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Stochastic Carbon Dioxide Forecasting Model for Concrete Durability Applications

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Abstract Over the Earth's history, the climate has changed considerably due to natural processes affecting directly the earth. In the last century, these changes have perpetrated global warming. Carbon dioxide is the main trigger for climate change as it represents approximately up to 80% of the total greenhouse gas emissions. Climate change and concrete carbonation accelerate the corrosion process increasing the infrastructure maintenance and repair costs of hundreds of billions of dollars annually. The concrete carbonation process is based on the presence of carbon dioxide and moisture, which lowers the pH value to around 9, in which the protective oxide layer surrounding the reinforcing steel bars is penetrated and corrosion takes place. Predicting the effective retained service life and the need for repairs of the concrete structure subjected to carbonation requires carbon dioxide forecasting in order to increase the lifespan of the bridge. In this paper, short term memory process models were used to analyze a historical carbon dioxide database, and specifically to fill in the missing database values and perform predictions. Various models were used and the accuracy of the models was compared. We found that the proposed Stochastic Markovian Seasonal Autoregressive Integrated Moving Average (MSARIMA) model provides R^2 value of 98.8%, accuracy in forecasting value of 89.7% and a variance in the value of the individual errors of 0.12. When compared with the CO_2 database values, the proposed MSARIMA model provides a variance value of −0.1 and a coefficient of variation value of $-8.0e^{-4}$.

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1 Introduction

Civil infrastructure investment in the European Union has been in a steady decline since the outbreak of the economic and financial crisis. Although the decrease appears to gradually level off from 2015 onwards with an increase of 5% [1]. The increase in the infrastructure investment from 2015 onwards was illustrated as an action by the European Union for the sake of designing and maintaining these systems for a certain service lifetime, which was recognized as critical issues worldwide.

Decision making in the civil infrastructure investment in the European Union utilizing the quality control plan is involved in the case of repairing or demolition of the reinforced concrete bridges, depending on the recent key performance indicators (KPI). The KPI are specified by engineering consultants regarding the current condition of the bridge and the strategies to be followed (Reference strategy/Representative strategy) taking into consideration the reliability, the cost and the availability of the bridge.

Reinforced concrete bridges are characterized by high durability, despite that, they are also vulnerable to natural hazards, as well as extreme events that affect their performance and serviceability. Statistics on bridge collapses worldwide reveal that natural hazards are the predominant cause of failure. French government revealed that among the 12,000 maintained bridges after the collapse of the motorway bridge located in Genoa, 840 are at risk of collapsing. This issue is common across Europe [2].

Carbonation of concrete is one of the main causes of corrosion and occurs by the reaction given in Eq. (1) between atmospheric CO_2 and the hydrated phases of concrete. This reaction generates calcium carbonate, leading to a drop in the pH value, in which the protective oxide layer of the reinforcing steel bars is broken and corrosion starts. Therefore, the life span of the concrete infrastructure is affected by the enhanced risk of carbonation induced corrosion [3].

$$\mathrm{Ca(OH)_2 + CO_2 = CaCO_3 + H_2O} \tag{1}$$

The temperature significantly affects the diffusion coefficient of CO_2 into concrete, the rate of reaction between CO_2 and Calcium Hydroxide ($Ca(OH)_2$), and their rate of dissolution in pore water [4]. The optimum relative humidity condition for the carbonation process is between 50 and 70%, including wetting and drying cycles that enhance the reaction [5].

The carbonation process is very sensitive to the local climate depending on the environmental conditions [6]. Climate change impacts the infrastructure as the increase in CO_2 levels associated with global warming will increase the carbonation-induced corrosion. Moreover, changes in humidity and temperature significantly affect the initiation time of corrosion [7]. Since studies on global warming have predicted several changes in climate, the impact of climate change on structural reliability should be considered. For example, Bastidas-Arteaga has calculated numerically in the oceanic environment a reduction in the lifetime of failure that ranges between 1.4 and 2.3% and up to 7% when cyclic loading is considered [8].

