

# A Data-Driven Approach on Bioconvection Flow

Bengisen Pekmen(✉) and Merve Gurbuz-Caldag

Department of Mathematics, TED University, 06420 Ankara, Turkey
bengisenpekmen@gmail.com, merve.gurbuz@tedu.edu.tr

**Abstract.** In this study, machine learning modeling is utilized on a bioconvection flow problem. The two dimensional, time independent natural convection flow problem in the presence of oxytactic bacteria is considered inside a unit square cavity. The dimensionless governing equations in terms of stream function, temperature, oxygen concentration, bacteria density and vorticity are numerically solved by radial basis function collocation method. In variation of Rayleigh, bioconvection Rayleigh, Peclet, Lewis and buoyancy ratio parameter, average Nusselt, Sherwood and bacteria density along the heated wall as well as average bacteria density throughout the entire cavity are calculated, and organized into a matrix to form a dataset. This dataset is used for neural network modeling to model the outcomes as averages. The obtained mean squared error metric results show the good fit even by one layer neural network. A feature importance analysis also approves the importance of Rayleigh number on average Nusselt number, and Peclet number on all other averages.

**Keywords:** Oxytactic Bacteria · Bioconvection Flow · Neural Network · Radial Basis Function · Feature Importance

## 1 Introduction

Bioconvection refers to the convective motion of a fluid induced by the directional swimming of microorganisms under the influence of gravity, a magnetic field, oxygen, or light. In the literature, various bioconvection problems have been examined in different channels, particularly involving gravitactic, oxytactic, or gyrotactic bacteria. Alloui et al. [1] investigated gravitactic bioconvection in a rectangular cavity, employing the control volume method to simulate contour plots of stream function, temperature, and concentration for various physical parameters. They also analyzed the bifurcation diagram of the stream function. Kuznetsov [8] applied the Galerkin finite element method to study bioconvection driven by gyrotactic microorganisms in a horizontal layer, concluding that the presence of these microorganisms has a destabilizing effect. Sheremet and Pop [10] examined heat and mass transfer in a nanofluid containing oxytactic bacteria within a square porous cavity. Using the finite difference method, they

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visualized streamlines, isotherms, and isoconcentrations of oxygen and bacteria for different values of Rayleigh, bioconvection Rayleigh, Peclet, and Lewis numbers. Their findings indicate that the average Nusselt number increases with higher Rayleigh numbers or lower Lewis numbers. Saini and Sharma [9] investigated thermo-bioconvection in porous media with gravitactic microorganisms, reporting that the Lewis number enhances bioconvection. Balla et al. [2] investigated the numerical solution of nanofluid flow in a porous square cavity with oxytactic bacteria by using weighted residual Galerkin finite element method. They showed that both the heat transfer and mass transfer increase with the augmentation of Lewis number and Brownian motion. Pekmen Geridonmez and Oztop [5] implemented radial basis function with finite difference (RBF-FD) to the bioconvection flow in a cavity with solid block field by $SiO_2$-water containing oxytactic bacteria subjected to the periodic magnetic field. They reported that mass transfer is a decreasing function of bioconvection Rayleigh number, but it is an increasing function of the other problem parameters. Habibishandiz et al. [6] studied the heat transfer characteristics of natural convection flow in a square porous cavity filled with a nanofluid containing oxytactic bacteria. They employed the finite element method to solve the nondimensional governing equations under constant and periodic temperature boundary conditions. Their results demonstrated that microorganisms enhance heat transfer, particularly under periodic temperature distributions. In [7], numerical and artificial neural network studies are investigated for the bioconvection flow in H-type cavity containing oxytactic bacteria and nano-enhanced phase change material. It is obtained that the rise in Hartmann number lessens the heat transfer, but improves the mass transfer. They also depicted that the artificial neural network (ANN) models are capable to predict each parameter with high accuracy.

In this study, a machine learning technique is integrated into the bioconvection flow in a square cavity including oxytactic bacteria. RBF is used to produce the dataset from the numerical results of the nondimensional governing equations. In neural network process, the inputs are Rayleigh, bioconvection Rayleigh, Peclet and Levis numbers, and the buoyancy ratio term. Outputs are the average Nusselt and Sherwood numbers, mean and average values of microorganism concentration. Feature importance analysis is also performed on the dataset.

