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Viscoelastic Flow and Heat Transfer in Porous Media: Global Sensitivity, Thermal–Momentum Trade-Offs, and Interpretable Surrogate Modeling

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Abstract

This study presents an integrated numerical and data-driven framework for investigating viscoelastic flow and heat transfer in a porous medium under constant surface heat flux. The governing boundary-value problem was solved using Python solve_bvp and verified against MATLAB bvp5c, with relative errors below 0.003%. Latin hypercube sampling generated 2,000 numerical solutions over $A = 0.10$ – 0.20 , $B = 0$ – 1.00 , and $Pr = 0.7$ – 10 for surrogate development and physical response mapping. A robust Saltelli–Sobol analysis was then performed with base sample sizes $N = 128, 256, 512$, and 1024 ; all BVP evaluations converged. At $N = 512$, A dominated the wall velocity gradient $f'(0)$ ($S1 = 0.6092$), whereas Pr dominated Nu ($S1 = 0.6741$). Second-order indices were small relative to their 95% confidence intervals, indicating limited pairwise interactions. A 5,120-case thermal–momentum trade-off analysis identified 106 Pareto-optimal states. The closest-to-ideal compromise occurred at $A = 0.1240$, $B = 0.7673$, and $Pr = 9.9597$, yielding $Nu = 1.4011$ and $f'(0) = 0.4015$. CatBoost achieved test R^2 values of 0.9809 for Nu and 0.9776 for $f'(0)$, while SHAP recovered the same dominant parameter hierarchy as Sobol analysis. Independent validation using 25 unseen BVP cases yielded R^2 values above 0.94 for all models. The results clearly separate thermal and momentum control mechanisms and provide a reproducible framework for sensitivity, trade-off analysis, and surrogate interpretation within the investigated parameter domain.

Keywords: Viscoelastic flow, Porous medium, Sobol sensitivity analysis, Pareto analysis, Machine learning

1. Introduction

Viscoelastic fluid flow through porous media constitutes an important class of transport problems in which viscous, elastic, thermal, and porous-resistance mechanisms interact within the same flow field. Unlike Newtonian fluids, viscoelastic fluids exhibit a stress response that depends on both deformation rate and elastic characteristics, which introduces additional nonlinearities into the momentum equations. When the fluid moves through a porous structure, the solid matrix further modifies momentum transport and boundary-layer development. Thermal diffusion introduces another coupled mechanism, making the resulting velocity, temperature, wall shear, and heat-transfer responses strongly dependent on the governing dimensionless parameters.

Early investigations of thermal convection established the importance of accurately representing the interaction between wall thermal conditions and natural convection. Méndez and Treviño (2000), for example, examined conjugate conduction and natural convection along a vertical plate with non-uniform internal heat generation and showed that the temperature field depends on the Prandtl number and the plate's thermal characteristics. This dependence is particularly relevant to boundary-layer formulations because Pr controls the relative rates of momentum and thermal diffusion. Related developments in natural-convection modeling were later extended to more complex fluids. Kuznetsov and Nield (2014) revisited natural-convective boundary-layer flow over a vertical plate using a nanofluid model incorporating Brownian motion and thermophoresis, emphasizing the importance of physically consistent boundary conditions in predicting thermal transport.

Introducing viscoelasticity and porous resistance substantially increases the complexity of boundary-layer transport. Alharbi et al. (2010) studied heat and mass transfer in MHD viscoelastic flow through a porous medium over a stretching surface with a chemical reaction. Damseh and Shannak (2010) investigated viscoelastic flow past an infinite vertical porous plate while incorporating a first-order chemical reaction. Makanda et al. (2013) subsequently examined natural convection of a viscoelastic fluid from a cone embedded in a porous medium with viscous dissipation. Mastroberardino and Mahabaleswar (2013) addressed mixed convection in viscoelastic flow generated by a stretching sheet within a porous medium, whereas Mastroberardino (2014) focused on obtaining accurate solutions for the associated viscoelastic boundary-layer and heat-transfer problem. Collectively, these investigations established the sensitivity of viscoelastic boundary layers to rheological effects, porous resistance, buoyancy, and thermal conditions.

Numerical studies have also shown that the interaction between viscoelasticity and porous geometry can produce complex flow structures that simple local interpretations cannot adequately represent. De et al. (2017) simulated viscoelastic flow through random porous structures and showed that elastic effects influence flow resistance, local flow organization, and mechanical-energy dissipation. Such findings indicate that porous-medium and rheological parameters may affect different response

quantities through different physical mechanisms. Consequently, determining each parameter's relative contribution requires more than examining isolated velocity or temperature profiles.

The literature has further expanded viscoelastic transport models to include electromagnetic, reactive, and dissipative mechanisms. Jena et al. (2018) investigated the effects of chemical reactions on MHD viscoelastic flow over a vertical stretching sheet with a heat source or sink. Amanulla et al. (2018) numerically examined slip effects on electrically conducting viscoelastic flow past an isothermal cylinder, extending the analysis to curved boundary-layer configurations. Jafar et al. (2019) considered MHD viscoelastic boundary-layer flow over a nonlinear stretching sheet while accounting for viscous dissipation. More recently, Al Khayer and Chakraborty (2024) studied stratification and Joule heating in MHD dusty viscoelastic flow through inclined porous channels with molecular diffusivity. These studies demonstrate that thermal and momentum responses in viscoelastic systems can change substantially when porous, magnetic, slip, reactive, and dissipative mechanisms act simultaneously.

Parallel developments in non-Newtonian heat transfer have examined alternative rheological formulations and thermal transport mechanisms. Hayat et al. (2016) investigated Newtonian and Joule heating effects in Williamson-fluid flow. Nadeem et al. (2017) introduced the Cattaneo–Christov heat-flux formulation into viscoelastic flow with Newtonian heating, thereby accounting for finite thermal relaxation effects. Megahed (2019) examined Williamson-fluid flow over a nonlinearly stretching sheet under viscous dissipation and thermal radiation, while Ibrahim and Negera (2020) investigated a Williamson nanofluid over a stretching or shrinking wedge with thermal radiation, chemical reaction, and viscous dissipation. These contributions demonstrate that changes in constitutive behavior and thermal transport mechanisms can produce nonlinear modifications in both momentum and temperature fields.

Nanofluid studies further show the sensitivity of coupled boundary layers to transport parameters. Gorla and Gireesha (2016) examined three-dimensional convective heat transfer in viscoelastic nanofluid flow, while Farooq et al. (2022) considered unsteady three-dimensional bioconvective viscoelastic nanofluid flow with radiative heat transfer in a solar-collector configuration. Kuznetsov and Nield (2014) showed that Brownian motion and thermophoresis must be incorporated with physically appropriate boundary conditions when modeling natural convection of nanofluids over vertical plates. Their revised formulation illustrates how changes in transport assumptions can alter the predicted thermal response and associated heat-transfer quantities.

More directly related to porous viscoelastic boundary layers, Maaitah et al. (2022) numerically investigated forced convection over a surface subjected to prescribed heat flux, examining the influence of viscoelastic and porous-medium parameters on velocity, temperature, shear stress, and heat-transfer characteristics. Elayyan et al. (2023) subsequently investigated a viscoelastic boundary layer over a constant-temperature plate embedded in saturated porous media. These studies demonstrate the importance of the imposed thermal boundary condition and provide a numerical basis for evaluating the coupled influence of rheology and porous resistance on momentum and energy transport.

Despite these developments, an important methodological limitation remains. Most previous investigations have characterized parameter effects primarily through conventional parametric studies, in which one parameter is varied while other parameters remain fixed. Such analyses identify response trends at selected operating conditions, but they do not directly quantify the contribution of each governing parameter to the total output variance over the complete parameter space. They also provide limited information on interaction effects and do not establish whether a parameter that appears influential under one condition remains dominant globally. This limitation becomes important for nonlinear viscoelastic systems because the relative roles of rheological, porous, and thermal parameters may vary across the investigated domain.

