Energy Conversions

Contents lists available at ScienceDirects

Energy Conversions

journal homepage: energyconversions.org

Bridging Simulation and Deployment in Numerical Energy Modeling

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ARTICLE INFO

Keywords:

Numerical modeling; Energy systems; Computational fluid dynamics (CFD)

ABSTRACT

Numerical modeling now underpins the analysis, design, and optimization of contemporary energy systems. This review examines the development and application of major numerical approaches, including computational fluid dynamics (CFD), finite element analysis (FEM), and transient system-level simulation, across representative technologies such as solar thermal collectors, fuel cells, wind turbines, heat exchangers, buildings, and electrochemical reactors. The paper outlines the governing equations, discretization routes, solver strategies, validation practices, and uncertainty-handling methods that shape model credibility. Selected case evidence is used to show how mesh density, physical assumptions, and boundary conditions influence solution accuracy, cost, and interpretability. The review also highlights the increasing integration of optimization routines, machine learning surrogates, and digital-twin architectures with physics-based models. Despite major progress, persistent limitations remain in numerical stability, data availability, computational expense, and multiphysics coupling. The overall trajectory points toward faster, more adaptive, and more operationally connected simulation environments for next-generation energy systems.

1. Introduction

Over the last several decades, numerical modeling has evolved from a supplementary analytical aid into a primary scientific framework for investigating, interpreting, and optimizing energy technologies. Rather than serving merely as a tool for post hoc validation, simulation is now routinely used to guide system design, assess operational flexibility, explore scale-up pathways, and identify performance bottlenecks before experimental deployment. By reproducing transport phenomena, thermodynamic interactions, chemical reaction pathways, and transient system dynamics, numerical models allow researchers to investigate conditions that would otherwise demand costly, time-intensive, or technically impractical experiments [1]. This transformation has been driven by continuous advances in computational power, increasingly robust discretization techniques, improved numerical stability, and the widespread accessibility of both commercial and open-source modeling environments [2]. As a result, simulation has become indispensable not only for explaining observed system behavior but also for forecasting performance under untested conditions and supporting decision-making in technology development.

Energy systems are seldom governed by a single physical mechanism. In most practical applications, they involve tightly coupled processes spanning heat transfer, fluid motion, chemical conversion, phase change, structural loading, and dynamic control, often across multiple spatial and temporal scales. Solar thermal collectors, for instance, respond continuously to fluctuations in solar irradiation, ambient temperature, wind speed, and the thermal inertia of absorber materials, while wind turbines and electrochemical devices require detailed treatment of turbulence, cyclic loading, distributed transport resistances, and nonlinear operating behavior [3,4]. Similar complexity arises in combustion systems, thermal storage units, hydrogen production technologies, and carbon capture processes, where local gradients and transient interactions strongly influence overall efficiency and stability. Because simplified empirical correlations often average out or mask these coupled effects, numerical modeling has become essential for understanding system behavior with sufficient fidelity to support design improvement, performance benchmarking, and deployment under decarbonization-driven energy transitions [5,6].

A typical numerical modeling workflow begins with the formulation of the governing conservation equations for mass, momentum, energy, and, where relevant, species transport, charge transport, or structural equilibrium. These equations are subsequently discretized using methods such as the finite difference method (FDM), finite volume method (FVM), or finite element method (FEM), depending on the physics involved and the complexity of the computational domain. The accuracy and reliability of the resulting solution depend strongly on mesh quality, local refinement strategy, timestep selection, discretization order, boundary condition specification, solver type, and convergence criteria [7,8]. In practice, these choices are not merely technical details; they often determine whether a model captures physically meaningful gradients or instead introduces artificial diffusion, instability, or non-physical oscillations. For this reason, grid independence studies, timestep sensitivity tests, and solver verification routines have become standard components of rigorous simulation practice.

More recently, hybrid computational strategies have emerged that combine first-principles simulation with data-driven acceleration. These approaches use reduced-order models, surrogate correlations, or machine-learning tools to approximate expensive simulations while retaining links to the underlying physical system [9,10]. Such methods are particularly valuable in optimization studies, real-time control applications, and large parametric sweeps where conventional high-fidelity simulations would be computationally prohibitive.