## 2 Problem in Mathematical Terms

This study investigates a steady, two-dimensional natural convection flow inside a unit square cavity, influenced by oxytactic bacteria. The problem setup is depicted in Fig. 1. The left wall acts as a heated boundary, while the right wall is maintained at a lower temperature. In contrast, the top and bottom walls are thermally insulated.

The buoyancy effect is incorporated using the Boussinesq approximation due to both temperature and density differences. Viscous dissipation and radiation effects are disregarded.

The dimensional equations consist of continuity, momentum, energy, oxygen concentration, and microorganism density, are formulated as follows

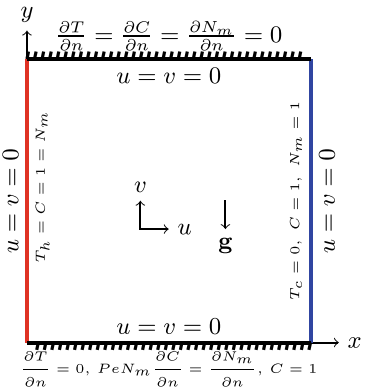



**Fig. 1.** Problem Setup and Boundary Conditions.

$$\frac{\partial u'}{\partial x'} + \frac{\partial v'}{\partial y'} = 0, \tag{1}$$

$$\nu \nabla^2 u' = u' \frac{\partial u'}{\partial x'} + v' \frac{\partial u'}{\partial y'} + \frac{1}{\rho} \frac{\partial p'}{\partial x'}, \tag{2}$$

$$\nu \nabla^2 v' = u' \frac{\partial v'}{\partial x'} + v' \frac{\partial v'}{\partial y'} + \frac{1}{\rho} \frac{\partial p'}{\partial y'} + \frac{g}{\rho} \left( \gamma \Delta \rho n' - \rho \beta (T' - T_c) + \rho_o \beta_o (C' - C^*) \right), \tag{3}$$

$$\nabla^2 T' = u' \frac{\partial T'}{\partial x'} + v' \frac{\partial T'}{\partial y'}, \tag{4}$$

$$D_c \nabla^2 C' = u' \frac{\partial C'}{\partial x'} + v' \frac{\partial C'}{\partial y'} + \delta n', \tag{5}$$

$$\frac{\partial}{\partial x'} \left( u' n' + \frac{b W_c}{\Delta C'} \frac{\partial C'}{\partial x'} n' - D_n \frac{\partial n'}{\partial x'} \right) + \frac{\partial}{\partial y'} \left( v' n' + \frac{b W_c}{\Delta C'} \frac{\partial C'}{\partial y'} n' - D_n \frac{\partial n'}{\partial y'} \right) = 0, \tag{6}$$

where $\rho$ is the density of water, $\rho_o$ is the density of oxygen, $\beta$ is the thermal expansion coefficient of water, $\beta_o$ is the thermal expansion coefficient of oxygen, $\alpha$ is the thermal diffusivity, $\nu$ is the kinematic viscosity, $u', v'$ are velocity components, $p'$ is the pressure, $g$ is the gravitational acceleration, $\gamma$ is the mean volume of microorganism, $D_c$ is the diffusivity of oxygen concentration, $n'$ is the density of bacteria, $W_c$ is the maximum cell swimming speed, $b$ is the chemotaxis constant, $D_n$ is the diffusivity of microorganism, $T'$ is the temperature, $C'$ is the concentration, $\delta n'$ is the oxygen consumption by the bacteria, and $\Delta C' = C - C^*$ with $C^* = C_{\min}$.

The dimensionless transformation parameters are defined as follows

$$(x, y) = \frac{(x', y')}{L}, \quad (u, v) = \frac{L}{\alpha}(u', v'), \quad p = \frac{L^2}{\rho\alpha^2}p', \tag{7}$$

$$T = \frac{T' - T_c}{\Delta T}, \quad C = \frac{C' - C^*}{\Delta C}, \quad N_m = \frac{n'}{n_0}, \tag{8}$$

where $L$ is the characteristic length, $\Delta T$ is the temperature difference, $\Delta C$ is the concentration difference, $\alpha$ is the thermal diffusivity and $n_0$ is the reference average density of bacteria.

