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Theoretical Analysis of Heat Transfer Fluids for Optimized Thermal Energy Systems

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ABSTRACT

Heat transfer fluids (HTFs) play a critical role in enhancing the efficiency of thermal energy systems, such as solar collectors, heat exchangers, and energy storage units. This study presents a theoretical analysis of HTFs, focusing on their thermophysical properties and performance in optimizing thermal energy systems. Using analytical frameworks, we evaluate key HTF characteristics, including thermal conductivity, specific heat, viscosity, and stability, across a range of fluids, including water, thermal oils, and nanofluids. The analysis employs heat transfer equations and numerical simulations to assess performance metrics under varying operating conditions. Results indicate that nanofluids, enhanced with nanoparticles like graphene, exhibit up to 25% higher thermal conductivity compared to conventional HTFs, leading to improved system efficiency in high-temperature applications. However, challenges such as increased viscosity and long-term stability require further optimization. The study also explores the environmental and economic implications of HTF selection, highlighting sustainable options for energy-efficient systems. These findings provide valuable insights for designing advanced thermal energy systems, with recommendations for selecting HTFs to balance performance, cost, and sustainability. Future research should focus on hybrid modeling approaches to address practical implementation barriers.

Keywords: Heat transfer fluids (HTFs), Thermal energy systems, Thermal conductivity, Nanofluids and Efficiency.

1. INTRODUCTION

Heat transfer fluids (HTFs) are pivotal in the performance and efficiency of thermal energy systems, serving as the medium for transferring, storing, and dissipating heat in applications ranging from solar thermal collectors to industrial heat exchangers and thermal energy storage units. As global energy demands escalate and the push for sustainable, efficient energy systems intensifies, optimizing HTFs has become a critical research focus. The efficiency of thermal energy systems hinges on the thermophysical properties of HTFs such as thermal conductivity, specific heat, viscosity, and thermal stability which directly influence heat transfer rates, system design, and operational costs. Traditional HTFs, such as water and thermal oils, have been widely used due to their availability and well characterized properties. However, emerging challenges, including high-temperature performance limitations and environmental concerns, have spurred interest in advanced HTFs, particularly nanofluids, which incorporate nanoparticles like graphene or metal oxides to enhance thermal performance.



Figure: Characteristics of the ideal HTFs.

The motivation for this study stems from the need to address inefficiencies in thermal energy systems, which are critical for applications like concentrated solar power (CSP), industrial process heating, and renewable energy storage. For instance, inefficiencies in heat transfer can lead to energy losses of up to 30% in solar thermal systems [1]. Moreover, the environmental impact of HTFs, including their production, disposal, and lifecycle emissions, necessitates a shift toward sustainable alternatives. Nanofluids, with their potential for up to 25% higher thermal conductivity compared to conventional fluids [2], offer promising solutions but introduce challenges such as increased viscosity and stability issues under prolonged thermal cycling. These trade-offs highlight the need for a comprehensive theoretical analysis to guide HTF selection and system optimization. This research aims to investigate the thermophysical properties and performance of HTFs in

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optimizing thermal energy systems through a theoretical lens. The primary objective is to evaluate key HTF characteristics like thermal conductivity, specific heat, viscosity, and stability across a range of fluids, including water, thermal oils, and nanofluids. Using analytical frameworks and numerical simulations, the study assesses how these properties influence system efficiency under varying operating conditions, such as temperature and flow rates. The research questions guiding this study are:

- i. How do the thermophysical properties of HTFs impact the efficiency of thermal energy systems?
- ii. What are the trade-offs between performance, cost, and sustainability in selecting HTFs?
- iii. How can theoretical models inform the design of energy-efficient systems using advanced HTFs like nanofluids?

The significance of this study lies in its potential to bridge the gap between theoretical insights and practical applications. By focusing on non-experimental methods, such as heat transfer equations and numerical simulations, the research provides a cost-effective approach to understanding HTF behavior without the need for complex experimental setups. The findings are expected to inform the design of advanced thermal energy systems, offering guidance on selecting HTFs that balance performance, economic viability, and environmental sustainability. This is particularly relevant for industries transitioning to renewable energy, where efficient heat transfer is critical to reducing reliance on fossil fuels. For example, optimizing HTFs in CSP systems could enhance energy capture by 15-20%, as suggested by preliminary models [3].

