Modelling and Simulation in Environmental Data Analysis

CLAUDIO GUARNACCIA, JOSEPH QUARTIERI

*Department of Industrial Engineering
University of Salerno
Via Giovanni Paolo II, I-84084 Fisciano (SA)
ITALY
cguarnaccia@unisa.it , quartieri@unisa.it

Abstract: - Environmental data analysis is one of the most important issue for assessing the impact of polluting agents in areas in which human activities have altered the standard natural development and evolution of air, water and ground. In particular, physical and chemical polluting agents need to be monitored and controlled, in order to reduce the dangers to human health due both to long term and to short term, but high level, exposures. In this paper, the attention will be mainly focused on the assessment and prediction of acoustical noise, and partially to air pollution data analysis. A review of some of the literature methods will be presented and two recent approaches will be sketched in the central section. The merging and intersection of more than one pollutant analysis will be finally discussed. In the author's opinion, these techniques should be encouraged and represent the future perspectives of environmental data analysis. In fact, the possibility of performing a complex field measurement campaign, able to record more than one pollutant data, can help in building reliable models, based on advanced mathematical and physical methods.

Key-Words: - Environment, Data Analysis, Acoustic Noise, Air Pollution, Modelling and Simulation.

1 Introduction

The study of physical and chemical polluting agents, such as acoustic noise, electromagnetic field, air pollution, etc., is a crucial point in environmental impact analysis nowadays. Both in urban and rural areas, several human activities affect the natural development of air, water and terrain. Several literature papers are focused on the analysis of environmental impact and some of them define indexes able to monitor a single pollutant. In [1], for instance, the authors proposed a complex index, able to consider the contribution of several pollutants in a single number, with appropriate weights.

The greatest risk perception is commonly related to air pollution, probably because it affects almost all the human senses. In [2], for instance, the effect produced by exposure to ozone concentration are reported, in order to motivate the need for an advanced modelling of this pollutant slope over time.

Besides air pollution, acoustical noise is also perceived as annoying, especially in urban areas, where noise levels are very high, and in rural areas, where, due to the very low background noise level, any noise source is felt as a high disturbance reason. In any case, the effect of the exposure to high noise levels are reported, for instance, in [3], regarding road traffic noise, and in [4], more in general, both from the auditory and non auditory point of view.

Because of these effects on human health, research on pollutants modelling and simulation has been largely pursued, with different approaches, producing many results, as reported in Section II. The aim of this paper is, on one side, to briefly report some of the literature adopted models and, on the other side, to present more recent procedures, that can be applied to different pollutants. The author will focus in particular on acoustical noise and air pollution: some of the results obtained in the last years will be presented and two recent models will be recalled. These are the Time Series Analysis model and the Poisson processes analysis. Then, future development possibilities and horizons will be briefly described, especially in terms of integrated models, that are models able to deal with more than one pollutant.

2 Literature review

Acoustical noise and air pollution have been deeply investigated from several points of view. Each scientist or engineering approached the problem from a personal experience and education starting point, producing a very large literature basis. For the sake of brevity, the author will not report all the possible approaches but will focus on some of them.

The most important problem in modelling and simulating acoustical phenomena is the intrinsic random feature of sound produced by almost any source present in urban areas. Since the most annoying sources are related to transportation systems and infrastructures, one cannot predict how many cars/sources will run on a certain road, and, when one can do that, for instance in the case of scheduled trains running on railways, it is very difficult to predict which will be the speed, the air density and temperature, the propagation conditions, etc.. Resuming, even if some parameters can be achieved, the noise production and propagation phenomenon is so complex that it is quite impossible to have an analytic and precise description. For this reason, statistical models have been firstly developed, for instance in the case of road traffic noise [5].

Even if at the beginning of Traffic Noise Models (TNMs) implementation, they had a quite good success, the growing of road infrastructures, of cars' number, the changes in driving habits, the development of new technologies, etc., lead to an increase of precision need. For instance, the statistical models didn't consider the speed of cars (except in some cases but only with additive correction) but only the number and the percentage of heavy vehicles. This means that if one has a certain number of cars, the statistical models do not distinguish if these cars are running on a highway, are braking because approaching a road intersection or are completely stopped because jammed during rush hours. Of course the noise produced in these three cases is much different. In [6] the comparison of some of these statistical models with experimental data is reported, with evident disagreements (Fig. 2).

