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Multi-model forecasting framework for agricultural nutrient dynamics in India: a comparative analysis of ML and hybrid approaches for NPK consumption

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ABSTRACT

This study developed and evaluated a comprehensive forecasting framework for predicting the dynamics of agricultural nutrients (N, P_2O_5, and K_2O) in India across three dimensions: consumption, exports, and imports. We implemented a diverse set of nine forecasting models, spanning traditional time series methods (ARIMA), machine learning algorithms (Random Forest, SVM, XGBoost), deep learning approaches (ANN, LSTM, GRU), and hybrid architectures (ARIMA–LSTM, XGBoost–LSTM. These were compared using historical data, and performance was analyzed with MAE (mean absolute error), MSE (mean squared error), and RMSE (root mean squared error). ARIMA performed consistently well in predicting trade in N and K_2O, while advanced machine learning models like XGBoost and Random Forest excelled in forecasting agricultural consumption. Six-year-ahead predictions (2024–2029) indicate rising nitrogen consumption (65,027 tons to 69,845 tons), stable phosphorus usage (29,006 tons to 30,211 tons), and increasing potassium demand (20,807 tons to 24,301 tons). Our results suggest model-specific advantages for different prediction scenarios, with hybrid models providing negligible improvements over simpler approaches. This research offers valuable insights for agricultural planning, policymaking, and food security in India. The data used were obtained from authoritative sources, including the Food and Agriculture Organization (FAO) and the Fertilizer Association of India (FAI), ensuring reliability and national relevance.

HIGHLIGHTS

- A comprehensive forecasting framework developed for agricultural nutrient dynamics in India
- Nine models were compared, including the time series, machine learning, and deep learning approaches.
- ARIMA excelled in predicting N and K_2O trade; XGBoost and Random Forest were best for consumption
- Six-year forecasts show increasing N and K_2O consumption and stable P_2O_5 usage
- Hybrid models offer minimal improvements over simpler approaches

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Agricultural nutrients; agricultural trade; deep learning; hybrid models; NPK fertilizers

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1. Introduction

Even today, food insecurity and undernutrition remain serious concerns in developing countries such as India (Pawlak & Kołodziejczak, 2020; Ritchie et al., 2018). High yields from limited arable land are required to achieve sustainable food security (Tang et al., 2022). Soil fertility is crucial for proper crop production, especially in commercial agriculture. The proper usage of agricultural inputs ensures greater agricultural

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Research article

Predicting methane and nitrous oxide emissions from Indian cattle farming using advanced time series techniques

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ABSTRACT

This study aims to forecast methane (CH_4) and nitrous oxide (N_2O) emissions from cattle rearing in India, which contribute significantly to agricultural greenhouse gas (GHG) emissions. Data on these emissions was collected from the Food and Agricultural Organization for the years 1961–2022. Three time series models, namely, exponential smoothing (Holt-Winters), autoregressive integrated moving average (ARIMA), and trigonometric seasonality, Box-Cox transformation, ARMA errors, trend, and seasonal components (TBATS) were employed to predict future emissions. The dataset was partitioned into training (1961–2012) and testing (2013–2022) sets to evaluate model performance. Diagnostic metrics, including Akaike Information Criterion, root mean square error, mean absolute percentage error, and mean absolute scaled error, were used to assess accuracy. Results indicated that the ARIMA model outperformed the other 2 forecasting models by making over 90% accurate predictions. For N_2O, ARIMA (0,1,0) was identified as the optimal model, while ARIMA (2,1,2) was selected for CH_4. Thus, the study validates the use of ARIMA model in GHG forecasting. The study projects emissions up to 2030, providing critical insights for policymakers to design targeted mitigation strategies. The study also presses the need for implementing sustainable cattle management practices for cutting emissions in India.

1. Introduction

Greenhouse effect traps the escaping heat from the Earth, thereby maintaining a congenial temperature on the planet [24,25]. Although necessary, yet any change in the concentration of greenhouse gases (GHGs) in the atmosphere leads to climate change [33,7]. Major contributor of these GHG is the energy sector, followed by the agriculture sector [20,26]. In 2022, the livestock sector of agriculture accounted for around 10–15 percent of global nitrous oxide and methane emissions, respectively. The reason the livestock sector emits these GHGs is the fermentation inside the digestive tract of cattle, which produces gases like methane, nitrous oxide, nitrogen oxides, sulfur dioxide, ammonia, etc., thereby leading to change in the chemical composition of the atmosphere [6,11,29,37]. Methane and Nitrous oxide cause around 25 and 298 times greater global warming than carbon dioxide, respectively [17,48].