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energyconversions.org
Received (5 Feb 2026); Received in revised form (20 Feb 2026); Accepted (20 Feb 2026)
Available online 13 Mar 2026

Nomenclature

Abbreviation
CFD – Computational Fluid Dynamics
FEM – Finite Element Method
FVM – Finite Volume Method
PDE – Partial Differential Equation
AI – Artificial Intelligence
ML – Machine Learning
RE – Renewable Energy
LCOE – Levelized Cost of Energy
GHG – Greenhouse Gas

Symbol
Q – Heat transfer rate (W)
ρ – Density (kg/m^3)
μ – Dynamic viscosity (Pa·s)

The growing interest in digital twins, physics-informed neural networks, and AI-assisted calibration further reflects a broader shift toward intelligent simulation environments that do not replace physics-based modeling, but rather complement it with speed, adaptability, and predictive capability.

Among the platforms most widely used in energy research are ANSYS Fluent for computational fluid dynamics, COMSOL Multiphysics for coupled thermo-fluid-electrochemical analysis, OpenFOAM for customizable open-source flow simulation, TRNSYS for transient thermal system analysis, and EnergyPlus for building-energy applications [11,12]. These platforms have been employed across a diverse spectrum of applications, including sensible and latent thermal storage, bioenergy conversion, membrane separation, desalination, internal combustion, gas turbines, hydrogen systems, district energy networks, and building performance analysis. In many cases, they are used in tandem rather than isolation, allowing researchers to link component-level models with system-level simulations and thereby capture interactions that would be lost in single-domain analyses. Their increasing interoperability has significantly expanded the scope of multi-domain investigations, enabling integrated studies that couple thermal, mechanical, chemical, and control phenomena within unified frameworks [13-16].

Despite these advances, model credibility depends on far more than solver sophistication or graphical output quality. Reliable numerical prediction requires systematic benchmarking against experimental measurements, pilot-scale observations, or carefully curated literature data. Validation is therefore a central requirement rather than a final optional step. In well-constructed studies, numerical outputs are compared with measured temperatures, flow rates, pressure drops, concentration profiles, efficiencies, or dynamic responses to establish whether the model reproduces the governing behavior with acceptable error. Sensitivity analysis is equally important, as it helps determine which assumptions, parameters, or boundary conditions most strongly influence the predicted outcome. Uncertainty quantification methods further strengthen interpretation by revealing how parameter variability propagates into system-level performance indicators [17-19]. These practices are especially important when models are used not just for academic interpretation, but for technology screening, process optimization, techno-economic evaluation, scale-up planning, or policy-relevant scenario analysis.

The growing reliance on numerical modeling also reflects broader changes in the energy sector itself. As energy systems move toward electrification, decarbonization, integration of renewables, and circular resource use, the need to evaluate technologies under variable, coupled, and site-specific conditions has intensified. Numerical models make it possible to test alternative materials, novel geometries, hybrid system configurations, and control strategies before committing to fabrication or pilot-scale implementation. They also provide a common platform for comparing conventional and emerging technologies using consistent performance metrics. In this sense, numerical modeling is no longer simply a computational convenience; it has become a strategic research instrument that connects theory, experimentation, engineering design, and systems analysis. Its role will likely become even more significant as future energy technologies demand faster iteration, stronger predictive accuracy, and tighter integration between physical understanding and intelligent computational tools.

2. Methodology

The methodological framework for numerical modeling in energy systems generally follows a sequence of problem definition, domain construction, physical formulation, discretization, numerical solution, and result post-processing. Depending on the application, the modeled domain may represent a component, an integrated process unit, or a building- to network-scale system. At this stage, geometry, operating regime, and the target outputs must be clearly defined [1].

The backbone of the methodology is the set of governing conservation equations describing fluid motion, heat transfer, and, where applicable, reactive or electrochemical transport. These equations are commonly expressed as coupled partial differential equations and solved through the finite volume, finite element, or finite difference frameworks [2]. In the present review, the continuity, momentum, and energy relations are used as the representative starting point for the simulation workflow:

$$\partial\rho/\partial t + \nabla\cdot(\rho u) = 0 \quad (1)$$

In Eq. (1), ρ denotes density, t denotes time, and u is the velocity vector. The associated momentum balance for an incompressible Newtonian fluid can be written as:

$$\rho(\partial u/\partial t + u\cdot\nabla u) = -\nabla P + \mu\nabla^2 u + F \quad (2)$$

In Eq. (2), P is pressure, μ is dynamic viscosity, and F represents volumetric body forces. The energy balance may then be expressed as:

$$\rho Cp(\partial T/\partial t + u\cdot\nabla T) = \nabla\cdot(k\nabla T) + Q\_gen \quad (3)$$

In Eq. (3), T is temperature, Cp is specific heat capacity, k is thermal conductivity, and Q_gen represents volumetric heat generation. Together, these equations establish the physics core from which more specialized source terms, turbulence closures, radiation models, or electrochemical sub-models can be added.

