National Seminar on Applications of Mathematics in Modern Science and Technology (20th May-2026)
Organized by: S.R. Government Arts & Science College Kothagudem, Telangana

International Journal of Science, Engineering and Technology
ISSN: 2348-4098, P-ISSN: 2395-4752

Mathematical Models in Heat and Mass Transfer Problems

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Abstract- The mathematical modeling of coupled heat and mass transfer is undergoing rapid transformation through fractional calculus, advanced lattice Boltzmann methods, machine learning surrogates, and generalized continuum theories. This review synthesizes peer-reviewed research from 2025–2026. Key advances include fractional-order models capturing memory effects with velocity enhancements up to 20%, a multi-speed lattice Boltzmann method achieving ≤1.5% error across ballistic-to-diffusive phonon transport, and machine learning models reaching R^2 > 0.9996 for temperature field prediction. Pore-scale simulations identify optimal porosity ranges, while generalized thermoelastic diffusion models predict stress reductions exceeding 70%. These developments enable next-generation thermal management, energy storage, and manufacturing design.

Keywords- heat transfer; mass transfer; fractional calculus; lattice Boltzmann method; machine learning; porous media

I. INTRODUCTION

Heat and mass transfer processes are central to engineering systems ranging from hypersonic vehicle thermal protection to biomedical cooling devices. Classical Fourier and Fick laws assume instantaneous response and infinite propagation speeds—assumptions that fail for ultrafast laser heating, micro-/nanoscale transport, and viscoelastic fluids. The period 2025–2026 has seen transformative advances: fractional calculus embeds memory effects, lattice Boltzmann methods (LBM) now unify ballistic and diffusive phonon transport, machine learning (ML) provides both fast surrogates and physical insights, and generalized continuum theories capture nonlocal and dual-phase-lag behavior. This review focuses exclusively on peer-reviewed Scopus-indexed publications from 2025–2026.

II. FRACTIONAL CALCULUS IN TRANSPORT PROCESSES:

Fractional derivatives replace integer-order time derivatives, capturing the fact that thermal or concentration disturbances propagate at finite speeds and that the system retains memory of past states.

A 2025 study in Scientific Reports investigated unsteady MHD flow of a Casson fluid in an inclined channel using Caputo time-fractional derivatives in generalized Fourier and Fick laws [8]. Fractional-order modeling predicted higher heat transfer rates but lower mass transfer efficiency compared to classical models, while effectively capturing the transition of Casson fluids toward Newtonian behavior. Stronger magnetic fields significantly suppressed fluid motion.

International Journal of Science, Engineering and Technology
ISSN: 2348-4098, P-ISSN: 2395-4752

Simultaneously, a study in the Journal of the Korean Physical Society (2025) applied the Caputo–Fabrizio fractional model to free convective flow of dusty nanofluids between parallel plates [7]. A fractional parameter $\alpha = 0.5$ yielded velocity enhancement of approximately 15%, while $\alpha = 1.5$ amplified nanofluid velocity by up to 20%. The Nusselt number reached values as high as 1.810, and higher dusty fluid parameters reduced thermodynamic irreversibility.

A third contribution in Alexandria Engineering Journal (2025) combined the Prabhakar fractional operator with Levenberg-Marquardt-trained neural networks to predict free convection in viscoelastic nanofluids under thermal radiation, achieving a mean squared error below 10^{-4} [6].

III. LATTICE BOLTZMANN METHODS FOR MULTISCALE HEAT TRANSFER

The lattice Boltzmann method has emerged as a powerful alternative to Navier-Stokes solvers, especially for flows with complex boundaries and multiphase interfaces.

A landmark advance in 2025–2026 is the multi-speed uniform propagation LBM (Msup-LBM) for unified phonon heat transport beyond Fourier's law [9]. By enforcing discrete conservation of energy and momentum and introducing a minimum-cost assignment scheme, the method achieves errors ≤ 1.5% in quasi-ballistic cases, ≤ 1% in the hydrodynamic regime (where conventional low-order lattices err by >50%), and ≤ 1% in the diffusive limit. This enables robust simulation of non-Fourier heat conduction in micro/nanoelectronics.

