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ARTICLE

Artificial intelligence, numerical simulation, and hybrid modeling in nanofluid heat transfer: A bibliometric and systematic decade review

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ABSTRACT

Recent advances in nanofluid heat-transfer research increasingly integrate computational fluid dynamics (CFD), artificial intelligence (AI), and hybrid modeling approaches to address complex, nonlinear transport phenomena. This study presents a systematic bibliometric and analytical review of nanofluid research combining numerical simulation and information technology (IT) over the past decade. Scopus-indexed publications from 2015 to 2024 were analyzed using bibliometric mapping to identify research trends, methodological evolution, and dominant modeling strategies. The results indicate a clear shift from standalone CFD-based analysis toward AI-assisted prediction and hybrid CFD-AI frameworks that balance physical fidelity and computational efficiency. Comparative assessment reveals that CFD remains essential for geometry-dependent and mechanistic analysis, AI enables rapid optimization and data-driven prediction, and hybrid approaches provide the most effective solution for complex multiphysics systems. Despite this progress, challenges persist in data availability, experimental validation, and modeling standardization. This study elevates bibliometric patterns into decision-oriented insights, providing practical guidance for selecting appropriate modeling strategies in nanofluid heat-transfer research and engineering applications.

INTRODUCTION

The continuous demand for high-efficiency thermal systems in engineering, automotive technologies, and renewable energy has intensified global interest in nanofluids as advanced heat-transfer media. Nanofluids (base fluids enhanced with nanoscale particles) offer superior thermal conductivity and convective performance, making them promising candidates for next-generation cooling and energy-conversion technologies (Al-Behadili & Al-Hajjaj, 2025; Nandiyanto et al., 2024). However, the thermophysical behaviour of nanofluids remains highly nonlinear and sensitive to particle size, shape, concentration, base-fluid properties, and flow environments. These complexities create substantial challenges for experimental characterization and system-level design.

To address these limitations, computational methods and information-technology-driven approaches have gained prominence. Extensive research has documented these developments (Ahmed et al., 2024; Reskianissa et al., 2022; Abidin et al., 2025; Al Husaeni & Wahyudin, 2023; Al Husaeni et al., 2024; Shaffiyah et al., 2022; Haristiani et al., 2025; Nandiyanto et al., 2023). Computational Fluid Dynamics (CFD), numerical simulation, and AI-based modelling enable researchers to explore nanofluid behaviour under diverse geometric, thermal, and flow conditions with higher precision and lower cost. CFD has been widely used to simulate nanofluid convection, turbulence, and multiphase interactions in complex systems such as heat exchangers, solar collectors, and porous media (Ramdaniah et al., 2023; Yang et al., 2024). Meanwhile, machine learning and artificial intelligence have emerged as powerful tools (Agarry et al., 2022; Abdulmuhsin et al., 2025; Nurjamin et al., 2026; Rahmiyanti, 2024; Ibrahim et al., 2025). In particular, these approaches accelerate thermal predictions, capturing hidden nonlinearities, and optimizing design parameters beyond the capabilities of conventional numerical approaches (Riyadi et al., 2024).

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artificial intelligence, bibliometric, computational fluid dynamics, machine learning, nanofluid

Despite increasing publications in this field, existing reviews exhibit several limitations. Prior studies tend to focus on isolated computational perspectives (either CFD-based modelling, experimental validation, or limited AI/ML applications) without offering an integrated understanding of how these approaches collectively evolve. Bibliometric analyses specific to nanofluid research are also limited, typically lacking thematic clustering, methodological comparison, and evaluation of emerging hybrid frameworks that combine CFD, AI, and experimental data. Given the rapid growth of intelligent simulation technologies and the shift toward data-driven thermal engineering, a comprehensive synthesis that integrates systematic review and bibliometric mapping is urgently needed.

Therefore, this study aims to provide a consolidated, systematic, and bibliometric review of nanofluid heat-transfer research from 2015 to 2024, focusing on the evolution of computational and information technology (IT) approaches. This work identifies methodological trends, thematic research clusters, hybrid modelling developments, and persistent gaps, particularly those related to dataset limitations, validation challenges, and cross-disciplinary integration. By highlighting these insights, the study offers a forward-looking perspective on the role of AI-CFD synergy in advancing efficient thermal systems and supporting innovation in sustainable energy technologies.