Utilizing these transformation parameters, the dimensional equations are converted into the following non-dimensional form

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{9}$$

$$Pr\nabla^2 u = u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x}, \tag{10}$$

$$Pr\nabla^2 v = u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} - RaPr\left(T - R_b N_m - NrC\right), \tag{11}$$

$$\nabla^2 T = u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y}, \tag{12}$$

$$\frac{1}{Le}\nabla^2 C = u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + \frac{1}{Le}N_m, \tag{13}$$

$$\frac{1}{Le}\nabla^2 N_m = \chi\left(u\frac{\partial N_m}{\partial x} + v\frac{\partial N_m}{\partial y}\right) + \frac{Pe}{Le}\left(N_m\nabla^2 C + \frac{\partial C}{\partial x}\frac{\partial N_m}{\partial x} + \frac{\partial C}{\partial y}\frac{\partial N_m}{\partial y}\right), \tag{14}$$

where $\chi = \dfrac{D_c}{D_n}$, $N_m$ is the number of microorganisms. Prandtl, Rayleigh, bioconvection Rayleigh, Peclet numbers, buoyancy ratio parameter and Lewis numbers are

$$Pr = \frac{\nu}{\alpha}, \quad Ra = \frac{g\beta\Delta T L^3}{\nu\alpha}, \quad R_b = \frac{\gamma n_0 \Delta\rho}{\rho\beta\Delta T}, \quad Pe = \frac{bW_c}{D_n},$$
$$Nr = \frac{(\rho_o - \rho)\beta_o \Delta C}{\rho\beta\Delta T}, \quad Le = \frac{\alpha}{D_c}.$$

By employing the stream function formulation, $(u, v) = \left(\dfrac{\partial\psi}{\partial y}, -\dfrac{\partial\psi}{\partial x}\right)$ and defining vorticity as $\omega = \dfrac{\partial v}{\partial x} - \dfrac{\partial u}{\partial y}$, the governing non-dimensional equations are

expressed in terms of the stream function and vorticity as follows

$$\nabla^2 \psi = -\omega, \tag{15}$$

$$\nabla^2 T = u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y}, \tag{16}$$

$$\frac{1}{Le}\nabla^2 C = u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + \frac{1}{Le}N_m, \tag{17}$$

$$\frac{1}{Le}\nabla^2 N_m = \chi\left(u\frac{\partial N_m}{\partial x} + v\frac{\partial N_m}{\partial y}\right) + \frac{Pe}{Le}\left(N_m\nabla^2 C + \frac{\partial C}{\partial x}\frac{\partial N_m}{\partial x} + \frac{\partial C}{\partial y}\frac{\partial N_m}{\partial y}\right), \tag{18}$$

$$Pr\nabla^2\omega = u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y} + RaPr\left(-\frac{\partial T}{\partial x} + R_b\frac{\partial N_m}{\partial x} + Nr\frac{\partial C}{\partial x}\right). \tag{19}$$

The boundary conditions are specified as follows

$$\text{on } x = 0 : u = v = \psi = 0,\ T = 1,\ C = N_m = 1, \tag{20}$$

$$\text{on } x = 1 : u = v = \psi = 0 = T,\ C = N_m = 1, \tag{21}$$

$$\text{on } y = 0 : u = v = \psi = 0,\ \frac{\partial T}{\partial y} = 0,\ C = 1,\ PeN_m\frac{\partial C}{\partial y} = \frac{\partial N_m}{\partial y}, \tag{22}$$

$$\text{on } y = 1 : u = v = \psi = 0,\ \frac{\partial T}{\partial y} = \frac{\partial C}{\partial y} = \frac{\partial N_m}{\partial y} = 0, \tag{23}$$

The following expressions are used to determine the average Nusselt number, Sherwood number, and the average bacterial density along the heated wall.

$$\overline{Nu} = -\int_0^1 \frac{\partial T}{\partial x}dy, \quad \overline{Sh} = -\int_0^1 \frac{\partial C}{\partial x}dy \quad \overline{N_m} = -\int_0^1 \frac{\partial N_m}{\partial x}dy \tag{24}$$

$\overline{Nu}$ represents the ratio of convective heat transfer to conductive heat transfer, while $\overline{Sh}$ denotes the ratio of convective mass transfer to conductive mass transfer. $\overline{Nm}$ along the heated wall represents the mean variation in bacterial density along the left heated boundary.

