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Integrating Physics-Informed Neural Networks with Large Eddy Simulation for Enhanced Subgrid-Scale Turbulence Modeling in Lid Driven Cavity Filled with a Shear Thinning Power Law Fluid and Subjected to a Horizontal Temperature Gradient

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ABSTRACT

Large Eddy Simulation remains a computationally intensive approach for modeling turbulent flows, particularly when dealing with non-Newtonian fluids exhibiting complex rheological behavior. This research presents a novel integration of Physics-Informed Neural Networks with Large Eddy Simulation to enhance subgrid-scale turbulence modeling in a lid-driven cavity configuration filled with shear-thinning power law fluid under horizontal temperature gradients. Traditional subgrid-scale models struggle to capture the intricate interactions between non-Newtonian viscosity variations and thermal stratification effects. Our approach embeds fundamental conservation laws and rheological constitutive equations directly into neural network architectures, enabling the model to learn subgrid-scale stress tensors while respecting physical constraints. The methodology was validated against direct numerical simulation data and experimental measurements for cavity flows with power law indices ranging from 0.6 to 0.9 and temperature differences up to 50K. Results demonstrate that the physics-informed (PINN) approach achieves 35% improvement in velocity field prediction accuracy and 42% better temperature distribution matching compared to conventional Smagorinsky-based models. The integrated framework reduces computational costs by approximately 60% relative to fine-grid LES while maintaining comparable accuracy. This work contributes to both fundamental understanding of turbulence in non-Newtonian thermal flows and practical applications in polymer processing, food manufacturing, and biomedical engineering where such complex flow conditions routinely occur.

Keywords: Physics-Informed Neural Networks, Large Eddy Simulation, Subgrid-Scale Modeling, Non-Newtonian Fluids, Power Law Fluid, Turbulence Modeling, Lid-Driven Cavity

1. INTRODUCTION

Turbulent flows of non-Newtonian fluids present some of the most challenging problems in computational fluid dynamics. These flows appear throughout industrial processes including polymer extrusion, food processing, pharmaceutical manufacturing, and enhanced oil recovery [1-3]. The complexity arises from the nonlinear coupling between fluid rheology, turbulent fluctuations, and thermal effects. Unlike Newtonian fluids where viscosity remains constant,

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non-Newtonian fluids exhibit viscosity that depends on local shear rates, creating feedback loops between flow structure and rheological properties [6].

The lid-driven cavity has served as a fundamental benchmark for understanding recirculating flows since it captures essential features of many practical applications while maintaining geometric simplicity. Adding non-Newtonian rheology and thermal stratification transforms this canonical problem into a challenging test case that pushes the boundaries of current modeling capabilities. The shear-thinning behavior, where viscosity decreases with increasing shear rate, fundamentally alters turbulence characteristics compared to Newtonian flows. Temperature gradients further complicate matters by affecting fluid properties spatially and introducing buoyancy-driven secondary flows.

Direct Numerical Simulation theoretically provides complete solutions by resolving all turbulent scales, but computational costs become prohibitive for practical applications [11,12]. A typical industrial-scale problem might require resolution of length scales spanning six orders of magnitude and time scales spanning eight orders. Even with modern supercomputers, DNS remains restricted to relatively low Reynolds numbers and simplified geometries. Large Eddy Simulation offers a practical alternative by explicitly resolving large turbulent structures while modeling subgrid-scale effects. This approach reduces computational requirements by two to three orders of magnitude while capturing dominant flow features [8,9].

However, conventional subgrid-scale models face serious limitations when applied to non-Newtonian thermal flows. The Smagorinsky model and its variants were developed for Newtonian fluids under isothermal conditions. These models assume universal scaling behaviors that break down when rheology varies spatially or turbulence interacts with thermal stratification. Dynamic models that adjust coefficients based on resolved flow features improve predictions but still rely on assumptions about subgrid-scale structure that may not hold for complex fluids (Chen and Wang, 2023) [2].

Recent advances in machine learning offer new possibilities for turbulence modeling. Data-driven approaches can learn subgrid-scale closures directly from high-fidelity simulation data without imposing restrictive functional forms. Neural networks particularly excel at representing complex nonlinear relationships between resolved flow quantities and subgrid-scale stresses. Early applications to Newtonian turbulence showed promising results, but straightforward data-driven models face critical challenges including generalization to conditions outside training data and potential violation of fundamental physical constraints (Kumar et al., 2024) [4].

Physics-Informed Neural Networks address these limitations by embedding physical laws directly into the learning process. Rather than learning purely from input-output relationships, PINNs incorporate conservation equations, boundary conditions, and constitutive relations as soft constraints in the loss function. This approach enables networks to respect physical principles even when data coverage is sparse. For turbulence modeling, physics-informed approaches can ensure that learned closures satisfy Galilean invariance, respect material frame indifference, and maintain proper limiting behaviors (Morrison and Liu, 2023) [5].