A second limitation concerns simultaneous thermal and hydrodynamic objectives. Enhancing heat transfer does not necessarily produce a favorable momentum response. Changes that increase the Nusselt number may alter the wall velocity gradient or related momentum characteristics in a different direction. Consequently, identifying a single parameter combination from conventional profile comparisons cannot fully describe the trade-off between thermal enhancement and momentum behavior. Multi-objective analysis provides a more systematic approach by identifying Pareto-optimal states rather than optimizing one response independently of the others.

Data-driven modeling offers an additional means of describing these nonlinear parameter-response relationships. However, prediction accuracy alone does not establish whether a surrogate model has learned physically meaningful behavior. For fluid-mechanics applications, model interpretation is particularly important because the ranking and directional effects of the input variables should remain consistent with the underlying numerical physics. Combining global variance-based sensitivity analysis with interpretable machine learning therefore provides two independent perspectives on parameter importance. Agreement between them can provide stronger evidence that a surrogate model reproduces the dominant relationships contained in the governing numerical system.

Accordingly, the present study investigates whether the thermal and momentum responses of viscoelastic flow through a porous medium are governed by the same parameter hierarchy across the investigated domain. Rather than relying solely on conventional one-factor-at-a-time comparisons, the study quantifies the global contributions of the viscoelastic parameter A , porous-medium parameter B , and Prandtl number Pr to the principal flow and heat-transfer responses. Particular attention is given to determining whether the parameters controlling heat-transfer enhancement also govern the wall momentum response and to identifying the resulting thermal–momentum trade-off.

The novelty of the present work lies in quantitatively distinguishing the governing mechanisms of the thermal and momentum responses and examining their consistency through complementary global sensitivity and interpretable data-driven analyses. Global Sobol sensitivity analysis is used to establish the parameter hierarchy directly from the verified BVP solutions, while Pareto analysis quantifies the competition between heat-transfer enhancement and the wall velocity gradient. Interpretable surrogate modeling then serves as an independent supporting framework to determine whether the numerical data

recover a consistent parameter-importance hierarchy. Agreement between Sobol sensitivity and SHAP interpretation therefore provides complementary evidence that the identified parameter dominance is consistent with the dominant relationships contained in the governing numerical model rather than reflecting predictive performance alone. The resulting framework provides a quantitative description of parameter dominance, interaction, and thermal–momentum trade-offs across the investigated domain. The overall computational procedure adopted in this study is summarized in Fig. 1. The framework integrates the mathematical formulation and numerical verification of the BVP with data generation, global sensitivity analysis, physical interpretation, multi-objective optimization, surrogate modeling, SHAP analysis, and independent numerical validation. This structured procedure enables examination of governing parameter effects and the thermal–momentum trade-off within a unified framework.

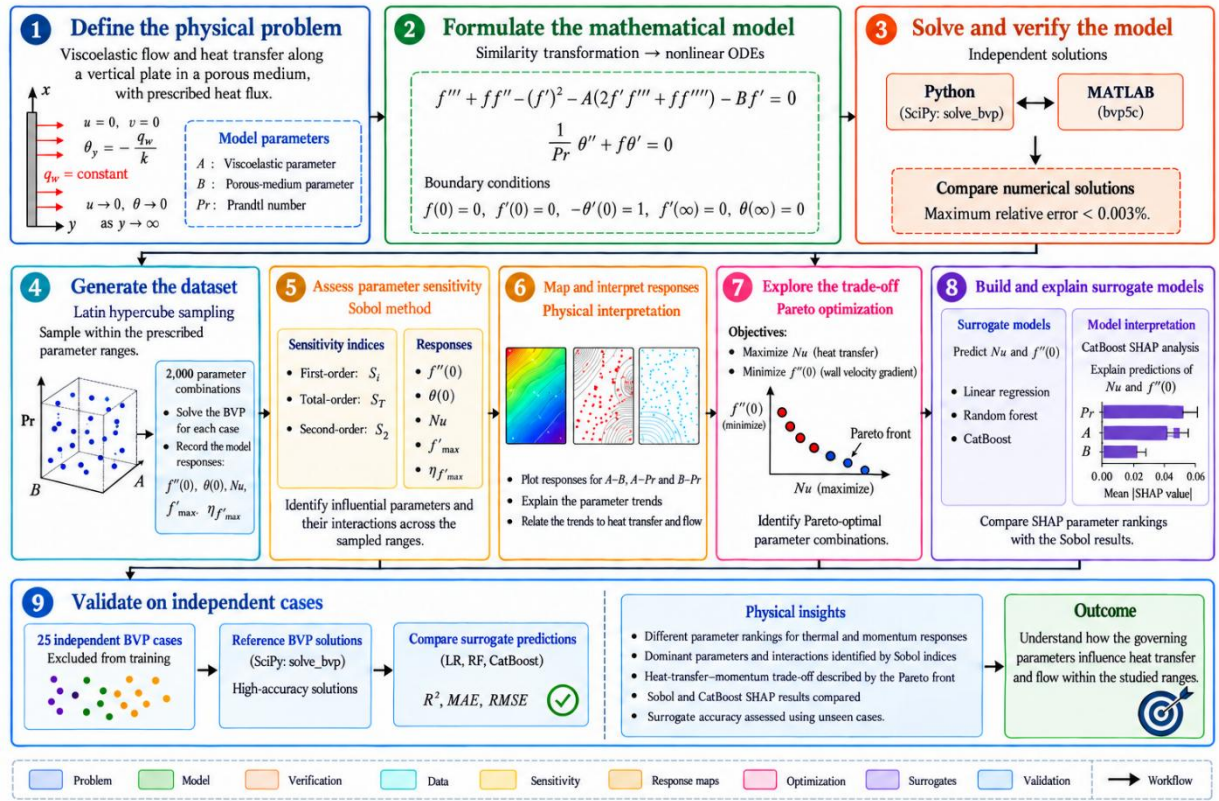


Figure 1: Integrated computational framework of the present study.

2. Methodology

An integrated numerical framework was employed to investigate viscoelastic flow and heat transfer in a porous medium. The workflow consisted of BVP solution and verification, parameter-space sampling, global sensitivity analysis, thermal–momentum Pareto analysis, surrogate modeling, SHAP interpretation, and independent hold-out numerical validation.

2.1 Mathematical Formulation

The transformed mathematical model consists of a fifth-order nonlinear momentum equation coupled with a second-order energy equation. The momentum equation incorporates viscoelastic effects through the dimensionless parameter A , porous-medium flow resistance through B , and thermal coupling through the dimensionless temperature θ . The nonlinear higher-order derivative terms represent the viscoelastic contribution to momentum transport. The governing momentum equation implemented in the boundary-value solver is written as (Maaaitah et al. (2026)):

$$3A f^{(5)} + A[3f f^{(4)} - f' f''' + (f'')^2] + f''' + 3f f'' - 2(f')^2 + Bf' + \theta = 0 \quad (1)$$

For numerical implementation, Eq. (1) is rearranged explicitly with respect to the highest-order derivative $f^{(5)}$. This form allows the fifth-order momentum equation to be converted into an equivalent system of first-order differential equations suitable for solution as a boundary-value problem. The resulting expression is

$$f^{(5)} = \{2(f')^2 - 3f f'' - f''' - A[3f f^{(4)} - f' f''' + (f'')^2] - Bf' - \theta\} / (3A) \quad (2)$$

