (sCO2) Power Cycles

The sCO2 Brayton cycle is a high-efficiency alternative to the standard steam-Rankine cycle, particularly suited for concentrated solar power (CSP) and nuclear reactors. Its primary advantage is the high fluid density near the critical point, which reduces compression work and allows for more compact turbomachinery (Qiu et al., 2025). Thermal efficiencies of over 50% are targeted, but sCO2 cycles are sensitive to the high ambient temperatures often found at solar sites (Wali et al., 2025). Research into sCO2 blends using dopants like TiCl4, R32, or Toluene has shown that these binary mixtures can maintain efficiencies above 50% even when minimum cycle temperatures are as high as 55 degrees C (Nguyen et al., 2025). Optimization of cycle layouts depends on whether the goal is maximum thermal efficiency, which peaks in the recompression cycle at approximately 55.95%, or maximum heat storage temperature difference, where the regenerative cycle excels (Na'im Abdullah, 2026).

Table 4: Performance Comparison of Supercritical CO2 Power Cycle Types

sCO2 Cycle Type	Key Advantage	Max Thermal Efficiency	Performance Factor
Simple Cycle	Layout simplicity	17.73%	Lowest exergy efficiency (Bakircioglu et al., 2025)
Recuperator Cycle	Improved heat recovery	19.26% - 32%	Standard benchmark (Bakircioglu et al., 2025)
Split Cycle	Enhanced exergy performance	23.56%	High pressure ratios (Bakircioglu et al., 2025)
Recompression	High-efficiency peak	55.95%	Requires complex split ratio (Bakircioglu et al., 2025)
Regenerative	High specific work	-	Ideal for heat storage (Bakircioglu et al., 2025)

7.4. Nuclear Microreactors and Autonomous Control

Nuclear microreactors, like the Holos-Quad design, provide self-contained power generation in 40-ft ISO containers for remote or emergency use. The system utilizes a helium-cooled direct Brayton cycle with an integrated bottoming Organic Rankine Cycle (ORC) to recover waste heat, increasing overall thermal efficiency from 45% to 60% (Avramova et al., 2021).

The optimization of these reactors involves autonomous load-following, achieved through the rotation of eight control drums containing boron carbide (B4C) neutron absorbers. Reinforcement learning (RL) algorithms have been successfully applied to this control problem, leveraging the microreactor's symmetry to reduce training time (Kim & Kihm, 2025). These RL-based controllers outcompete traditional standards, especially in scenarios with imperfect reactor feedback, taking a significant step toward real-time automated nuclear control (He et al., 2025).

8. The Emergence of Intelligent Digital Twins

The culmination of coupled computational and experimental frameworks is the Intelligent Digital Twin (DT). A DT is a virtual replica that mirrors the state and behavior of a physical asset in real-time, enabling monitoring, simulation, and analysis throughout its lifecycle (Ali et al., 2025).