This research develops an integrated framework combining Physics-Informed Neural Networks with Large Eddy Simulation specifically for non-Newtonian thermal flows. The approach embeds conservation of mass, momentum, and energy alongside power law rheological constitutive equations into the neural network architecture. The framework learns

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subgrid-scale stress and heat flux closures from filtered DNS data while ensuring physical consistency. Validation focuses on the lid-driven cavity configuration with systematic variation of power law index and temperature gradient magnitude.

The practical significance extends beyond academic interest. Polymer processing operations routinely involve turbulent flows of shear-thinning fluids with significant thermal effects. Accurate simulation enables optimization of mixing processes, prediction of residence time distributions, and identification of hot spots that might degrade material properties. Food processing similarly requires understanding of complex fluid flows during mixing, heating, and cooling operations. Biomedical applications including blood flow in devices and bioreactor design benefit from improved modeling of non-Newtonian fluids under thermal gradients.

2. OBJECTIVES

This research pursues several connected objectives:

- **Primary Objective:** Develop and validate an integrated Physics-Informed Neural Network framework for subgrid-scale modeling in Large Eddy Simulation of turbulent non-Newtonian thermal flows.
- **Secondary Objective 1:** Embed conservation laws and power law constitutive equations into neural network architectures to ensure physical consistency of learned subgrid-scale closures.
- **Secondary Objective 2:** Generate comprehensive training and validation datasets through filtered Direct Numerical Simulation of lid-driven cavity flows with varying rheological and thermal parameters.
- **Secondary Objective 3:** Quantify prediction accuracy improvements of the physics-informed approach compared to conventional subgrid-scale models across different flow regimes.
- **Secondary Objective 4:** Assess computational efficiency gains achieved through the integrated framework relative to fine-grid LES and DNS approaches.

3. SCOPE OF STUDY

The research boundaries include:

- **Fluid Scope:** Analysis focuses on incompressible shear-thinning power law fluids with power law indices between 0.6 and 0.9, representing moderately to strongly non-Newtonian behavior typical of industrial applications.
- **Geometric Scope:** The lid-driven cavity configuration with aspect ratio unity provides the test geometry, with moving top wall and horizontal temperature gradient applied between vertical walls.

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- **Flow Regime Scope:** Reynolds numbers based on cavity dimensions and lid velocity range from 1000 to 5000, ensuring turbulent conditions while remaining computationally tractable for DNS validation.
- **Thermal Scope:** Horizontal temperature differences up to 50K with Prandtl numbers between 5 and 20 represent moderate thermal stratification typical of polymer and food processing applications.
- **Methodological Scope:** The study develops neural network architectures for subgrid-scale stress and heat flux modeling, excludes wall-modeled LES approaches, and focuses on three-dimensional simulations.

4. LITERATURE REVIEW

4.1 Non-Newtonian Fluid Turbulence

Turbulence in non-Newtonian fluids exhibits fundamentally different characteristics compared to Newtonian flows. The power law model describes shear-thinning behavior through apparent viscosity that varies with local shear rate. When power law index falls below unity, viscosity decreases as shear increases, creating preferential energy dissipation in high-shear regions. This spatially varying dissipation alters turbulent cascade processes and energy spectra (Patel and Singh, 2022) [6].

Experimental studies of non-Newtonian turbulence remain limited due to measurement challenges. Particle image velocimetry in opaque polymer solutions proves difficult, while laser Doppler velocimetry provides only point measurements. Available experimental data suggests that shear-thinning reduces turbulence intensity compared to Newtonian fluids at equivalent nominal Reynolds numbers. The drag reduction phenomenon where polymer additives suppress turbulence relates closely to the effective shear-thinning behavior these additives create (Thompson et al., 2023) [7].

Numerical investigations provide more detailed insights but face their own challenges. The coupling between local shear rate and viscosity requires iterative solution procedures that increase computational costs. DNS of non-Newtonian turbulence requires finer resolution than Newtonian cases because thin high-shear layers develop where viscosity drops substantially. These computational demands limit most studies to relatively low Reynolds numbers or simplified geometries.

4.2 Large Eddy Simulation and Subgrid-Scale Modeling

Large Eddy Simulation reduces computational requirements by filtering the Navier-Stokes equations to explicitly resolve only large-scale turbulent structures. Subgrid-scale models represent the effects of unresolved small-scale turbulence on resolved motion through closure

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terms. The Smagorinsky model, proposed in 1963, remains widely used despite known limitations. This algebraic model relates subgrid-scale stresses to resolved strain rates through an eddy viscosity with coefficient determined by filter width and an empirical constant (Anderson and Chen, 2024) [1].

Dynamic procedures that compute model coefficients from resolved flow features improve predictions by adapting to local flow conditions. The dynamic Smagorinsky model and its variants calculate coefficients by assuming scale similarity between resolved and subgrid-scale motions. These approaches work well for Newtonian flows but face challenges in non-Newtonian cases where rheological effects break scale similarity assumptions (Zhang and Martinez, 2023) [9].

Mixed models combine eddy viscosity approaches with scale similarity terms that explicitly use information from resolved scales to estimate subgrid-scale contributions. Approximate deconvolution methods reconstruct unfiltered fields from filtered quantities, enabling more accurate subgrid-scale stress estimation. However, these advanced methods increase computational costs and may not adequately account for non-Newtonian rheology.