A carbon dioxide database is essential to study the influence of realistic exposure conditions on concrete carbonation. Databases could be also used to establish probabilistic prediction models. Therefore, this study proposes a prediction model that is established based on the time-domain analysis of the database and evaluated with a short memory process. The model is also compared with other autoregressive models. The proposed Stochastic Markovian Seasonal Autoregressive Integrated Moving Average model (MSARIMA) is also used to fill the missing database and to perform predictions, taking into account the statistical analysis on the previously existing historical database and seasonality.

Climate models are based on well-notarized physical processes that simulate the transfer of energy and materials through the climate system. Climate models, also known as general circulation models, use mathematical equations to characterize how energy and matter interact in different parts of the ocean, atmosphere and land [9]. Climate models are operated using variability that is driving the climate and predicting the climate change in the future. External factors are the main inputs into the climate models that affect the amount of the solar energy absorbed by the Earth or the amount trapped by the atmosphere, these external factors are called "forcing". They include variations in the sun's output, greenhouse gases and tiny particles called aerosols that are emitted from burning fossil fuels, forest fires and volcanic eruptions. The aerosols reflect incoming sunlight and influence cloud formation except the black carbon.

Climate models provide results that vary with respect to the actual historical database; those variations are at the expense of each model differences in: (ensemble, data source, forcing, the initial state of run, driving model, aerosols influence and jet stream impact). However, the proposed model is based on stochastic time series analysis that avoids the climate models variations and provides database that is statistically related to the existing historical database.

2 Carbon Dioxide Forecasting

Time series forecasting is a quantitative approach that uses information based on historical values and associated patterns to predict future observations. Time series analysis comprises methods for analyzing time-series data to extract meaningful statistics and other characteristics of the data. The analysis includes trend, seasonality and irregular components. A time-series analysis quantifies the main features in data and random variation. These reasons, combined with improved computing power, have made time series methods widely applicable.

2.1 Methodology

2.1.1 Time Series Analysis

Time series analysis for carbon dioxide database is based on the time-domain analysis (autocorrelation analysis and cross-correlation analysis), in which the type of the process deduced is a short-term memory process with short-range dependence that is characterized by an exponential decay of the autocorrelation function (Acf) for the historical database.

2.1.2 Decomposition

Time series consists of two systematic components: trend and seasonality, and a non-systematic component called noise. A multiplicative nonlinear model is used as the seasonality increases with the increase in the trend. The autocorrelation function of the non-systematic component demonstrates the characteristics of the autoregressive model in terms of damaged cosine shape.

2.1.3 Stationarity

Stationarity of the database is essential to maintain the statistical properties of the time series, a stationarized series is relatively easy to predict, the stationarity is achieved through differencing and log transformation. The basic idea of stationarity is that the probability laws that govern the behavior of the process do not change over time. In a sense, the process is in statistical equilibrium. Specifically, a process is strictly stationary if the distribution of existed state is the same as the distribution of the previous state for all choices of time points and all choices of time step lag. The stationarity of the time series is checked using Kwiatkowski–Phillips–Schmidt–Shin (KPSS) test and augmented Dickey–Fuller (ADF) test [10].

2.1.4 Models

The statistical technique utilized for forecasting the carbon dioxide is Seasonal Stochastic Markovian Autoregressive Integrated Moving Average (MSARIMA) which provides high accuracy and precise results. Moreover, other statistical techniques that include moving average based methods, such as Autoregressive Moving

Average (ARMA), Autoregressive Integrated Moving Average (ARIMA), Holt-Winters' Triple Exponential Smoothing and Seasonal Autoregressive Integrated Moving Average (SARIMA) were performed in order to compare the variations in the accuracy of the models.