A cumulant-based thermal LBM (CuLBM) was developed for two-dimensional natural convection and implemented on GPUs using CUDA [10]. It was validated for Rayleigh numbers up to 10^9 for Newtonian fluids and 10^6 for non-Newtonian fluids, covering power-law indices from 0.6 to 1.4 and Bingham numbers up to 15, offering superior numerical stability at high Rayleigh numbers.
For multiphase problems, a phase-field-based LBM was developed to handle interfacial heat and mass transfer with liquid–vapor phase change and volume change [11]. GPU-accelerated simulations of film boiling and rising bubbles validated the model's accuracy without unphysical leakage.

IV. MACHINE LEARNING AS SURROGATE AND PHYSICAL INTERPRETER

Machine learning is now integrated into the modeling pipeline for both rapid prediction and interpretability.

A 2026 study in International Communications in Heat and Mass Transfer combined finite element simulations with ML to predict concentration and temperature fields in flows with varying Richardson numbers [2]. Random Forest models achieved near-perfect predictive accuracy ($R^2 > 0.9996$). The average Nusselt number increased by 125% at the highest Reynolds and Richardson numbers.

A second study in the same journal (2026) investigated unsteady double-diffusive convection in curved porous enclosures saturated with nano-encapsulated phase change materials (NEPCM) [1]. An XGBoost regression surrogate achieved RMSE of 0.012 for Nusselt number and 0.015 for Sherwood number, with feature importance highlighting boundary conditions and cross-diffusion interactions as dominant drivers. Dual heating enhanced peak Nusselt number by about 27% and Sherwood number by 19% compared with single-wall heating.

A 2025 framework combined Wasserstein GANs for porous structure generation, LBM for high-fidelity thermal simulation, and XGBoost with SHAP analysis for prediction and interpretation [12]. The XGBoost

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model achieved $R^2 = 0.9981$ for predicting the average Nusselt number under oscillatory flow. SHAP analysis identified critical thresholds—Re > 75, Strouhal number > 100, porosity > 0.63, specific surface area > 0.12, and pore-size dispersion > 5.6—as conditions that boost oscillating flow heat transfer.
The Hammerhead framework, published in Machine Learning: Science and Technology (December 2025), integrates CFD with surrogate-based optimization for pipe flow heat and mass transfer in tokamak cooling systems, reducing computational cost while maintaining high fidelity [13].

V. POROUS MEDIA: PORE-SCALE DYNAMICS AND TRANSFORMED METAMATERIALS

A 2025 study in Thermal Science and Engineering Progress conducted pore-scale numerical simulations in randomly generated heterogeneous porous structures with porosities from 0.4 to 0.9 [14]. Vortices preferentially emerge in pore-throat expansion zones, with stability duration strongly dependent on porosity. Higher porosity reduces pressure drop and promotes convective heat transfer but decreases temperature uniformity. The average temperature decreases significantly with rising mass flux, with diminishing returns beyond 4.5 kg/(m²·s). Thermal resistance remained below 0.8 K/W across all operating conditions.

An innovative transformation optics approach was proposed in the Journal of Engineering Thermophysics (2025) for single-parameter regulation of heat and mass transport in porous media [19]. Unlike existing methods requiring complex transformations of multiple parameters, the new method enables functional control (thermal cloaks, concentrators, rotators) through a single parameter, simplifying metamaterial design.

Nanofluids and Non-Newtonian Rheology:
A 2025 study in Results in Engineering developed the first mathematical framework for entropy and energy transport of non-Newtonian Sutterby nanofluid flow through intersecting planes, extending the classical Jeffery-Hamel problem to Sutterby rheology with viscous dissipation [15]. The Reynolds number was found to have diametrically opposite effects on velocity for convergent versus divergent channels.
A comprehensive 2025 study in International Journal of Thermal Sciences compared Carreau and power-law models for shear-thinning nanofluids in differentially heated enclosures [16]. The key finding was the identification of critical thresholds where nanoparticle effects switch from enhancement to deterioration. Enhancement maps in the (Rayleigh number, power-law index) plane were constructed to identify optimal operating conditions.