METHODS

This study employed a Systematic Literature Review (SLR) combined with bibliometric analysis to examine the evolution of computational and information-technology-based approaches in nanofluid heat-transfer research. The methodological procedure followed a structured, transparent, and reproducible workflow that included database selection, development of a search strategy, screening through predefined inclusion and exclusion criteria, data extraction, thematic synthesis, and bibliometric mapping.

Data Sources and Search Strategy

The Scopus database was selected as the primary source due to its comprehensive coverage of peer-reviewed literature in the fields of engineering, computational sciences, and thermal-fluid sciences. A search strategy was constructed using Boolean operators to capture studies involving nanofluids, computational fluid dynamics (CFD), numerical simulation, artificial intelligence, and machine learning. The final search syntax was: TITLE-ABS-KEY (nanofluid AND ("computational fluid dynamics" OR "numerical simulation" OR "machine learning" OR "artificial intelligence")).

The bibliometric dataset was retrieved from Scopus on 21 July 2025 and updated on 21 November 2025 at 14:00 GMT+7. Only 'articles' and 'reviews' were included, while conference papers, book chapters, notes, and errata were excluded. The subject areas were restricted to Engineering, Chemical Engineering, and Computer Science to ensure thematic relevance.

Inclusion and Exclusion Criteria

A multi-stage screening process was applied to ensure the relevance, quality, and analytical consistency of the selected publications. The following inclusion criteria were used:

(i) Publication period (2015–2024): to capture recent developments in computational and AI-assisted nanofluid research (Result: 226 articles retained).
(ii) Language (English): to ensure consistency of analytical interpretation (Result: 52 articles retained).
(iii) Scientific domains (Engineering, Chemical Engineering, Computer Science): reflecting direct relevance to thermal modelling, simulation techniques, and AI/ML integration

Publications outside the thematic scope, such as purely biological studies, descriptive reports, or non-technical manuscripts, were excluded at earlier stages.

In addition, the Open Access (OA) filter was applied solely to ensure full-text availability for methodological inspection at the time of screening. Non-OA papers were not intentionally excluded for theoretical reasons; rather, the OA status reflected accessibility constraints during retrieval. Nonetheless, the inclusion criteria remain aligned with SLR standards, focusing on relevance, quality, and thematic alignment.

Systematic Literature Review Procedure

The articles that passed the screening were analyzed through a four-phase SLR workflow:

(i) Methodological Classification. Publications were categorized into several approach types: Experimental, Numerical/CFD-based, AI/ML-based, and Hybrid (CFD-AI or CFD–experimental)
(ii) Thematic Analysis. A deductive-inductive coding strategy was used to identify dominant themes, including heat-transfer enhancement, numerical modelling, AI-driven prediction, porous media dynamics, and hybrid nanofluid optimization.
(iii) Evaluation of Technological Contributions. Each article was examined to determine how computational or IT-based methods improved prediction accuracy, system design efficiency, or modelling capabilities beyond classical thermal-fluid analysis.
(iv) Identification of Research Gaps. Gaps were mapped across three domains: Dataset limitations for AI training, Weak experimental validation of AI models, and Limited cross-disciplinary collaboration.

This procedure ensured that both the qualitative thematic structure and methodological evolution were captured systematically.

Bibliometric Analysis

Bibliometric mapping was conducted using VOSviewer, a widely adopted software for network visualization and scientometric analysis. The bibliometric workflow included: Publication Trend Analysis (Annual publication growth was evaluated to identify emerging patterns and shifts in research focus), Co-authorship and Country Productivity (Leading countries, institutions, and collaborative networks were mapped), Keyword Co-occurrence Analysis (Keywords were clustered into research themes to uncover intellectual structures and identify emerging directions such as machine learning, hybrid nanofluids, entropy analysis, and complex multiphysics modelling), and Overlay Visualization (Temporal mapping was used to distinguish early CFD-focused work from recent AI and hybrid-modelling trends). Integrating SLR and bibliometric techniques provided both depth and breadth in understanding the evolution and current directions of nanofluid research from computational and IT perspectives.

