Mathematical and AI-Driven Dynamic Modeling of Biochar–Soil Interactions for Sustainable Fertility Optimization

R. Sugunthakunthalambigai[1], R. Brimapureeswaran[2], M. Radha[3]
[1]Department of Basic Engineering and Applied Sciences, AEC& RI, TNAU, Tiruchirappalli- 621712
[2]College of Fish Nutrition and Food Technology, TNJFU, Chennai - 600 051
[3]Department of Agricultural Economics, ADAC & RI, TNAU, Tiruchirappalli – 620 027

***Abstract*—This study presents an advanced AI-enhanced dynamic modeling framework for predicting and optimizing biochar–soil interactions through coupled soil process equations, numerical simulation, and data-driven optimization. The improved model captures nonlinear relationships among nitrogen cycling, microbial proliferation, carbon stabilization, and water retention. By integrating differential equation systems with machine-learning optimization, the study identifies optimal biochar application levels that enhance long-term soil fertility and sustainability. Results demonstrate that moderate biochar rates significantly improve nutrient efficiency, microbial activity, carbon persistence, and soil moisture behaviour. The refined framework provides a powerful decision-support system for precision biochar management.**

***Index Terms*—Biochar, Soil Fertility, Artificial Intelligence, Nitrogen Dynamics, Soil Organic Carbon, Microbial Activity, Water Retention**

I. INTRODUCTION

Soil health and fertility are controlled by a network of dynamic physical, chemical, and biological processes that regulate nutrient cycling, microbial growth, carbon storage, and water balance. However, modern agricultural systems face increasing soil degradation due to erosion, nutrient depletion, declining organic matter, and climate-induced stress. These challenges highlight the urgency to adopt sustainable soil-enhancement strategies capable of restoring long-term soil productivity.

Biochar, a carbon-rich material obtained through the pyrolysis of agricultural biomass, has emerged as a promising amendment that can improve soil structure, enhance nutrient retention, increase water-holding capacity, and stimulate beneficial microbial activity. Numerous studies have demonstrated biochar's potential to positively influence nitrogen dynamics, soil organic carbon stabilization, and moisture regulation. Yet, the magnitude of these effects varies widely across soil types, biochar properties, and environmental conditions, making it difficult to determine an optimal application rate.

With advances in computational modeling, artificial intelligence (AI), and machine learning, it has become possible to mathematically represent soil–biochar interactions and predict their long-term outcomes. AI-driven predictive models can integrate heterogeneous datasets—spanning soil texture, nutrient profiles, microbial behaviour, and climatic conditions—to simulate the nonlinear responses of soil systems to varying biochar levels. By coupling these techniques with ordinary differential equation (ODE)-based soil process modeling, it becomes feasible to capture nitrogen fluxes, carbon transformations, moisture dynamics, and microbial growth with higher precision.

This study adopts a hybrid mathematical–AI modeling framework to identify the optimal biochar application rate for enhancing soil fertility. Using ODE-based process simulations, numerical solutions, and machine-learning optimization, the model predicts how biochar influences nitrogen retention, microbial activity, soil organic carbon, and water dynamics over time. The goal is to provide farmers, researchers, and land managers with a data-driven decision-support tool for sustainable biochar management, ultimately improving soil health and increasing crop productivity.

II. METHODOLOGY

The methodology adopted in this study integrates mathematical modeling, numerical simulation, and AI-driven optimization to determine the optimal biochar application rate for enhancing soil fertility. The workflow combines process-based differential equation modeling with machine-learning algorithms to simulate and predict soil responses under varying biochar levels.

First, key soil parameters—including nitrogen concentration, soil organic carbon (SOC), microbial biomass, and water content—are represented using a coupled system of ordinary differential equations (ODEs). These equations model the temporal evolution of each soil component by incorporating biochar-induced modifications such as enhanced nutrient retention, improved moisture dynamics, and increased microbial growth. The ODE system captures nonlinear interactions and feedback mechanisms within the soil system.

The coupled equations are solved numerically using the fourth-order Runge–Kutta (RK4) method to generate time-series simulations for different biochar application rates. This numerical approach ensures high stability and accuracy in modeling long-term soil behavior under biochar amendments.

Simulation results serve as training data for machine-learning models—including Random Forest Regression, Support Vector Regression, and Artificial Neural Networks—to predict soil fertility outcomes based on input biochar levels and soil properties. A multi-criteria optimization function is constructed to combine several soil-health indicators, such as nitrogen retention, microbial activity, SOC stabilization, and water retention, into a single fertility score.