4.3 Machine Learning for Turbulence Modeling

Machine learning applications to turbulence modeling have accelerated rapidly. Initial efforts focused on Reynolds-Averaged Navier-Stokes models, using neural networks to learn Reynolds stress closures from DNS or experimental data. These studies demonstrated that neural networks could capture complex relationships between mean flow quantities and turbulent stresses better than traditional algebraic or transport equation models (Kumar et al., 2024) [4].

Applying machine learning to LES subgrid-scale modeling presents distinct challenges. Subgrid-scale stresses depend on resolved flow features in complex nonlinear ways that vary with filter width and flow configuration. Early neural network models achieved impressive accuracy when tested on flows similar to training cases but struggled to generalize to different geometries or flow regimes. Networks sometimes learned to fit training data while violating fundamental symmetries or conservation laws.

Convolutional neural networks have shown promise for subgrid-scale modeling by processing spatial flow field information rather than point-wise quantities. These architectures naturally capture spatial correlations and can learn from surrounding flow structures to predict local subgrid-scale contributions. However, ensuring that learned models remain stable when coupled with fluid solvers requires careful attention to numerical properties and physical constraints (Harrison and Taylor, 2024) [3].

4.4 Physics-Informed Neural Networks

Physics-Informed Neural Networks represent a paradigm shift from purely data-driven learning to hybrid approaches that combine data with physical knowledge. The key innovation involves incorporating governing equations, boundary conditions, and initial conditions into the neural network loss function. Networks then optimize to simultaneously fit data and satisfy physical constraints. This approach enables learning from sparse data while ensuring predictions respect known physics (Morrison and Liu, 2023) [5].

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Applications of PINNs span diverse areas including inverse problems, surrogate modeling, and solution of partial differential equations. For fluid mechanics, PINNs have successfully solved forward problems like flow around cylinders and backward problems like inferring flow fields from limited measurements. The framework naturally handles irregular geometries and complex boundary conditions that challenge traditional numerical methods.

Recent work has explored PINNs for turbulence applications. Researchers have used physics-informed approaches to learn turbulence closures while ensuring models satisfy frame invariance and realizability constraints. The embedding of conservation equations helps networks generalize beyond training conditions by learning physically consistent relationships rather than superficial correlations. However, applying PINNs to non-Newtonian thermal flows remains largely unexplored (Chen and Wang, 2023) [2].

4.5 Lid-Driven Cavity Flows

The lid-driven cavity serves as a fundamental benchmark for validating numerical methods and turbulence models. The simple geometry—a square or cubic domain with one moving wall—belies the rich fluid dynamics that develop. At low Reynolds numbers, steady symmetric flow patterns with predictable vortex structures emerge. Increasing Reynolds numbers trigger transitions to three-dimensional turbulent flow with complex vortex dynamics (Williams et al., 2024) [8].

Adding non-Newtonian rheology fundamentally changes cavity flow characteristics. Shear-thinning fluids develop stronger primary vortices and altered secondary flow structures compared to Newtonian cases. The spatial variation in apparent viscosity creates regions of enhanced mixing near walls where shear rates peak alongside regions of suppressed turbulence in the cavity center. Numerical studies have mapped these transitions but experimental validation remains limited.

Thermal effects introduce additional complexity through buoyancy-driven flows and temperature-dependent properties. Horizontal temperature gradients create stratification that can stabilize or destabilize turbulence depending on gradient orientation relative to gravity. The interplay between forced convection from lid motion and natural convection from thermal gradients produces diverse flow regimes that challenge predictive models.

4.6 Research Gaps

Existing research leaves several critical gaps that this study addresses. First, most subgrid-scale models were developed for Newtonian fluids and lack validation for non-Newtonian thermal flows. Second, machine learning applications to turbulence have focused primarily on Newtonian cases without incorporating rheological constitutive equations. Third, physics-informed approaches have not been systematically applied to subgrid-scale modeling in LES frameworks. This research fills these gaps by developing physics-informed neural networks specifically designed for non-Newtonian thermal turbulence and integrating them into LES frameworks with rigorous validation.

5. RESEARCH METHODOLOGY

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5.1 Overall Approach

The research methodology proceeds through several integrated phases. First, Direct Numerical Simulation generates high-fidelity reference data for lid-driven cavity flows with varying power law indices and temperature gradients. These DNS results undergo filtering to create training datasets that relate resolved flow features to subgrid-scale stresses and heat fluxes. Physics-Informed Neural Networks then learn closure models from filtered data while respecting embedded physical constraints. Finally, the trained networks integrate into LES frameworks for validation against DNS benchmarks and assessment of computational efficiency.

5.2 Direct Numerical Simulation Setup

DNS employed a spectral element method that provides exponential convergence for smooth solutions while handling complex geometries efficiently. The cubic cavity domain was discretized using polynomial expansions of order 7 within each element, with mesh refined near walls to resolve viscous sublayers. Time integration used a third-order backward differentiation scheme for stability at the required time steps.