A typical, three parameters formula for a statistical TNM is:

$$L_{eq} = A \log Q\left[1 + \frac{P}{100}(n-1)\right] + b\log(d) + C \quad (1)$$

where L_{eq} is the hourly acoustic equivalent level, Q is traffic volume (flow) in vehicles per hour, P is the percentage of heavy vehicles, n is the acoustical equivalent and d is the distance from observation point to center of the traffic lane. The A, b and C coefficients may be derived, for a fixed investigated area, by linear regression methods on many L_{eq} data taken at different traffic flows (Q, P) and distances (d). The acoustical equivalent, n, (defined as the number of light vehicle that generate the same acoustic energy of a heavy one) can be estimated both by regression method or by single vehicle emission measurements.

Improvements to formula (1) have been proposed by the author, for instance in [7]. The introduction of the dependence of source power level from speed, both for light and heavy vehicles, is the key point of this paper:

$$\begin{aligned} L_{w,L}(v) &= \alpha_L + \beta_L \, Log(v) \\ L_{w,P}(v) &= \alpha_P + \beta_P \, v \end{aligned} \quad (2)$$

α and β are parameters of experimental data fit, reported in the study of Steven, performed for the German Environmental Agency [8].

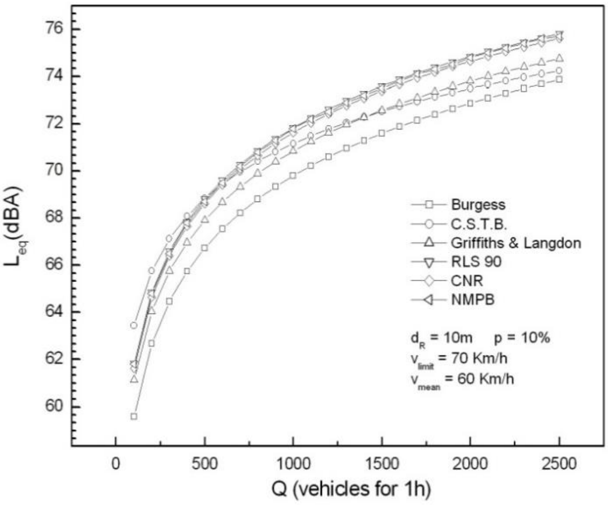

Fig. 1: Comparison between different Traffic Noise Models, with fixed parameters (see legenda) [5].

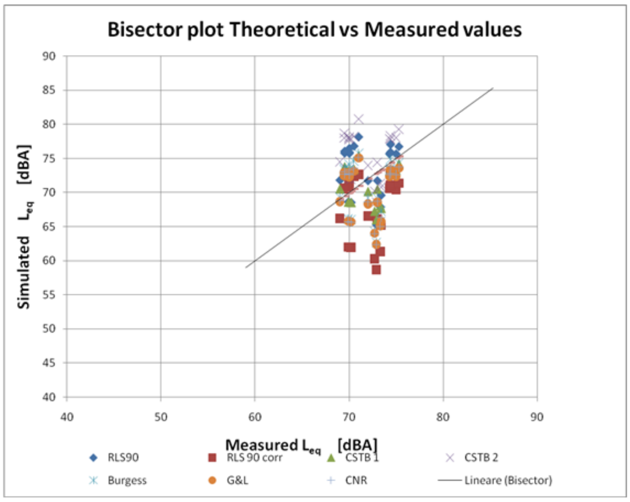

Fig. 2: Simulated versus Measured Leq, for both sites and all the measurements, [6].

The final expression for the equivalent level is:

$$L_{eq}^{(1h)} = 10Log[N_L + n(v)N_P] + \alpha_L + \beta_L Log(v) + \\ -20Log(d) - 47{,}563 \qquad (3)$$

that can be related to formula (1) by the position:

$$Q_{eq}^{1h} = N_L + n(v)N_P\,,$$
$$A = 10,\quad b = -20,$$
$$C = \alpha_L + \beta_L Log(v) - 47{,}5638.$$

This time the traffic flow Q (in particular the acoustic equivalent) and the C parameter depend on speed.

In [9-22], several different approaches are reported regarding road traffic noise (resumed in [23]), considering predictive software, field measurements, intersections, non standard conditions, etc., and other noise sources, such as railways, wind turbines, industrial settlements, etc..

