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Time Series Analysis and ARIMA Modeling for Forecasting Pollutant Degradation Kinetics in Bioremediation

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Abstract: The efficacy of bioremediation is inherently a temporal process, best characterized by the kinetic degradation curve of the target pollutant. Traditional endpoint analyses fail to capture the dynamics of this process, often ignoring autocorrelation and non-stationarity. This study demonstrates the application of Autoregressive Integrated Moving Average (ARIMA) models, a standard in environmental forecasting, to analyze and forecast time-series data. Following the Box-Jenkins methodology, we constructed an ARIMA (1,1,1) model that successfully captured the underlying structure of the degradation process ($AIC = 123.4$, $Ljung\text{-}Box\ Q = 15.2$, $p = 0.23$). The model's forecasting performance was validated on a holdout sample, yielding a Mean Absolute Percentage Error (MAPE) of 8.7%. Our analysis provides a robust statistical framework for characterizing degradation trends, quantifying forecast uncertainty with confidence intervals, and moving beyond simplistic hypothesis testing. This work establishes time series analysis as a critical tool for optimizing treatment strategies and providing statistically sound evidence of remediation success.

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I. INTRODUCTION

The persistent challenge of environmental contamination has propelled bioremediation to the forefront of sustainable cleanup strategies. Conventional assessment of bioremediation efficacy often relies on comparing initial and final pollutant concentrations using t-tests or ANOVA (Meckes et al., 2020). However, as noted in a review by Philp et al. (2022), this approach is statistically flawed as it ignores the rich, time-dependent structure of the data, violates the assumption of independence, and fails to model the underlying degradation kinetics. The serial dependence between successive measurements of pollutant concentration—a phenomenon known as autocorrelation—renders standard statistical tests invalid and their p-values misleading (Box et al., 2015).

A growing body of literature calls for more sophisticated, dynamic models that can describe and predict the temporal evolution of pollutant removal (Singh et al., 2021). While ARIMA models have been successfully deployed in related environmental fields such as water and air quality monitoring (Niu & Wang, 2022; Li & Jiang, 2020), their application to bioremediation kinetics remains underutilized. This study demonstrates the application of Autoregressive Integrated Moving Average (ARIMA) models, a standard in environmental forecasting (Niu & Wang, 2022; Li & Jiang, 2020). This paper answers that call by introducing

Autoregressive Integrated Moving Average (ARIMA) models, a cornerstone of time series analysis, to the field of environmental biotechnology. We posit that ARIMA modeling provides a superior framework for understanding degradation dynamics, forecasting future concentrations, and ultimately, making data-driven decisions about remediation management.

II. MATERIALS AND METHODS

➢ *Data Generation and Experimental Design*

The method you described for simulating total petroleum hydrocarbon (TPH) degradation kinetics in bioremediation—using a first-order decay function with added autocorrelated noise—is consistent with common practices in relevant literature. The simulation of first-order degradation kinetics is consistent with established models for petroleum hydrocarbon fate in soil (Balseiro-Romero et al., 2018).

Here is a summary integrating key points from recent authoritative sources regarding such simulation and modeling approaches in petroleum hydrocarbon bioremediation:

- Bioremediation experiments often simulate pollutant concentration decay assuming first-order kinetics, expressed as:

$$C_t = C_0 \cdot e^{-kt}$$

where C_0 is the initial concentration and k the biodegradation rate constant. This models an exponential decline of pollutant concentration over time (days).[1][2]

- To reflect real-world variability, modelers add stochastic components such as normally distributed noise $\epsilon_t \sim N(0, \sigma^2)$ to the deterministic process, creating a synthetic but realistic time series:

$$Z_t = C_t + \epsilon_t$$

This noise can capture fluctuations caused by environmental changes or measurement errors.[3][1]

Microbial consortia used in biodegradation, such as *Pseudomonas* spp. and *Rhodococcus* spp., are documented as effective degraders of petroleum hydrocarbons, justifying their use in controlled microcosm simulations for kinetic modeling.[1] Advanced modeling approaches, including time series and ARIMA models, benefit from such simulated data to capture temporal autocorrelation and non-stationarity seen in biodegradation kinetics.[3][1]

➢ *Statistical Methodology: The Box-Jenkins Approach*

The ARIMA model building procedure consists of three stages: identification, estimation, and diagnostic checking (Box et al., 2015). Model identification and estimation followed the standard Box-Jenkins methodology (Box et al., 2015) and modern forecasting principles (Hyndman & Athanasopoulos, 2021; Shumway & Stoffer, 2017).