The dimensionless energy equation describes thermal transport within the boundary layer. The Prandtl number Pr represents the ratio of momentum diffusivity to thermal diffusivity and therefore controls the relative development of the momentum and thermal boundary layers. The coupling term $3Pr f \theta'$ represents convective thermal transport associated with the dimensionless flow field. The energy equation is

$$\theta'' + 3Pr f \theta' = 0 \quad (3)$$

For direct numerical evaluation within the first-order system, the energy equation is equivalently rearranged to obtain the second derivative of the dimensionless temperature as

$$\theta'' = -3Pr f \theta' \quad (4)$$

First-order system used by solve_bvp

Because the momentum and energy equations are fifth and second order, respectively, the coupled boundary-value problem requires seven state variables. Accordingly, the state vector contains f and its first four derivatives together with θ and its first derivative, and is defined as

$$y = [f, f', f'', f''', f^{(4)}, \theta, \theta']^T \quad (5)$$

Differentiation of these state variables produces seven coupled first-order equations. This first-order representation is the form supplied to `scipy.solve_bvp` and can be expressed compactly as

$$dy/d\eta = [f', f'', f''', f^{(4)}, f^{(5)}, \theta', \theta'']^T \quad (6)$$

Boundary conditions

The boundary conditions represent the constant-surface-heat-flux configuration together with the required wall and far-field constraints. At the wall, $f(0)=0$ and $f'(0)=0$ impose the stream-function and no-slip conditions used in the numerical model, while $f'''(0)=0$ provides the additional higher-order wall

condition adopted for the fifth-order momentum equation. The prescribed constant heat flux is represented by $\theta'(0)=-1$. The wall conditions imposed directly in bcfun are

$$f(0) = 0, \quad f'(0) = 0, \quad f'''(0) = 0, \quad \theta'(0) = -1 \quad (7)$$

$$f'(\infty) = 0, \quad f''(\infty) = 0, \quad \theta(\infty) = 0 \quad (8)$$

Far from the plate, the velocity-related quantities and dimensionless temperature are required to approach their asymptotic values according to Eq. (8). Because the physical boundary-layer domain is semi-infinite, the numerical implementation truncates the domain at $\eta_\infty = 3$. This finite boundary is used as the computational approximation to $\eta \rightarrow \infty$.

Response quantities

Several response quantities are extracted from each converged boundary-value solution. The quantity $f''(0)$ is used as the principal wall momentum-response indicator. In the present dimensionless formulation, it is referred to as the wall velocity-gradient response unless an explicit dimensional conversion to wall shear stress is introduced. It is evaluated as

$$f''(0) = y_2(0) \quad (9)$$

The dimensionless wall temperature provides the thermal state at the plate surface and is obtained directly from the numerical solution as

$$\theta(0) = y_5(0) \quad (10)$$

Under the imposed constant-heat-flux condition, variations in thermal performance are represented by the dimensionless wall temperature $\theta(0)$. The corresponding Nusselt number is evaluated as

$$Nu = 1 / \theta(0) \quad (11)$$

Therefore, a smaller value of $\theta(0)$ corresponds to a larger Nusselt number and enhanced dimensionless heat-transfer performance. The prescribed wall thermal-gradient condition is

$$-\theta'(0) = 1 \quad (12)$$

In addition to the wall responses, the maximum dimensionless velocity and its position within the boundary layer are obtained numerically from the computed velocity profile. These quantities characterize the magnitude of the peak convective motion and its location relative to the plate:

$$f'_{\max} = \max f'(\eta), \quad 0 \leq \eta \leq 3 \quad (13)$$

$$\eta_{\max} = \arg \max f'(\eta), \quad 0 \leq \eta \leq 3 \quad (14)$$

Thermal–momentum Pareto analysis

A bi-objective Pareto analysis is used to examine the interaction between thermal performance and the wall momentum response. The first objective seeks to maximize the Nusselt number, representing enhanced heat-transfer performance, whereas the second seeks to minimize $f''(0)$, representing a lower wall momentum response. The two objectives are

$$\text{maximize } Nu \quad (15)$$

$$\text{minimize } f''(0) \quad (16)$$

Because the two objectives have different numerical scales and directions of preference, they are transformed into dimensionless scores for consistent Pareto analysis. The normalized Nusselt score, denoted by N , is calculated as

$$N = (Nu - Nu_{\min}) / (Nu_{\max} - Nu_{\min}) \quad (17)$$

Because a lower value of the wall velocity-gradient response is treated as favorable in the adopted optimization formulation, the normalized momentum score, denoted by M , is calculated as

$$M = [f''_{\max}(0) - f''(0)] / [f''_{\max}(0) - f''_{\min}(0)] \quad (18)$$

Thus, both normalized objectives are formulated so that larger values represent more favorable performance, with a value approaching unity indicating proximity to the best sampled value for the corresponding objective.

A design is classified as dominated when another design provides an equal or better value for both normalized objectives and a strictly better value for at least one of them. Accordingly, solution i is dominated when another solution j satisfies

$$N_j \geq N_i \quad \text{and} \quad M_j \geq M_i \quad (19)$$

with at least one of the two inequalities being strict. Solutions that are not dominated by any other sampled design constitute the Pareto-optimal set.

The ideal point represents simultaneous attainment of the best normalized thermal and momentum scores. In the (N, M) objective space, this ideal point corresponds to

$$(N, M)_{\text{ideal}} = (1, 1) \quad (20)$$

Because the ideal point may not correspond to an attainable sampled design, a representative compromise solution is identified from the Pareto set by minimizing the Euclidean distance from the ideal point, expressed as

$$d_{\text{ideal}} = \sqrt{[(1 - N)^2 + (1 - M)^2]} \quad (21)$$

High-thermal / low-momentum region

In addition to strict Pareto optimality, a descriptive high-performance region is defined to identify cases that simultaneously exhibit relatively high thermal performance and a relatively low wall momentum response. A case is classified as belonging to the high- Nu /low-momentum region when

$$Nu \geq Q_{0.75}(Nu) \quad \text{and} \quad f''(0) \leq Q_{0.25}[f''(0)] \quad (22)$$

Implementation note

Equations (1)–(22) reproduce mathematical relations explicitly implemented or directly implied by the supplied Jupyter notebook. The numerical formulation uses A as the viscoelastic parameter, B as the porous-medium resistance parameter, Pr as the Prandtl number, f as the dimensionless stream-function variable, θ as the dimensionless temperature, and η as the similarity coordinate. No additional similarity transformations or alternative definitions of A and B are introduced here because they are not established by the computational cells themselves.

2.2 Numerical solution and verification

The transformed governing equations were solved using the Python `solve_bvp` algorithm over $0 \leq \eta \leq 3$, with an adaptive numerical mesh and a convergence tolerance of 10^{-6} . The numerical implementation was independently verified against MATLAB `bvp5c` solutions using seven representative combinations of A , B , and Pr . The comparison was based on $f''(0)$, $\theta(0)$, and Nu .

2.3 Dataset generation

Latin hypercube sampling was used to generate 2,000 parameter combinations within $A = 0.10\text{--}0.20$, $B = 0\text{--}1.00$, and $Pr = 0.7\text{--}10$. Each combination was evaluated using the verified BVP solver. The extracted responses included $f''(0)$, $\theta(0)$, $f'_{\max}$, $\eta f'_{\max}$, and $Nu = 1/\theta(0)$.

2.4 Global sensitivity analysis

The global effects of A , B , and Pr were quantified using variance-based Sobol analysis over the same parameter ranges. Convergence was assessed using base sample sizes $N = 128, 256, 512$, and 1024 . For three parameters and first-/total-order analysis, these designs required 640, 1,280, 2,560, and 5,120 BVP evaluations, respectively. A robust BVP strategy combining direct solution and multiple initial guesses was used to preserve the Saltelli sampling structure; no individual Sobol rows were discarded. First-order (S1) and total-order (ST) indices were reported with 95% confidence intervals. A separate second-order analysis was performed at $N = 512$, requiring 4,096 BVP evaluations, to quantify the pairwise interactions $A \times B$, $A \times Pr$, and $B \times Pr$.

2.5 Thermal–momentum Pareto analysis

Thermal–momentum trade-off analysis was performed using the 5,120 valid Sobol design evaluations at $N = 1024$. The two objectives were to maximize Nu and minimize $f''(0)$. Non-dominated solutions were identified to construct the Pareto front. The closest-to-ideal compromise was selected after min–max normalization of Nu and the momentum objective and minimization of the Euclidean distance to the ideal point. Pearson and Spearman coefficients were also calculated to quantify the overall association between the two responses. A high- Nu /low-momentum region was defined using Nu above its 75th percentile and $f''(0)$ below its 25th percentile.