These studies, together with the growth of available data and computing resources, represent the starting point of an increasing interest in dynamical modelling. Dynamical models, many of them developed in traffic theory framework, are starting to be implemented in road traffic noise control [24-27]. Even if there is a bigger effort in setting up the model, in the parameters identification and in the computational part, the preliminary results are very encouraging.

Regarding air pollution, the need for modelling and control is strictly related to the growing of industrial activities and transportation duties. In [28], for instance, a detailed analysis on of benzene, toluene, ethylbenzene, and xylenes (BTEX) field measurements taken in Mexico, is performed. The Principal Component Analysis method is adopted and very interesting results are reported, in terms of correlation between different pollutants and between certain human activities and highest concentrations.

More analysis can be found in [29-34] where several approaches are adopted, such as neural network, multivariate analysis, principal component analysis, etc..

3 Recent models

Besides the models presented in section II, different procedures have been recently developed. In this section, two approaches will be presented because they represent the connection point between different pollutants analysis. Both of them, in fact, have been adopted on acoustical noise and air pollution separately.

3.1 Time Series Analysis

The first procedure is the Time Series Analysis (TSA). These models, largely adopted in several disciplines, have been applied to road traffic noise data in [35] and [36] and to carbon monoxide concentration in [37].

The main aims of these kind of models are basically the recognition of the phenomenon under study by means of data trend and periodicities reconstruction, and the prediction of future values of the time series. Thus, a general procedure may be resumed as follows:

- Possible seasonal effect detection in the data set
- Lag (periodicity) evaluation
- Smoothing (removal of periodicity) of the calibration data time series
- Trend and seasonality evaluation
- Error evaluation (difference between observed and forecasted values in the calibration dataset)
- Final model drawing and validation

The description of the steps listed above can be found in details in [35] and references therein, where different approaches, in particular additive and multiplicative, are presented and briefly discussed. The choice the author generally adopts is a mixed approach, that is multiplicative between trend and seasonality, and additive for the error component:

$$F_t = T_t \bar{S}_i + m_e \qquad (4)$$

where F_t is the model prediction, T_t is the trend, $\bar{S}_i$ is the seasonal coefficient, m_e is the mean of the error e_t, defined as actual value (A_t) minus forecast (F_t):

$$e_t = A_t - F_t \qquad (5)$$

Let us underline that TSA models are mostly adopted when the data sets follow recurring seasonal patterns.

A common plot that can be reported is the superposition of observed values and model forecasts. In Figure 3, for instance, the two models presented in [36] are plotted versus the night noise levels used in the calibration phase. The two models are characterized respectively by a single and a double seasonality implementation. In this case, in fact, the data exploit a short term periodicity (daily) and a long term one (about 4 months).

It is interesting to notice that the double seasonality model is much better than the single one, because of the ability to reproduce the low frequency (long term) periodicity.

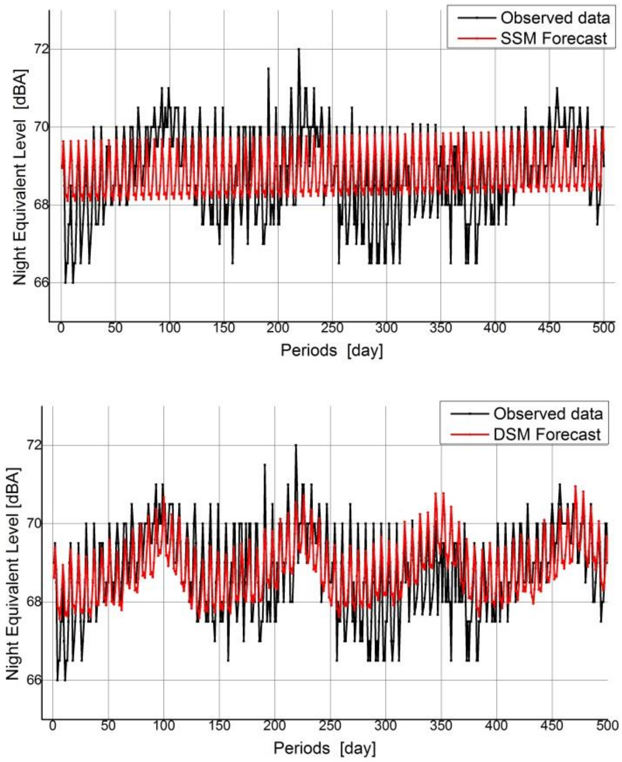

Fig. 3: Single (top) and Double (bottom) seasonality Time Series model plotted versus time, together with observed nightly noise level data [36].

