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A Nested Monte Carlo Simulation Model for Enhancing Dynamic Air Pollution Risk Assessment

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***Abstract*—The risk assessment of air pollution is an essential matter in the area of air quality computing. It provides useful information supporting air quality (AQ) measurement and pollution control. The outcomes of the evaluation have societal and technical influences on people and decision-makers. The existing air pollution risk assessment employs different qualitative and quantitative methods. This study aims to develop an AQ-risk model based on the Nested Monte Carlo Simulation (NMCS) and concentrations of several air pollutant parameters for forecasting daily AQ in the atmosphere. The main idea of NMCS lies in two main parts, which are the Outer and Inner parts. The Outer part interacts with the data sources and extracts a proper sampling from vast data. It then generates a scenario based on the data samples. On the other hand, the Inner part handles the assessment of the processed risk from each scenario and estimates future risk. The AQ-risk model is tested and evaluated using real data sources representing crucial pollution. The data is collected from an Italian city over a period of one year. The performance of the proposed model is evaluated based on statistical indices, coefficient of determination (R2), and mean square error (MSE). R2 measures the prediction ability in the testing stage for both parameters, resulting in 0.9462 and 0.9073 prediction accuracy. Meanwhile, MSE produced average results of 9.7 and 10.3, denoting that the AQ-risk model provides a considerably high prediction accuracy.**

***Keywords*—Air pollution; dynamic risk; Monte Carlo simulation; nested Monte Carlo Simulation.**

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I. INTRODUCTION

Risk assessment estimates risks posed by inseparable hazards involved in certain processes or situations [1]–[5]. Commonly, risks fluctuate within a period of risk assessment depending on the processes involved, whether in manufacturing, in usage such as driving a car, or in disposals such as water and air pollution. Dynamic Risk Assessment (DRA) entails methods that repeatedly and cumulatively perform risk assessment processes in order to cater to dynamic environmental factors or dynamic decisions needed in such an environment [6]–[8]. DRA is frequently performed over time in which the risk assessment changes over an attempt's measurements and assessment decisions. Examples of DRA include assessing the risk of air pollution or the supply chain of products.

Air pollution, in particular, has posed a great threat to the environment as the industrial world continues to contribute to the environmental decline [9]–[11]. Due to the critical influences of air pollution, air quality prediction and monitoring are important tasks of Air Quality Systems (AQS). Air pollution in many cities is rising in parallel with economic surges, thus, observing, forecasting, and controlling air pollution becomes increasingly important to safeguard the health impact.

Nonetheless, the prediction of air pollution risks is a complex problem in DRA due to the dynamic nature of the pollution data, such as high spatiotemporal unevenness. Different DRA methods can predict the uncertainties in the input data [12], including the Monte Carlo simulation, Markov chain, and Bayesian networks [13]. In addition, numerous aspects of Artificial Intelligence (AI) techniques have been implemented in various domains of risk assessments, such as Fuzzy Logic, Neural Networks, Genetic Algorithms, Nearest neighbors, and Software agents [14].

Monte Carlo Simulation (MCS) is a statistical technique that depends on random numbers. With this technique, approximate solutions to different kinds of mathematical problems can be obtained. Monte Carlo is able to provide these solutions by carrying out statistical sampling experiments on a computer. The experiments are applied to problems with no probabilistic content as well as to those that naturally have a probabilistic structure. This technique falls under computational algorithms, which rely on repetitive random sampling and the user's ability to generate a truly random sequence of numbers in principle. Usually, these methods are employed to simulate a physical system based on mathematical models. The reliance of the Monte Carlo techniques on random numbers and repeated computation makes them the most appropriate means of performing calculations on a computer because they can provide an efficient, valuable, and acceptably approximate methodology, especially when an exact solution with a deterministic algorithm is not feasible.