After establishing the governing equations and boundary conditions that describe the flow behavior, we next turn to the numerical strategy adopted to solve these equations. The radial basis function (RBF) collocation method is utilized due to its meshfree nature and flexibility in handling complex geometries.

## 3 Numerical Method

The Radial basis function (RBF) method [3,4] is a meshfree collocation technique, where the problem domain and its boundary are discretized using $N_d$ number of interior and $N_b$ number of boundary points. In this method, the unknown $\zeta$ is approximated using an RBF $g(r)$ as follows

$$\zeta(x, y) = \sum_{i=1}^{N_d+N_b} a_i g(||x - x_i||), \tag{25}$$

in which $r = ||x - x_i||$ represents the Euclidean norm between the field point $x$ and collocation point $x_i$. The collocation form of (25) is expressed by $\zeta = Ga$, where the matrix $G$ has dimensions $(N_d + N_b)^2$, while the vector $a$ is of length $(N_d + N_b)$.

By treating the partial derivatives of the RBF $g(r)$ as the matrices $G_x$, $G_y$, $G_{xx}$ and $G_{yy}$, the differentiation matrices are straightforwardly obtained as $P_x = G_x G^{-1}$, $P_y = G_y G^{-1}$, $P_L = (G_{xx} + G_{yy})G^{-1}$.

In the current study, polyharmonic spline RBF $g(r) = r^7$ is used to solve the equations (15)–(19). The equations in their discretized form can be written as follows

$$P_L \psi^{k+1} = -\omega^k, \tag{26}$$

$$(P_L - K)\, T^{k+1} = 0, \tag{27}$$

$$(P_L - LeK)\, C^{k+1} = N_m^k, \tag{28}$$

$$\left(P_L - Le\chi K - PeP_L[C^{k+1}]_d - Pe(P_x[C^{k+1}]_d P_x + [P_y C^{k+1}]_d P_y)\right) N_m^{k+1} = 0, \tag{29}$$

$$(PrP_L - K)\, \omega^{k+1} = RaPrP_x(-T^{k+1} + R_b N_m^{k+1} + NrC^{k+1}), \tag{30}$$

where $K = ([P_y\psi]_d P_x + [P_x\psi]_d P_y)$, $P_x = G_x G^{-1}$, $P_y = G_y G^{-1}$ and $P_L = (G_{xx} + G_{yy})G^{-1}$. $[.]_d$ represents the diagonal matrix, $k$ denotes the iteration level. The iterative process proceeds until the stopping condition is met

$$\sum_{\Xi=\psi,T,C,N_m,\omega} \frac{||\Xi^{k+1} - \Xi^k||_\infty}{||\Xi^{k+1}||_\infty} < 10^{-5}, \tag{31}$$

During this iterative process, the vorticity boundary conditions are obtained from the definition of vorticity as follows

$$\omega^{k+1} = P_x v^{k+1} - P_y u^{k+1}, \tag{32}$$

and a relaxation parameter $\tilde{\gamma} \in (0, 1)$ is applied to the vorticity, as shown below

$$\omega^{k+1} = (1 - \tilde{\gamma})\omega^k + \tilde{\gamma}\omega^{k+1}, \tag{33}$$

where k is the iteration level. $\overline{Nu}$, $\overline{Sh}$ and $\overline{Nm}$ are evaluated using the Composite Simpson's 1/3 rule for numerical integration.

A bioconvection problem previously solved in [10] is revisited for validation of the method, and the obtained $\overline{Nu}$ and $\overline{Sh}$ along the heated left vertical wall are compared in Table 1. Our results demonstrate a strong agreement with those presented in the reference.

Once the numerical simulations are conducted across a broad parametric space, the results are structured into a dataset suitable for machine learning. To extract deeper insights and predict outcomes more efficiently, we employ neural network modeling as described below.