Evaluating the error, i.e. the difference between observed data and model forecast in each time period *t*, a quantitative analysis of the model performance can be done. In particular, time series models have a very good performance when data have an intrinsic periodic feature, such as in [35]. Looking at the histogram of the errors (Figure 4) and at the error statistics (Table 1), it is easy to notice a very narrow error distribution and the null error mean value, with very low standard deviation. In [35], the error was always below 1 dBA. This is an outstanding result, almost never achieved by common noise models. In [36], Figure 5 and Table 2, the performance are a little worse than the previous case, but still very good in terms of prediction ability of the model.

Let us remind that these histograms and statistics are evaluated on the calibration datasets. The real test of the model is done during the validation phase, that is evaluating the performance of the model compared with data not used in the calibration. This generally furnishes the real ability of the model to predict the future behaviour of the data.

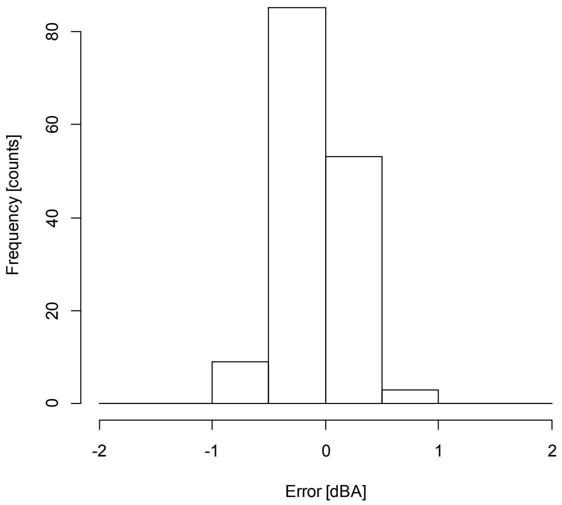

Fig. 4: Frequency histogram of the errors calculated on the model calibration, performed on the first 150 daily noise level data [35].

Table 1: Summary of statistics of the error distribution evaluated on the calibration daily noise levels [35].

Mean [dBA]	Std.dev [dBA]	Median [dBA]	Min [dBA]	Max [dBA]	skew	kurt
0.00	0.30	-0.09	-0.81	0.72	-0.03	-0.1

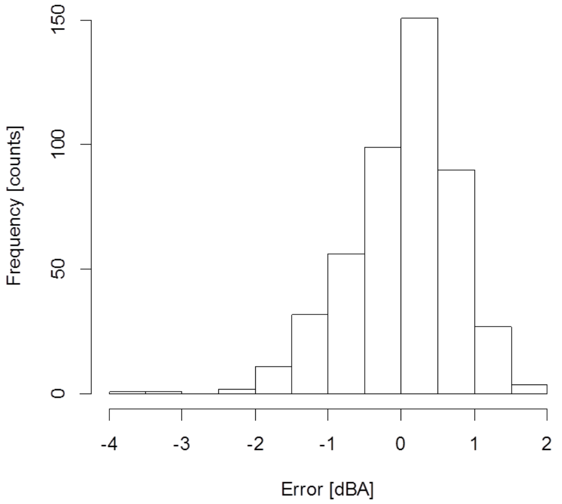

Fig. 5: Frequency histogram of the errors calculated on the model calibration dataset, performed on the 474 night noise levels dataset [36].

Table 2: Double seasonality model summary statistics of the error distribution evaluated on the calibration night noise levels dataset [36].

Mean [dBA]	Std.dev [dBA]	Median [dBA]	Min [dBA]	Max [dBA]	skew	kurt
0.02	0.74	0.15	-3.93	1.99	-0.79	1.72

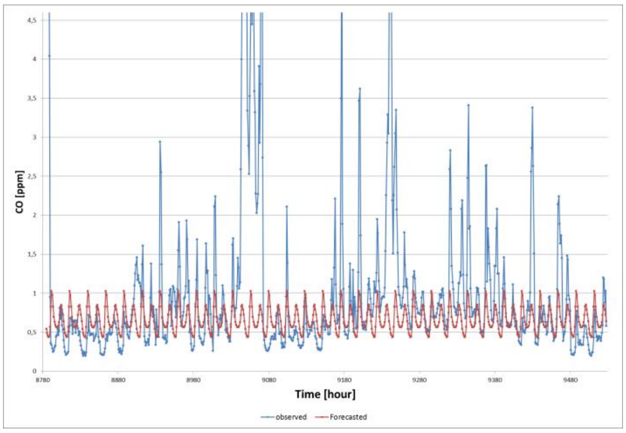

Fig. 6: Observed and predicted CO concentrations, during January 2013 (i.e. first validation dataset) [37].