Research by Dhammapala, Bowman, and Schulte [15] integrated the Monte Carlo (MCs) method with the American Meteorological Society/U.S. Environmental Protection Agency Regulatory Model (AERMOD) output along with the background concentrations, taking into consideration their seasonality. In the MC method, data from the same months are randomly combined with replacement and then used to compute 1000 estimates of the 98th or 99th percentiles. Gao et al. [16] performed sensitivity and uncertainty analysis using MCS. In Joerss et al. [17], MCS was applied in assessing the uncertainties in German 2005 emissions of particulate matter (PM10 & PM2.5) and aerosol precursors (SO2, NOx, NH3, and NMVOC) carried out in the PAREST (PArticle REduction STrategies) research project. In the uncertainty analysis, an amendment was made to the German Federal Environment Agency's emission inventory, which was then combined with a model on the disaggregation of energy balance data.

The literature also showed different kinds of algorithms developed along with expert judgment data to predict uncertainties efficiently and pragmatically in model input data emission. Pineda et al. [18] presented a methodology for the evaluation of uncertainty in modeled concentrations related to probable errors of the input data. The proposed methodology was also based on MC. Tong et al. [19] presented a probabilistic risk assessment model designed to explore the effects of construction dust on employees in the construction industry based on the United States Environmental Protection Agency (USEPA).

To this end, the risk assessment of a particular problem, operation, or operator is a complex process that is mainly based on probabilistic or estimation methods. The availability and accuracy of this depend on the algorithms used underneath. This paper proposes an AQ-risk model based on the statistical method of Nested Monte Carlo Simulation (NMCS) for air pollution of DRA. The contributions of this paper encompass two points: (1) the prediction of air pollutant levels by the AQ-risk model and (2) the evaluation of the model by experimenting with real data.

The structure of the paper is arranged as follows. Section 2 provides details about the related work. Section 3 presents the methods and materials that explain the risk domains, including air pollution, and presents and details the methods and materials that are used in this paper, including NMCS, evaluation methods, and the testing dataset. Section 4 provides details of the proposed AQ-risk model application in air pollution risk assessment. Section 5 presents the experimental and mathematical examples along with the results and evaluations of these examples. Finally, Section 6 provides a concluding summary and presents the potential areas of DRA as future work.

II. Materials and Methods

A. Air Pollution Risk Assessment

Environmental problems have escalated globally, thus imposing high risks to human lives. The concerned authorities (both governments and experts) have successfully managed to control air pollution. The major source of air pollution has always been burning fossil fuels in automobiles and industries. Air pollution causes severe health problems such as asthma, bronchitis, and wheezing. Although the use of Air Quality Systems (AQS) to monitor air quality has been the common way of determining ambient air quality and checking compliance with regulations and standards, such data are incomplete in time and space. Air pollutants prediction can improve the existing knowledge regarding air pollution and provide useful information to facilitate optimal emission control techniques [20]. The predictive capability can also enhance the acceptability of the nature and contributions of several sources of air pollutants.

Appropriate air pollutant prediction models can provide the required information to public establishments in times of emergency. Several air pollutant prediction models have been proposed and developed over the years. However, the complexity of the factors involved in predicting air pollutants has made the process more difficult. Hence, there is a need to develop appropriate methods or models that can accurately predict air pollutants' future trends.

Table I presents the major air pollutants and their sources. The pollution parameters include Carbon dioxide (CO2), Carbon monoxide (CO), Sulphur dioxide (SO2), Nitrogen oxides (NOx), Ozone (O3), Hydrocarbons (HC), and particulate matter PM10 as well PM2.5.

TABLE I
MAJOR SOURCES OF AIR POLLUTION

No.	Pollution parameter	Sources
1.	Carbon dioxide (CO2)	The burning of fossil fuels (coal, oil, etc.) in furnaces of thermal power plants, industries, etc.
2.	Carbon monoxide (CO)	Automobile, industrial furnaces, open fires, forest fires, and combustion of domestic fuel.
3.	Sulfur dioxide (SO2)	The burning of fossil fuels, industries, and automobiles.
4.	Nitrogen oxides (NOx)	Industries manufacturing HNO3 and other chemicals and automobile exhaust.
5.	Ozone (O3)	Automobile, specific industrial operations.