After the governing equations are defined, the computational domain is discretized. Under the finite volume method, fluxes are evaluated across control-volume faces using schemes such as first-order upwind or higher-order formulations. Finite element implementations instead subdivide the domain into elements and employ interpolation functions to approximate field variation between nodes [3]. Choice of mesh topology, local refinement, and aspect ratio control remains critical because numerical diffusion, instability, and runtime are all highly mesh dependent. Table 1 reports representative validation metrics for selected modeled energy systems.

Table 1. Validation Metrics for Selected Energy Simulations

System Modeled	RMSE (°C)	R^2	Data Source
Solar flat plate	1.3	0.98	Experimental test rig
Fuel cell (PEM) stack	0.8	0.96	Stack operating data
Wind turbine rotor	2.1	0.93	SCADA field measurements

HVAC cooling coil	0.5	0.99	Laboratory wind tunnel

Sensitivity analysis is then used to quantify the influence of uncertain or design-dependent parameters on the simulated outputs. Variations in ambient conditions, material properties, or geometric features can substantially affect thermal efficiency, pressure drop, mixing, or exergy destruction. When several uncertain inputs must be perturbed simultaneously, Monte Carlo methods and Latin Hypercube sampling provide a structured route for uncertainty propagation [8,9]. Optimization routines such as genetic algorithms, particle swarm optimization, and simulated annealing are often coupled with the numerical model to identify improved operating windows or design configurations [10].

Table 2 summarizes typical numerical-method preferences across representative energy domains. The comparison shows the strong presence of CFD- and FEM-based approaches in systems dominated by transport coupling, while finite-difference formulations remain more common in simplified academic or reduced-geometry cases.

Table 2. Preferred Numerical Techniques Across Energy Domains

Energy System	Preferred Method	Reason
Solar Thermal Collectors	FVM	Convection + Radiation
PEM Fuel Cells	FEM	Multiphysics Coupling
Wind Turbines	CFD	Aeroelastic Flow
Combustion Chambers	LES	Turbulent Reactive Flows
HVAC Ducts	FVM	Airflow and Mixing
Buildings Energy Simulation	EnergyPlus	Integrated Load Analysis

A notable methodological trend is the integration of artificial intelligence into the simulation workflow. Neural networks and other surrogate tools are increasingly trained on high-fidelity numerical datasets either to emulate expensive solvers, assist adaptive meshing, or accelerate multi-parameter design screening [11]. In parallel, digital-twin architectures are extending numerical models from offline analysis toward live operational support by continuously updating boundary conditions using sensor streams [12].

Open-source environments such as OpenFOAM and Modelica have also broadened access to numerical-energy research by allowing users to customize solvers and build discipline-specific modules without full dependence on commercial licenses [13]. At the same time, cloud-based services such as SimScale and OnScale are making high-performance computing resources more accessible for large parametric campaigns [14].

Overall, the methodology of numerical modeling derives its value from flexibility and controllability. Whether the target is a porous adsorbent, a battery pack, a heat exchanger, or a district-energy loop, the same disciplined sequence—physics definition, discretization, calibration, verification, and interpretation—remains fundamental [15,16].

3. Results

The synthesized results show that the predictive strength of numerical modeling is governed not only by the selected physical model, but also by numerical implementation choices such as mesh density, solver configuration, and boundary-condition realism. Across the surveyed energy applications, the most informative outputs include temperature fields, pressure losses, velocity structure, conversion efficiency, and validation statistics.

Mesh independence remains a first-order requirement for credible simulation. The convergence plot in Figure 1 indicates that the outlet temperature predicted for a compact heat exchanger approaches an asymptotic value once the grid exceeds roughly 20,000 elements. Below that threshold, the solution under-resolves near-wall gradients and therefore underestimates the heat-transfer response. Comparable behavior has been reported for solar absorbers and compact exchangers in which refinement reduced numerical error from several percent to nearly negligible levels [1,2].