Lately, Autoregressive Integrated Moving Average (ARIMA) model has been used to study the short time-varying processes. However, one limitation of ARIMA is its natural tendency to concentrate on the mean values of the past series data. Therefore, it remains challenging to capture a rapidly changing process, in which the proposed model (MSARIMA) solves this issue by triggering a Markovian step when the value of the integration part is >1 and the probability of occurrence is related to the previous seasonal events.

2.2 Models Description

Models presented are divided into two categories: auto regression (AR) moving average (MA) parameters and exponential smoothing parameters. The proposed MSARIMA model is based on the AR and MA parameters. In addition, it accounts for seasonality and Markovian step technique.

The autoregressive model of order p, which is denoted as AR(p), writes:

$$X_t = c + \sum_{i=1}^{p} \varphi_i X_{t-i} + \varepsilon_t; \varepsilon_t \sim \mathrm{WN}\left(0, \sigma_\varepsilon^2\right) \tag{2}$$

where X_t is the state, φ is a parameter of the model, c is constant, ε_t is a random white noise WN and σ_ε^2 is the variance of the random white noise.

In this case, we denote by $\{X_t\} \sim$ AR (p). In the same way, we can rewrite a process AR(p) with a polynomial φ (B).

$$\varphi(B)X_t = \varepsilon_t; \varphi(B) = 1 - \varphi_1 B - \varphi_2 B^2 - \cdots - \varphi_p B^p \tag{3}$$

The moving average model of order q, which is denoted as MA(q), writes:

$$X_t = \omega + \sum_{i=1}^{q} \theta_i \varepsilon_{t-i} + \varepsilon_t \tag{4}$$

where θ is a parameter of the model and ω is the expectation of X_t, often equals to zero.

Use the backshift operator B to rewrite Eq. (4).

$$X_t = \theta(B)\varepsilon_t; \theta(B) = 1 + \theta_1 B + \theta_2 B^2 + \cdots + \theta_q B^q \tag{5}$$

2.2.1 Autoregressive Moving Average Model (ARMA)

The general ARMA model was described in the 1951 by Peter Whittle [11].

$$X_t = c + \omega + \sum_{i=1}^{q} \theta_i \varepsilon_{t-i} + \sum_{i=1}^{p} \varphi_i X_{t-i} + \varepsilon_t \tag{6}$$

The model could be written using the polynomials φ(B) and θ(B) in which the constant c and ω are zero values:

$$X_t - \sum_{i=1}^{p} \varphi_i X_{t-i} = \sum_{j=1}^{q} \theta_j \varepsilon_{t-j} + \varepsilon_t \tag{7}$$

$$\varphi(B)X_t = \theta(B)\varepsilon_t \therefore \left(1 - \sum_{i=1}^{p} \varphi_i B^i\right)X_t = \left(1 + \sum_{j=1}^{q} \theta_j B^j\right)\varepsilon_t \tag{8}$$

The ARMA model omits the integration part of its calculation leading to a non-stationary time series model in which statistical parameters will vary with time. On the contrary, embedding the integration part in the time series will control the stationarity in which the statistical properties such as mean, variance, autocorrelation, etc. are all constant over time.

2.2.2 Autoregressive Integrated Moving Average Model (ARIMA)

The ARIMA is an advanced ARMA model that solves the stationarity of the time series by using difference operation, this value is up to the second-order of integration ($d_{\max} = 2$) based on the backshift operator Eq. (9). Otherwise, it is solved using log transformation.

$$B(X_t) = X_{t-1};\ B^d(X_t) = X_{t-d} \tag{9}$$

The general equation taking into account the constant c and ω as a non-zero value, in which $c = \omega\left(1 - \varphi_1 - \cdots - \varphi_p\right)$ and ω is the mean of $(1 - B)^d X_t$, is as follows:

$$(1 - \varphi_1 B - \cdots - \varphi_p B^p)(1 - B)^d (X_t - \omega t^d / d!) = \left(1 + \theta_1 B + \cdots + \theta_q B^q\right)\varepsilon_t \tag{10}$$