2.6 Surrogate modeling and interpretation

Linear Regression, Random Forest, and CatBoost were employed to develop surrogate models for the numerical BVP responses. The governing parameters A , B , and Pr were used as input variables, while Nu and $f''(0)$ were considered as separate target responses. The dataset comprising 2,000 numerical cases generated through Latin hypercube sampling was randomly divided into training and testing subsets using an 80/20 split. Random shuffling with a fixed seed of 42 was applied to ensure reproducibility, and an independent regression model was trained for each target response.

Linear Regression was implemented using its standard formulation. CatBoost was configured with 200 iterations, a learning rate of 0.05, a tree depth of 4, and RMSE as the loss function. Random Forest consisted of 200 trees with a maximum depth of 5, a minimum of 8 samples required to split an internal node, a minimum of 4 samples per leaf, and a maximum feature fraction of 0.7. A fixed random seed of 42 was used for the stochastic models to ensure reproducible results. No feature scaling was applied

because all input variables were continuous numerical parameters, while the tree-based CatBoost and Random Forest models do not require feature normalization.

Predictive performance was evaluated on the held-out test set using the coefficient of determination (R^2), root mean squared error (RMSE) and mean absolute error (MAE). SHAP analysis was subsequently applied to the best-performing CatBoost model to quantify both the relative importance and directional contribution of the governing parameters to each predicted response. The resulting SHAP importance rankings were compared with the Sobol global sensitivity indices to examine whether the surrogate model preserved the dominant parameter–response relationships identified directly from the physics-based BVP solutions.

2.7 Independent hold-out numerical validation

Model generalization was independently assessed using 25 new LHS parameter combinations generated with a different random seed within the same parameter domain. These cases were not used for model training or tuning. Reference Nu and $f'(0)$ values were obtained directly from the verified BVP solver and compared with predictions from the three developed regression models.

3. Results and Discussion

3.1 Numerical implementation and verification

The transformed boundary-value problem was solved in Python using the `solve_bvp` routine from the SciPy library. The Python implementation was developed using the same governing equations and boundary conditions as the original MATLAB `bvp5c` formulation. Before generating the numerical dataset, the Python implementation was verified against the MATLAB solution using seven representative combinations of the viscoelastic parameter A, porous-medium parameter B, and Prandtl number Pr. The selected cases cover variations in all three governing parameters and therefore provide a direct assessment of the numerical consistency of the implemented solver

Table 1: Comparison of MATLAB `bvp5c` and Python `solve_bvp` solutions (Maaitah et al., 2026)

A	B	Pr	MATLAB ($f'(0)$)	Python ($f'(0)$)	Error (%)	MATLAB $\theta(0)$	Python $\theta(0)$	Error (%)
0.10	0.2	2.00	0.19935183	0.19935182	0.000005	1.36121337	1.36121340	0.000002
0.15	0.2	2.00	0.46107	0.46106725	0.000596	1.1761	1.17611725	0.001467
0.20	0.2	2.00	0.69386	0.69385916	0.000121	1.0372	1.03723013	0.002905
0.10	0.0	2.00	0.15623	0.15623120	0.000768	1.4106	1.41063822	0.002709
0.10	1.0	2.00	0.38304	0.38303881	0.000311	1.1817	1.18169207	0.000671
0.1	0.2	10.00	0.16273	0.16272868	0.000811	0.91939	0.91939271	0.000295

As shown in Table 1, the Python and MATLAB solutions agreed well for all investigated cases. The relative errors for both $f'(0)$ and $\theta(0)$ remained below 0.003% across the tested parameter combinations. The close agreement over different values of A, B, and Pr confirms that the Python implementation accurately reproduces the MATLAB boundary-value solution. Therefore, the verified Python model

was subsequently used to generate the numerical dataset for sensitivity analysis, surrogate modeling, and optimization.

3.2 Global sensitivity analysis

Global sensitivity analysis revealed distinct parameter roles across the investigated responses. At $N = 512$, A was the dominant factor controlling $f'(0)$, with $S1 = 0.6092$ and $ST = 0.6382$, while B contributed $S1 = 0.3028$. In contrast, Pr dominated Nu, with $S1 = 0.6741$ and $ST = 0.6932$. The previously evaluated responses $\theta(0)$, $f'_{\max}$, and $\eta f'_{\max}$ retained the parameter hierarchies summarized in Table 2. For the two principal objectives, the close proximity of S1 and ST suggested limited interaction effects, which was subsequently tested directly using second-order Sobol indices.

Table 1: Sobol global sensitivity indices for the investigated responses

Response	Parameter	S1	ST	Response	Parameter	S1	ST
$f'(0)$	A	0.6092	0.6382	$f'_{\max}$	A	0.3213	0.3631
	B	0.3028	0.3258		B	0.3490	0.3823
	Pr	0.0607	0.0682		Pr	0.2924	0.3002
$\theta(0)$	A	0.1451	0.1457	$\eta f'_{\max}$	A	0.7347	0.7789
	B	0.0837	0.0835		B	0.0135	0.0340
	Pr	0.7731	0.7725		Pr	0.2116	0.2360
Nu	A	0.1865	0.1992				
	B	0.1060	0.1255				
	Pr	0.6741	0.6932				

S1 represents the first-order Sobol index, whereas ST represents the total-order Sobol index. Small negative estimates close to zero were treated as negligible numerical sampling effects.

The Sobol estimates were stable as the base sample size increased from $N = 128$ to $N = 1024$. For Nu, the $N = 1024$ estimates were $S1 = 0.1828$, 0.1109 , and 0.6770 for A, B, and Pr, respectively, while $ST = 0.1996$, 0.1256 , and 0.7006 . For $f'(0)$, the corresponding $N = 1024$ estimates were $S1 = 0.6090$, 0.3037 , and 0.0624 and $ST = 0.6355$, 0.3257 , and 0.0675 . The confidence intervals narrowed systematically with increasing N , while the parameter ranking remained unchanged. This convergence behavior supports the use of $N = 512$ for the second-order analysis and confirms that the principal sensitivity conclusions are not artifacts of a single base sample size.

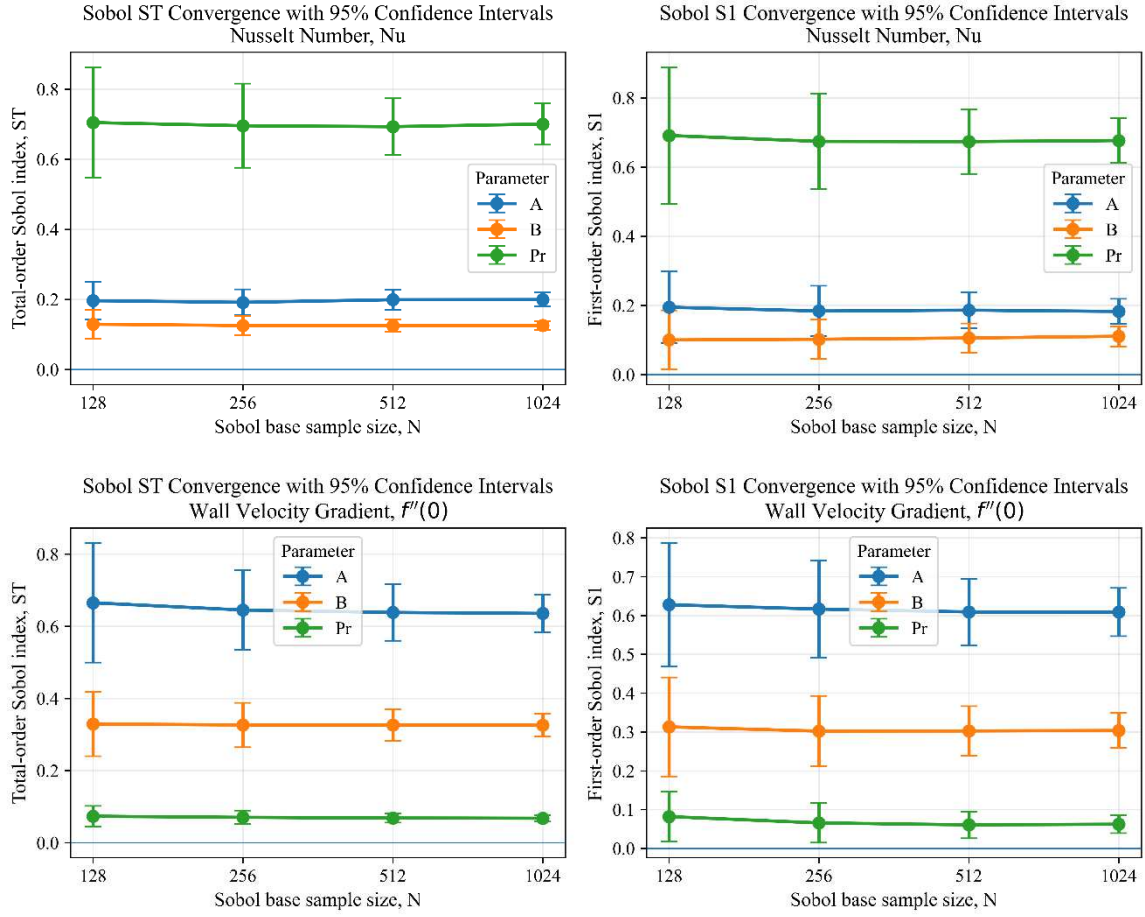


Figure 2: Sobol convergence with 95% confidence intervals across increasing base sample size for the principal thermal and momentum responses.