6.	Hydrocarbons (HC)	Motor vehicles, industrial operations.
7.	Particulate matter PM10 and PM2.5	Fuel combustion and industrial operations, nonindustrial fugitive emissions like road dust, agricultural, construction, and transportation.

Air pollutants prediction models are classified into stochastic and deterministic models; the deterministic models predict and model air pollutants' chemical and physical transport procedures with respect to the influence of atmospheric factors like temperatures, wind speed, and relative humidity when predicting and modeling air pollutants. They provide air pollutant predictions on either a long-term or short-term basis, and their performance depends on a detailed mechanism of pollutant formation.

Several studies have strived to develop AQS, which can mimic evolution processes and environmental influences. However, the challenges of developing a precise air pollutant level prediction model still exist due to the complexity of the processes that control the formation and movement of air pollutants. The performance of the predictive models is influenced by their related parameters, in which the higher number of parameters causes difficulty in processing big and dynamic data resources.

The statistical prediction model learns from historical data to predict future circumstances. Several statistical models are used to predict air pollution levels in time and space and are reliant on certain parameters [5]. Although it is not important to model the physical relation between pollutants and ambient levels, nevertheless, time series analysis is necessary. Some deployed statistical methods include time-series analysis, Neural networks, and Bayesian Networks [21].

Various factors, such as historical data and weather conditions, influence the distribution of pollutants. Criteria pollutants are a group of major pollutants such as nitrogen oxides, carbon monoxide, photochemical oxidants, hydrocarbons, sulfur dioxide, particulates, and lead, which contribute significantly to air pollution. They are considered the highest threat to air quality as they hugely affect humans and the environment. Since 1970, the Clean Air Act in the USA has set permissible limits for air pollutant levels in the air, especially in the cities. They also monitor the unconventional air pollutants, which are less produced (although still toxic and harmful) compared to the established air pollutants.

B. Nested Monte Carlo Simulation Model

Monte Carlo simulations (MCS) and Nested Monte Carlo Simulation (NMCS) are mainly used in three problem classes: optimization, numerical integration, and generating draws from a probability distribution. MCS is one of the most common methods that have been used to reconcile uncertainties associated with risk-related problems. In addition, it is also well known as a means of quantifying variability, uncertainty, and unevenness in Dynamic Risk Assessments (DRA). MCS provides a quantitative way to estimate the probability distributions for exposure to the risks and supply more information for decision-makers related to risk safeguarding. The widespread use of this method efficiently promises a considerable improvement in the scientific rigor of risk assessments [22].

Many researchers used NMCS in different domains of risk. Dickmann and Schweizer [23] proposed an approach to estimate widely employed portfolio risk metrics value-at-risk (VaR) and conditional value-at-risk (cVaR) employing NMCS. Their work combined theoretical with software and hardware implementation to investigate performance on heterogeneous computing systems across different computing platforms, namely central processing unit (CPU), Many Integrated Core (MIC) architecture XeonPhi, graphics processing unit (GPU), and a field-programmable gate array (FPGA). Giles and Haji-Ali [24] used the NMCS model in the probability of a large loss from a financial portfolio. NMCS also has some nested expectations with the idea of adaptively selecting the number of samples to approximate the Inner expectation.

In this NMCS model, an Outer simulation is used to generate risk scenarios, and an Inner simulation is used to estimate future risk values in each scenario. Other models in the literature include different Artificial Intelligence techniques for approximation and decision-making [25]–[27]. The MCS consists of three main steps. The first step is to determine a suitable probability model for the characteristic of simulation footing. The summary is to find the appropriate solution and distribution function. The second step is to produce a random vector of implementation or a sample that establishes the sampling method of the random distribution. The third and final step is to establish various estimators that determine a random variable as a solution to the object problem after simulating an unbiased estimator, as shown in Fig. 1.