**Table 1.** Validation with Ref. [10]

| | | | | Sheremet and Pop [10] | | Current Study | |
|---|---|---|---|---|---|---|---|
| $Ra$ | $R_b$ | $Le$ | $Pe$ | $\overline{Nu}$ | $\overline{Sh}$ | $\overline{Nu}$ | $\overline{Sh}$ |
| 10 | 10 | 1 | 0.1 | 1.0775 | 0.3368 | 1.0772 | 0.3366 |
| | | | 1 | 1.0720 | 0.3296 | 1.0715 | 0.3293 |
| | | 10 | 0.1 | 1.0771 | 0.2556 | 1.0769 | 0.2553 |
| | | | 1 | 1.0397 | 0.2298 | 1.0393 | 0.2295 |
| | 100 | 1 | 0.1 | 1.0717 | 0.3447 | 1.0711 | 0.3444 |
| | | | 1 | 1.1723 | 0.3650 | 1.1806 | 0.3675 |
| 100 | 10 | 1 | 0.1 | 3.0910 | 0.2506 | 3.1236 | 0.2494 |
| | | | 1 | 2.6560 | 0.2270 | 2.6563 | 0.2261 |

## 4 Modelling

In this part, investigation on neural network modeling is presented. The input features in the range of $Ra \in [100, 10^4]$, $Rb \in [10, 100]$, $Pe \in [0.1, 5]$, $Le \in [1, 10]$, $Nr \in [0, 1]$ are combined in a set. The target variables are considered as $\overline{Nu}$, $\overline{Sh}$, $\overline{Nm}$, $mean(Nm)$. By this means, a dataset of dimension $1895 \times 9$ with 5 input columns and 4 output columns is saved performing the numerical method in each input combination. The numerical results are obtained by setting $Pr = 6.8$, $\chi = 1$. Additionally, $mean(Nm)$ is the statistical mean of density of bacteria all around the cavity.

Neural network modeling by using 'fitrnet' in Matlab is utilized. The activation function is adopted as rectified linear unit (ReLU). The input data is standardized (z-score standardization).

The data is divided into train (70%), validation (15%) and test (15%) sets. The dimension of these sets is $1327, 284, 284$, respectively. Firstly, models are trained with train dataset, and tested with validation set in 10 runs. The best model inside these runs is saved. Then, the saved best model is used for prediction on test dataset. In order to assess the quality of the model, mean squared error (MSE/mse) metric is used. We used Mean Squared Error (MSE) to evaluate how well the model performed on both the training and test data, ensuring that the results reflect the model's accuracy and ability to generalize to new, unseen data. The obtained MSE metric results on both train and test datasets are compared in different number of hidden layers in Table 2. The column of layer info corresponds to the number of hidden layers as well as the size of the hidden layer. As is noted that the rise in the number of layers reduces both the train and test MSE metric results. However, one layer neural network is also enough to get satisfying MSE metric results.

Figure 2 illustrates NN modeling on test dataset with one layer of size 100. In the first column, black dots very close to the perfect prediction line show the good fit. Also, the residuals changing between small intervals verifies the fine

**Table 2.** MSE metric results in different layer sizes.

| LayerInfo | MSE | $\overline{Nu}$ | $\overline{Sh}$ | $\overline{Nm}$ | $mean(Nm)$ |
|---|---|---|---|---|---|
| 100 | train | 5.4e–4 | 8.4e–5 | 1.3e–4 | 1.3e–5 |
| | test | 6.8e–4 | 1.1e–4 | 2.2e–4 | 1.4e–5 |
| 100,100 | train | 1.8e-4 | 6.6e-5 | 1.1e–4 | 9.0e–6 |
| | test | 3.0e–4 | 8.2e–5 | 1.7e–4 | 1.0e–5 |
| 100,100,100 | train | 8.7e–5 | 5.8e–5 | 1.0e–4 | 6.6e-6 |
| | test | 1.9e–4 | 7.5e–5 | 1.7e–4 | 6.9e–6 |

modeling. MSE metric results on the test data for each output is also given on the residual plots, and these also confirm the good quality of fitting.