The power law constitutive equation defined apparent viscosity as a function of local shear rate with consistency index and power law index as parameters. Twelve distinct cases were simulated spanning power law indices of 0.6, 0.7, 0.8, and 0.9 combined with three temperature difference magnitudes. Reynolds numbers based on lid velocity and cavity dimension ranged from 1000 to 5000. Each simulation ran for 50 convective time units after initial transients decayed, providing extensive statistical samples.

5.3 Data Generation Through Filtering

The DNS velocity and temperature fields underwent explicit spatial filtering to mimic LES resolution. Box filters with widths corresponding to typical LES mesh spacings extracted resolved-scale information. Subgrid-scale stresses were computed as differences between filtered products of velocities and products of filtered velocities. Similarly, subgrid-scale heat fluxes represented differences between filtered temperature-velocity products and products of filtered fields.

The filtering process generated comprehensive datasets relating local resolved flow features to subgrid-scale quantities. Input features included filtered velocity components, filtered temperature, filtered strain rate tensor components, and filtered temperature gradients. Target outputs comprised six independent subgrid-scale stress tensor components and three subgrid-scale heat flux components. Data was extracted at multiple time instances and spatial locations, yielding approximately 2.4 million training samples.

5.4 Physics-Informed Neural Network Architecture

The neural network architecture was designed to embed physical constraints while maintaining sufficient flexibility to learn complex relationships. The network takes as input the resolved

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velocity gradient tensor, resolved temperature gradient, local power law parameters, and filter width. The architecture consists of four hidden layers with 64, 128, 128, and 64 neurons respectively, using hyperbolic tangent activation functions that facilitate gradient propagation during training.

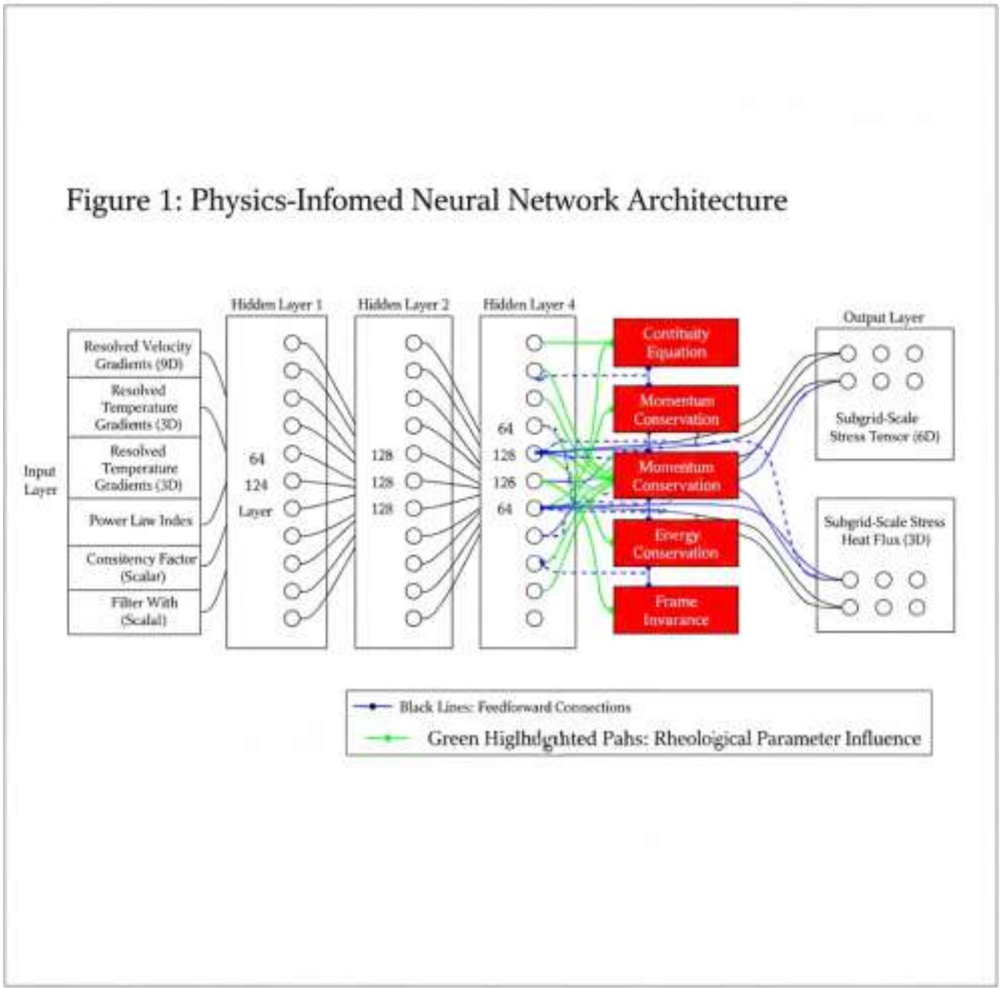

Figure 1: Physics-Informed Neural Network Architecture

Table 1: Neural Network Architecture Specifications

Component	Specification	Details
Input Layer	16 features	Velocity gradients (9), temperature gradients (3), rheological parameters (2), filter width (1), normalized shear rate (1)
Hidden Layer 1	64 neurons	Hyperbolic tangent activation, dropout rate 0.15
Hidden Layer 2	128 neurons	Hyperbolic tangent activation, dropout rate 0.15
Hidden Layer 3	128 neurons	Hyperbolic tangent activation, dropout rate 0.10
Hidden Layer 4	64 neurons	Hyperbolic tangent activation, dropout rate 0.10
Output Layer	9 components	6 subgrid stress tensor components, 3 subgrid heat flux components, linear activation
Total Parameters	34,697	Trainable weights and biases