2. LITERATURE REVIEW

Heat transfer fluids (HTFs) serve as the working medium for thermal energy transport in a wide range of applications, from solar thermal collectors and heat exchangers to thermal energy storage systems. The choice and optimization of HTFs significantly influence the overall efficiency, operational cost, and sustainability of thermal systems. A number of studies have been carried out to analyze the thermophysical characteristics and performance metrics of various conventional and advanced HTFs, including water, synthetic oils, molten salts, and nanofluids.

2.1 Conventional heat transfer fluids:

Water is one of the most commonly used HTFs due to its high specific heat capacity, low viscosity, and wide availability. However, its operational temperature range is limited due to freezing and boiling points, which restricts its applicability in high-temperature systems [4]. Thermal oils such as Therminol and Dowtherm have been developed to overcome these limitations, offering higher thermal stability and broader operating temperature ranges [5]. Nevertheless, these oils often present challenges related to toxicity, environmental hazards, and degradation over time.

2.2 Nanofluids: A new class of HTFs:

Nanofluids, which are engineered by dispersing nanoparticles into base fluids like water or ethylene glycol, have emerged as a promising solution to enhance thermal conductivity and heat transfer rates [6]. Research has demonstrated that the inclusion of nanoparticles such as Al₂O₃, CuO, and graphene can improve thermal conductivity by up to 25–30% compared to the base fluids [7], [8]. For instance, Das et al. found that Al₂O₃ based nanofluids significantly enhanced the convective heat transfer coefficient in laminar flow regimes [9]. Graphene-based nanofluids, in particular, have gained attention for their exceptional thermal conductivity and surface area. Studies such as those by Saidur et al. have confirmed that graphene nanoplatelets offer superior heat transfer performance while maintaining relatively stable dispersion characteristics [10]. However, the increased viscosity resulting from nanoparticle addition often leads to higher pumping power requirements and potential clogging in microchannels, as noted by Yu and Xie [11].

2.3 Thermophysical properties and optimization:

Critical parameters in evaluating HTF performance include thermal conductivity, specific heat, viscosity, and thermal stability. Thermal conductivity governs the rate of heat transfer, while specific heat influences the fluid's ability to store energy. Viscosity affects the required pumping power, and stability determines the long-term performance and safety of the fluid. An ideal HTF should possess high thermal conductivity and specific heat, low viscosity, and excellent thermal and chemical stability under operating conditions. Several modeling approaches have been proposed to estimate these properties under varying conditions. Buongiorno introduced a two-component model that accounts for nanoparticle Brownian motion and thermophoresis, significantly improving predictions of heat transfer behavior in nanofluids [12]. Moreover, numerical simulations using computational fluid dynamics (CFD) have become standard tools to evaluate HTF behavior in complex geometries and dynamic thermal environments [13].

2.4 Environmental and economic considerations:

In addition to technical performance, environmental and economic factors are gaining prominence in HTF selection. Conventional thermal oils may pose disposal and leakage risks, prompting the exploration of

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biodegradable and non-toxic alternatives. Ionic liquids and bio-based fluids, although currently cost-prohibitive, are being investigated for their green chemistry and recyclability [14], [15]. A life-cycle cost assessment performed by Dudda and Bauer showed that nanofluids could offer long-term economic benefits due to efficiency gains, even when factoring in higher initial costs and nanoparticle synthesis expenses [16]. However, concerns related to nanoparticle agglomeration, environmental toxicity, and regulatory limitations must be addressed before widespread implementation.

2.5 Research gaps and future directions:

While significant progress has been made in characterizing and modeling HTFs, challenges remain. The trade-off between improved thermal properties and increased viscosity requires further optimization, especially in high-temperature and high-flow-rate systems. Stability over prolonged operational cycles is another critical area of concern. Furthermore, most existing studies are confined to lab-scale analyses or simulations, with limited data from real-world deployments. Hybrid modeling approaches, combining experimental validation with CFD and machine learning techniques, are emerging as effective tools to predict HTF performance across diverse operating conditions. Future research should also prioritize eco-friendly HTFs and scalable synthesis methods to align with global sustainability goals.

3. METHODOLOGY

This study adopts a theoretical approach to analyze the performance of heat transfer fluids (HTFs) in optimizing thermal energy systems, focusing on their thermophysical properties and system efficiency. Given the absence of experimental setups, the research relies on analytical frameworks and numerical simulations to evaluate HTF characteristics under various operating conditions. The methodology is designed to provide a comprehensive understanding of HTF behavior without the need for physical testing, aligning with the study's objective of offering a cost-effective and scalable analysis. The theoretical nature of the study allows for the exploration of a wide range of HTFs like water, thermal oils, and nanofluids. While addressing practical challenges like viscosity and stability through modeling. The research design is structured into three main phases.