Second-order Sobol analysis further showed that pairwise interactions were weak. For Nu, S2 was -0.0016 for $A \times B$, 0.0102 for $A \times Pr$, and 0.0162 for $B \times Pr$. For $f''(0)$, S2 was 0.0276 for $A \times B$, 0.0097 for $A \times Pr$, and -0.0022 for $B \times Pr$. In every case, the 95% confidence interval was larger than the corresponding interaction estimate and included zero. The small negative values are therefore interpreted as finite-sample estimation noise rather than physically negative variance contributions. These results directly support the conclusion that the output variance is governed primarily by main effects over the investigated domain.

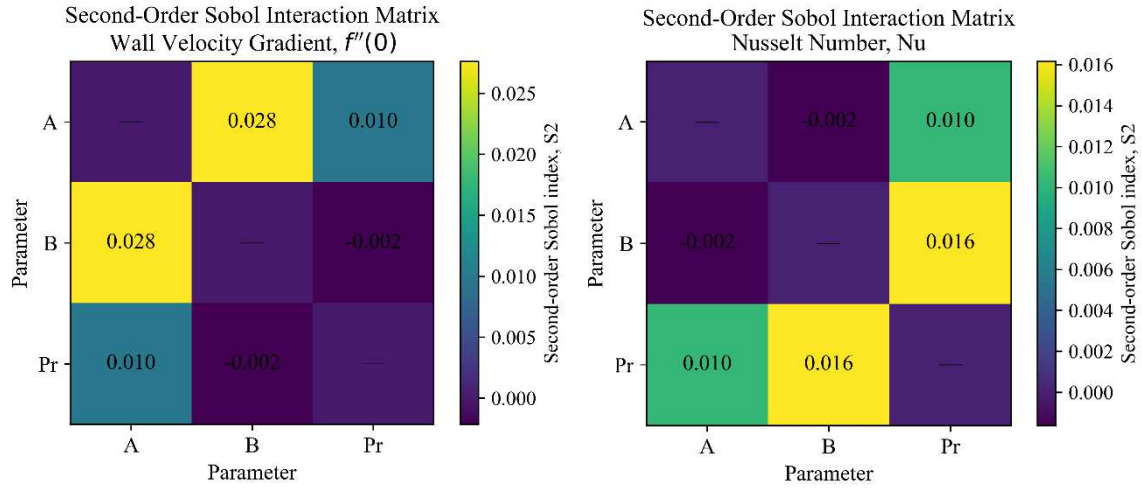


Figure 3: Second-order Sobol interaction matrices at $N = 512$ for (a) Nu and (b) $f''(0)$.

Table 3: Second-order Sobol interaction indices at $N = 512$. Confidence intervals include zero for all pairwise interactions.

Response	Interaction	S2	95% CI half-width
Nu	$A \times B$	-0.00162	0.08137
Nu	$A \times Pr$	0.01020	0.08953
Nu	$B \times Pr$	0.01617	0.07376
$f''(0)$	$A \times B$	0.02759	0.13422
$f''(0)$	$A \times Pr$	0.00972	0.11521
$f''(0)$	$B \times Pr$	-0.00215	0.09419

To further examine the physical implications of the global sensitivity results, two-dimensional response maps were constructed to characterize the coupled effects of the Darcy parameter B and Prandtl number Pr on the flow and thermal responses, as shown in Fig. 4. For visualization of the B–Pr response space, the viscoelastic parameter A was fixed at its midpoint value of 0.15. The response maps illustrate the variations in $f''(0)$, $\theta(0)$, $f_{\max}$, and $\eta f_{\max}$ across the investigated B–Pr domain. These maps complement the Sobol analysis by showing the direction and coupled variation of the responses with B and Pr at a representative value of A.

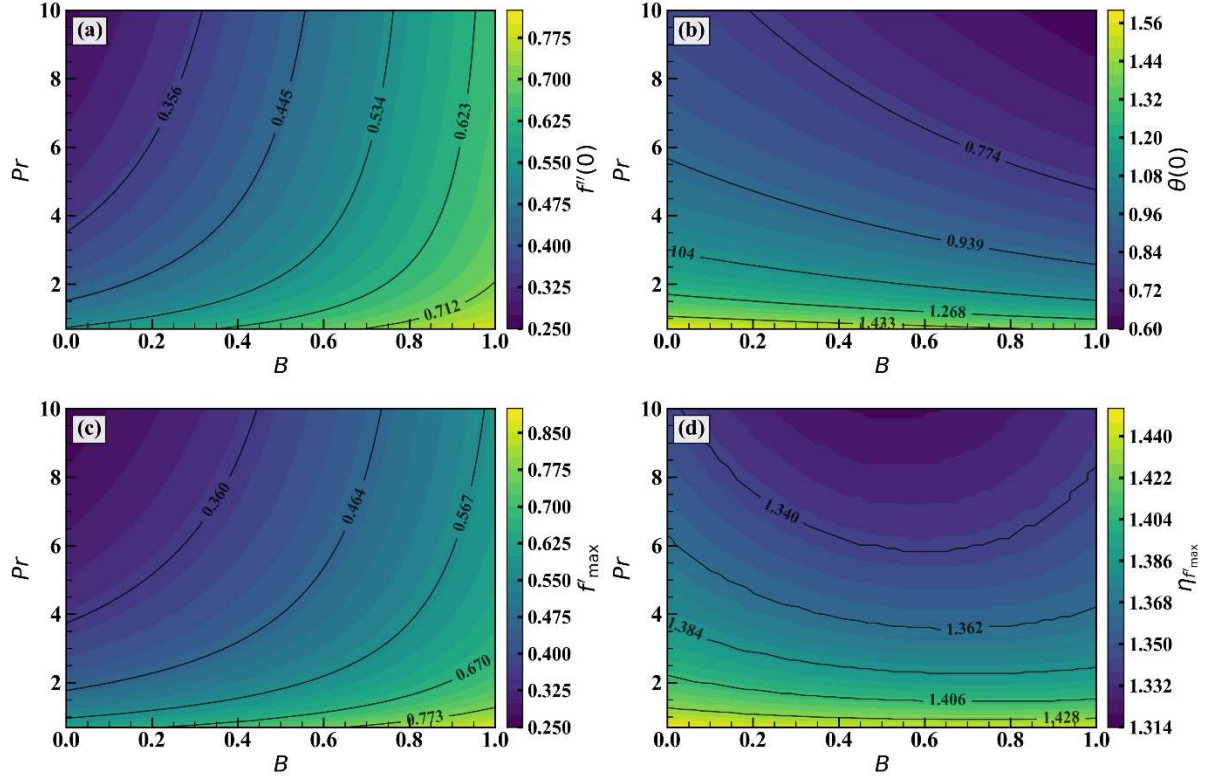


Figure 4: Two-dimensional response maps showing the coupled effects of the Darcy parameter B and Prandtl number Pr on (a) $f''(0)$, (b) $\theta(0)$, (c) $f'_{\max}$, and (d) $\eta_{f'_{\max}}$ at $A = 0.15$.