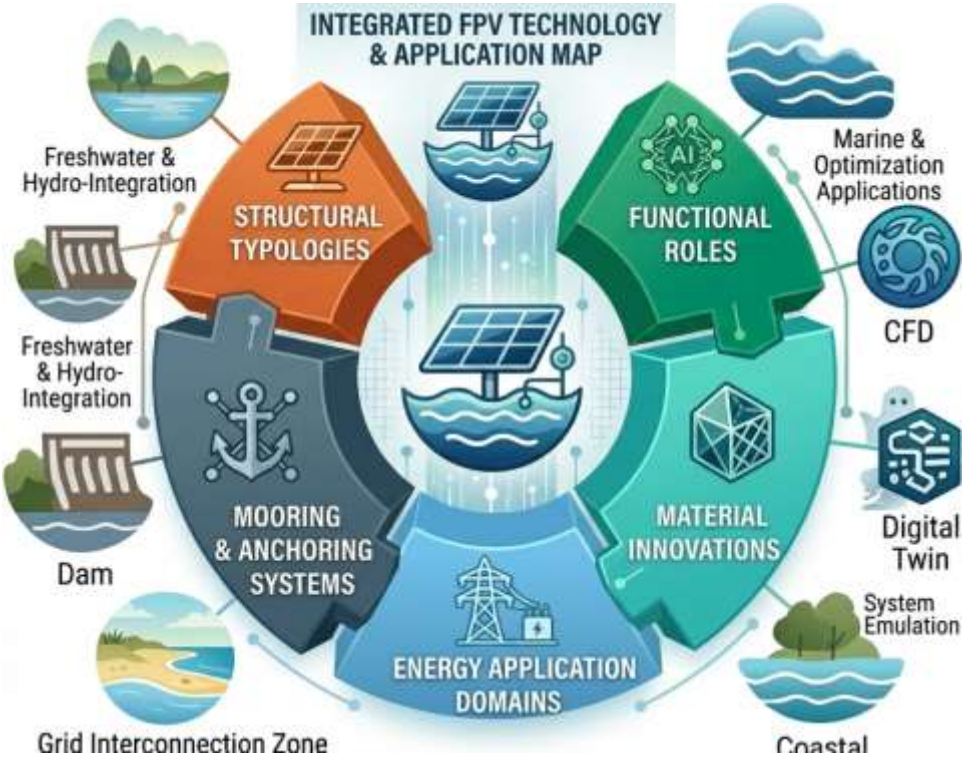


Figure 2. Integrated Floating Photovoltaic (FPV) Technology Application Map and System Interconnection Domains

8.1. DT Methodology and Architectures

In the nuclear industry, Argonne National Laboratory has developed DT methodology using Graph Neural Networks (GNNs) (Hiromasa et al., 2023). GNNs represent the reactor system as a network of connected parts (nodes and edges), facilitating a comprehensive understanding of dynamic behavior and the prediction of transients based on sparse sensor data (Furlong et al., 2025). These twins can rapidly predict reactor response to changes in power output or cooling performance, outperforming traditional system codes in speed and accuracy (Liu et al., 2025).

For gas turbines, hybrid AI methodologies for DTs are classified into four mature levels:

- **ANN-Augmented Thermodynamic Models**: These couple classical GPA (Gas Path Analysis) with neural networks for component-level diagnostics and health tracking (Preprints.org, 2025).
- **Physics-Integrated Operational Architectures**: These integrate live SCADA data with modular physics models for fleet-wide optimization (Ranjbarzadeh et al., 2025).
- **Generative and Model-Discovery Approaches**: These utilize techniques like GANs for synthetic data generation for rare fault events or SINDy for extracting governing equations from data (Xie & Li, 2023).

8.2. Operational Impact and Savings

The integration of digital twins into building energy models (BEMs) and industrial cooling systems has demonstrated significant efficiency gains (Nguyen et al., 2025). Using containerized BEMs and surrogate models, heating energy savings of 10-15% have been achieved during winter operation without any HVAC retrofit (French et al., 2010). In droplet microfluidics and microchannel cooling, deep reinforcement learning-enabled digital twins have achieved droplet size control within a CV% below 5%, outperforming systems without such control (Palley et al., 2025). The reliability of these systems is strongly dependent on the underlying meteorological data base used for sizing (Beyer, 2025).

9. Conclusions

The multi-scale thermo-fluid optimization framework presented in this review establishes a new paradigm for the design and operation of high-efficiency energy conversion systems by tightly coupling fundamental molecular and interfacial science with continuum-scale transport phenomena and system-level performance. Through the integration of topology optimization, physics-informed reduced-order models, machine learning surrogates, and advanced experimental diagnostics (micro-PIV/LIF, thermographic PIV, hybrid IR techniques), the framework overcomes longstanding limitations in predicting and controlling nonlinear, multi-physics behaviors under realistic dynamic conditions.

Demonstrated performance improvements such as 15% lower peak temperatures in microelectronic cooling, 2–25% gains in low-temperature thermal energy conversion, and the pathway to >70% electrical efficiency in hybrid fuel-cell systems highlight the framework's ability to deliver tangible efficiency, compactness, and resilience gains without requiring hardware overhauls. The emergence of intelligent digital twins, enabled by data assimilation and real-time state estimation, further transforms these systems from static designs into adaptive, self-optimizing assets capable of autonomous load-following and fault-tolerant operation.