Holding layer size at 100 with one hidden layer, feature importance analysis is also addressed in the following steps:

* Our best model and MSE metric results on test data, say $mse_test$, are kept.
* An input column, say $i$, $i = 1, 2, 3, 4, 5$, both in train and test datasets, is shuffled.
* The shuffled form of dataset is predicted by the model.
* The result of the MSE metric as a result of model prediction on shuffled case, say $mse_shuffled_i$, are computed.
* The absolute difference between $mse_test$ and $mse_shuffled_i$ is stored.
* Since shuffling is randomly done, the process is returned 50 times.
* The average of absolute differences are calculated for each $i$.
* The highest value of these mean results refers to the most important feature causing the target to be predicted in difficulty.

In view of these steps, the same importance order of parameters $Ra, Rb, Pe, Le, Nr$ is found both in train and test datesets. Table 3 demonstrates the order of parameter importance on the corresponding target variable. As is expected that $Ra$ is the most important parameter in $\overline{Nu}$ prediction. Peclet number is revealed the most important feature in all other target variables. In each cases, the least effect emerges in the presence of buoyancy ratio term $Nr$.

**Table 3.** Feature Importance Analysis

| Output | Feature Order |
|---|---|
| $\overline{Nu}$ | $Ra > Pe > Rb > Le > Nr$ |
| $\overline{Sh}$ | $Pe$, $Ra$, $Rb$, $Le$, $Nr$ |
| $\overline{Nm}$ | $Pe$, $Rb$, $Ra$, $Le$, $Nr$ |
| $mean(Nm)$ | $Pe$, $Ra$, $Rb$, $Le$, $Nr$ |

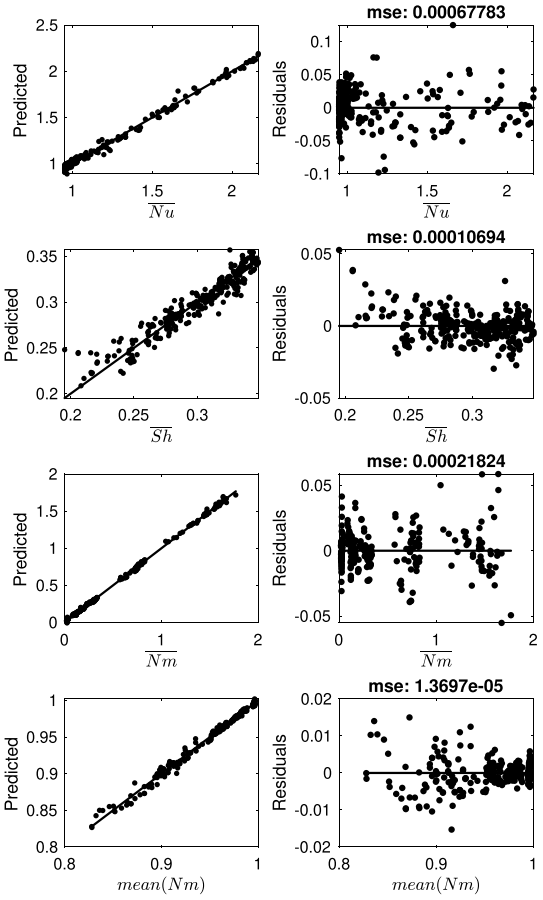



**Fig. 2.** One layer NN modeling.

## 5 Conclusion

This study successfully applies machine learning modeling to a bioconvection flow problem, demonstrating its effectiveness in capturing the complex behavior of natural convection in the presence of oxytactic bacteria. The two-dimensional, steady-state flow inside a unit square cavity is analyzed using the radial basis function collocation method to numerically solve the dimensionless governing equations for stream function, temperature, oxygen concentration, bacterial density, and vorticity.

A detailed dataset is generated by varying key dimensionless parameters, including the Rayleigh, bioconvection Rayleigh, Peclet, Lewis, and buoyancy ratio numbers. The corresponding average Nusselt number, Sherwood number, and bacterial density along the heated wall, as well as the average bacterial

density throughout the entire cavity, are computed and structured into a matrix for neural network modeling.

The results indicate that even a single-layer neural network achieves a good fit, as reflected in the mean squared error metric. Furthermore, a feature importance analysis highlights the dominant influence of the Rayleigh number on the average Nusselt number and the Peclet number on all other computed averages. These findings underscore the potential of machine learning in modeling complex bioconvection phenomena, offering a data-driven approach for predicting flow characteristics with high accuracy.

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