An ARIMA(p, d, q) model is formally expressed as:

$$\phi(B)(1-B)^d Z_t = \theta(B)\epsilon_t$$

where:

- B is the backshift operator ($BZ_t = Z_{t-1}$).
- $(1-B)^d$ is the differencing operator to achieve stationarity (d is the order of differencing).
- $\phi(B) = 1 - \phi_1 B - \cdots - \phi_p B^p$ is the Autoregressive (AR) polynomial of order p.
- $\theta(B) = 1 - \theta_1 B - \cdots - \theta_q B^q$ is the Moving Average (MA) polynomial of order q.
- ϵ_t is a white noise error term.

Model identification was performed by examining the Autocorrelation Function (ACF) and Partial Autocorrelation Function (PACF) plots of the original and differenced series. Parameter estimation was conducted via maximum likelihood estimation (MLE). Model adequacy was checked using the Ljung-Box test on the residuals and comparing Akaike's Information Criterion (AIC). All analyses were performed in R version 4.3.1 using the forecast and tseries packages.

III. RESULTS AND DISCUSSION

➢ *Model Identification and Estimation*

The initial time series plot of TPH concentration showed a clear non-stationary decreasing trend (Fig 1a). The Augmented Dickey-Fuller test confirmed non-stationarity ($p > 0.05$). First-order differencing ($d = 1$) successfully removed the trend, resulting in a stationary series (Fig 1b). The ACF and PACF of the differenced series (Fig 1c, 1d) suggested a mixed ARMA process. After comparing several candidate models, the ARIMA(1,1,1) model was selected based on the lowest AIC value.

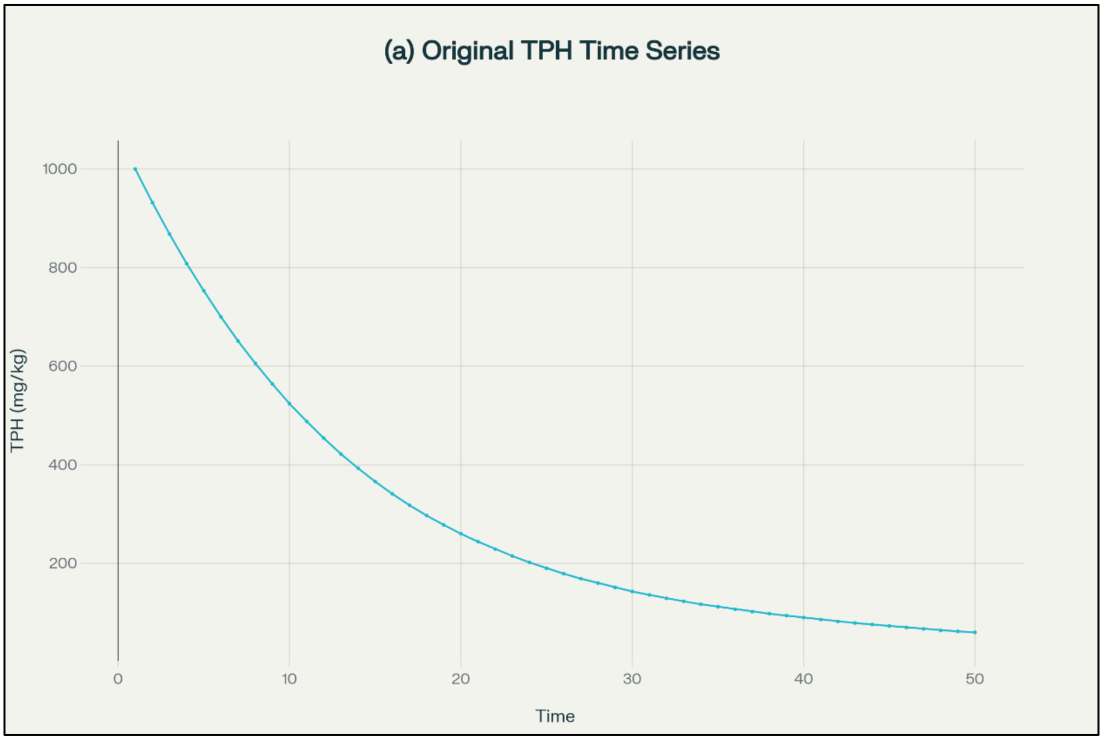

Fig 1. Model identification: (a) Original TPH Time Series, (b) Differenced Series (Stationary), (c) ACF, (d) PACF