As global energy systems increasingly rely on variable renewables and low-grade waste heat recovery, this coupled computational-experimental approach provides the essential scientific and engineering foundation for accelerating the deployment of next-generation technologies, including small modular reactors, supercritical CO_2 cycles, and advanced fuel cells. Future progress will hinge on continued refinement of cross-scale bridging methods, enhanced uncertainty quantification, and broader industry adoption of digital-twin platforms. Ultimately, the framework offers a powerful, scalable route to decarbonized, high-density, and resilient energy conversion critical for meeting the intertwined challenges of rising demand, climate imperatives, and system flexibility in the decades ahead.

References

Bakırcıoğlu, V., Jond, H. B., & Yılmaz, F. (2025). Multi-objective optimization and thermodynamic analysis of a supercritical CO_2 Brayton cycle in a solar-powered multigeneration plant for net-zero emission goals. Energies, 17(23), Article 6001. https://doi.org/10.3390/en17236001

Beyer, H.-G. (2025). Repercussions of interannual variability in irradiance on sizing PV for autonomous renewable energy systems. *PURE Faroe Islands*. https://www.pure.fo/en/publications/beyer-hans-georg-repercussions-of-interannual-variability-in-irra/

Carlomagno, G. M., & Cardone, G. (Eds.). (2013). *Infrared thermography for thermo-fluid-dynamics*. Springer. https://doi.org/10.1007/978-3-642-29508-9

Tunkle, L., Abdulraheem, K., Lin, L., & Radaideh, M. I. (2025). Nuclear microreactor control with deep reinforcement learning. arXiv. https://doi.org/10.48550/arXiv.2504.00156

Energies. (2025). Fluid flow and heat transfer in porous media: A multiscale perspective that bridges molecular, pore, and macroscopic levels. *Energies*, *18*(4), 976. https://www.mdpi.com/1996-1073/18/4/976

Ilgen, A. G., Borguet, E., Geiger, F. M., Gibbs, J. M., Grassian, V. H., Jun, Y.-S., Kabengi, N., & Kubicki, J. D. (2024). Bridging molecular-scale interfacial science with continuum-scale models. Nature Communications, 15(1), Article 5326. https://doi.org/10.1038/s41467-024-49598-y

Kim, H. J., & Kihm, K. D. (2005). Measurements of temperature and flow fields with sub-millimeter spatial resolution using two-color laser induced fluorescence (LIF) and micro-particle image velocimetry (PIV). Journal of Mechanical Science and Technology, 19(2), 716–728. https://doi.org/10.1007/BF02916193

Liu, Y., Alsafadi, F., Mui, T., O'Grady, D., & Hu, R. (2025). Development of whole system digital twins for advanced reactors: Leveraging graph neural networks and SAM simulations. *Nuclear Technology*. https://doi.org/10.1080/00295450.2024.2385214

OECD Nuclear Energy Agency. (2025). *SMR dashboard - Third edition*. https://www.oecd-nea.org/upload/docs/application/pdf/2025-09/web_-smr_dashboard-_third_edition.pdf

Palley, B., Martins, J. P., Bernardo, H., & Rossetti, R. (2025). Integrating machine learning and digital twins for enhanced smart building operation and energy management: A systematic review. *Applied Sciences*, *9*(6), 202. https://www.mdpi.com/2413-8851/9/6/202

Preprints.org. (2025). *Survey of current research and industrial practices for gas turbine intelligent digital twins*. https://www.preprints.org/manuscript/202509.1360

ResearchGate. (2025). *Data assimilation: New impetus in experimental fluid dynamics*.(https://www.researchgate.net/publication/390832640_Data_assimilation_new_impetus_in_experimental_fluid_dynamics)

ResearchGate. (2025). *Performance improvement of low-temperature thermal energy conversion systems via physics-based control and optimization*. https://www.researchgate.net/publication/400352497