RESULTS AND DISCUSSION

Bibliometric Publication Trends and Thematic Research Clusters

The bibliometric analysis reveals a strong and sustained expansion of nanofluid research integrating computational and IT-based approaches over the past two decades. As shown in **Figure 1**, global publications increased from fewer than 20 studies per year in the early 2000s to 649 documents by 2025, with a pronounced acceleration after 2020. This growth coincides with the rapid adoption of machine learning, hybrid modeling frameworks, and high-performance computational tools in thermal-fluid engineering, highlighting the increasing reliance on intelligent simulation for heat-transfer optimization and energy-related applications.

Keyword co-occurrence mapping identifies four dominant thematic clusters: (i) classical heat-transfer and fluid-dynamic parameters, (ii) numerical simulation and nanoparticle-related modeling, (iii) AI-driven and hybrid predictive frameworks, and (iv) foundational CFD and material-related concepts. Collectively, these clusters indicate a maturing research landscape that is progressively shifting from standalone CFD studies toward integrated, data-informed, and hybrid modeling strategies. This evolution reflects the growing role of IT-enabled simulation in addressing complex, nonlinear, and multiphysics challenges in next-generation nanofluid applications.

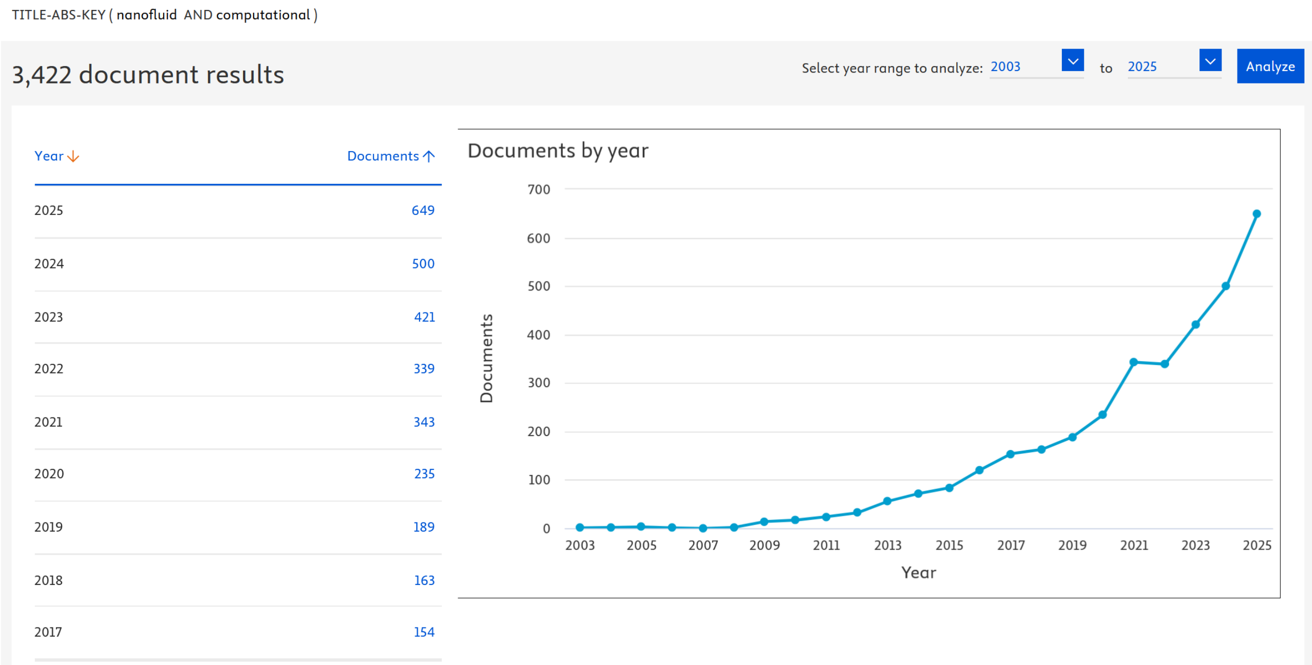

Figure 1: Global publication trends for nanofluid research using computational approaches (2003–2025). Data was retrieved from the Scopus database, updated on 21 November 2025.

Evolution of Computational Approaches in Nanofluid Research

Research on nanofluid heat transfer has shifted from single-method numerical studies toward integrated modeling ecosystems that combine physics-based simulation, data-driven prediction, and hybrid learning frameworks. Four methodological groups (experimental, numerical/CFD, AI/ML, and hybrid (CFD-AI or CFD–experimental)) capture the field's dominant strategy evolution and are summarized in Table 1.