2.2.3 Seasonal Autoregressive Integrated Moving Average Model (SARIMA)

The seasonality of a model is detected using an autocorrelation function in which the peaks evolve over the lag values of a defined time series with a scale value >24. The monthly seasonal stationarity of a model is based on a lag value of $s = 12$ and is known as the seasonal monthly differencing operator in Eq. (11).

$$(1 - B)^s X_t = X_t - X_{t-s} \tag{11}$$

$$\emptyset\left(B^s\right)\varphi(B)(X_t - \omega) = \Theta\left(B^s\right)\theta(B)\varepsilon_t \tag{12}$$

The SARIMA model without the differencing operations is mentioned in Eq. (12) and the terms are illustrated below:

$$\varphi(B) = 1 - \varphi_1 B - \varphi_2 B^2 - \cdots - \varphi_p B^p \tag{13}$$

$$\emptyset\left(B^s\right) = 1 - \emptyset_1 B^s - \emptyset_2 B^{2s} - \cdots - \emptyset_p B^{ps} \tag{14}$$

$$\theta(B) = 1 + \theta_1 B + \theta_2 B^2 + \cdots + \theta_q B^q \tag{15}$$

$$\Theta\left(B^s\right) = 1 + \Theta_1 B^s + \Theta_2 B^{2s} + \cdots + \Theta_q B^{qs} \tag{16}$$

where $\emptyset$ is the seasonal AR parameter, φ is the AR parameter,Θ is the seasonal MA parameter and θ is the MA parameter.

2.2.4 Markovian Seasonal Autoregressive Integrated Moving Average model (MSARIMA)

The proposed model is based on the SARIMA model. The MSARIMA solves the SARIMA only limitation with its tendency to concentrate on the mean values of the past series data by working on a sequence of time intervals changing their mean value in each time and by triggering a Markovian step Eq. (17).

$$\delta = P\{S_n | S_{n-12} = i_{n-12}\} = \begin{cases} \mathrm{E}\left(\varepsilon_{\sum i-12}\right) > 1, & X = x_{n-i} + \mu \\ \mathrm{E}\left(\varepsilon_{\sum i-12}\right) < 1, & X = x_{n-i} + 1 \end{cases} \tag{17}$$

where $\mathcal{S}$ is the state, μ is the mean value of the monthly seasonal errors of the value X and δ is the Markovian step value.

The MSARIMA model is developed based on the SARIMA model with a triggering condition when the integration value >1, the model works on increasing the accuracy of the prediction regarding the seasonal errors for the current state.

The step process depends on the most recent past event and the Markovian step is a renewable process because it presents only positive values. This model neglects the ω values in the previous equations and presents the Markovian step process value δ for more accurate results. The equation is as follows:

$$\emptyset\left(B^{s}\right)\varphi(B)(X_t) = \Theta\left(B^{s}\right)\theta(B)\varepsilon_t + \delta \tag{18}$$

2.2.5 Holt-Winters' Multiplicative Seasonal Model

Winters (1960) extended Holt's method to capture seasonality [12]. The Holt-Winters' seasonal method comprises the forecast equation and three smoothing equations. The multiplicative method is used when the seasonal variations are changing proportionally to the trend of the series. The seasonal component is expressed in relative terms and the series is seasonally adjusted by dividing through by the seasonal component. Within each year, the seasonal component will sum up to approximately the seasonal frequency value.

$$\hat{X}_{t+h|t} = (l_t + \mathrm{h} \cdot b_t) S_{t+\mathrm{h}-\mathrm{m}(\mathrm{k}+1)} \tag{19}$$

$$l_t = \alpha \frac{X_t}{S_{t-m}} + (1-\alpha)(l_{t-1} + b_{t-1}) \tag{20}$$

$$b_t = \beta(l_t - l_{t-1}) + (1-\beta) b_{t-1} \tag{21}$$

$$S\mathrm{t} = \gamma \frac{\mathrm{Xt}}{l_{t-1} - \mathrm{b}_{t-1}} + (1-\gamma) S_{t-m} \tag{22}$$

where l_t is the level, bt is the trend, St is the seasonal component, m is the seasonal frequency, and α, β and γ are the model smoothing parameters.