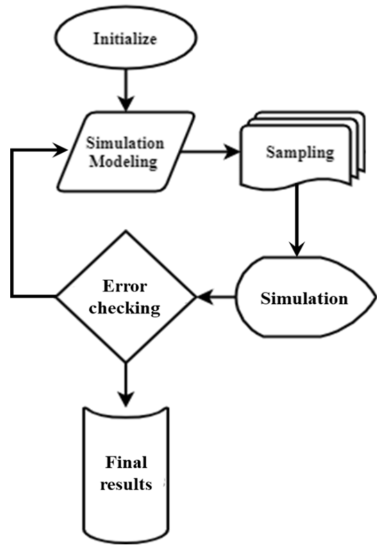

Fig. 1 The MCS Procedure

Many statistical problems include overlapping expectations; therefore, they do not allow the traditional MCS estimate. Such problems entail adapting to the capabilities so that the terms in the external evaluator include a separate, interrelated, and estimated account.

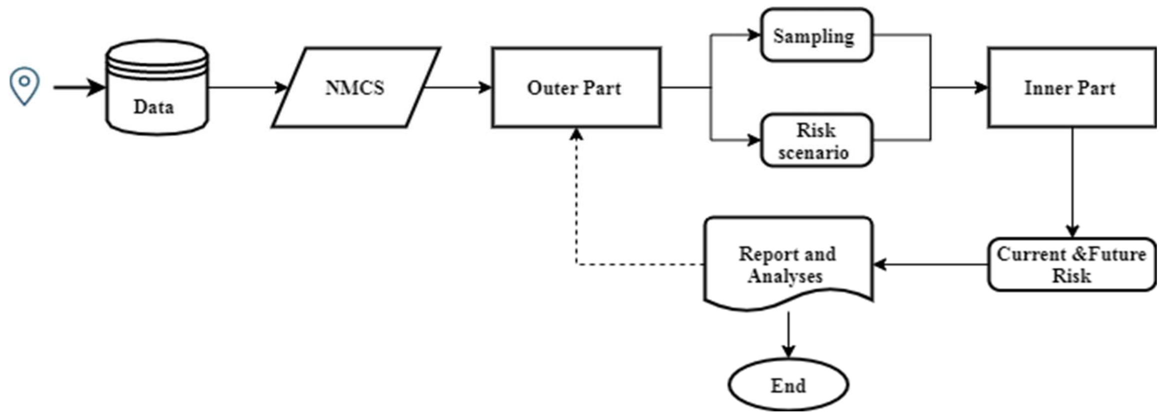

Fig. 2 The NMCS Procedure

Nested expectations also occur in various problems, such as risk management. Tackling such problems requires some form of nested estimation scheme like NMCS. NMCS is interested in estimating quantities of the form as shown in Eq. (1) and Eq. (2).

$$E_Z = [F(E(Z))] \tag{1}$$

where Z represents different risk scenarios, and E[W|Z] represents exposure, conditional on the scenario.

$$\gamma = \frac{1}{N}\sum_{n=1}^{N} \quad F\left[\frac{1}{M}\sum_{m=1}^{M} \quad W^{(n,m)}\right] \tag{2}$$

where N is the Outer samples Z^n, Minner samples $W^{m,n}$, conditional on Z^n.

C. Nested Monte Carlo Simulation for AQ Risk Assessment

Owing to the capability of the statistical models to produce accurate predictions [18], the NMCS is proposed in this paper to predict and assess future air pollution risks based on different air pollution parameters. The NMCS is not widely used in many applications, but nested expectations occur in several problems, such as portfolio risk management, where it is performed accurately. Based on the above superiority, NMCS is believed to predict the risk of air pollution. To our best knowledge, no report exists on the use of NMCS for air pollution risk prediction based on different parameters measurement.