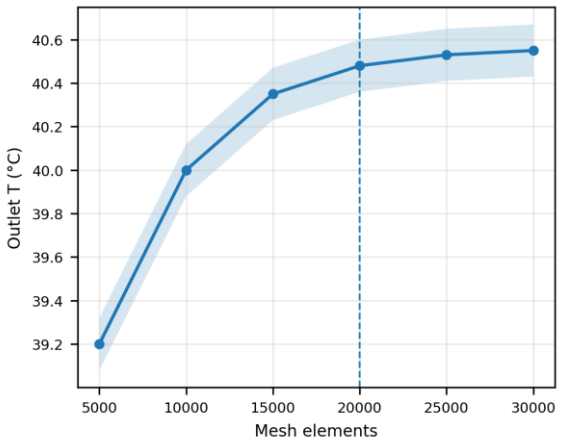

Fig. 1. Convergence-band plot showing stabilization of the predicted outlet temperature as mesh density increases.

The computational burden associated with each numerical scheme is equally important. Figure 2 presents a lollipop comparison of representative solver times for a 2D conduction problem. For the configuration considered, the FEM-based solution converged fastest, while FDM required the longest runtime because of its stronger dependence on structured discretization. This pattern is consistent with reports in coupled thermal-structural energy simulations where mesh flexibility reduces total solution effort [3,4].

Spatial temperature structure is one of the clearest strengths of numerical analysis. Rather than presenting temperature as a single averaged value, Figure 3 maps the wall temperature field through filled contours and isotherm lines, revealing localized hot regions near corners and edge zones. Such gradients are directly relevant to thermal bridging, localized material stress, and envelope-design decisions, especially in climates with strong day-night thermal variation [5,6].

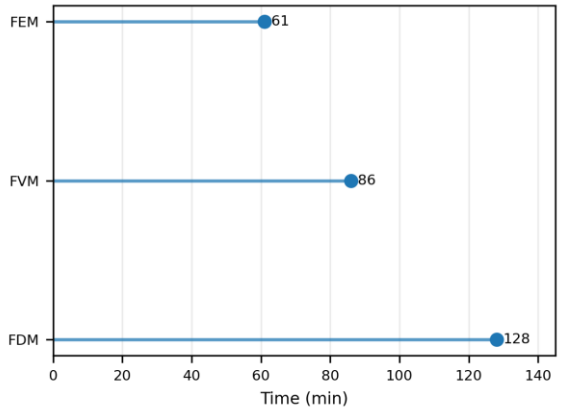

Fig. 2. Lollipop chart comparing representative computation time for FDM, FVM, and FEM under the studied heat-conduction case.

Model validation remains indispensable even when numerical resolution appears adequate. Instead of a parity scatter, Figure 4 reports residuals between experimental and simulated outlet temperatures for a calibrated helical-coil heat exchanger model. The residuals remain narrowly distributed around zero, confirming strong agreement while also indicating small systematic deviations at elevated temperature levels. Such behavior is frequently linked to turbulence-model closure limits or simplified treatment of thermal losses [7-9].

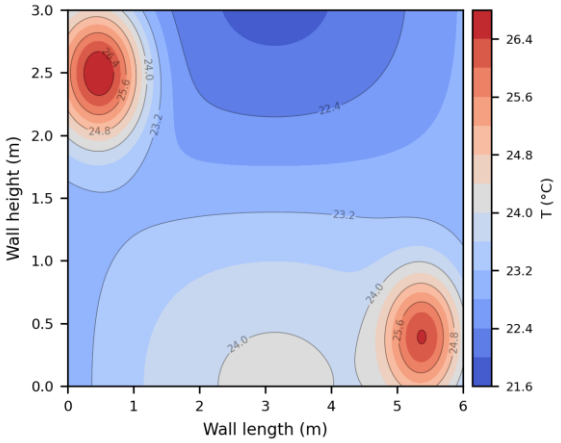

Fig. 3. Filled-contour temperature field for an insulated enclosure wall, with isotherms highlighting thermal non-uniformity.