3 Results and Discussion

The main objective of this section is to estimate the ability of the proposed approach in forecasting carbon dioxide concentration using an incomplete database. The forecasting and prediction of the missing values are performed using the following mathematical and stochastic models: ARMA, ARIMA, SARIMA, Holt-Winters' and MSARIMA.

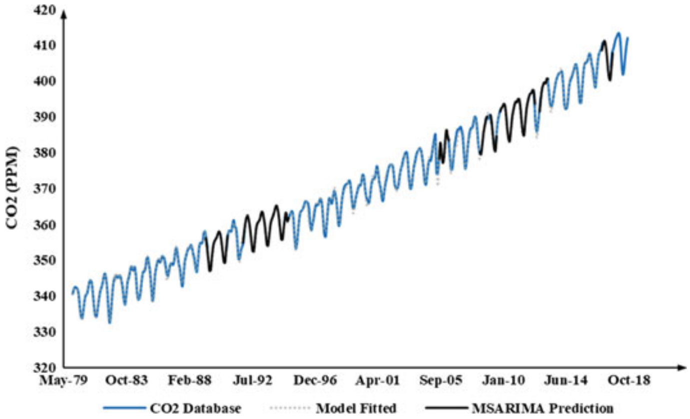

Fig. 1 Example of CO_2 assessment based on previous database

3.1 *Database Description*

The concentration of greenhouse gases in Portugal is measured on the island of Terceira, which is one of the nine islands in the archipelago of the Azores, located in the middle of the Atlantic Ocean. The database is available since 1979 for different greenhouse gases. In particular, for the three main gases, carbon monoxide (CO) since 1990, carbon dioxide (CO_2) since 1979, and methane (CH_4) since 1983. However, the carbon dioxide database includes missing values. The samples are collected on the island of Terceira and the analysis is carried out in NOAA lab, Hawaii, in the scope of the Cooperative Global Air Sampling Network.

3.2 *MSARIMA CO_2 Database Prediction*

The database offered by NOAA lab, Hawaii, in the scope of the Cooperative Global Air Sampling Network includes missing values. Therefore, a stochastic MSARIMA model presents accurate results in filling the database shown in Fig. 1 and can be used in for forecasting purposes.

3.3 *Stochastic Models Analysis*

3.3.1 Stochastic Models Predictions

In this section, the prediction of the MSARIMA model is compared with SARIMA and Holt-Winters' models as both include seasonal components. This is implemented

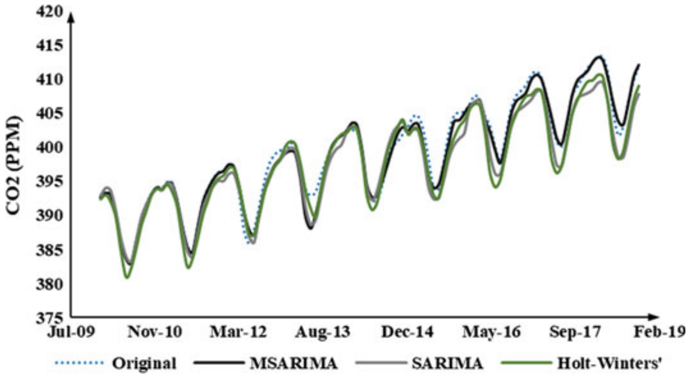

Fig. 2 Stochastic models comparison

by forecasting a historical CO_2 starting from 2010 through 2018 Fig. 2. The prediction of the MSARIMA model seems to provide the best fitting results to the original database compared to the other models. The errors associated with the predictions will be further studied in the next section.