Fig. 2 shows the flow diagram of the NMCS model. Based on this figure, the NMCS consists of two main parts. The first part is the interactive outer part with the data source, and it is employed to extract a suitable sampling from a huge dataset. In addition, the Outer part is responsible for generating scenarios. On the other hand, the second part is the Inner which is responsible for assessing the current risk from each scenario and estimating the future risk.

Fig. 3 shows the proposed AQ-risk model based on NMCS in air pollution risk assessment. The NMCS first calculates the average and standard deviation between each parameter and prepares the sampling of data using Eq. (3) – Eq. (5), where M is the mean of the dataset, N is the number of data points in the population, and σ represents the probability of a normal distribution.

$$STD = \sqrt{\frac{\sum \quad CO2 - M|NOx - M}{N}} \tag{3}$$

$$f(CO_2|NO_x, \mu, o) = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{(CO2|NOx-\mu)^2}{2\sigma^2}} \tag{4}$$

$$\mu = \frac{\sum \quad CO2 - M|NOx - M}{N} \tag{5}$$

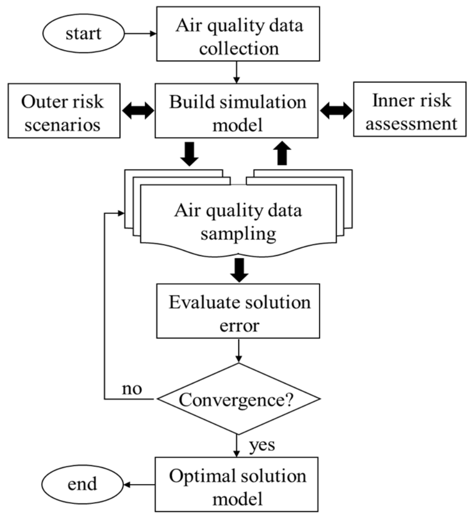

Fig. 3 The AQ-risk model

Fig. 3 explains that the Outer and Inner procedures begin from the data recorder, followed by the Outer procedure's processing. Next, the Inner part proceeds to predict risks from different scenarios. If there is an error in any steps, the process returns to the first step to make a new sampling and pre-processing.

III. Result and Discussion

The dataset used in this work has been recorded from an Italian city over a period of one year. The samples include two air pollution parameters: carbon dioxide (CO2) and Nitrogen oxides (NOx). The measurements are obtained every hour from sensors. The dataset has several parameters used to assess the scale of air pollution. In this paper, we test a new method to predict the dynamic time data of AQI. Fig.

4 shows the projection of 24 hours data based on the two parameters of AQI.

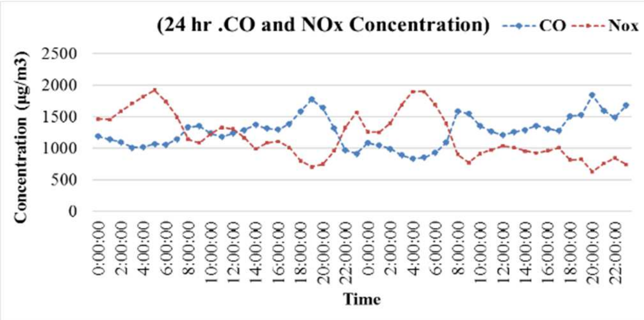

Fig. 4 Variation of CO and NOx concentration (mg/m3) for 24 hours

Subsequently, the performances of the proposed model are evaluated based on statistical indices of coefficient of determination (R2) and mean square error (MSE). The AQ-risk model predicts the risk based on NOx parameters and CO concentrations in the air. The results show that NMCS analyzed and predicted the NOx, and CO risk with a minor error. Table II shows the prediction results of the proposed NMCS model for CO, while Table III shows NOx's results.