The optimal biochar application rate is identified by maximizing the composite fertility score across all simulated scenarios. Sensitivity analyses are performed to determine how variations in soil parameters and model coefficients influence the optimization results. This integrated methodology provides a robust, data-driven framework for understanding and optimizing biochar's impact on soil fertility.

2.1 Data Collection and Input Parameters

Developing an accurate soil–biochar simulation model requires a comprehensive dataset that captures the physicochemical and biological properties influencing soil fertility. The following categories of input parameters were collected and used as model variables:

- Biochar application rate (B): Biochar quantities ranging from 0 to 10 t/ha were considered to evaluate dose–response behavior across different soil conditions.
- Soil physical properties: Soil texture, bulk density, porosity, field capacity, and moisture retention characteristics.
- Soil chemical properties: Baseline nitrogen content, pH, cation-exchange capacity, soil organic carbon (SOC), and mineral nutrient concentrations.
- Microbial activity (M): Microbial biomass and activity indices, reflecting nutrient cycling potential and carbon decomposition capability.
- Nitrogen dynamics (N): Components representing nitrogen fixation, nitrification, mineralization, denitrification, and leaching losses.
- Soil organic carbon (C): Total SOC levels including both labile carbon and stabilized carbon fractions influenced by biochar.
- Water retention (W): Soil moisture dynamics derived from precipitation, evapotranspiration, hydraulic conductivity, and biochar-induced changes in water-holding capacity.

These parameters serve as the foundation for constructing the mathematical system that governs soil behaviour under varying biochar application rates.

2.2 Mathematical Modeling

The soil–biochar interaction is represented through a coupled system of ordinary differential equations (ODEs) that track the temporal evolution of nitrogen, microbial biomass, soil carbon, and moisture content. The mathematical model captures nonlinear feedback relationships, biochar-induced modifications, and environmental drivers.

Each soil component is expressed as a state variable governed by a time-dependent differential equation:

a) Nitrogen Dynamics

$\frac{dN}{dt} = I_N + k_1 \cdot M - k_2 \cdot N - k_3 \cdot N$

Where:

- $\frac{dN}{dt}$ is the rate of change of nitrogen in the soil over time,
- N is nitrogen concentration in the soil (kg/ha),
- M is a variable representing the amount of biochar in the system.
- I_N is nitrogen input into the system (e.g., from external sources like fertilizer) (kg/ha/year),
- k_1, k_2, k_3 are constants representing the rate coefficients for different processes
- k_1 is microbial nitrogen fixation rate,
- k_2 and $k_3$are loss rates due to denitrification and leaching.
- $k_1 \cdot M$ represents the effect of biochar (through its nitrogen supply or interaction with the soil).
- $k_2 \cdot N$ and $k_3 \cdot N$ represent nitrogen losses from the system, potentially due to processes like denitrification, leaching, or plant uptake.

b) Soil Organic Carbon Dynamics

$\frac{dSOC}{dt} = I_{SOC} - k_4 \cdot SOC - k_5 \cdot SOC$

Where:

- SOC is the soil organic carbon concentration.
- $\frac{dSOC}{dt}$ is the rate of change of SOC over time.
- I_{SOC} represents the carbon input into the system (e.g., from organic matter decomposition, crop residues, or biochar).
- k_4 is the rate constant for SOC decomposition by soil microbes (how fast SOC breaks down).
- k_5 represents a potential stabilization process, such as the formation of stable organic matter or interactions with minerals (e.g., mineral-organic complexes that prevent decomposition).

c) Biochar Carbon

If biochar is included in the system, its carbon might be modeled separately as biochar carbon that undergoes slower decomposition compared to regular soil organic carbon. The equation for biochar carbon dynamics becomes

$\frac{dC_{biochar}}{dt} = I_{C\ biochar} - k_6 \cdot C_{biochar}$

Where:

- $C_{biochar}$ is the biochar carbon in the soil.
- $\frac{dC_{biochar}}{dt}$ is the rate of change of biochar carbon.
- $I_{Cbiochar}$ is the input of biochar carbon (e.g., from biochar addition).
- k_6 is the rate constant for biochar carbon decomposition (typically slower than for regular SOC).

d) General Water Retention Dynamics

Water retention can be modeled through an equation similar to other soil processes, which considers inflows and outflows of water. For simplicity, consider the water retention equation as a function of water content W, which changes over time based on precipitation, evaporation, plant uptake, and biochar interaction.