Abd Ali, S. A. M. (2026). Experimental configuration and operating parameters of the thermo-fluid energy conversion system. Al-Rafidain Journal of Engineering Sciences, 4(1), 296–328. https://doi.org/10.61268/yhg4cc67

Smith, O. J. M., & Kantor, K. N. (2025). Coupled thermo-fluid models for heat transfer optimization in microelectronic cooling systems. Journal of Applied Mathematical Models in Engineering, 1(4), 41–47. https://doi.org/10.17051/JAMME/01.04.06

Thermal-Fluid Topology Optimization for Heat Sink Design. (2025). https://lirias.kuleuven.be/retrieve/4437f016-9b3e-48c2-8fde-11f247f4442e

Wu, Z., Zhu, P., Huang, Y., Yao, J., Yang, F., Zhang, Z., & Ni, M. (2025). A comprehensive review of modeling of solid oxide fuel cells: From large systems to fine electrodes. Chemical Reviews, 125(4), 2184–2268. https://doi.org/10.1021/acs.chemrev.4c00614

Corigliano, O., Pagnotta, L., & Fragiacomo, P. (2022). On the technology of solid oxide fuel cell (SOFC) energy systems for stationary power generation: A review. Sustainability, 14(22), 15276.

Chen, G. (2005). Nanoscale energy transport and conversion: a parallel treatment of electrons, molecules, phonons, and photons. Oxford university press.

French, R. H., Parsegian, V. A., Podgornik, R., Rajter, R. F., Jagota, A., Luo, J., ... & Zemb, T. (2010). Long range interactions in nanoscale science. Reviews of Modern Physics, 82(2), 1887-1944.

French, R. H., Parsegian, V. A., Podgornik, R., Rajter, R. F., Jagota, A., Luo, J., ... & Zemb, T. (2010). Long range interactions in nanoscale science. Reviews of Modern Physics, 82(2), 1887-1944.

Qiu, C., Brinck, T., & Wang, J. (2025). Modeling Potential Energy Surface by Force Fields for Heterogeneous Catalysis: Classification, Applications, and Challenges. Chemical Science.

Becker, M. (2025). Dynamic solvation fields: a paradigm shift in solvent effects on chemical reactivity. Physical Chemistry Chemical Physics, 27(45), 24146-24158.

Mehmani, A., Kelly, S., & Torres-Verdin, C. (2019). Review of micro/nanofluidic insights on fluid transport controls in tight rocks. Petrophysics, 60(06), 872-890.

Xie, C., & Li, H. (2023). Multiscale simulations of nanofluidics: Recent progress and perspective. Wiley Interdisciplinary Reviews: Computational Molecular Science, 13(5), e1661.

Yu, J., Du, M., Zhang, Y., Chen, X., & Yang, Z. (2025). Research progress on micro/nanopore flow behavior. Molecules, 30(8), 1807.

Fraux, G., Coudert, F. X., Boutin, A., & Fuchs, A. H. (2017). Forced intrusion of water and aqueous solutions in microporous materials: from fundamental thermodynamics to energy storage devices. Chemical Society Reviews, 46(23), 7421-7437.

Nguyen, A. T., & Piri, M. (2025). Selective adsorption of fluid mixtures in nanoporous materials: Effects of confinement and wettability. Chemical Engineering Journal, 168885.

Ranjbarzadeh, R., & Sappa, G. (2025). Numerical and experimental study of fluid flow and heat transfer in porous media: A review article. Energies, 18(4), 976.

Wali, S. A., Abubakar, A. M., Abubakar, H., Kareem, S. A., & Ellouze, M. (2025). Compressible fluid flow and heat transfer. Flow Dynamics and Heat Transfer: Computational Fluid Dynamics, Thermal Analysis, Numerical Simulations, 29.

Ahmad, S., Liu, D., Cham, B. M., Xu, W., & Yang, S. (2025). Optimization of heat transfer efficiency of electronic device through conjugate heat transfer using Darcy-Forchheimer modelled base plate: 2D versus 3D computations. Applied Thermal Engineering, 265, 125535.