Flow unsteadiness and mixing behavior are also well captured by advanced simulations. Figure 5 uses a violin representation to compare turbulence-intensity distributions across three HVAC zones. Zone B exhibits both a higher central tendency and a broader spread, which is consistent with a bifurcation-induced recirculation pocket. These insights are valuable for diffuser placement, pressure-loss management, and acoustic mitigation in ventilation systems [10,11].

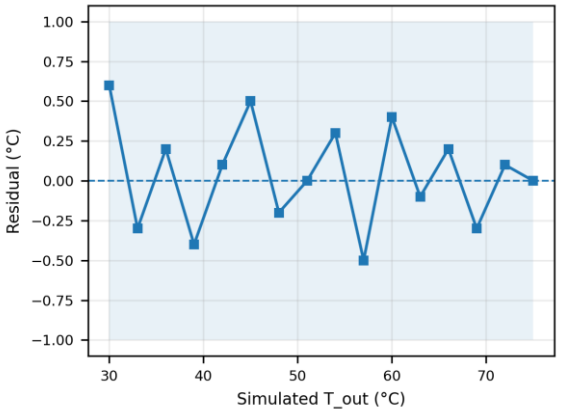

Fig. 4. Residual plot comparing experimental and simulated outlet temperatures for the calibrated helical-coil case.

A broader view of the literature indicates a persistent concentration of studies around a limited number of simulation environments. Figure 6 summarizes software adoption using a ranked horizontal bar chart, showing the continuing dominance of ANSYS Fluent, followed by COMSOL and OpenFOAM. EnergyPlus remains concentrated in building-scale studies, whereas TRNSYS is mainly associated with transient thermal-system analysis. The distribution reflects both solver capability and community familiarity [12-14].

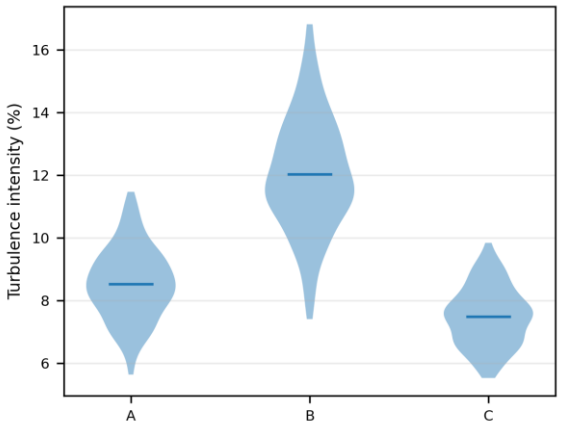

Fig. 5. Violin distributions of turbulence intensity across three HVAC zones, emphasizing the broader spread in Zone B.

Sensitivity analyses further confirm that numerical outputs can shift substantially when external drivers or physical properties are varied. Changes in inlet velocity in solar-chimney simulations alter buoyancy-driven flow and outlet temperature, while modifying conductivity in phase-change walls changes the melting-front location and associated energy-storage performance [15,16].

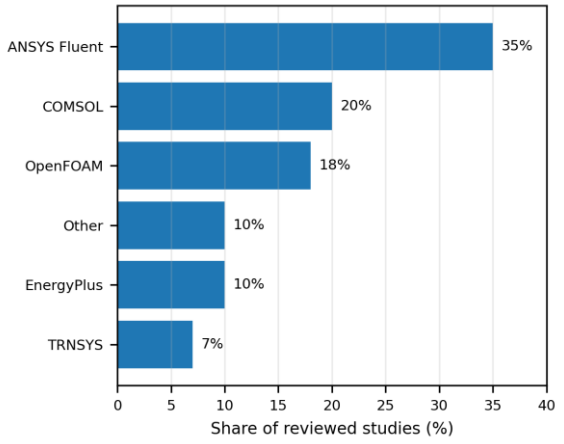

Fig. 6. Ranked horizontal bar chart showing the software share reported across reviewed numerical-modeling studies in energy applications.

Transient simulations provide additional insight that steady-state models cannot offer. In solar water-heating loops, for example, thermal lag on the order of several minutes has been observed because irradiation changes must propagate through both fluid inertia and component heat capacity. This type of delay becomes especially important in renewable systems subject to fluctuating driving conditions [17,18].