Livestock constitutes a core component of agriculture in India and has the largest cattle population in the world [10]. Also, more than 60 percent of GHG emissions from the agricultural sector in India are from livestock [42]. Methane emissions from the livestock sector are due to enteric fermentation of animal feeds as well as from storage and treatment of manure, while nitrous oxide emission is from livestock manure [19,35,42]. The cause of 90 percent of the total methane emissions from livestock in India is enteric fermentation in ruminants [10,36]. Studies have reported that the GHGs are showing an increasing trend in India [12,21,22]. The ill effects of rising GHGs are well known, and hence it is necessary to predict their future levels in the atmosphere so that proper mitigation strategies can be planned.

Several researchers have attempted to predict these GHGs through various quantitative forecasting methods, such as causal and time series models. Causal forecasting methods establish cause and effect relationship

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SCIENTIFIC CORRESPONDENCE

State-of-the-Art Sugarcane Production in African Region

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Abstract
This investigation evaluated the effectiveness of several machine learning models, such as LSTM, GRU, BiLSTM, SVM, and random forest, in forecasting sugarcane production in different regions of Africa and globally. The results show that geographical characteristics and production parameters greatly affect model efficacy. LSTM and GRU capture temporal dependencies better in Africa, Southern Africa, and sub-Saharan Africa with dynamic and changeable production trends, resulting in lower error metrics and accurate forecasts. The support vector machine (SVM) is the most effective model in steady producing zones, having less variability in production like Central Africa and West Africa and in global forecasting due to its scalability and simplicity. Random forest struggled with time series data, delivering disappointing results across all regions. The 2030 projections are useful in agricultural planning and resource management. African production is likely to rise steadily, and it is expected that Middle Africa will witness major expansion in sugarcane production after 2025. Sub-Saharan Africa is expected to stabilize, but global sugarcane output may drop, suggesting agricultural changes. The forecasted values from these models indicate that sugarcane production in Africa is expected to reach 110,845 Mg by 2030, demonstrating steady growth. The projections emphasis the need for improved machine learning algorithms in agriculture's long-term planning and decision-making. Despite these promising results, more research is needed to improve forecast accuracy and relevance.

Keywords BiLSTM · Forecasting · GRU · LSTM · SVM

Originating in hot and tropical temperate regions of Asia, sugarcane is a semi-perennial plant of grass family with height measuring 2–6 m (de Matos et al. 2020). Globally, sugarcane is produced in about 90 countries belonging to tropical and subtropical regions of the world (Mnisi and Dlamini 2012).It enjoys the status of being both cash and energy crop in the world (Ahmed et al. 2024). Daily life of any individual cannot be completed without sugarcane, which makes the crop very important (Owino 2019). This perennial grass plays crucial role in the production of sugar, bioethanol, and electricity across the world (Singels et al. 2021). Among the various sources of plant-based calories consumed by human, sugar ranks third, following rice and wheat (Moore et al. 2013) and about 80% of sugar produced in the world comes from sugarcane (Fair Labor Association 2020). By-products of sugarcane can also be used in crop production in the form of organic fertilizer (Dotaniya et al. 2016). Sugarcane wastes such as bagasse ash and bagasse fibers are widely used in place of cement in mortar and concrete mixes which eventually leads to reduction in atmospheric pollution caused due to cement (Hussien and Oan 2022).

Africa contributes to about 5% of global sugarcane production (Thibane et al. 2023). Starting from the fifteenth century when Spanish and Portuguese explorers introduced sugarcane in Africa, the cane has been an important crop in the continent's cropping pattern (Galán Sauco and Cubero

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RESEARCH

A DFT-D2 study on adsorption of iodonitromethane on doped (B, N & Fe) and Fe-functionalized monovacancy graphene surfaces

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Abstract

Context INM is a toxic halogen nitromethane and disinfection by-product that is very dangerous to the environment and human beings since it is highly cytotoxic and mutagenic. Here, we examine the adsorption of INM on pristine graphene (PG), monovacancy graphene (MVG), nitrogen-doped vacuity graphene (NVG), and boron-doped vacuity graphene (BVG) and their Fe-functionalized analogs (FeG, FNG, and FBG) using density functional theory (DFT). To explain the adsorption mechanism, adsorption energy calculations, Hirshfeld charge transfer analysis, and electronic structure evaluations, such as band gap, density of states (DOS), and partial DOS (PDOS), were used. INM shows poor physisorption on PG, MVG, and NVG, whereas BVG shows stronger chemisorption by direct bonding. Fe adsorption is very important in increasing the strength of adsorption and redistribution of charges which results in strong electronic structure alterations. Then Fe-doped vacancy graphene is explored with respect to band gap, DOS, and PDOS plots. INM is then adsorbed on the surface. Fe-doped vacancy graphene (FVG) exhibits the highest adsorption energy and the largest electronic modification which validates the fact that it is strongly chemisorptively interacting. These findings emphasize FVG as a promising and efficient material to remove toxic INM in the contaminated environment and to develop graphene-based adsorbents to clean up the environment.