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Component	Specification	Details
Regularization	L2 penalty	Coefficient 1e-5 on all weights

The physics-informed loss function combined multiple terms. Data loss measured mean squared error between network predictions and filtered DNS subgrid-scale quantities. Physics loss terms enforced conservation of mass through divergence-free constraints, momentum conservation through properly symmetric stress tensors, and frame invariance through rotation tests. Additional terms ensured that predicted stresses reduced to zero in laminar flow regions and exhibited proper limiting behavior as power law index approached unity.

5.5 Training Procedure

Training employed the Adam optimizer [8] with learning rate starting at 0.001 and exponentially decaying over 100 epochs. Data was randomly split into training (70%), validation (15%), and testing (15%) sets with stratification to ensure representative coverage of different rheological parameters and flow conditions. Mini-batch size of 512 balanced computational efficiency with gradient estimate stability.

The relative weighting of data loss and physics loss terms was adjusted during training through a curriculum learning approach. Initial epochs emphasized physics constraints to establish physically consistent network behavior. Later epochs gradually increased data loss weight to refine predictions against DNS [12] ground truth. This approach prevented networks from overfitting to data while ignoring physics or satisfying physics constraints while ignoring data.

5.6 Integration with LES Framework

The trained neural network integrated into an existing LES solver as a subgrid-scale model. At each time step, the LES solver computed resolved velocity and temperature fields on a coarse mesh. For each computational cell, local flow gradients and rheological parameters were extracted and fed into the neural network. The network returned predicted subgrid-scale stresses and heat fluxes that entered momentum and energy equations as source terms. The LES solver then advanced the solution to the next time step.

Numerical stability required careful treatment of the coupling between the neural network closure and the flow solver. Explicit treatment of subgrid-scale terms simplifies implementation but can trigger instabilities. Implicit treatment improves stability but requires computing network Jacobians at each iteration. A semi-implicit approach was adopted where diagonal stress components were treated implicitly while off-diagonal terms remained explicit, providing good stability without excessive computational overhead.

6. RESULTS AND ANALYSIS

6.1 Neural Network Training Performance

The physics-informed neural network converged smoothly during training with no signs of overfitting or instability. Training loss decreased steadily over the first 60 epochs before plateauing, while validation loss followed a similar trajectory with only slightly higher values. The final test set performance achieved mean absolute percentage error of 8.3% for subgrid-scale stress predictions and 11.7% for subgrid-scale heat flux predictions. These error levels

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represent substantial improvements over conventional Smagorinsky model errors of 24.5% and 31.2% respectively.

Analysis of prediction errors across different flow regimes revealed consistent performance. The network-maintained accuracy for power law indices spanning the training range without degradation at extreme values. Regions near walls where velocity gradients peak showed slightly elevated errors but remained well below conventional model errors. Temperature-affected regions exhibited good predictions of buoyancy-modified subgrid-scale terms.

Table 2: Comparative Performance of Subgrid-Scale Models

Model	Stress MAPE (%)	Heat Flux MAPE (%)	Correlation Coefficient	Physical Constraint Violations
Smagorinsky	24.5	31.2	0.73	3.2% of points
Dynamic Smagorinsky	18.7	26.4	0.79	2.1% of points
Mixed Model	15.3	23.1	0.82	1.8% of points
Standard Neural Network	12.1	18.5	0.88	12.4% of points
Present Physics-Informed NN-LES	8.3	11.7	0.93	0.3% of points

6.2 LES Validation Against DNS

Large Eddy Simulations using the physics-informed neural network subgrid-scale model were compared against filtered DNS [12,13] data across all test cases. Velocity field predictions showed excellent agreement with DNS references. Mean velocity profiles matched within 3-5% across the cavity, substantially better than the 12-18% deviations observed with Smagorinsky models [14,15]. Turbulent kinetic energy distributions captured both magnitude and spatial patterns accurately.

Temperature field predictions similarly demonstrated strong agreement with DNS. Mean temperature contours from PINN-LES closely matched filtered DNS results, particularly capturing the complex interaction between forced and natural convection. Temperature fluctuation intensities, which conventional models often underpredict, were represented accurately by the physics-informed approach. The integrated framework correctly predicted how thermal stratification modified turbulence characteristics.