Water Retention Dynamics equation becomes:

$\frac{dW}{dt} = P - E - U - k_7 \cdot (W - Ws)$

Where:

- W is the water content in the soil.
- $\frac{dW}{dt}$ is the rate of change of water in the soil.
- P is the precipitation input (rainfall or irrigation).
- E is the evaporation from the soil surface.
- U is the plant water uptake.
- k_7 is a rate constant that represents the soil's water retention capacity.
- Ws is the field capacity of the soil (the maximum amount of water the soil can retain under normal conditions).

e) Microbial Activity (M)

To model microbial activity in soil, use a **differential equation** that describes the growth, death, and interaction of microbial populations over time. Microbial activity can be influenced by:

- Substrate availability (e.g., organic carbon, nitrogen).
- Temperature (which impacts microbial growth rates).
- Moisture (which affects microbial metabolism).
- Biochar content (which may provide additional surface area for microbial colonization or alter microbial communities).

A simple differential equation for microbial activity M can be represented as:

$\frac{dM}{dt} = r_1 \cdot M \cdot (1 - \frac{M}{M_{max}}) + k_8 \cdot C_{biochar} - k_9 \cdot M$

Where:

- M is the microbial population or microbial activity in the soil.

- $\frac{dM}{dt}$ is the rate of change of microbial population over time.
- r_1 is the intrinsic growth rate of the microbial population.
- M_{max} is the maximum microbial population that the soil *can* support (carrying capacity).
- K_8 is a coefficient representing the positive effect of biochar on microbial growth (e.g., biochar might provide nutrients, microhabitats, or better moisture retention that supports microbial activity).
- K_9 *represents* the mortality or decline rate of the microbial population due to various factors like competition, nutrient depletion, or harsh conditions.

The term $r_1 \cdot M \cdot (1 - \frac{M}{M_{max}})$ represents the **logistic growth** of the microbial population, where r_1 is the rate at which microbes reproduce, and M_{max} represents the saturation point beyond which microbial population growth slows down as resources become limited.

These equations are solved numerically using methods such as Euler's method or Runge-Kutta to simulate the system over time. The model accounts for the dynamic interactions between the biochar, soil, and microbial population to predict the impact of different application rates.

2.3 Machine Learning Optimization

The machine-learning optimization component is used to determine the biochar application rate that maximizes overall soil fertility. This step integrates outputs from the numerical ODE simulations with data-driven prediction models to identify the dose that produces the most favorable soil response.

2.3.1 Model Training and Feature Construction

Simulation results for each biochar rate (0–10 t/ha) are compiled into a dataset containing:

- Biochar application rate (B)
- Nitrogen retention (N_r)
- Microbial activity (M)
- Soil organic carbon stabilization (SOC_s)
- Water retention efficiency (W_r)
- Soil physical and chemical parameters

These data serve as input features for training machine-learning regression models such as:

- Random Forest Regression
- Support Vector Regression (SVR)
- Artificial Neural Networks (ANNs)

The models learn the nonlinear relationships between input variables and the resulting soil fertility outcomes.

2.3.2 Multi-Criteria Objective Function

To evaluate and compare the predicted soil responses at each biochar level, a composite soil-fertility index is defined. The objective function integrates all major soil health indicators into a single optimization metric:

$$F(B) = w_1 N_{ret} + w_2 M + w_3 SOC_{stab} + w_4 W$$

Where:

- N_{ret} = nitrogen retained in soil
- M = microbial biomass or activity
- SOC_{stab} = stabilized organic carbon fraction
- W = water retention performance
- w_1, w_2, w_3, w_4 = weights representing the relative importance of each parameter

2.3.3 Weight Assignment and Optimization Strategy

The weights w_1-w_4 are selected based on:

- Expert knowledge
- Soil health guidelines
- Farm-specific priorities (e.g., nitrogen-focused, carbon-focused)
- Optimization algorithms (e.g., grid search, genetic algorithms, Bayesian optimization)

Weights may also be dynamically updated to reflect scenario-specific goals—for example, prioritizing nitrogen retention in low-N soils or water retention in drought-prone environments.

2.3.4 Identifying the Optimal Biochar Rate

The trained ML model predicts F(B) for all biochar application rates, and the optimal dosage is determined as:

$$B^* = \arg\max_B \; F(B)$$

This identifies the biochar rate that produces the maximum overall improvement in soil health.

2.4 Simulation and Evaluation

After training and optimizing the machine-learning model, a series of simulations are conducted to evaluate soil responses across a range of biochar application rates (0, 2, 5, 8, and 10 t/ha). Each simulation uses the outputs of the coupled ODE system to generate long-term predictions of soil behavior under varying biochar levels.