Phase Change Materials: Refining Close-Contact Melting:
A 2025 study in the International Journal of Heat and Mass Transfer addressed a critical flaw in the enthalpy-porosity method for close-contact melting (CCM) of phase change materials [17]. The conventional method fails to capture the rigid body descent of the solid PCM block. By incorporating an additional source term into the momentum equation, allowing gravity to act selectively on the solid phase, the upgraded model overcomes the damping limitations. It was validated against experimental data, establishing a robust simulation framework for thermal energy storage.
An adaptive physics-driven deep learning framework was developed for the two-phase Stefan problem (2025), using three specialized deep neural networks in parallel, constrained by energy conservation and interface conditions [18]. The model captures the parametric influence of geometrical parameters on solidification rates without requiring mesh regeneration.

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Generalized Thermoelastic Diffusion Models:
A 2026 study in International Communications in Heat and Mass Transfer presented a novel generalized thermoelastic diffusion model integrating dual-phase-lag heat and mass transfer with Soret and Dufour cross-effects [4]. Applied to an infinite hollow cylinder under thermal shock, the model predicts significantly lower peak radial and hoop stresses, faster equilibrium attainment, and smoother chemical potential profiles compared to classical models. This is critical for thermochemical metal treatments, semiconductor manufacturing, and battery design.

A second study in the same journal (2026) proposed a nonlocal photo-thermoelastic model integrating the Moore–Gibson–Thompson heat equation with a Guyer-Krumhansl-type extension of Green-Naghdi Type III heat conduction [5]. For a rotating semiconductor half-space under magnetic field and photothermal excitation, nonlocality reduces peak normal stress by over 70% and enhances thermal penetration depth by more than sixfold. Rotation induces phase reversal in displacement and amplifies subsurface carrier density by up to 75 times, while the magnetic field modulates shear stress by over 200%.

VI. CONCLUSION

Mathematical models for heat and mass transfer have advanced dramatically in 2025–2026. Fractional calculus provides memory-aware formulations achieving velocity enhancements up to 20% and MSE below 10^{-4}. Lattice Boltzmann methods now span ballistic phonon transport (error ≤1.5%) to diffusive regimes with GPU-accelerated multiphase capability. Machine learning surrogates achieve $R^2 > 0.9996$, and explainable AI reveals critical thresholds for heat transfer enhancement. Pore-scale simulations identify optimal porosity ranges and mass flux limits. Nanofluid models quantify viscosity-induced trade-offs and provide enhancement maps. Phase change material models overcome enthalpy-porosity limitations, and generalized thermoelastic diffusion models predict stress reductions exceeding 70% and penetration depth enhancements over sixfold. These advances enable next-generation thermal management, energy storage, and manufacturing design with unprecedented predictive accuracy.

REFERENCES

1. A. M. Alotaibi and A. M. Aly (2026). International Communications in Heat and Mass Transfer, Vol. 172, Part 2.
2. S. Hussain et al. (2026). International Communications in Heat and Mass Transfer, Vol. 174.
3. R. Su, Y. Shen et al. (2026). International Journal of Heat and Mass Transfer, Vol. 259.
4. A. E. Abouelregal and H. M. Sedighi (2026). International Communications in Heat and Mass Transfer, Vol. 172, Part 1.
5. A. E. Abouelregal et al. (2026). International Communications in Heat and Mass Transfer, Vol. 172, Part 2
6. S. A. Shehzad et al. (2025). Alexandria Engineering Journal.
7. M. I. Khan et al. (2025). Journal of the Korean Physical Society.
8. M. I. Khan et al. (2025). Scientific Reports, Vol. 15, Article 39790.
9. Multi-speed uniform propagation LBM (2025). International Communications in Heat and Mass Transfer.
10. CuLBM development (2025). Results in Engineering, Vol. 27, 106225.
11. Phase-field LBM (2025). International Journal of Heat and Mass Transfer.
12. Generative deep learning and XGBoost framework (2025). International Journal of Heat and Fluid Flow.
13. Hammerhead (2025). Machine Learning: Science and Technology.

International Journal of Science, Engineering and Technology
ISSN: 2348-4098, P-ISSN: 2395-4752

14. B. Liu et al. (2025). Thermal Science and Engineering Progress, Vol. 68.
15. Non-Newtonian Sutterby nanofluid (2025). Results in Engineering.
16. Carreau nanofluid (2025). International Journal of Thermal Sciences.
17. Close-contact melting (2025). International Journal of Heat and Mass Transfer.
18. Adaptive PDDL framework (2025). arXiv preprint.
19. Single-parameter regulation (2025). Journal of Engineering Thermophysics, Vol. 46(11), 3753-3760.