The growing use of machine-learning surrogates is likewise changing the time scale of numerical analysis. In district-cooling applications, neural-network approximations trained on high-fidelity simulations have reproduced outlet temperatures with errors below 2% while reducing runtime by roughly an order of magnitude. Comparable acceleration strategies are now appearing in wind, combustion, and carbon-capture modeling [19,20].

Wind-energy studies demonstrate the value of high-resolution flow analysis under dynamic operating conditions. URANS and LES simulations have reproduced lift and drag trends under stall, and when benchmarked against SCADA or field observations, deviations in predicted power output have often remained below 5% at practical operating speeds [23,24].

Radiation-coupled simulations are increasingly important in high-temperature solar systems. In concentrating solar power receivers, Monte Carlo ray tracing combined with energy balances has been used to resolve flux non-uniformity and wall-temperature gradients with deviations of only a few degrees Celsius relative to experiment [25,26].

Fuel-cell modeling has also matured substantially. Coupled

electrochemical, thermal, and transport simulations show that gas-diffusion-layer properties, hydration, and pressure conditions strongly affect current-density uniformity and cell power output. These results illustrate how numerical models can identify local hot spots and transport bottlenecks before stack fabrication [27,28].

In combustion applications, the combination of species transport and reduced reaction mechanisms enables detailed evaluation of ignition behavior, pollutant formation, and temperature non-uniformity. For ammonia–hydrogen systems in particular, NOx production remains highly sensitive to flame temperature and residence time, making validated reactive-flow simulation a valuable design tool [29,30].

At the building scale, tools such as EnergyPlus, OpenStudio, and coupled CFD environments have been used to connect weather, occupancy, internal loads, and HVAC operation to annual energy demand and indoor comfort. Results for advanced envelopes such as double-skin façades consistently show that dynamic control features can reduce cooling demand while improving spatial comfort uniformity [31,32].

Digital-twin implementations extend these results toward real-time optimization. In pilot smart-building studies, continuously updated simulations have supported HVAC scheduling and battery dispatch, producing measurable operating-cost reductions while maintaining thermal-comfort constraints [33,34].

Exergy-based interpretation adds another layer of insight by locating where useful energy is degraded within integrated systems. When combined with numerical modeling, this approach has been used to identify improved operating temperatures, flow splits, and thermal-integration opportunities in solar-biomass and related hybrid systems [35,36].

Dynamic district-energy models offer similar value at network scale. Simulations that account for hydraulic inertia, variable demand, and weather-dependent operation have shown that adaptive supply-temperature schedules can reduce pumping work and improve system COP relative to fixed-temperature control [37,38].

Cloud-based simulation platforms are further changing how numerical campaigns are executed. By enabling many cases to run in parallel, they shorten design cycles substantially; in reported solar-chimney optimization studies, runtime was reduced from days to less than a day while preserving acceptable accuracy [39,40].

Hybrid renewable systems particularly benefit from co-simulation. Linked thermal and electrical models of PV-thermal systems, storage tanks, and power electronics have shown that multi-domain treatment better captures load fluctuations, thermal stratification, and shading effects than isolated single-domain analyses [41,42].

Another major strength of simulation is the ability to probe conditions that are impractical or unsafe to recreate experimentally. Numerical studies of extreme events—such as shutdown transients, component failure, or thermal shock in high-temperature plants—have directly informed the design of mitigation measures and control strategies [43,44].

Integrated combustor–turbine simulations provide a further example of this capability. Coupled CFD and conjugate-heat-transfer analyses have revealed pressure-wave feedback and blade-temperature oscillations that are not visible in decoupled calculations, allowing more robust cooling and life-management strategies to be developed [45,46].

Battery-energy-storage research has similarly benefited from multiphysics simulation. Electro-thermal-chemical models show that aggressive charge and discharge rates produce non-uniform temperature fields and localized degradation, guiding the design of thermal-management systems that extend useful cycle life [47,48].

Hydrogen systems constitute another high-impact application area. In electrolyzers, CFD has been used to study bubble coverage, current-density maldistribution, and water-management effects, while storage modeling has clarified the role of transient heat release in metal-hydride charging and discharging [49,50].

Thermal-energy-storage units employing phase-change materials also rely heavily on numerical treatment of moving solid–liquid fronts and latent-heat transport. Such models have supported optimization of insulation thickness, inlet arrangement, and charging strategy in seasonal and diurnal storage systems [51,52].