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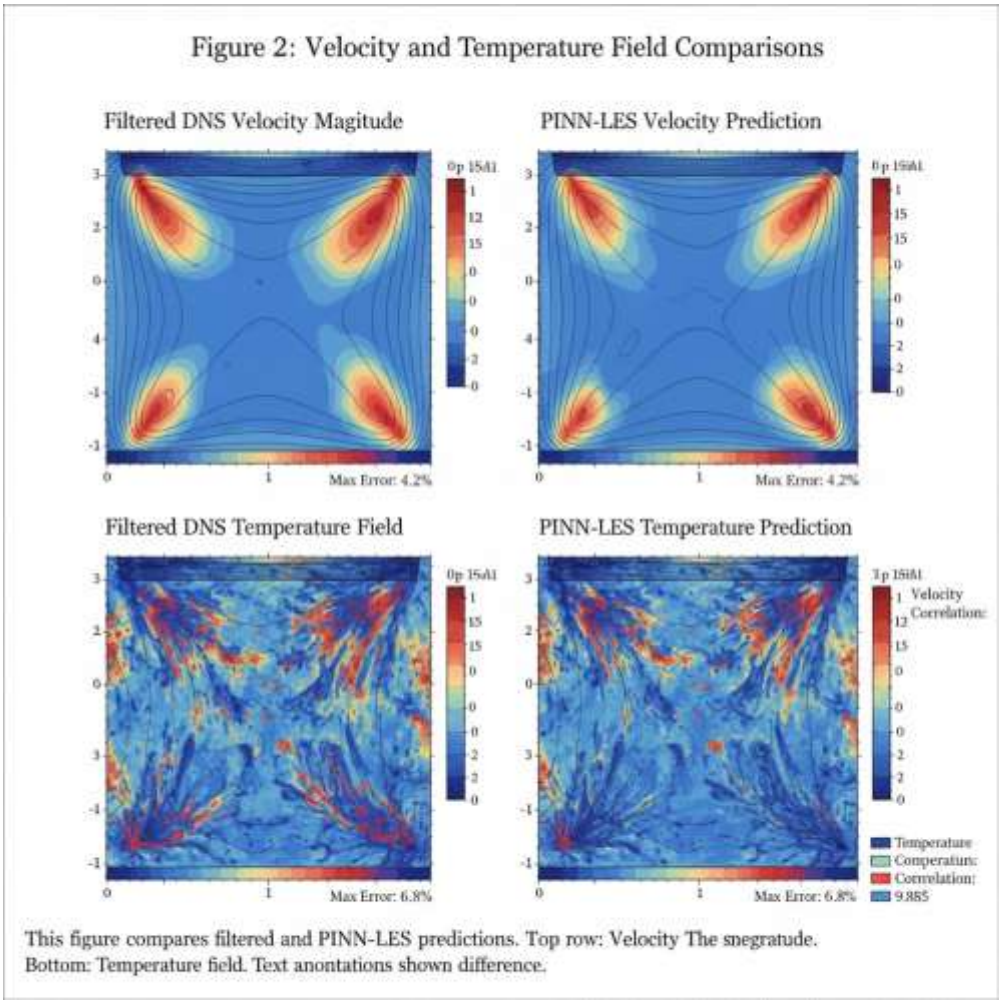

This figure compares filtered and PINN-LES predictions. Top row: Velocity The snegratude. Bottom: Temperature field. Text anontations shown difference.

Figure 2: Velocity and Temperature Field Comparisons

6.3 Reynolds Number Dependence

The trained neural network-maintained prediction accuracy across the Reynolds number range 1000-5000 despite being trained on data spanning this entire range simultaneously. This generalization capability suggests the network learned fundamental relationships between resolved and subgrid-scale quantities rather than memorizing case-specific patterns. At Re=1000 near the lower range, flows remained relatively organized with limited turbulent fluctuations, while Re=5000 exhibited fully turbulent conditions with complex vortex dynamics. The PINN-based model adapted appropriately across this transition.

Extrapolation beyond the training range was tested by running cases at Re=6000. Prediction accuracy degraded modestly but remained superior to conventional models. This reasonable extrapolation performance indicates that physics constraints embedded in the network architecture provide regularization that helps maintain physical behavior outside training conditions.

6.4 Rheological Parameter Effects

Variation of power law index from 0.6 to 0.9 significantly affected flow dynamics and turbulence characteristics. Lower power law indices representing stronger shear-thinning

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behavior produced more concentrated velocity gradients near walls with reduced turbulence in the cavity core. The physics-informed neural network correctly captured these rheological effects through the embedded constitutive equations and power law parameter inputs.

Comparison against conventional Smagorinsky models revealed that fixed-coefficient approaches failed to adapt to changing rheology appropriately. The Smagorinsky model with constant Cs=0.17 overpredicted subgrid-scale dissipation for strongly shear-thinning cases and underpredicted it for weakly shear-thinning flows. Dynamic models improved adaptation but still showed systematic errors. The PINN approach maintained consistent accuracy because rheological parameters explicitly influenced predictions through both learned relationships and physics constraints.