Table 3: Summary of statistics of the error distribution, evaluated on the first validation dataset of CO concentrations (January 2013) [37].

Mean [ppm]	Std.dev [ppm]	Median [ppm]	Min [ppm]	Max [ppm]
0.34	1.09	0.03	-0.75	8.00

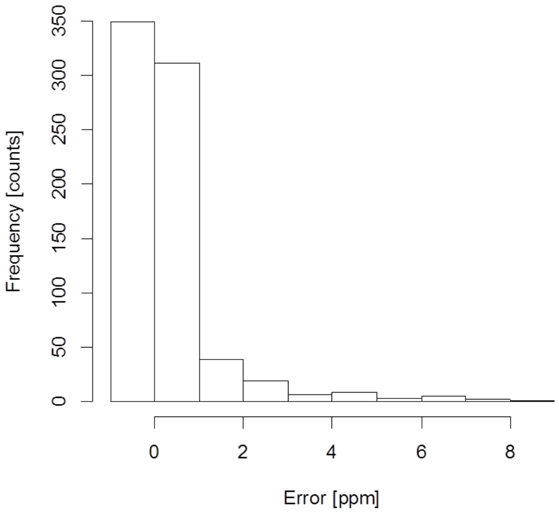

Fig. 7: Frequency histogram of the errors calculated on the first validation dataset of CO concentrations, performed on the 744 January data [37].

For instance, in [37], in the carbon monoxide application, even if the general results in the calibration phase are not very encouraging, because of strong local variations, there are some months in which the model, calibrated on the entire 2012 year, gives good results. This is the case of the validation done on January 2013, with respect to the validation done on May 2013. In the former case, January, probably because of climate conditions and variations, the CO concentrations strongly oscillated, with respect to the general trend and periodicity, resulting in an evident underestimation of the model, confirmed by plot of the forecasts (Figure 6), error statistics (Table 3) and histogram (Figure 7).

In May 2013, instead, the model better approximates the observed data, probably because in this period of the year, the phenomena that caused the local oscillations are negligible. Results of the model forecasts evidently improve in this case, as reported in Figure 8, Table 4 and Figure 9.

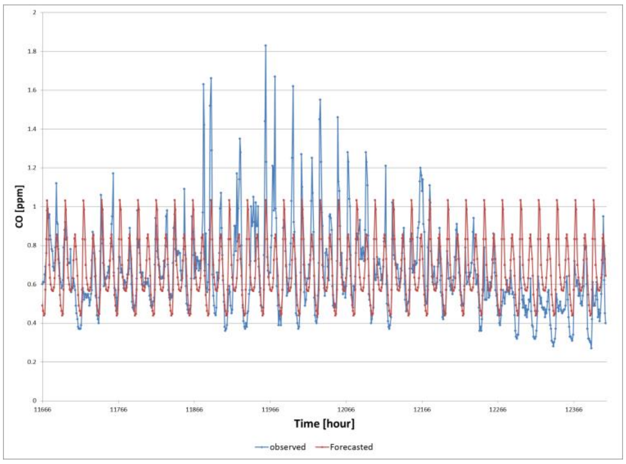

Fig. 8: Observed and predicted CO concentrations, during May 2013 (i.e. second validation dataset) [37].

Table 4: Summary of statistics of the error distribution, evaluated on the second validation dataset of CO concentrations (May 2013) [37].

Mean [ppm]	Std.dev [ppm]	Median [ppm]	Min [ppm]	Max [ppm]
-0.01	0.20	-0.02	-0.58	0.84

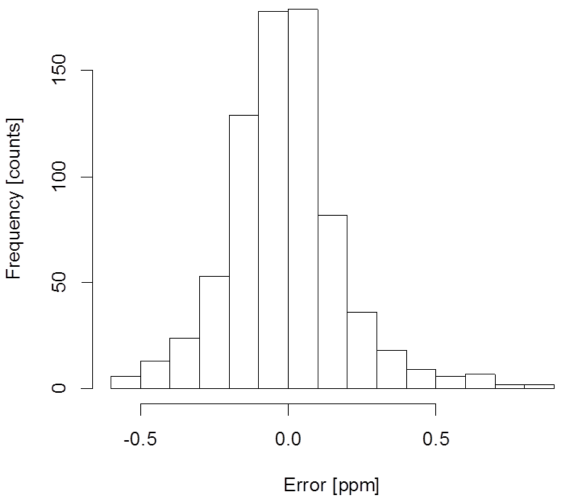

Fig. 9: Frequency histogram of the errors calculated on the second validation dataset of CO concentrations, performed on the 744 May data [37].