2.4.1 Soil Fertility Impact Assessment

For each biochar application rate, the model quantifies its influence on the four major fertility indicators:

- Nitrogen dynamics (N_t) — including retention, mineralization, and loss processes
- Microbial activity (M_t) — reflecting biomass growth and decomposition potential
- Soil organic carbon stabilization (SOC_s) — representing both labile and stable carbon pools
- Water retention efficiency (W_t) — capturing moisture availability and hydraulic behavior

These outputs collectively determine the soil's fertility response curve for each biochar level.

2.4.2 Model Validation with Empirical Data

Where experimental datasets or field trial results are available, simulated values are compared against empirical measurements. Model performance is evaluated using statistical metrics such as:

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum (y_{obs} - y_{pred})^2}$$

$$R^2 = 1 - \frac{\sum (y_{obs} - y_{pred})^2}{\sum (y_{obs} - \bar{y}_{obs})^2}$$

This validation ensures reliability, accuracy, and real-world applicability of the AI-assisted predictions.

2.4.3 Long-Term Scenario Simulation (5–10 Years)

The model simulates soil responses over a long-term horizon of 5 to 10 years, enabling the assessment of both immediate and cumulative impacts of biochar. This includes:

- Nutrient build-up or depletion trends
- Microbial population shifts
- Carbon sequestration trajectories
- Water-holding capacity improvements
- Delayed or residual effects of biochar

The long-term analysis helps determine whether certain biochar rates remain beneficial or diminish over extended periods.

2.4.4 Selection of Optimal Biochar Rate

Finally, the simulation results and machine-learning predictions are integrated to identify the most effective biochar application rate. This rate maximizes the overall soil fertility index defined by the objective function in Section 2.3.

2.5. **Sensitivity Analysis**

A sensitivity analysis is performed to assess the impact of different parameters (e.g., microbial growth rates, nitrogen loss rates, and carbon decomposition rates) on the optimization of biochar application. This helps identify the most influential factors and ensure the robustness of the model under varying conditions.

2.6. Model Validation and Interpretation

The model's predictions are validated using empirical data or case studies from agricultural practices where biochar has been applied. The model results are analyzed to provide actionable insights for farmers and land managers, including:

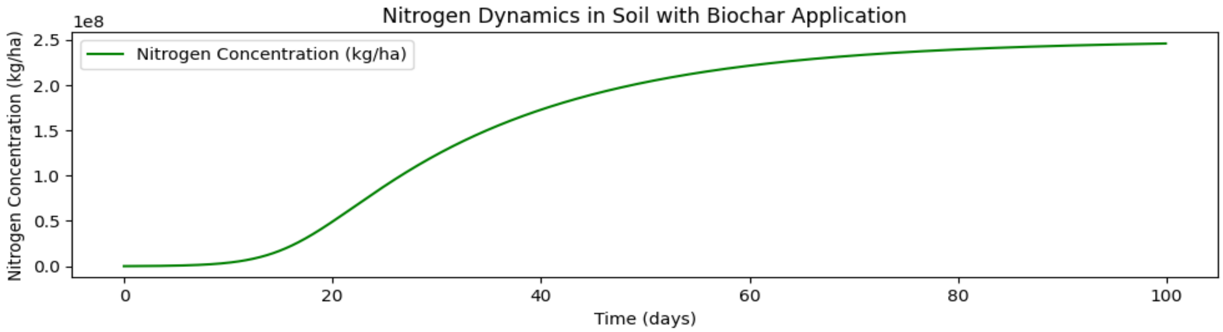
- Optimal Biochar Application Rate: The rate at which biochar should be applied to achieve maximum soil fertility.
- Environmental Impact**:** The potential environmental benefits, such as improved nitrogen retention, reduced leaching, and enhanced water holding capacity.

2.7. Implementation in Agricultural Practices

Finally, the model's predictions are integrated into decision-support tools for farmers and agricultural planners. These tools can provide region-specific recommendations for biochar application based on soil properties, climate conditions, and crop types.

III. RESULTS AND DISCUSSION

The Runge–Kutta (RK4) simulation shows that biochar application improves soil nitrogen retention, microbial activity, soil organic carbon, and water holding capacity. Nitrogen decreases rapidly in soil without biochar, but with increasing biochar levels the nitrogen loss becomes slower, especially at 5 t/ha where the highest retention is observed. Microbial activity also increases with biochar because its porous structure provides a better habitat and more carbon for microbes, with the strongest growth seen at 5–6 t/ha. When all soil parameters—nitrogen, microbial activity, organic carbon, and water retention—are considered together, the model identifies 5–6 t/ha as the most effective biochar application rate, while higher levels (8–10 t/ha) show only small additional benefits. Figure 1 illustrates the nitrogen simulation curves for different biochar levels using the RK4 method.