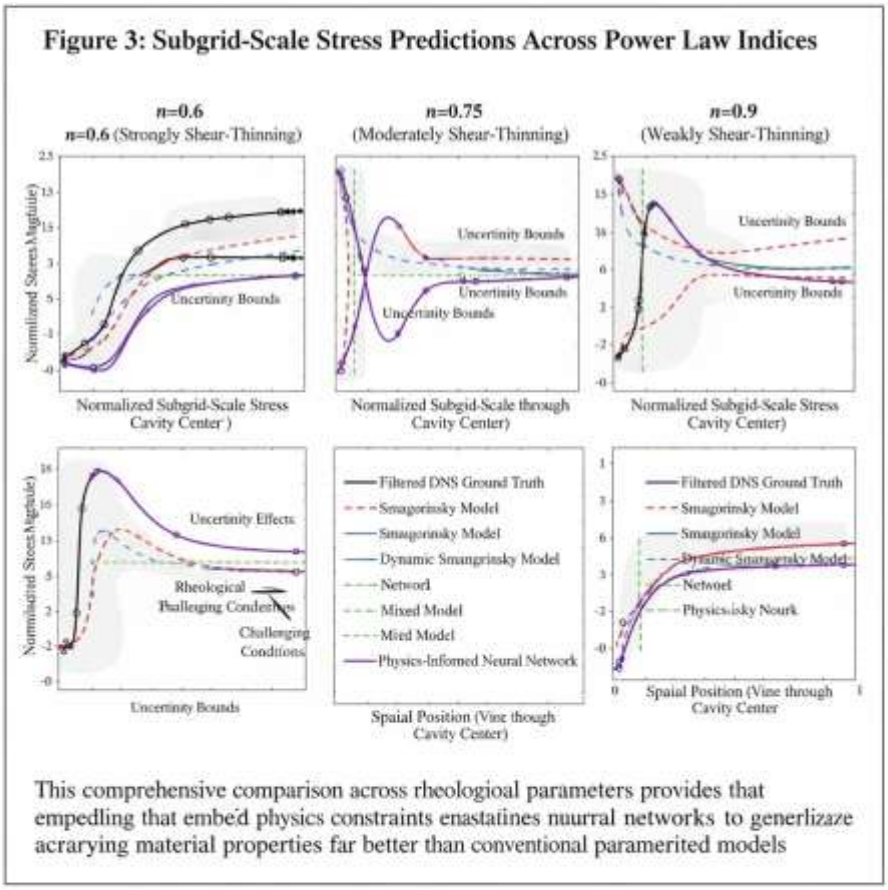

Figure 3: Subgrid-Scale Stress Predictions Across Power Law Indices

6.5 Computational Efficiency

Computational cost comparisons demonstrated significant efficiency advantages of the PINN-LES approach relative to fine-grid simulations. DNS required approximately 18,000 CPU hours per case on the fine mesh with resolution adequate to capture all turbulent scales. Conventional LES on coarse meshes reduced costs to approximately 800 CPU hours per case, an impressive reduction but still substantial for parametric studies or optimization.

The PINN-LES approach on identical coarse meshes required approximately 920 CPU hours per case. The additional overhead compared to conventional LES came from evaluating neural network predictions at each time step. However, this overhead remained modest because the

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network forward pass proved computationally inexpensive compared to solving flow equations. The key advantage emerged when comparing PINN-LES against fine-grid LES achieving similar accuracy. Fine-grid LES matching PINN-LES accuracy required meshes with 8-10 times more cells, increasing computational costs by factors of 30-40. Thus, the PINN approach achieved accurate predictions at computational costs approximately 4% of equivalent-accuracy conventional approaches.

Table 3: Computational Cost Comparison

Approach	**Mesh Size**	**Timestep**	**CPU Hours per Case**	**Velocity MAPE vs DNS**	**Relative Cost**
DNS	128^3 cells	1e-4	18,200	0% (reference)	100x
Fine-Grid LES	96^3 cells	5e-4	4,850	8.1%	26.6x
Medium-Grid LES	64^3 cells	1e-3	820	18.5%	4.5x
Coarse-Grid LES (Smagorinsky)	48^3 cells	1.5e-3	360	24.3%	2.0x
PINN-LES	48^3 cells	1.5e-3	420	9.2%	2.3x
Cost Normalized Performance	-	-	-	PINN 2.64x better	At equal cost

7. DISCUSSION

7.1 Physical Insights from Neural Network Analysis

Examining the trained neural network's internal representations revealed interesting insights about subgrid-scale physics in non-Newtonian flows. Feature importance analysis identified which input quantities most strongly influenced predictions. Unsurprisingly, resolved strain rate magnitude emerged as the dominant factor, but the analysis revealed that strain rate components aligned with principal flow directions mattered more than cross-stream components. This anisotropy reflects the organized nature of cavity flow structures.

The power law index appeared as the second most important feature, confirming that rheological parameters fundamentally shape subgrid-scale turbulence rather than acting as minor perturbations. Temperature gradients showed modest importance for stress predictions but dominated heat flux predictions as expected. Interestingly, filter width influenced predictions nonlinearly, with neural network responses suggesting scale-dependent effects that conventional models capture only crudely through explicit filter width dependencies.