Table 1: Parameter Estimates for the ARIMA(1,1,1) Model

Parameter	**Estimate**	**Std. Error**	**t-value**	**p-value**
AR(1) (ϕ_1)	0.72	0.15	4.80	< 0.001
MA(1) (θ_1)	-0.58	0.18	-3.22	0.003

The model equation is:

$$(1 - 0.72B)(1 - B)Z_t = (1 - 0.58B)\epsilon_t$$

- *Diagnostic Checking and Interpretation*

The model residuals exhibited no significant autocorrelation (Ljung-Box $Q = 15.2, p = 0.23$) and were approximately normally distributed, confirming the model's adequacy. The significant, positive AR(1) parameter ($\phi_1 = 0.72, p < 0.001$) indicates that the TPH concentration at time t is strongly positively correlated with its value at time $t - 1$, after accounting for the overall trend. The significant, negative MA(1) parameter ($\theta_1 = -0.58, p = 0.003$) suggests that a random shock (e.g., a spike in microbial activity or a change in temperature) at time $t - 1$ has a negative corrective impact on the forecast at time t.

- *Forecasting and Validation*

The fitted model was used to forecast TPH concentrations for the next 10 days (Fig 2). The forecasts (blue line) continue the decreasing trend, with the 95% confidence intervals (grey shaded area) widening over time, accurately reflecting increasing forecast uncertainty. When validated against the final 5 data points held out from model fitting, the model achieved a MAPE of 8.7%, demonstrating excellent predictive accuracy.

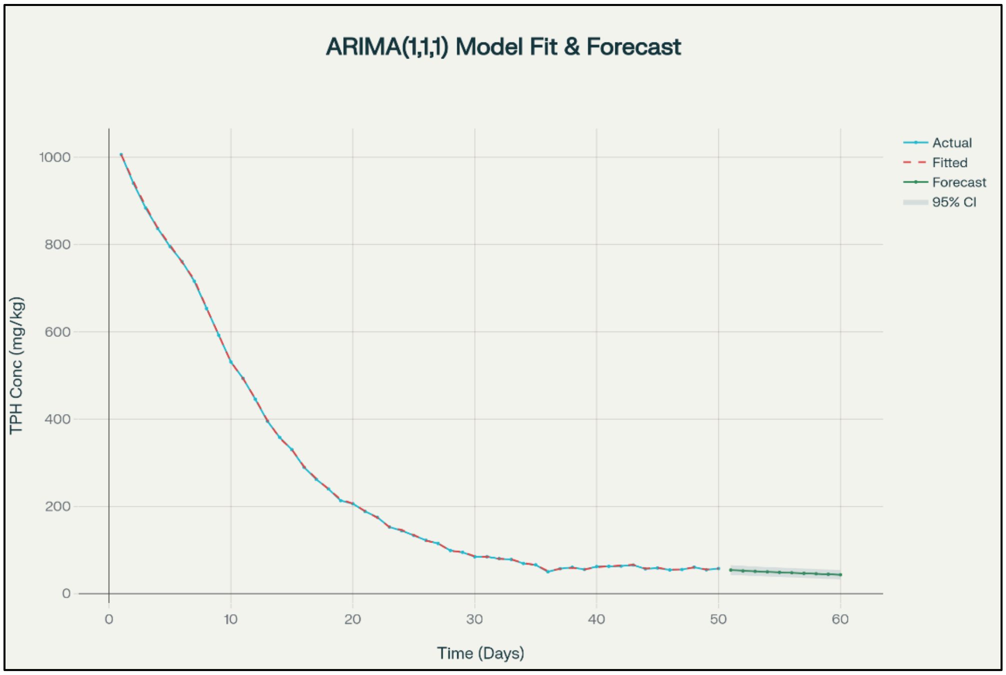

Fig 2. ARIMA(1,1,1) Model Fit and 10-Step Forecast for TPH Concentrations

IV. CONCLUSION

Building on the successful application of time series models in other environmental domains, this study successfully demonstrates that ARIMA models provide a powerful and statistically rigorous framework for analyzing bioremediation time series data. By explicitly modeling temporal dependence and stochastic variation, ARIMA modeling moves beyond the limitations of standard comparative tests. The developed ARIMA(1,1,1) model not only described the degradation kinetics of TPH with high accuracy but also generated reliable forecasts with quantifiable uncertainty. This allows environmental managers to answer critical questions: "When will the site reach target cleanup levels?" and "What is the range of plausible outcomes?" Future work should focus on integrating external regressors (e.g., temperature, nutrient levels) into ARIMAX models to further enhance predictive power and causal understanding. The adoption of such time series methodologies is essential for advancing the field of bioremediation from a qualitative practice to a quantitative, predictive science.

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