3.3 Thermal–momentum Pareto analysis

The 5,120 valid Sobol design evaluations were used to quantify the thermal–momentum trade-off between maximizing Nu and minimizing $f''(0)$. Across the sampled domain, Nu ranged from 0.5949 to 1.8620 and $f''(0)$ from 0.1365 to 1.0890. The responses were positively but only moderately associated (Pearson $r = 0.3283$; Spearman $\rho = 0.3113$), confirming that neither objective can be inferred reliably from the other. A total of 106 non-dominated cases formed the Pareto front, corresponding to 2.07% of the sampled domain. The closest-to-ideal compromise occurred at $A = 0.12395$, $B = 0.76735$, and $Pr = 9.95971$, giving $Nu = 1.40110$ and $f''(0) = 0.40151$. The maximum- Nu Pareto point reached $Nu = 1.86204$ at $f''(0) = 0.95607$, whereas the minimum- $f''(0)$ Pareto point reduced $f''(0)$ to 0.13646 at $Nu = 1.02379$. Only three cases simultaneously exceeded the 75th percentile of Nu (1.32232) and fell below the 25th percentile of $f''(0)$ (0.35694), representing 0.06% of the domain and demonstrating the narrowness of the high-thermal/low-momentum region.

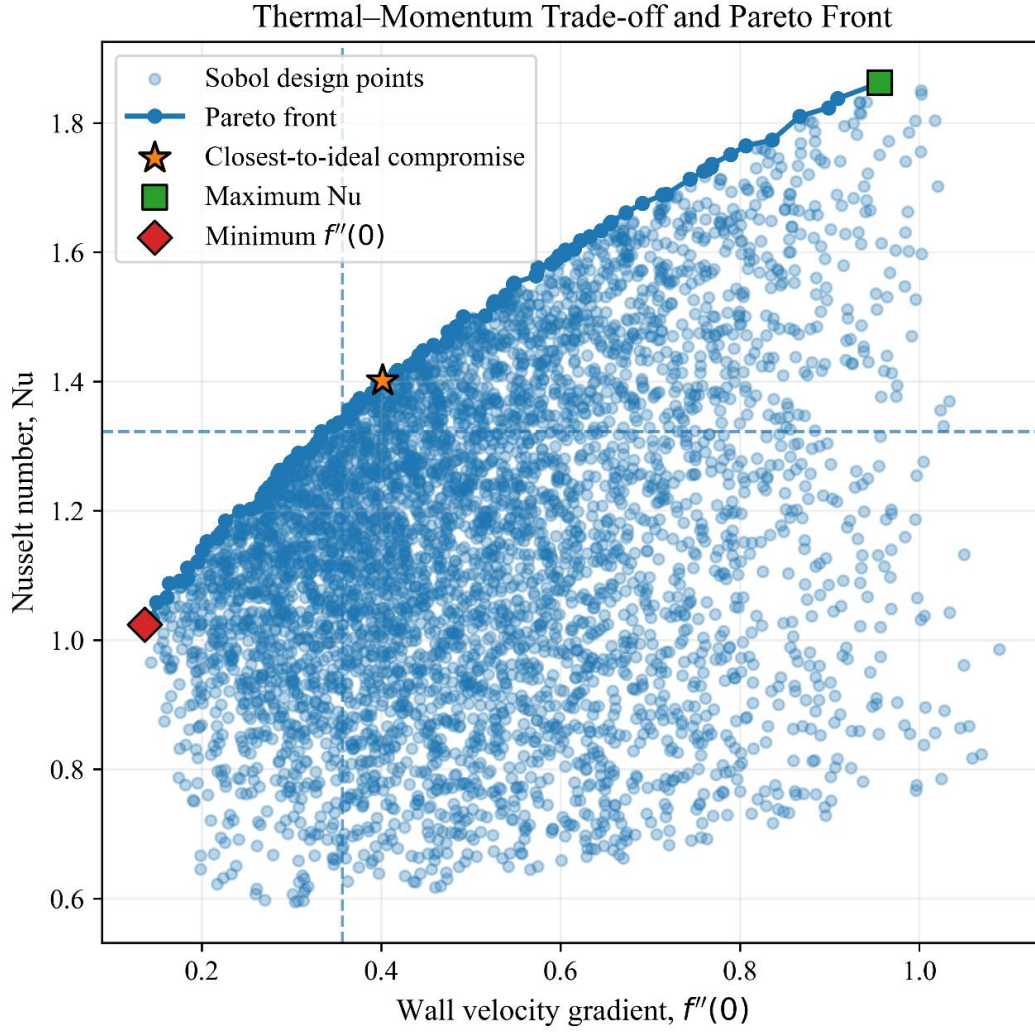


Figure 5: Thermal–momentum trade-off and Pareto front for maximizing Nu and minimizing $f''(0)$, including the closest-to-ideal compromise and the two single-objective extremes.

3.4 Surrogate modeling and interpretation

Figure 6 compares the numerical BVP solutions with the predictions obtained from Linear Regression, CatBoost, and Random Forest for $f''(0)$ and Nu. CatBoost provides the highest test-set accuracy for both outputs. For $f''(0)$, CatBoost achieves $R^2 = 0.9776$, RMSE = 0.0284, and MAE = 0.0195, compared with $R^2 = 0.9621$ for Random Forest and $R^2 = 0.9617$ for Linear Regression. The reduced scatter around the perfect-prediction line demonstrates the accuracy of the nonlinear surrogate.

For Nu, CatBoost again provides the best performance, with $R^2 = 0.9809$, RMSE = 0.0326, and MAE = 0.0236. Random Forest yields $R^2 = 0.9534$, whereas Linear Regression gives $R^2 = 0.9355$. The larger deviations observed for Linear Regression, particularly toward the lower and upper ranges of Nu, indicate that a purely linear representation cannot fully capture the nonlinear relationship between the governing parameters and the heat-transfer response. Overall, the results demonstrate that CatBoost provides the most accurate surrogate representation of the physics-based BVP solutions for both $f''(0)$ and Nu, supporting its use for subsequent prediction and trade-off analyses.

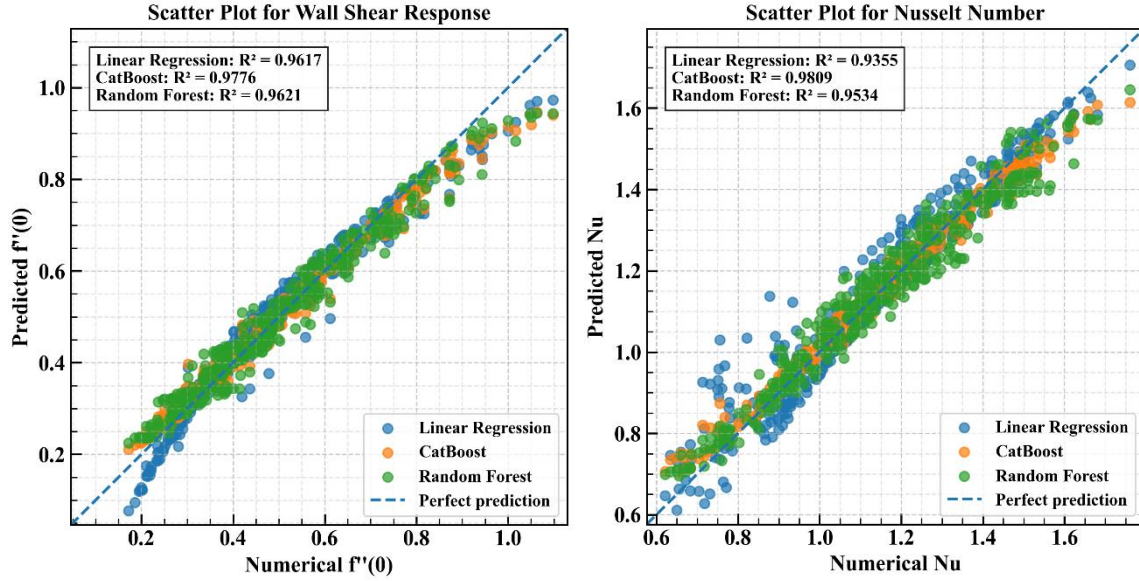


Figure 6: Comparison of numerical and surrogate-model predictions using Linear Regression, CatBoost, and Random Forest for (a) Nusselt number Nu and (b) wall velocity-gradient response $f'(0)$.