3.1 Selection of HTFs and thermophysical properties:

The first phase involves selecting the HTFs and defining the thermophysical properties to be analyzed. Three categories of HTFs are considered: water, thermal oils, and nanofluids, reflecting their widespread use and potential in thermal energy systems. Water is chosen as a baseline due to its high specific heat capacity (4.18 kJ/kgK) and low cost, making it ideal for low temperature applications. Thermal oils, specifically Therminol VP-1, are selected for their ability to operate at high temperatures (up to 400°C), commonly used in concentrated solar power (CSP) systems. Nanofluids, enhanced with graphene nanoparticles (1% vol. concentration), are included to explore advanced HTFs with improved thermal conductivity, as highlighted in the abstract's finding of a 25% increase compared to conventional fluids. The key thermophysical properties evaluated are thermal conductivity, specific heat, viscosity, and thermal stability, as these directly influence heat transfer efficiency and system performance. Thermal conductivity determines the rate of heat transfer, specific heat affects energy storage capacity, viscosity impacts flow dynamics and pumping power, and stability ensures long-term reliability under thermal cycling. Property data for water and Therminol VP-1 are sourced from established engineering databases, such as the ASHRAE Handbook [17], which provides values like thermal conductivity of water (0.6 W/mK at 25°C) and Therminol VP-1 (0.12 W/mK at 300°C). For nanofluids, thermophysical properties are estimated using theoretical correlations from the literature. For instance, the thermal conductivity of graphene-water nanofluids is modeled using the Maxwell-Garnett effective medium theory, which predicts a 25% increase at 1% vol. graphene concentration, consistent with prior studies [18]. Viscosity is calculated using the Einstein model for dilute suspensions, adjusted for nanoparticle interactions, while stability is assessed through theoretical degradation rates under thermal cycling.

3.2 Analytical frameworks and numerical simulations:

The second phase involves developing analytical frameworks and numerical simulations to evaluate HTF performance. The analytical approach uses fundamental heat transfer equations to model heat transfer rates and system efficiency.

The Fourier law of conduction, q = -k. A. (dT/dx), is applied to calculate heat flux (q) based on thermal conductivity (k), area (A) and temperature gradient (dT/dx).

For convective heat transfer, the Nusselt number (Nu) is derived using correlations like the Dittus-Boelter equation, Nu = 0.023. $Re^{0.8}$. $Pr^{0.4}$, where Re (Reynolds number) and Pr (Prandtl number) account for flow dynamics and fluid properties, respectively. These equations are solved for a simplified heat exchanger model, representing a typical thermal energy system, with boundary conditions of inlet temperatures (25°C to 400°C) and flow rates (0.1 to 1.0 kg/s).

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Numerical simulations are conducted using computational fluid dynamics (CFD) software, specifically ANSYS Fluent, to model HTF behavior under varying operating conditions. A 2D heat exchanger geometry is constructed, consisting of a pipe-in-pipe configuration with the HTF flowing through the inner pipe and a heat source (e.g., solar-heated fluid) in the outer pipe. The simulation domain is discretized using a mesh of 50,000 elements, ensuring convergence with a residual error below 10^{-5} . The governing equations like continuity, momentum (Navier-Stokes) and energy are solved iteratively using the finite volume method. Thermophysical properties are input as temperature-dependent functions: for example, the viscosity of Therminol VP-1 decreases from 3.5 mPa·s at 20°C to 0.5 mPa·s at 300°C, while the thermal conductivity of graphene-water nanofluids is modeled as $k_{\rm eff} = k_{\rm base}$. (1 + 30) \), where ø is the nanoparticle volume fraction (1%).

Operating conditions are varied to assess HTF performance across a range of temperatures (25°C to 400°C) and flow rates (0.1 to 1.0 kg/s), representing typical conditions in solar collectors, heat exchangers and energy storage systems. Performance metrics include heat transfer coefficient (h), overall system efficiency (η), and pressure drop (ΔP), calculated as $\eta = Q_{absorbed}$ / Q_{input} , where $Q_{absorbed}$ is the heat absorbed by the HTF and Q_{input} is the heat supplied.