John, B., Senthilkumar, P., & Sadasivan, S. (2019). Applied and theoretical aspects of conjugate heat transfer analysis: A review. Archives of Computational Methods in Engineering, 26(2), 475-489.

Delpisheh, M., Ebrahimpour, B., Fattahi, A., Siavashi, M., Mir, H., Mashhadimoslem, H., ... & Mamlouk, M. (2024). Leveraging machine learning in porous media. Journal of Materials Chemistry A, 12(32), 20717-20782.

Bhattacharyya, S., Khatri, S., Biswas, N., Moiduddin, K., Mian, S. H., & Almutairi, Z. (2025). Thermal management of sodium-ion and lithium-ion battery of electric vehicle using magnetic nanofluid and vortex generators with magnetic virtual baffles. The European Physical Journal Special Topics, 1-27.

Bertram, A., Othmer, C., & Zimmermann, R. (2018). Towards real-time vehicle aerodynamic design via multi-fidelity data-driven reduced order modeling. In 2018 AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference (p. 0916).

Mao, R., Lan, Y., Liang, L., Yu, T., Mu, M., Leng, W., & Long, Z. (2025). Rapid CFD prediction based on machine learning surrogate model in built environment: A review. Fluids, 10(8), 193.

Na'im Abdullah, M. (2026). Enhanced reduced-order modeling and accelerated direct numerical simulation. In Artificial Intelligence for Computational Fluid Dynamics (pp. 91-129). Academic Press.

Rajashekaraiah, T., Dulabhai, H. P., Kiran, K., Ravikumar, R., Shivakumar, S., Girisha, K. B., ... & Santosh, V. (2025). Recent Advances in Computational Fluid Dynamics Using Artificial Intelligence, Machine Learning, and Deep Learning: A Comprehensive Review. Journal of Mines, Metals & Fuels, 73(11).

Alwafi, A., Nguyen, T., Hassan, Y., & Anand, N. K. (2022). Experimental analysis of a non-isothermal confined impinging single plume using time-resolved particle image velocimetry and planar laser induced fluorescence measurements. International Journal of Heat and Mass Transfer, 193, 122952.

Voulgaropoulos, V., Aguiar, G. M., Markides, C. N., & Bucci, M. (2022). Simultaneous laser-induced fluorescence, particle image velocimetry and infrared thermography for the investigation of the flow and heat transfer characteristics of nucleating vapour bubbles. International Journal of Heat and Mass Transfer, 187, 122525.

Hiromasa, S., Hara, S., & Inaoka, K. (2023). The velocity and thermal fields of two parallel plane jets using simultaneous PIV and two-color LIF measurements. International Journal of Heat and Fluid Flow, 103, 109192.

Naumann, C., Käufer, T., Stark, N., & Cierpka, C. (2026). Improving simultaneous two-color PLIF and PIV temperature and velocity field measurements through a single three-chip color camera. Experiments in Fluids, 67(2), 21.

Shi, Y., Wei, P., Feng, K., Feng, D. C., & Beer, M. (2025). A survey on machine learning approaches for uncertainty quantification of engineering systems. Machine learning for computational science and engineering, 1(1), 11.

He, W., Jiang, Z., Xiao, T., Xu, Z., & Li, Y. (2025). A survey on uncertainty quantification methods for deep learning. ACM Computing Surveys.

Ali, H., Safdar, R., Liu, J., Binti Abd Manan, T. S., Hu, G., Rasool, M. H., ... & Gao, F. (2025). Hybrid fusion paradigm in advanced process monitoring: a panoramic review and future perspectives. Industrial & Engineering Chemistry Research, 64(47), 22465-22514.

Avramova, M., Abarca, A., Hou, J., & Ivanov, K. (2021). Innovations in multi-physics methods development, validation, and uncertainty quantification. Journal of Nuclear Engineering, 2(1), 44-56.

Furlong, A., Zhao, X., Salko, R. K., & Wu, X. (2025). Physics-based hybrid machine learning for critical heat flux prediction with uncertainty quantification. Applied Thermal Engineering, 127447.