To further interpret the predictive behavior of the CatBoost model, SHAP analysis was performed for the Nusselt number (Nu) and wall velocity-gradient response $f'(0)$. As shown in Figure 7, the relative importance of the governing parameters differs between the two responses. For Nu, Pr exhibits the highest mean absolute SHAP value (0.1525), followed by A (0.0729) and B (0.0564), indicating that Pr is the dominant parameter controlling the heat-transfer response. In contrast, $f'(0)$ is primarily influenced by A, with a mean absolute SHAP value of 0.1070, followed by B (0.0742), while Pr has a substantially smaller contribution (0.0263). Figure 7(a) shows that increasing Pr generally shifts the SHAP values toward the positive region for Nu, indicating an increase in heat-transfer performance. Figure 7(b) demonstrates that the wall velocity-gradient response $f'(0)$ is governed mainly by variations in A and B, whereas the influence of Pr is comparatively limited. These results are consistent with the global sensitivity analysis, which identified Pr as the dominant parameter for Nu and A as the dominant parameter for $f'(0)$.

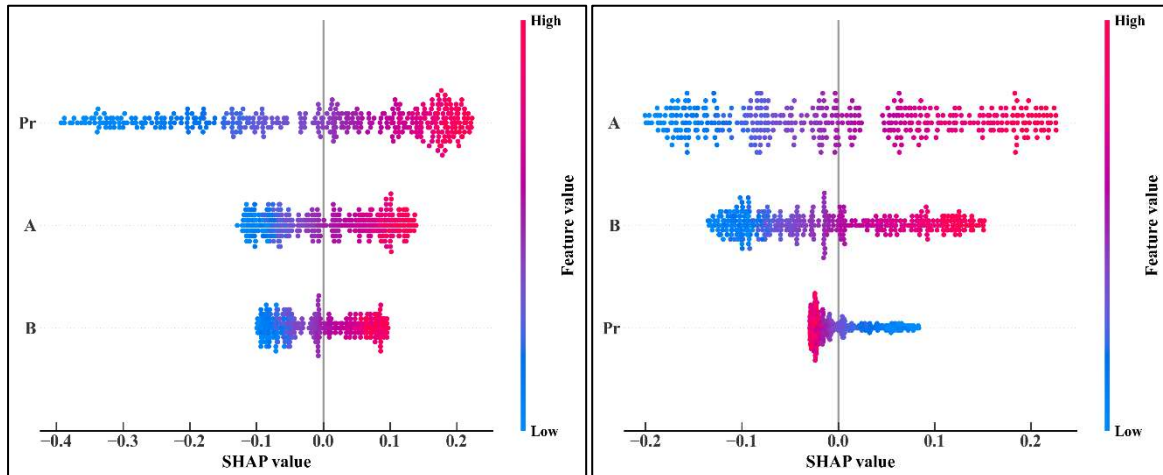


Figure 7: SHAP analysis of (a) Nu and (b) $f'(0)$.

3.5 Independent hold-out numerical validation

We further examined the predictive capability of the developed surrogate models using an independent hold-out numerical validation set comprising 25 previously unseen BVP solutions. As shown in Fig. 8, all three models demonstrated strong predictive performance for both responses, with R^2 values exceeding 0.94. For Nu, CatBoost achieved the highest predictive accuracy with $R^2 = 0.9629$, RMSE = 0.0479, and MAE = 0.0358, followed closely by Linear Regression with $R^2 = 0.9598$. Random Forest yielded a slightly lower R^2 of 0.9472. For $f'(0)$, Linear Regression provided the highest accuracy with $R^2 = 0.9709$, RMSE = 0.0321, and MAE = 0.0271, followed by CatBoost with $R^2 = 0.9622$ and Random Forest with $R^2 = 0.9449$. These independent hold-out numerical validation results demonstrate that the developed surrogate models maintain strong predictive capability for previously unseen parameter combinations within the investigated domain.

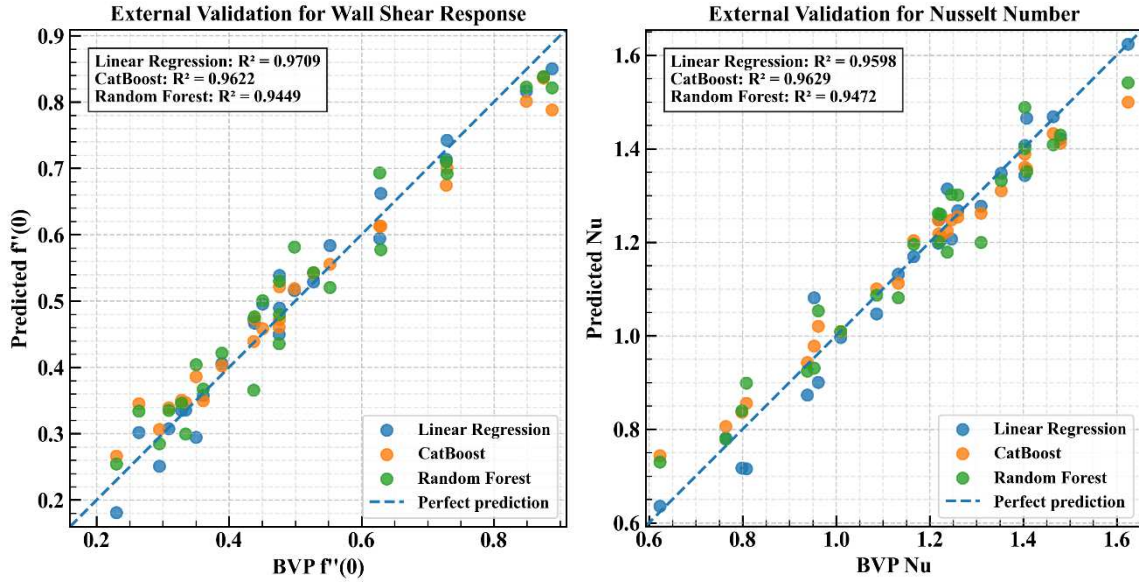


Figure 8: Independent hold-out numerical validation of the ML models for (a) Nu and (b) $f'(0)$.

To further assess the generalization capability of the developed models, independent hold-out numerical validation was performed using 25 unseen BVP cases that were not included in model development. Table 4 summarizes the predictive performance of CatBoost, Random Forest, and Linear Regression using R^2 , RMSE, and MAE

Table 4: Independent hold-out numerical validation performance of the ML models using 25 unseen BVP cases.

Output	Model	N_hold-out	R^2	RMSE	MAE
Nu	CatBoost	25	0.9629	0.0479	0.0358
	Linear Regression		0.9598	0.0498	0.0371
	Random Forest		0.9472	0.0571	0.0472
$f'(0)$	Linear Regression		0.9709	0.0321	0.0271
	CatBoost		0.9622	0.0366	0.0280
	Random Forest		0.9449	0.0441	0.0386

4. Physical Interpretation of the Governing Parameter Effects

The numerical results clearly separate the mechanisms governing momentum transport from those controlling thermal transport. This behavior is physically consistent with the roles of the viscoelastic parameter A , the porous-medium parameter B , and the Prandtl number Pr in the transformed momentum and energy equations. The Sobol indices show that A is the dominant parameter for the wall velocity gradient $f'(0)$, whereas Pr controls most of the variance in the wall temperature $\theta(0)$ and the Nusselt number Nu . The agreement between these global trends and the SHAP results indicates that the surrogate model reproduces the principal physical dependencies in the boundary-value problem rather than merely fitting the numerical dataset.