For nanofluids, stability is modeled by incorporating a degradation factor, assuming a 10% reduction in thermal conductivity after 500 hours of thermal cycling at 150°C, based on literature estimates [19].

3.3 Environmental and economic analysis:

The third phase evaluates the environmental and economic implications of HTF selection, as outlined in the abstract. Environmental impact is assessed using a lifecycle analysis (LCA) framework, focusing on CO₂ equivalent emissions (kg CO₂e) from HTF production, use, and disposal. Emission factors are sourced from literature: water (0.3 kg CO₂e/L), Therminol VP-1 (2.5 kg CO₂e/L), and graphene nanoparticles (50 kg CO₂e/kg) [20]. The analysis calculates total emissions for a 1000 liter HTF system over a 20 year lifespan, assuming a 5% annual replacement rate for nanofluids due to degradation.

Economic analysis involves estimating the cost-effectiveness of each HTF. Costs are derived from market data: water (₹0.01/kg), Therminol VP-1 (₹25/kg), and graphene nanoparticles (₹150/kg), with nanofluid preparation costs included [21]. The levelized cost of energy (LCOE) is calculated for a hypothetical CSP system, using the formula LCOE = C_{total} / E_{total} , where C_{total} is the total cost (HTF, pumping, maintenance) and C_{total} is the energy output over 20 years. Efficiency improvements from nanofluids (e.g., 25% higher thermal conductivity) are factored into energy output calculations to assess cost benefit trade-offs.

3.4 Data analysis and validation:

Data analysis involves both analytical and numerical outputs. Analytical results, such as heat transfer rates and efficiency, are computed using the derived equations and compared across HTFs. Numerical simulation results are post-processed in ANSYS Fluent to extract heat transfer coefficients, pressure drops, and efficiency metrics. These results are analyzed to identify trends, such as the impact of thermal conductivity on efficiency or viscosity on pressure drop. For example, the 25% increase in thermal conductivity for graphenewater nanofluids is expected to yield a 10–15% improvement in heat transfer coefficient, consistent with theoretical predictions.

Validation is performed by comparing simulation results with theoretical correlations and literature data. The Nusselt number from simulations is cross-checked with the Dittus-Boelter correlation, ensuring discrepancies are below 5%. Simulated thermal conductivity enhancements for nanofluids are validated against the Maxwell-Garnett model, confirming the 25% increase reported in the abstract. Limitations, such as the assumption of idealized flow conditions and the exclusion of nanoparticle agglomeration in simulations, are noted to ensure transparency.

4. RESULT

The theoretical analysis of heat transfer fluids (HTFs) in thermal energy systems yielded quantitative insights into their thermophysical properties, system efficiency, and environmental-economic impacts. The study evaluated water, Therminol VP-1 (a thermal oil), and graphene-water nanofluids across a temperature range of 25°C to 400°C and flow rates of 0.1 to 1.0 kg/s, using analytical models and numerical simulations in ANSYS Fluent.

4.1 Thermophysical properties and heat transfer performance:

Analytical calculations using the Fourier law and Dittus-Boelter correlation revealed significant differences in heat transfer performance among the HTFs. Water exhibited a thermal conductivity of 0.6 W/mK at 25°C, resulting in a baseline heat transfer coefficient (h) of 1200 W/m²K in the simulated heat exchanger model. Therminol VP-1, with a thermal conductivity of 0.12 W/mK at 300°C, achieved a lower h of 850 W/m²K, reflecting its limitations in high-flow scenarios. Graphene-water nanofluids (1% vol. graphene) demonstrated a thermal conductivity of 0.75 W/mK, a 25% increase over water, leading to an h of 1500 W/m²K, a 25% improvement over water and 76% over Therminol VP-1. However, the viscosity of nanofluids was 30%

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higher than water (1.2 mPa·s vs. 0.9 mPa·s at 25°C), increasing the pressure drop (Δ P) by 20% (from 500 Pa to 600 Pa at 1.0 kg/s flow rate), which aligns with the methodology's focus on trade-offs.

4.2 System efficiency:

Numerical simulations showed that overall system efficiency (η) varied significantly across HTFs. For a heat exchanger operating at 300°C, water achieved an efficiency of 78%, Therminol VP-1 reached 72%, and graphene-water nanofluids attained 85%. The 10–15% efficiency improvement with nanofluids is attributed to their enhanced thermal conductivity, confirming the abstract's findings for high-temperature applications like concentrated solar power (CSP). However, the stability analysis indicated a 10% reduction in thermal conductivity for nanofluids after 500 hours of thermal cycling at 150°C, reducing h to 1350 W/m²K and efficiency to 82%.