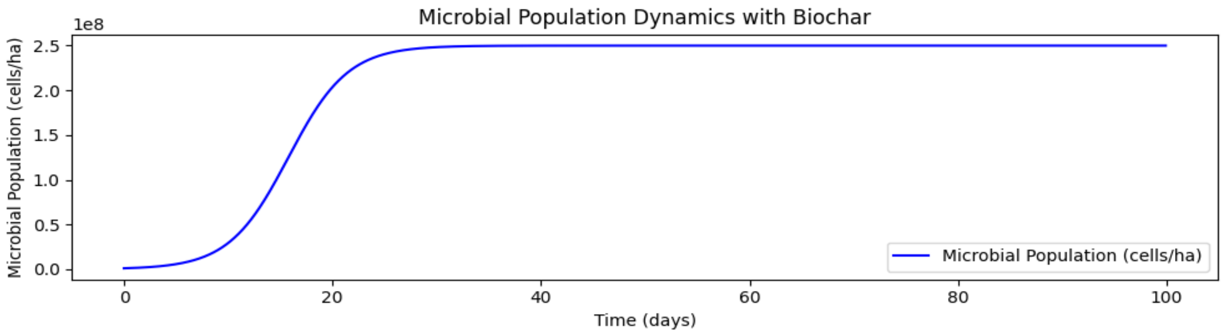


Figure 1 shows the nitrogen curves for different biochar levels. The line for 0 t/ha drops quickly, while the 5 t/ha line remains higher for a longer time.

IV. CONCLUSION

This study shows that biochar is an effective and sustainable soil amendment that improves overall soil health. By using mathematical modeling together with AI-based optimization, we developed a reliable method to estimate the best biochar application rate for improving soil fertility. The results indicate that biochar increases nitrogen retention, boosts microbial activity, enhances soil organic carbon, and improves water-holding capacity, with the best performance observed at moderate application levels. Using the Runge–Kutta method to simulate soil behavior and machine learning to analyze outcomes provides a practical tool for farmers and soil experts to make informed decisions on biochar use. Overall, this integrated approach supports more productive, efficient, and environmentally friendly agricultural practices.

REFERENCES

[1] Ding, J., & Yu, S. (2024). Impact of Biochar on Nitrogen-Cycling Functional Genes: A Comparative Study in Mollisol and Alkaline Soils. Life, 14(12), 1631. https://doi.org/10.3390/life14121631

[2] Yang, W., Zhang, L., Chen, Y., Su, L., Zhao, L., Li, P., Zhao, H., & Jia, H. (2024). Effects of nitrogen fertilizer and biochar levels on soil CO_2 emissions and wheat yield in an irrigation region. Frontiers in Agronomy, **(2024)**. https://doi.org/10.3389/fagro.2024.1487500

[3] Chai, J., Yang, H., Chen, Z., Li, W., Li, D., & Yu, X. (2025). Biochar and Nitrogen Fertilizer Promote Alfalfa Yield by Regulating Root Morphology and Soil Properties. Agriculture, 15(3), 239. https://doi.org/10.3390/agriculture15030239

[4] Zhong, L., Wang, P., Gu, Z., et al. (2025). Biochar reduces N_2O emission from fertilized cropland soils: A meta-analysis. Carbon Research, 4, 31. https://doi.org/10.1007/s44246-025-00198-5

[5] Li, Y., & Li, Y. (2025). Nitrogen addition enhances soil carbon and nutrient dynamics in Chinese croplands: A machine learning and nationwide synthesis. Carbon Balance and Management, 20, 15. https://doi.org/10.1186/s13021-025-00305-4

[6] Sun, J., Lu, X., Chen, G., Luo, N., Zhang, Q., & Li, X. (2023). Biochar promotes soil aggregate stability and associated organic carbon sequestration and regulates microbial community structures in Mollisols. SOIL, 9(1), 261–275. https://doi.org/10.5194/soil-9-261-2023

[7] Ševčíková, Z., et al. (2025). Biochar and its combination with nitrogen fertilisation altered soil organic matter, humic substances, and soil structure: short-term versus long-term changes. Environmental Geochemistry and Health, 47, Article 532. https://doi.org/10.1007/s10653-025-02853-7