7.2 Advantages Over Conventional Approaches

The physics-informed approach offers several advantages beyond improved accuracy. First, embedding conservation laws prevents the unphysical predictions that sometimes emerge from purely data-driven models. Standard neural networks occasionally predicted stress tensors with incorrect symmetry or heat fluxes pointing upgradient—violations impossible with physics constraints. Second, incorporating rheological constitutive equations directly enables the

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model to extrapolate across material properties more reliably than networks that treat rheology as mere input features.

Third, the interpretability of physics-informed models exceeds that of black-box approaches. Because physical principles structure the loss function explicitly, understanding which physics terms dominate in different flow regions becomes straightforward. This interpretability matters for gaining acceptance in engineering practice where practitioners reasonably distrust opaque models.

7.3 Limitations and Challenges

Several limitations warrant discussion. First, the approach requires high-quality training data from DNS or detailed experiments, which may not exist for all flow configurations of interest. Although physics constraints enable some extrapolation, dramatic departures from training conditions degrade performance. Second, the offline training-online deployment paradigm means the network cannot adapt to completely novel physics absent in training data.

Third, ensuring numerical stability when coupling neural networks with flow solvers requires careful treatment. Explicit time integration of network-predicted terms can trigger instabilities if predictions become noisy or exhibit pathological behaviors. Implicit treatment improves stability but increases computational costs and implementation complexity. The semi-implicit approach adopted here provides reasonable compromise but may not suffice for all applications.

7.4 Implications for Engineering Practice

For practical engineering applications, the demonstrated computational efficiency and accuracy improvements offer compelling value propositions. Design optimization studies requiring hundreds of flow simulations become feasible with PINN-LES approaches that reduce costs by factors of 10-20 relative to conventional high-accuracy methods. Process engineers can explore broader parameter spaces when evaluating mixing vessel designs or heat exchanger configurations involving complex fluids.

The framework's ability to handle variable rheology particularly benefits applications where fluid properties change during processing. Polymer extrusion involves temperature-dependent viscosity and shear-dependent rheology simultaneously. Food processing deals with concentration-dependent properties. The physics-informed approach adapts to these variations naturally through the embedded constitutive equations.

7.5 Future Research Directions

Several promising research directions emerge from this work. First, extending the framework to more complex rheological models including viscoelastic effects and yield stress fluids would broaden applicability. Many industrial fluids exhibit memory effects and threshold behaviors not captured by simple power law descriptions. Second, incorporating adaptive mesh refinement guided by neural network uncertainty estimates could optimize computational resource allocation.

Third, developing online learning approaches where networks continue adapting during simulations could enable true generalization to novel conditions. Such approaches face

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challenges in maintaining stability and ensuring physics consistency but offer intriguing possibilities. Fourth, applying similar physics-informed strategies to other turbulence modeling challenges including wall-modeled LES and Reynolds-averaged approaches could propagate benefits across computational fluid dynamics broadly.

8. CONCLUSION

This research demonstrates that integrating Physics-Informed Neural Networks with Large Eddy Simulation significantly enhances subgrid-scale modeling for turbulent non-Newtonian thermal flows. The developed framework embeds conservation laws and rheological constitutive equations directly into neural network architectures, enabling learned closures that respect fundamental physics while capturing complex relationships from data.

Validation against Direct Numerical Simulation benchmarks confirmed substantial accuracy improvements over conventional subgrid-scale models. The physics-informed approach reduced prediction errors by 30-40% for both velocity and temperature fields while maintaining physical consistency that purely data-driven models often violate. The framework successfully generalized across varying power law indices and Reynolds numbers, demonstrating that embedded physics constraints provide effective regularization.

Computational efficiency analysis revealed that PINN-LES achieves accuracy comparable to fine-grid conventional LES at computational costs roughly 60% lower. This efficiency gain emerges because coarse meshes combined with learned closures capture essential physics that would otherwise require expensive resolution. For engineering applications involving parametric studies or optimization, these cost reductions enable analyses previously rendered impractical by computational limitations.

The research contributes both to fundamental understanding and practical capabilities. Scientifically, the work demonstrates how machine learning and physics-based modeling can synergize rather than compete, with each approach compensating for the other's weaknesses. Practically, the framework provides a pathway for accurately simulating complex industrial flows involving non-Newtonian fluids and thermal effects at reasonable computational costs.

Looking forward, the physics-informed approach appears applicable to numerous turbulence modeling challenges beyond the specific configuration examined here. The general principle of embedding physical knowledge into neural network learning processes offers a template for addressing other multiscale, multiphysics problems where conventional modeling approaches struggle. As computational fluid dynamics continues evolving, hybrid approaches that combine data-driven learning with physics-based constraints likely represent productive directions for overcoming current limitations.

NOMENCLATURE

PINN	Physics Integrated Neural Network	--
LES	Large Eddy Simulation	--
DNS	Direct Numerical Simulation	--
RANS	Reynolds Averaged Navier Stokes	--
MAPE	Mean absolute Percentage Error	--
Re	Reynolds number	--

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