3.3.2 Stochastic Models Accuracy

A statistical study was performed to derive the variations between the mathematical stochastic models and the meteorological station's database. The difference of the relative frequencies for CO_2 presented in Fig. 3 was performed for a time series starting from 01/2010 to 01/2018 to describe the variations in the models. The proposed MSARIMA model presents the lowest variations. Moreover, ARIMA and

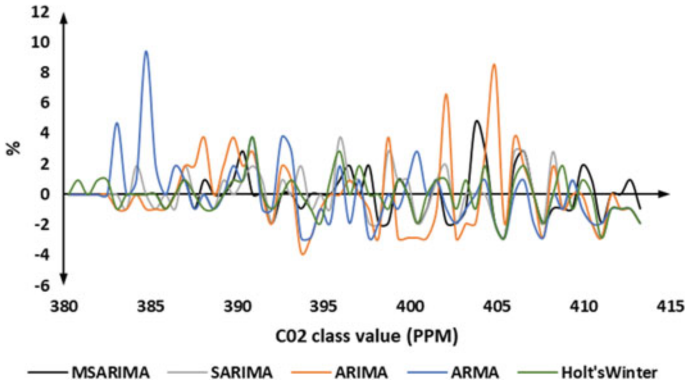

Fig. 3 Difference in relative frequency

Table 1 Statistical differences with meteorological station's CO_2 database

Model	Mean value	Variance	Coefficient of variation (%)
MSARIMA	−0.32	−0.1	−0.0008
SARIMA	−1.567	−11.94	−0.20
Holt-Winters'	−1.562	−7.07	−0.11
ARIMA	−1.27	−5.48	−0.08
ARMA	−4.82	3.05	0.07

Table 2 Accuracy between MSARIMA and SARIMA models

Model	ME	RMSE-MAE	1-MAPE [%]	R^2 [%]
MSARIMA	9.78	0.12	89.7	98.8
SARIMA	24.0	0.16	85.3	97.8

ARMA models show higher variations than the other models as seasonality is not considered.

The stochastic models' statistical study in Table 1 illustrates the variation of the models with the original database in terms of mean value, variance and coefficient of variation, in which the MSARIMA model shows the lowest variation with the meteorological station's CO_2 database. On the contrary, the others present higher variations in the results.

The accuracy of the stochastic models is finally demonstrated by comparing SARIMA and MSARIMA models with the original database for the data given in Fig. 2. This study will be carried out in terms of the error indicators in Table 2. In this table ME is the mean error, RMSE is the square root of the average of the square errors, MAE is the mean absolute error, MAPE is the mean absolute percentage error and R^2 is the proportion of the fitted model variation with the original database.

The MSARIMA model presents the highest R^2 value in which 98.8% of the CO_2 database variation is explained by the fitted model. The mean error refers to the average of all errors, it is also described as the uncertainty in measurements, the proposed MSARIMA model provides the lowest value in errors. The variation in the errors in the set of forecasts is diagnosed by the difference between RMSE and MAE, in which lower values in RMSE-MAE show lower variance in the individual errors, as shown in Table 2 the MSARIMA model has the lowest RMSE-MAE values. The accuracy of a model prediction is presented by the 1-MAPE value, as it calculates the relation between forecasted values and original values, in which the MSARIMA model has the highest accuracy in forecasting.

4 Conclusions

The prediction of the proposed Stochastic Markovian Seasonal Autoregressive Integrated Moving Average (MSARIMA) model seems to provide the best fitting results to the original CO_2 database compared to the other models.

The proposed MSARIMA model provides R^2 value of 98.8%, accuracy in forecasting value of 89.7% higher than all the other models and variance in the individual errors value of 0.12. When compared with the CO_2 database values, the proposed MSARIMA model provides a mean value of −0.32, a variance value of −0.1 and a coefficient of variation value of $-8.0e^{-4}$.

The provided results demonstrate that there is no overestimation in the predictions using the proposed MSARIMA model, which might be an obstacle due to the proposed step methodology. On the contrary, the MSARIMA model provided the best fit in predictions when compared with the original CO_2 database.

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