Across the reviewed literature, CFD remains central for interpreting geometry-dependent transport behavior and evaluating design modifications in channels, porous media, solar collectors, and heat-exchanger configurations, where controlled experiments can be costly or difficult to replicate (Alshukri et al., 2024; Epandi et al., 2022). In parallel, AI/ML approaches have expanded rapidly as decision-support tools for fast prediction and optimization of key outputs (e.g., heat-transfer indicators, pressure-related metrics, and entropy-linked performance) across nonlinear and multivariable parameter spaces (Riyadi et al., 2024; Swamy et al., 2024; Zhao, 2024). Rather than replacing physics-based modeling, these approaches primarily reduce evaluation time and enable broader parametric exploration.

More recently, hybrid frameworks have emerged to balance physical fidelity and computational efficiency by combining simulation-driven datasets with learning-based surrogates, particularly for multiphysics cases involving porous structures, magnetic effects, microchannel systems, and bioconvection behavior (Kamsuwan et al., 2023; Alizadeh et al., 2021). The increasing use of established multiphysics platforms for model integration further indicates a transition toward workflow-level coupling between simulation and prediction rather than isolated single-method studies. A consolidated categorization of computational and IT-based modeling, including representative studies and application focuses, is presented in Table 2.

The evidence indicates a clear progression from CFD-centered analysis to AI-enabled prediction and, increasingly, to hybrid CFD-AI pipelines that support efficient design-space exploration and system-level decision-making. This progression is driven by practical constraints (high computational cost, limited experimental coverage, and the need to represent coupled transport mechanisms) alongside expanding application demands in renewable energy systems, microthermal devices, and adaptive thermal-management technologies.

Contributions and Added Value of IT in Nanofluid Research

IT has reshaped nanofluid heat-transfer research by shifting modeling practices from computationally intensive, single-case simulations toward scalable, data-assisted decision frameworks. Across the reviewed studies, three dominant contributions of IT integration emerge: improved computational efficiency, enhanced predictive capability for nonlinear systems, and expanded feasibility of multiphysics analysis.

Table 1: Classification of research approaches in nanofluid studies. Data was obtained from references (Sreelakshmi et al., 2024; Alshukri et al., 2024; Epandi et al., 2022; Riyadi et al., 2024; Swamy et al., 2024; Kamsuwan et al., 2023; Zhao, 2024; Alizadeh et al., 2021)

No	Research Approach	Short Description
1	Experimental	Direct evaluation of heat transfer performance using laboratory measurements, typically used to validate simulation or AI models.
2	Numerical Simulation (CFD & Thermal)	Modeling of nanofluid flow and heat transfer using CFD techniques in various geometries and boundary conditions.
3	AI/ML Integration	Utilization of machine learning algorithms to accelerate prediction and optimization of nanofluid systems.
4	Hybrid (Numerical–AI or CFD–Experimental)	Combining two approaches to improve the validity, simulation speed, and prediction accuracy of thermal systems.

Table 2: Classification of Computational Approaches and IT in Nanofluid Studies. Data was obtained from references (Alshukri et al., 2024; Sreelakshmi et al., 2024; Shahini et al., 2021; Epandi et al., 2022; Yang et al., 2024; Riyadi et al., 2024; Swamy et al., 2024; Zhao, 2024; Marjani et al., 2020; Ahmad et al., 2023; Kamsuwan et al., 2023; Hussain et al., 2024)

Approach Category	Main Description	Application Focus
CFD and Numerical Methods	Mainly used for modeling flow and heat transfer using FVM, FDM, and FEM; covering complex geometries, porous systems, and heat exchangers.	Channel optimization, passive heating, heat exchangers, and solar collectors
Machine Learning and Data-Driven Modeling	Used for historical data-based thermal performance prediction, classification, and optimization, including CNN, LightGBM, ANFIS, and fuzzy logic.	Performance prediction, optimal geometric design, viscosity, pressure, and bioconvection
Simulation Software	CFD tools such as ANSYS Fluent, COMSOL, OpenFOAM, and STAR-CCM+ are used for multiphysics analysis and integration with AI.	Complex fluid simulation, microthermal system design, and CFD-AI coupling
IoT and Real-Time Data Integration	Focus on adaptive monitoring and dynamic response to changing operational conditions using real-time sensors and AI.	Adaptive cooling systems, renewable energy, and feedback-based systems