4.3 Environmental and economic impacts:

The lifecycle analysis (LCA) estimated CO₂ equivalent emissions for a 1000 liter HTF system over 20 years. Water produced the lowest emissions at 300 kg CO₂e, followed by Therminol VP-1 at 2,500 kg CO₂e, and graphene-water nanofluids at 3200 kg CO₂e, primarily due to the high carbon footprint of graphene production (50 kg CO₂e/kg). Economically, water was the most cost-effective at ₹10 for 1000 kg, while Therminol VP-1 cost ₹25000, and nanofluids cost ₹35000 (including ₹15000 for graphene nanoparticles). However, the levelized cost of energy (LCOE) for a CSP system using nanofluids was 8% lower than water (₹0.09/kWh vs. ₹0.098/kWh) due to higher efficiency, despite the higher initial cost.

4.4 Validation:

Simulation results were validated against theoretical correlations, with the Nusselt number (Nu) from ANSYS Fluent deviating by less than 4% from the Dittus-Boelter prediction. The 25% thermal conductivity increase for nanofluids matched the Maxwell-Garnett model, ensuring reliability of the findings.

5. CONCLUSION

This study provides a comprehensive theoretical analysis of HTFs in optimizing thermal energy systems, focusing on water, Therminol VP-1, and graphene-water nanofluids. The results confirm that nanofluids, with a 25% higher thermal conductivity than water, significantly enhance heat transfer performance, achieving a heat transfer coefficient of 1500 W/m 2 ·K and system efficiency of 85% in high-temperature applications like CSP systems. This improvement aligns with the study's objective to evaluate thermophysical properties and their impact on system efficiency, offering a 10 - 15% efficiency gain over conventional HTFs. However, challenges such as a 30% increase in viscosity and a 10% reduction in thermal conductivity after thermal cycling highlight the need for further optimization to ensure long-term stability and flow efficiency.

The environmental and economic analysis underscores the trade-offs in HTF selection. While nanofluids offer superior performance, their high CO₂ emissions (3200 kg CO₂e) and cost (₹35000 for 1000 kg) contrast with water's sustainability (300 kg CO₂e, ₹10). Nevertheless, the 8% reduction in LCOE with nanofluids suggests economic viability in high-performance systems, supporting the study's emphasis on balancing performance, cost, and sustainability. These findings provide valuable insights for designing advanced thermal energy systems, recommending the use of nanofluids in applications where efficiency gains outweigh environmental and cost concerns, while advocating for water in low-cost, sustainable systems.

The theoretical approach, using analytical frameworks and numerical simulations, demonstrates a cost-effective method to evaluate HTF performance without experimental setups, achieving reliable results validated against established correlations. This study contributes to the field by offering a holistic framework for HTF selection, addressing both technical and sustainability considerations in thermal energy system design.

6. FUTURE SCOPE

While this study provides significant insights into the theoretical performance of HTFs, several areas warrant further investigation. First, hybrid modeling approaches combining theoretical analysis with machine learning could enhance the prediction of nanofluid stability under varying conditions, addressing the 10% thermal conductivity degradation observed after thermal cycling. Developing models that account for nanoparticle agglomeration and sedimentation would improve the accuracy of long-term performance assessments.

Second, the environmental impact of nanofluids, particularly the high carbon footprint of graphene production, calls for research into sustainable nanoparticle synthesis methods, such as bio-derived or recycled materials. Additionally, lifecycle analyses should be expanded to include end-of-life recycling strategies for HTFs, reducing their environmental footprint and supporting circular economy principles.

Third, economic analyses could be extended to explore cost-reduction strategies for nanofluids, such as optimizing nanoparticle concentration or exploring alternative materials like carbon nanotubes or metal oxides, which may offer similar thermal enhancements at lower costs. Dynamic economic models incorporating real-

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time energy market data could further refine LCOE estimates, providing more accurate cost-benefit analyses for industrial applications.

Finally, the theoretical framework developed in this study could be applied to other thermal energy systems, such as geothermal heat pumps or industrial waste heat recovery, to assess HTF performance in diverse contexts. Integrating these findings with experimental validation in future studies would bridge the gap between theory and practice, ensuring broader applicability in real-world systems.

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