TABLE II
AQ-RISK MODEL RESULTS OF MSE FOR CO

Time	CO	CO Prediction	MSE (CO)
0:00:00	1185	1183	9.2195
1:00:00	1136	1137	11.672
2:00:00	1094	1090	13.928
3:00:00	1010	1008	11.390
4:00:00	1011	1010	10.535
5:00:00	1066	1060	11.224
6:00:00	1052	1050	12.318
7:00:00	1144	1140	6.6332
8:00:00	1333	1330	12.379
9:00:00	1351	1350	12.288
10:00:00	1233	1230	6.5764
11:00:00	1179	1170	8.8745
12:00:00	1236	1234	8.7177
13:00:00	1286	1280	10.271
14:00:00	1371	1370	12.688
15:00:00	1310	1306	7.0710
16:00:00	1292	1290	10.087
17:00:00	1383	1380	13.152
18:00:00	1581	1581	13.444
19:00:00	1776	1779	13.619
20:00:00	1640	1645	7.7459
21:00:00	1313	1315	7.9214
22:00:00	965	970	9.1923
23:00:00	913	915	6.5383

TABLE III
AQ-RISK MODEL RESULTS OF MSE FOR NOX

Time	NOx	NOx Prediction	MSE (NOx)
0:00:00	1462	1465	7.858
1:00:00	1453	1456	7.858
2:00:00	1579	1550	11.35
3:00:00	1705	1690	9.746
4:00:00	1818	1796	10.79
5:00:00	1918	1897	4.582
6:00:00	1738	1700	10.68
7:00:00	1490	1520	11.82
8:00:00	1136	1200	11.66
9:00:00	1079	1100	10.90
10:00:00	1218	1200	6.164
11:00:00	1328	1290	11.29
12:00:00	1301	1300	11.88
13:00:00	1162	1180	9.069
14:00:00	983	1000	9.656
15:00:00	1082	1070	9.578
16:00:00	1103	1100	10.12
17:00:00	1008	1006	4.24
18:00:00	799	800	12.18
19:00:00	702	700	9.069
20:00:00	743	740	7.262
21:00:00	957	940	12.53
22:00:00	1325	1320	11.19
23:00:00	1565	1560	12.82

Based on the MSE results for the proposed DRA model in Table II and Table III, the correlations between the measured and predicted values in the testing stage through the AQ-risk model have been drawn in Fig. 5 and Fig. 6. The values of R2 are obtained by the NMCS model in the testing stage for both parameters (0.9462 and 0.9073), denoting that the NMCS model performs in DRA.

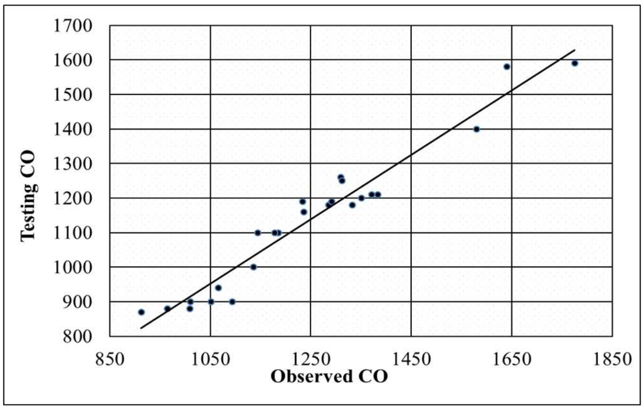

Fig. 5 R2 for CO

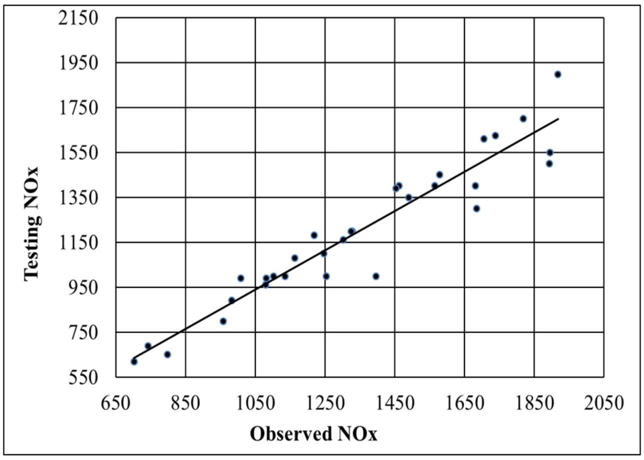

Fig. 6 R2 for NOx

Fig. 7 compares the real data of NOx parameter and NOx prediction by the proposed model. A prediction depends on historical data on pollution, and the model has training on the past pollution data, then predicts the air pollution risk.