Table 3: Challenges and gaps in the current research, especially in IT and nanofluid-related research. Data was obtained from references (Riyadi et al., 2024; Zhao, 2024; Swamy et al., 2024)

No.	Challenge or Research Gap	Explanation and Supporting Literature
1	Limited availability of open datasets for AI model training	One of the major barriers to integrating artificial intelligence is the scarcity of publicly accessible datasets that include consistent experimental or simulation parameters. This shortage slows down the training, benchmarking, and validation of machine-learning models.
2	Difficulties in validating AI-based simulations against real experimental data	Many AI models have not been validated using real experimental measurements, making their outputs largely predictive and not yet fully reliable for practical implementation in thermal systems.
3	Weak multidisciplinary collaboration between material scientists, engineers, and IT specialists	Modern nanofluid research requires strong synergy among multiple disciplines. However, cross-disciplinary collaboration remains limited, slowing the integration of AI techniques with physics-based models into a unified and comprehensive framework.

Comparative Assessment of CFD, AI, and Hybrid Modeling Approaches

CFD, AI, and hybrid modeling approaches constitute three dominant paradigms in nanofluid heat transfer analysis, each suited to different modeling objectives and system complexities, as summarized in **Table 4**. CFD remains the most physically interpretable approach, as it directly resolves governing equations and boundary conditions, making it well-suited for geometry-dependent design analysis and mechanistic investigation, albeit at high computational cost and sensitivity to constitutive property models. In contrast, AI-based approaches emphasize data-driven prediction, enabling rapid optimization, parameter sensitivity analysis, and real-time performance estimation once trained; however, they typically require large datasets, lack physical transparency, and exhibit limited extrapolation capability beyond the training domain. Hybrid modeling approaches integrate physics-based CFD with AI-driven learning to balance physical fidelity and computational efficiency, often by embedding physical constraints into learning architectures or using AI as surrogate solvers. Consequently, method selection should follow decision-oriented criteria: CFD for mechanistic and design-stage analysis, AI for fast optimization and control when data are available, and hybrid approaches for complex real-world systems requiring both accuracy and efficiency. This comparison translates bibliometric trends into actionable guidance for modeling strategy selection in nanofluid heat transfer research.

Table 4: Decision-Oriented Comparison of Modeling Approaches in Nanofluid Heat Transfer

Aspect	CFD	AI	Hybrid
Primary focus	Physics-based simulation	Data-driven prediction	Physics-informed learning
Physical interpretability	High	Low	Medium–High
Data requirement	Low–Medium	High	Medium
Computational cost	High	Low (after training)	Medium

Generalization ability	Strong within physics assumptions	Limited beyond training data	Improved via physical constraints
Suitability	Design analysis, mechanism study	Optimization, control, prediction	Complex systems, real-world deployment
Key limitation	High computational expense	Lack of physical transparency	Model integration complexity

CONCLUSION

This study shows that nanofluid heat-transfer research has evolved from standalone CFD-based analysis toward integrated modeling strategies that combine CFD, artificial intelligence (AI), and hybrid frameworks. Bibliometric evidence indicates that CFD remains essential for mechanistic and geometry-dependent analysis, while AI enables rapid prediction and optimization in data-rich contexts. Hybrid CFD-AI approaches increasingly provide the most balanced solution by preserving physical fidelity while reducing computational cost for complex multiphysics systems. From an engineering perspective, modeling strategy selection should be objective-driven: CFD for detailed design and physical interpretation, AI for fast optimization and control, and hybrid methods for complex or real-time applications. Despite this progress, broader implementation is limited by data scarcity, insufficient experimental validation, and the lack of standardized modeling protocols. Addressing these constraints through integrated physics–data approaches and collaborative benchmarking will be critical for advancing reliable and scalable nanofluid-based thermal systems.

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CONFLICT OF INTEREST

Authors confirm that there is no conflict of interest.

CONTRIBUTIONS OF INDIVIDUAL AUTHORS

ABDN prepared the manuscript and analysis data, NACS revised draft, and SRN prepared funds and final check for draft.

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