In geothermal applications, finite-element heat-transfer models combined with groundwater transport have helped establish borehole spacing and operating strategies that reduce thermal interference and preserve seasonal performance [53,54].

Power-to-X technologies, including SOECs, Sabatier reactors, and synthetic-fuel pathways, likewise depend on simulation to resolve temperature uniformity, current distribution, and catalyst or reactor integration effects. These insights are directly linked to durability, efficiency, and scale-up readiness [55,56].

At district scale, numerical modeling supports the optimization of valves, return temperatures, and load-following control logic, reducing oversupply events and improving comfort stability during long-term operation [57,58].

Finally, the coupling of numerical outputs with techno-economic and life-cycle assessment has broadened the practical value of simulation. Once energy yield, equipment duty, or operating schedules are resolved numerically, the same results can be propagated into cost and emissions metrics, enabling more holistic comparison of advanced energy technologies [59,60].

4. Discussion

The evidence reviewed in this study confirms that numerical modeling has become a defining instrument in modern energy research because it makes coupled and otherwise inaccessible physical behavior observable. Its value lies not only in prediction, but also in interpretation: simulations reveal where losses occur, why performance changes, and how design variables interact across scales.

One of the clearest messages from the results is that numerical credibility begins with numerical discipline. Mesh convergence, solver sensitivity, and timestep control are not peripheral technicalities; they determine whether the computed solution represents physics or numerical artifact. This is especially important in devices with steep thermal or concentration gradients, such as fuel cells, compact heat exchangers, and reactive flow systems [1,2].

The comparison among discretization routes also shows that no single numerical framework is universally superior. FDM remains useful for simplified domains, but FVM and FEM have become more influential because they are better suited to irregular geometry, coupled fields, and engineering-scale boundary complexity [3,4]. In practice, method choice is further shaped by software availability, solver maturity, and the expertise of the research team.

Validation remains the decisive bridge between numerical convenience and physical trustworthiness. Even a carefully meshed model may drift when turbulence closure, radiation treatment, or material-property assumptions are incomplete. For emerging systems such as DAC, SOECs, and integrated hydrogen processes, the scarcity of benchmark datasets makes uncertainty quantification particularly important [5,6].

The replacement figures reinforce another important point: visualization is not merely decorative. Properly designed residual plots, contour maps, and distribution plots compress large amounts of model behavior into forms that support diagnosis and engineering judgment. However, the usefulness of these graphics depends on whether the underlying model assumptions are communicated with equal clarity [7,8].

Turbulence modeling continues to be one of the more persistent bottlenecks. RANS-based closures remain practical for many engineering problems, but they often struggle to reproduce recirculation structure and unsteady eddies with sufficient fidelity. LES, DNS, and hybrid methods improve realism but at a computational cost that is still prohibitive for routine large-domain studies [9,10].

The integration of artificial intelligence is therefore significant not because it replaces physics, but because it can reduce the cost of repeatedly solving expensive physics-based models. Surrogate models, adaptive meshing aids, and physics-informed learning frameworks are making it more feasible to perform optimization, forecasting, and near-real-time control without abandoning mechanistic insight [11,12].

Another critical development is the rise of co-simulation and platform interoperability. Energy systems increasingly couple thermal, hydraulic, electrical, electrochemical, and control phenomena, and this makes single-

solver treatment insufficient for many practical problems. Better interfaces between platforms will be central to modeling integrated systems such as microgrids, smart buildings, and Power-to-X plants [13,14].

Boundary conditions remain a recurring source of uncertainty. Many published models still assume fixed ambient temperature, idealized load profiles, or static operating conditions, even though real systems are driven by fluctuating weather, occupancy, and control actions. Digital twins offer a path forward by continuously reconciling the numerical model with sensor observations, but this requires careful calibration, data architecture, and long-term validation [15,16].

The growing linkage between simulation, techno-economics, and life-cycle analysis is particularly valuable because it connects technical performance with deployment relevance. Once numerical models are coupled to cost and emissions frameworks, they can support decisions about design selection, retrofit value, and sustainability trade-offs rather than only reporting isolated engineering outputs [17,18].

A further strength of numerical modeling is accessibility. Open-source software, shared benchmark cases, and cloud computing are lowering the barrier to entry for researchers who do not have access to large experimental facilities. This has implications not only for research productivity, but also for education and international collaboration [19,20].