3.2 Time Series Analysis

The second method that will be presented in this section regards the application of homogeneous or non-homogeneous Poisson processes.

In [38] and [39], Rodrigues et al. developed and applied the model to air pollution, in particular to ozone concentration, while in [40] and [41] the same procedure is applied to environmental noise data, produced by road traffic noise [40] and measured in proximity of an airport [41].

The Poisson process, counting the number of times that a pollutant level surpasses a given threshold, is used to estimate the probability that a population is exposed to high levels of the selected pollutant, a certain number of times in a given time interval. The rate function of the Poisson process can be assumed to be of different functional forms. For instance, in [40] and [41] a Weibull type (power law) is chosen.

In general, the first step is the calibration of the model, i.e. the evaluation of model parameters, that are the coefficients of the rate function. This evaluation can be performed in different ways, such as maximization of the likelihood function or MonteCarlo Markov Chain (MCMC) methods. In the latter methods, the prior distribution for the parameters can be non-informative or informative, depending on the knowledge of the phenomenon under study. The maximization of the likelihood function can be used in order to have better starting points for the Markov Chains of the MCMC method.

Once the rate function's parameters are obtained, the number of exceedances of the given threshold can be calculated and, consequently, the probability of exposure to the considered pollutant can be estimated. More details on this method can be found in [29, 30] and [40, 41], where complete analyses of the model results are reported, together with comparison with field measurements.

4 Integrated analysis of pollutants

Besides these analyses of single pollutants, the real new horizon of environmental impact assessment is the integration of different pollutants modelling and prediction.

An application of this idea can be found in [42], where the evaluation of the impact of urban development trends in mobility patterns of a Portuguese city and air quality consequences is presented, adopting a sequential modelling process, that includes land use and transportation, road traffic air pollutants emissions and air quality models. This integrated methodology has been applied to a medium sized Portuguese city and showed a good predicting performances for PM10 concentrations, while the CO concentrations are underestimated. With this method, different mobility patterns and vehicle technology characteristics can be simulated. The authors of [42], for instance, simulated a "car pooling" and the "Euro 6" scenarios, that correspond respectively to a reduction in total running vehicles number and to a reduction in the vehicle average pollutant emissions.

In [43], a prototype system for modelling noise and air pollution is developed for the Macao Peninsula. A road traffic noise model, an operational air pollution model, digital maps, an urban landscape model and a Geographic Information System (GIS) are integrated in the same model framework. This preliminary model investigates how the existing urban scenario influence vehicle transport and street environment. The interesting result is that the historical areas, characterized by narrower roads, complex road networks and a higher density of intersections, lead to lower traffic volumes and thus to lower noise pollution, but the greater street canyon effects lead to higher carbon monoxide (CO) concentrations. This means that a government policy aimed at the reduction of one of the pollutant that affects a certain area, could lead to a worsening with respect to other agents. This is probably one of the most important reason why integrated predictive models should be strongly encouraged and largely developed.

5 Conclusions

In this paper, a review of some techniques of physical and chemical polluting agents modelling and simulation is presented. In particular, mainly regarding acoustical noise, the authors briefly reviewed some of the models developed in the last years, in order to present more recent techniques, based on Time Series Analysis and Poisson processes. With respect to some of the literature approaches, these models can be easily used for more pollutants, since they are mainly based on dataset analysis. The success of the model depends on the features of the dataset and on the calibration process, during which the parameters are tuned and the forecasting model is built.

Special attention is given to integrated models, that join the analysis of more than one pollutant. Even if some approaches are present in literature, more has still to be done and a strong research activity has to be pursued in this direction. Acting on one pollutant, in fact, can lead to worsening of other agents effects. On the contrary, a complex field measurement campaign, able to record different pollutants data, can help in building reliable models, based on advanced mathematical and physical methods.

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