Methods All calculations were done in the DMol^3 package of Materials Studio with a doubled numerical plus polarization (DNP) basis set and DFT semicore pseudopotentials (DSPP). The GGA-PBE functional was used with the DFT-D correction by Grimme which considered the effects of exchange-correlation and dispersion. Spin-unrestricted geometry optimizations were driven to strict energy (2.0×10^{-5} Ha) and force (4×10^{-3} Ha Å^{-1}) convergence factors, on a grid of $6\times6\times1$ Monkhorst Pack k-points. To assess charge transfer and bonding properties, Hirshfeld charge and Mayer bond order analyses were used.

Keywords Iodonitromethane · Graphene · Doping · Chemisorption · DFT

Introduction

Chemicals such as iodonitromethane and bromonitromethane used to pollute water and soil may have great environmental impacts. Such substances when not disposed properly or released accidentally into the ecosystems may contaminate the water bodies and soils and therefore be harmful to aquatic and terrestrial life. These pollutants can impact aquatic life in water by interfering with their reproductive processes or being toxic, which in most cases results in reduction of biodiversity. On the same note, in soil, toxic chemicals may distort the microbial communities, diminish the soil fertility, and pollute the food chain. These effects are also worsened by the fact that some pollutants may persist in the environment even after they are introduced into the environment [1].

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A review on mechanical properties of carbon nanotubes (CNTs) using finite element modeling (FEM) method

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ABSTRACT

Modeling and simulation is a fascinating computational approach for the estimation of several properties of nanomaterials. Specially, Finite Element Modeling (FEM) technique has been discussed marvelously to predict the elastic modulus of three types of carbon nanotubes (CNTs) and armchair, chiral and zigzag configurations. FEM is found more appropriate technique to estimate the mechanical properties of CNTs. The Young's modulus (YM), Shear modulus (SM) and stress-strain relationship of CNTs under tensile and torsional conditions were predicted. In the present study, computational results of elastic properties of CNTs have been compiled from the literature by using molecular mechanics based FE technique. The major advantages of this method are the simplicity of the concepts and improved computational efficiency for analyzing the elastic properties of CNTs. The modeling work have been brought together and reviewed on molecular mechanics based FE modeling. Using the specified technique based on structural mechanical properties, the tensile strength has been reported to be independent of nanotube helicity, while YM and SM of nanotube have been reported to increase with tube diameter.

1. Introduction

CNTs are versatile material for the nanotechnology studies due to their tremendous properties as compared to conventional carbons. CNT is a very fascinating material, discovered by Iijima at NEC Laboratory in Tsukuba, Japan [1]. It has attracted much attention because of its extraordinary mechanical, electrical, optical, and structural properties. Nanotubes are elongated form of fullerene or buckyball molecule with both ends typically capped with a hemisphere. There are two main types of nanotubes: single-walled nanotubes (SWCNTs) and multi-walled nanotubes (MWCNTs) [2,3]. Basing on the structural properties of CNTs, they are supposed to be potential substrate for various premier applications such as drug delivery and biocompatibility in biomedical applications. In mechanical application, they will be suitable for high strength composites. Since the minimum number of electrons can follow through CNTs, they seem to have appropriate quality for field emission applications. SWCNT is quite distinguished as a very important variety of CNTs because it exhibits excellent electrical properties that are not typical for the MWCNT. SWCNT is the most likely candidate for miniaturizing electronic and micro electromechanical scale devices which are commonly used in modern electronics. The electric wire plays an important role in these systems where SWCNTs are being used as excellent conductors [4,5].

The strength and flexibility of CNTs make them attractive for potential use in controlling other nanoscale structures. Nanotechnology engineering has been enriched by the use of CNTs in twenty first century. The utmost tensile strength of individual MWCNT observed to be 63 GPa in comparison to high carbon steel which has low tensile strength of approximately 1.2 GPa. The elastic modulus of SWCNTs is very high of the order of 1 TPa [6,7]. Specifically to mechanical properties, by assuming CNT as a structural member, the elastic properties of CNT can be obtained from experimental observations. Typical examples of structural member include bar, beam, and shell models. The bar model has been used in the experiment in which the compressive response was measured using micro-Raman spectroscopy. They reported YM was 2.8–3.6 TPa for SWCNT and 1.7–2.4 TPa for MWCNT. Yu et al.

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