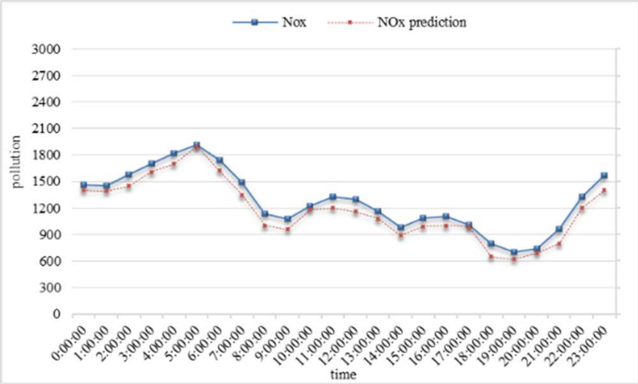

Fig. 7 The NOx prediction results

Next, Fig. 8 compares real data of CO pollution with CO prediction by the proposed model. The model has training on the past pollution data, then predicts the future air pollution risk. The DRA and risk analysis of air pollution are essential matters in the zone of AQ systems. Note that we compared the forecasting data with real data and computed the MSE and R2 to illustrate the proposed method's ability. The results showed that the NMCS model provides dynamic air pollution risk assessment and prediction as required and with adequate accuracy.

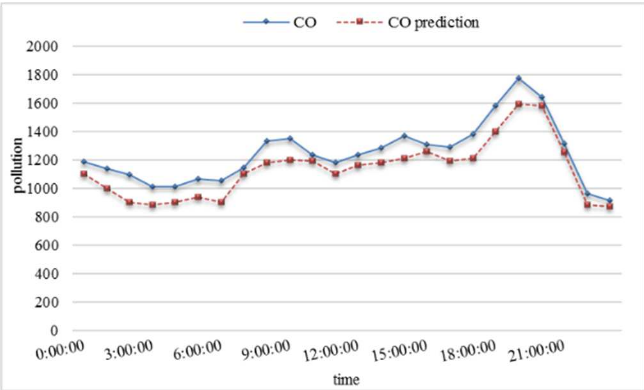

Fig. 8 The CO prediction results

R2 measures the prediction ability in the testing stage for both parameters, resulting in 0.9462 and 0.9073. MAE measures the prediction ability in the testing stage for both parameters, which therefore average results in 9.7 and 10.3, denoting that the AQ-risk model provides highly accurate predictions.

IV. Conclusions

Dynamic Risk Assessment (DRA) and risk analysis of air pollution are essential matters in the zone of Air Quality (AQ) systems, and it can provide highly beneficial information to related parties of AQS. Many existing works solve these problems individually by different qualitative and quantitative methods. Accordingly, a Nested Monte Carlo simulation (NMCS) has been used to propose an AQ-risk model as an efficient and adaptive method for overcoming air pollution measures' complex and dynamic risk assessment processes. The proposed AQ-risk model is evaluated by experimenting with real data collected from a significantly polluted area in an Italian city from 2004 to 2005.

The results showed that the model analyzed and predicted the NOx, and CO risk with high accuracy. R2 measures the prediction ability in the testing stage for both parameters, which accordingly results in 0.9462 and 0.9073, denoting that the AQ-risk model provides highly accurate prediction results. Future work considers improving the AQ-risk model by including multilevel Monte Carlo Simulation (MLMCS) to decrease the simulation cost and considering more testing parameters, including O3, SO2, and PM10, which is regarded as the most influential parameters on health in general, based on previous studies.

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