Cheng, S., Quilodrán-Casas, C., Ouala, S., Farchi, A., Liu, C., Tandeo, P., ... & Arcucci, R. (2023). Machine learning with data assimilation and uncertainty quantification for dynamical systems: a review. IEEE/CAA Journal of Automatica Sinica, 10(6), 1361-1387.

Succetti, F., Panella, M., Giannitrapani, P., Rigo, J. C., & Colonnese, S. (2025). Machine Learning for Fluid Thermodynamics: State of the Art and Open Challenges. IEEE Access.

Shu, D. (2024). Deep Generative Models for Fluid Flow Modeling. Carnegie Mellon University.

Adumene, S., Islam, R., Amin, M. T., Nitonye, S., Yazdi, M., & Johnson, K. T. (2022). Advances in nuclear power system design and fault-based condition monitoring towards safety of nuclear-powered ships. Ocean engineering, 251, 111156.

Luo, F., Shuai, C., Du, Y., Gao, C., Ren, F., & Zhao, Y. (2024). Reconstruction of physical field characteristics of underwater vehicle wake based on data-driven approach. Physics of Fluids, 36(11).

Hu, S., Jin, Q., Gao, C., Zhang, X., Lu, M., He, Y., ... & Bai, W. (2025). The new paradigm of computational fluid dynamics: Empowering computational fluid dynamics with machine learning. Physics of Fluids, 37(8).

Kadeethum, T., O'malley, D., Ballarin, F., Ang, I., Fuhg, J. N., Bouklas, N., ... & Yoon, H. (2022). Enhancing high-fidelity nonlinear solver with reduced order model. Scientific reports, 12(1), 20229.

Faraji, F., & Reza, M. (2025). Machine learning applications to computational plasma physics and reduced-order plasma modeling: a perspective. Journal of Physics D: Applied Physics, 58(10), 102002.

Sarkar, S. (2024). Computational Thermo-Fluid Dynamics Modeling For Process Optimization In Hydrogen-Integrated Industrial Heat Systems. Journal of Sustainable Development and Policy, 3(03), 87-133.

Šturek, D., & Lazarova-Molnar, S. (2025). Surrogate Modeling: Review and Opportunities for Expert Knowledge Integration. Procedia Computer Science, 257, 826-833.

Bergström, L., & Nkosi, T. (2025). Surrogate-Assisted Global Optimization for Expensive Engineering Systems: From Trust Regions to Bayesian Optimization. Multidisciplinary Engineering Science Open, 2, 1-11.

Vargas-Salgado, C., Hurtado-Pérez, E., Alfonso-Solar, D., & Malmquist, A. (2021). Empirical design, construction, and experimental test of a small-scale bubbling fluidized bed reactor. Sustainability, 13(3), 1061.

Veza, I. (2025). Fuel-cell thermal management strategies for enhanced performance: review of fuel-cell thermal Management in Proton-Exchange Membrane Fuel Cells (PEMFCs) and solid-oxide fuel cells (SOFCs). Hydrogen, 6(3), 65.

Saeed, M., El-Hameed, M. A., Al-Hajri, E., & Kabbani, A. (2025). Water Management Strategies for Proton Exchange Membrane Fuel Cells: A Comprehensive Review. Electrochem, 6(4), 38.

Haider, R., Wen, Y., Ma, Z. F., Wilkinson, D. P., Zhang, L., Yuan, X., ... & Zhang, J. (2021). High temperature proton exchange membrane fuel cells: progress in advanced materials and key technologies. Chemical Society Reviews, 50(2), 1138-1187.

Jang, S., Kang, Y., Bae, K. T., Park, S. H., Park, Y. J., Kim, D., ... & Lee, K. T. (2025). Digital Twin of Solid Oxide Electrochemical Cells: From 3D Microstructure Reconstruction to Multiphysics Modeling. Advanced Energy Materials, 15(47), e03842.

Alfaifi, S. M., Balu, R., Chiang, K., Choudhury, N. R., & Dutta, N. K. (2025). Electrocatalysts for the oxygen reduction reaction in proton exchange membrane fuel cells: significant advances, major challenges, and future directions. ACS Catalysis, 15(11), 9301-9345.