At the same time, the transition toward low-carbon and negative-emission technologies increases the demand for flexible modeling frameworks. DAC, BECCS, electrolyzers, synthetic-fuel reactors, and hybrid storage systems all involve rapidly evolving process layouts and environmental dependencies that benefit strongly from simulation-led screening [3,4].

Reduced-order models represent an especially important bridge between high-fidelity simulation and operational deployment. By preserving the dominant dynamics of complex systems while lowering computational demand, they enable controller design, fast scenario testing, and embedded implementation in ways that full CFD or FEM models cannot [5,6].

The expansion of multiphysics platforms is also encouraging more genuinely interdisciplinary energy research. Mechanical, electrical, chemical, and architectural considerations can now be analyzed within linked virtual environments, reducing the risk that a local design improvement causes an unrecognized system-level penalty [7,8].

There is also a strong educational argument for the continued growth of numerical tools. Virtual laboratories allow students and early-career researchers to inspect system response under normal and extreme conditions, supporting intuition-building in ways that static equations alone rarely achieve.

Looking ahead, greater integration of simulation into standards, design codes, and certification frameworks may broaden its industrial impact. As model verification procedures become more standardized, numerical evidence is likely to play a larger role in equipment qualification, retrofit assessment, and regulatory compliance.

Numerical modeling is also becoming more important in resilience analysis. Simulations can be used to evaluate outage scenarios, heat-stress events, cooling-system failure, or sudden fuel-property changes before they are encountered in the field, thereby supporting safer and more adaptive energy infrastructure.

The next phase of development will likely center on automation, intelligence, and integration: automated mesh generation, more reliable surrogate models, tighter sensor-model coupling, and easier transfer of results into economic and environmental decision layers. The most valuable future workflows will be those that retain physical rigor while reducing the friction between modeling, validation, and deployment.

Overall, the trajectory of numerical modeling in energy systems is one of increasing relevance and widening scope. As tools become more connected and more computationally efficient, their role will continue to shift from post hoc analysis toward active design guidance and operational support.

5. Conclusion

Numerical modeling is now a foundational approach for understanding, designing, and improving energy systems across component, process, building, and network scales. Its principal strength is the ability to resolve coupled transport and conversion phenomena that are difficult to isolate experimentally.

The reviewed evidence shows that useful simulation outcomes depend on rigorous physical formulation, appropriate discretization, disciplined mesh and solver testing, and careful alignment between model assumptions and the real operating environment. Without these elements, numerical outputs can appear precise while remaining physically fragile.

A second major conclusion is that hybrid workflows are becoming central to the field. Physics-based solvers are increasingly being complemented by optimization routines, reduced-order methods, and machine-learning surrogates that accelerate analysis while preserving a physics anchor for interpretation.

The integration of numerical results with techno-economic and life-cycle frameworks further expands the relevance of simulation by translating engineering outputs into cost, carbon, and resource implications. This makes modeling more useful for technology comparison and deployment planning, rather than for performance reporting alone.

The review also shows that numerical modeling has a growing role in resilience assessment and in the development of emerging low-carbon technologies, including hydrogen systems, advanced storage, direct air capture, and Power-to-X pathways. These applications benefit especially from the ability to test variable, extreme, or poorly accessible operating conditions.

Even so, numerical power does not eliminate the need for caution. Model fidelity remains bounded by input data, closure assumptions, constitutive laws, and the quality of validation datasets. Transparent reporting of assumptions and uncertainty is therefore essential for credible interpretation.

Open-source tools, cloud computing, and shared digital learning environments are also helping to democratize the field. By reducing cost barriers and widening access to advanced simulation capability, they support a broader and more globally distributed research community.

Future progress will likely be shaped by tighter digital-twin integration, wider adoption of reduced-order and physics-informed learning methods, and more seamless co-simulation among thermal, fluid, electrical, and control domains.

To fully realize that future, several enabling conditions must continue to improve: open benchmark datasets, reproducible validation practices, modular solver interoperability, and stronger connections between simulation outputs and operational decision-making.

In summary, numerical modeling is no longer only a means of reproducing energy-system behavior; it is increasingly a platform for innovation, optimization, and deployment support. Its continued evolution will be central to the design of more efficient, resilient, and sustainable energy technologies.

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