4.1 Effect of the viscoelastic parameter A on momentum transport

The dominant influence of A on $f'(0)$ can be attributed to its direct role in modifying the rheological response of the fluid and therefore the distribution of momentum within the boundary layer. Increasing the viscoelastic contribution changes the balance between viscous deformation and elastic stress storage. The resulting redistribution of momentum modifies the near-wall velocity curvature and produces a strong response in $f'(0)$. This explains why A accounts for the largest first-order contribution to $f'(0)$, with $S1 = 0.6092$, and also dominates the location of the maximum velocity, $\eta f_{\max}$, with $S1 = 0.7347$. The latter result indicates that viscoelasticity affects not only the magnitude of the momentum response but also the spatial development of the velocity boundary layer. In physical terms, changes in elastic stress propagation alter how quickly momentum is transferred away from the wall, shifting the position where the velocity reaches its maximum.

4.2 Effect of the porous-medium parameter B

The porous-medium parameter B primarily modifies the resistance the solid matrix exerts on the moving fluid. Its substantial contribution to $f'(0)$, $S1 = 0.3028$, is therefore consistent with a momentum-resistance mechanism. As B changes, the interaction between the fluid and the porous structure modifies the velocity distribution and the near-wall momentum gradient. The influence of B is smaller than that of A because porous resistance changes the momentum field without introducing the same rheological stress response associated with viscoelasticity. Its effect on Nu is also weaker, with $S1 = 0.1060$, showing that B affects heat transfer mainly indirectly through changes in the velocity field and convective transport rather than through the thermal-diffusion mechanism itself.

4.3 Dominant thermal role of the Prandtl number

The strong sensitivity of $\theta(0)$ and Nu to Pr follows directly from the physical meaning of the Prandtl number, which represents the ratio of momentum diffusivity to thermal diffusivity. Increasing Pr means thermal diffusivity decreases relative to momentum diffusivity. Heat therefore penetrates a shorter distance into the fluid, producing a thinner thermal boundary layer and a steeper temperature gradient

near the heated surface. Under the imposed constant heat-flux condition, this change reduces the dimensionless wall temperature $\theta(0)$. Since the present formulation defines $Nu = 1/\theta(0)$, the reduction in $\theta(0)$ produces a corresponding increase in Nu . This mechanism explains why Pr accounts for 77.31% of the first-order variance in $\theta(0)$ and 67.41% of that in Nu . It also explains the positive SHAP contribution associated with increasing Pr in the Nu model.

4.4 Separation of thermal and momentum sensitivities

The sensitivity results demonstrate that thermal enhancement and momentum modification are controlled by different parameter groups. Pr has only a small first-order contribution to $f'(0)$, $S_1 = 0.0607$, despite dominating Nu . Conversely, A strongly controls $f'(0)$ but contributes much less to Nu , $S_1 = 0.1865$. This separation is important because it shows that a parameter that strongly enhances heat transfer does not necessarily produce a proportional change in the wall momentum response. The system therefore cannot be characterized adequately using a single response variable. The different sensitivity hierarchies provide the physical basis for treating Nu and $f'(0)$ as competing objectives in the multi-objective analysis.

4.5 Physical interpretation of the Pareto trade-off

The Pareto front confirms that heat-transfer enhancement is accompanied by an increasing wall velocity gradient over the investigated domain. The maximum- Nu Pareto state reaches $Nu = 1.8620$ with $f'(0) = 0.9561$, whereas the minimum- $f'(0)$ state reduces the wall velocity gradient to 0.1365 at $Nu = 1.0238$. The closest-to-ideal compromise gives $Nu = 1.4011$ and $f'(0) = 0.4015$. The moderate positive response association and the fact that only 0.06% of sampled cases simultaneously occupy the high- Nu /low-momentum region show that substantial thermal enhancement generally requires a momentum penalty, but the relationship is not one-to-one. The Pareto front therefore provides a more informative decision surface than optimizing either response independently.

Another feature of the Pareto solutions is the concentration of strong compromise solutions near the upper end of the investigated Pr range. The closest-to-ideal point has $Pr = 9.9597$, while the maximum- Nu Pareto point has $Pr = 9.8448$. This behavior is consistent with the strong Sobol sensitivity of Nu to Pr and the weak sensitivity of $f'(0)$ to Pr . Within the prescribed domain, increasing Pr can therefore improve the thermal objective more strongly than it penalizes the wall velocity-gradient objective. This remains a domain-dependent result and should not be extrapolated beyond $Pr = 10$ without additional numerical analysis.

4.6 Consistency between Sobol and SHAP interpretations

The agreement between Sobol and SHAP provides an additional physical consistency check. Sobol analysis evaluates parameter importance directly from the variance of the physics-based BVP outputs, whereas SHAP evaluates how the trained surrogate attributes its predictions to the input variables. Both approaches independently identify Pr as the principal control of Nu and A as the principal control of

$f'(0)$. This agreement indicates that CatBoost preserved the governing numerical model's dominant parameter-response structure. It also strengthens the interpretation of the surrogate as a computational approximation of the resolved BVP behavior within the sampled parameter domain.

4.7 Overall physical implication

Taken together, the results show that the investigated system is governed by two coupled but distinguishable mechanisms. Viscoelasticity and porous resistance primarily regulate momentum redistribution and the near-wall velocity response, while the Prandtl number primarily regulates thermal diffusion and heat-transfer intensity. Their coupling determines the final velocity and temperature fields and produces the observed thermal-momentum trade-off. This mechanistic interpretation explains the sensitivity rankings, the response maps, the Pareto front, and the surrogate-model behavior within a single consistent physical framework.

5. Conclusions

An integrated numerical, sensitivity, optimization, and machine-learning framework was developed to characterize viscoelastic flow and heat transfer in a porous medium under constant surface heat flux. The Python `solve_bvp` implementation reproduced the MATLAB `bvp5c` solutions with relative errors below 0.003%, providing a verified numerical basis for the subsequent analyses.

The Sobol results demonstrated that the governing parameters affect the thermal and momentum responses differently. At $N = 512$, A was the principal factor controlling $f'(0)$, with $S1 = 0.6092$ and $ST = 0.6382$, whereas Pr dominated Nu with $S1 = 0.6741$ and $ST = 0.6932$. Convergence analysis from $N = 128$ to $N = 1024$ preserved these rankings while progressively narrowing the 95% confidence intervals. Direct second-order analysis showed small pairwise $S2$ estimates with confidence intervals that included zero, confirming that main effects dominate output variance over the investigated domain. The 5,120-case Pareto analysis identified 106 non-dominated states and quantified a clear trade-off between heat-transfer enhancement and the wall velocity gradient. The closest-to-ideal compromise was $A = 0.12395$, $B = 0.76735$, and $Pr = 9.95971$, yielding $Nu = 1.40110$ and $f'(0) = 0.40151$. The maximum- Nu Pareto state reached $Nu = 1.86204$ at $f'(0) = 0.95607$, whereas the minimum- $f'(0)$ state achieved $f'(0) = 0.13646$ at $Nu = 1.02379$. Only 0.06% of sampled cases simultaneously satisfied the high- Nu and low-momentum percentile criteria, demonstrating that this favorable region is narrow within the investigated domain.

CatBoost provided the highest test-set predictive accuracy for both modeled responses, achieving $R^2 = 0.9809$ for Nu and $R^2 = 0.9776$ for $f'(0)$. SHAP interpretation was consistent with the global sensitivity analysis, identifying Pr as the dominant predictor of Nu and A as the dominant predictor of $f'(0)$. This agreement indicates that the nonlinear surrogate captured the numerical model's principal parameter-response relationships.

Independent hold-out numerical validation using 25 previously unseen BVP cases confirmed model generalization within the investigated parameter domain. All three surrogate models achieved R^2 values

above 0.94. CatBoost provided the highest hold-out accuracy for Nu with $R^2 = 0.9629$, whereas Linear Regression achieved the highest accuracy for $f'(0)$ with $R^2 = 0.9709$. These results support using the developed framework for rapid parameter assessment and identifying thermal-momentum trade-offs without replacing direct numerical verification outside the investigated parameter ranges.

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Data Availability

The datasets generated and analysed during the current study are available from the corresponding author on reasonable request.

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