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Back-forward Model Analysis for Spatial Localization of Pollutant Sources

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Abstract

The present paper deals with the implementation, calibration and validation of a back-forward mathematical model for pollutant source spatial localization and characterization.

In particular, a Gaussian model, used as a sort of reverse engineering tool, was implemented to analyse plume dispersion. In this paper particulate matter was the pollutant agent.

In order to calibrate model parameters and verify its accuracy, an extensive experimental campaign of plume dispersion was carried out in a controlled environment. In details, a wind tunnel was used to generate wind effect on plume and aerosol particles spatial concentrations were measured by means of a sensor network.

On the basis of the obtained results it is possible to state that the implemented model is able to identify position of the sources and emission rate with low errors.

Keywords: Pollutants dispersion, Gaussian model, genetic algorithm, wind tunnel chamber.

Nomenclature

Variable	UOM	Description
x	[cm]	Downwind direction
y	[cm]	Crosswind direction
z	[cm]	Vertical direction
Q	[µg/s]	Source mass flow rate
U	[m/s]	Wind speed at the source
L	[cm]	Source height
σ_y	[-]	Horizontal dispersion coefficient
σ_z	[-]	Vertical dispersion coefficient
C_{PM10}	[µg/m^3]	Concentration of PM_{10}

INTRODUCTION

The dispersion of air pollution both in urban areas and open spaces is becoming of great concern in the scientific community. In last decades the normal levels of air pollution have increased especially in urban areas [1-2] and many countries have started to pay attention to monitoring systems for air pollution. The rapid economic and industrial growth has led to an expansion of urban areas, and above all, a tremendous increase of energy consumption and emissions of air pollutants [3-4]. Air pollution has become one of the world's worst problems of toxic pollution particularly for its consequences on sociomedical systems [5]. In accordance to it some short-term and long-term strategies have been development in order to reduce and control pollutant emissions in urban areas [6]. Perhaps, one of the most important is the European Directive 2008/50/CE whose aim is to adopt a standardized method to control, monitor and study air pollutants in urban areas. In such scenario many air pollutants have been regulated and different limits imposed to European countries. The main important air pollutants are: Carbon Monoxide (CO), Nitrogen oxides (NO_x), Sulphur dioxide (SO_2), Ozone (O_3), Benzene (C_6H_6), particular matters ($PM_{2.5}$, PM_{10}, TSP). The dispersion phenomenon of these pollutants depends on their chemical compositions. While pollutants such as CO, NO_x, SO_2, O_3, C_6H_6 are basically gases, the particular matters pollutants are usually made up of solid particles or liquid droplets [7]. The diffusion of air pollutants depends also on their sources. Typically, there are four main types of air pollution sources: mobile sources, any types of transports, stationary sources, such as power plants or industrial facilities, area sources, such as agricultural areas, cities or wood burning fireplaces and natural sources such as wind-blown dust, wildfires or volcanoes. Generally, the most common sources are industrial sources [8], hazard chemical released due to accidents or natural events [9], and vehicular urban traffic [10-11]. In such scenario, many air quality models to predict, study and evaluate the pollution dispersion have been studied and implemented [12-14]. Air quality models are able to predict the pollutant gases or aerosol trajectories in atmosphere. The evaluation and calibration of dispersion models is of a crucial importance, because their results often influence decisions that have large public-health and economic consequences. Obviously there are different types of models and their performances depend on many variables. The classification of these models may refer about the source type (point source, line source, area source), the adopted scale (large or small scale), the input type (deterministic models and stochastic models), the dynamic conditions (steady or unsteady state), the pollutant sources (gases or particles). Many reviews [15, 16] have already classified and studied these models, trying to focus about performance in respect with the variables stated before. Among all these possible models the most used are probably Lagrangian [17] and Gaussian models [18]. Both of them are able to estimate the downwind ambient concentration of air pollutants from different sources types. Lagrangian models work well both for homogeneous and stationary conditions over the flat terrain [19] and unstable media condition for the complex terrain [20] but they usually suffer for computational calculation and they cannot be used for real time applications [21]. Gaussian models are widely used in atmospheric dispersion modelling, usually in regulatory purposes because of their easy implementation and their near real-time responds. They generally are used in large scale applications [22] and although they have been shown to over-predict concentrations in low wind conditions [23], since the plume models are calculated with steady state approximations they do not take into account the time required for the pollutant to move from the source to the receptor.

While these models previously treated basically refer to the direct processes of propagation of pollutants, the problem of the identification of unknown sources could be treated with inverse models. Usually, the concentration measurements are the starting points thanks to which with back forward analysis it is possible to recognize the source of pollution. In order to resolve this inverse problem, many methods have been developed. Among them, optimization methods have been widely used to identify sources [24-26]. These methods suffer the uncertainty of estimation results. Another approach is the stochastic approximation method with probability density functions [27, 28] which could find reasonable solutions in terms of tolerance by comparing the simulated data with measurements. Usually, the stochastic approximation methods are based on different theories: Bayesian inferences theory [29, 30], Markov Chain Monte Carlo (MCMC) methods [31], kalman filter methods [32]. However, the above stochastic approximation methods are very computationally expensive and cannot be used in real/near-real time applications. Additionally, a lot of prior information such as measurement errors, parameter bounds and expected inputs should be determined previously in Bayesian estimation and MRE methods, but they are hard to be known in the real condition. Another class of methods used for identification sources is based on Genetic Algorithms. GAs are successfully applied to a number of optimization problems in different sectors, where more traditional methods are often found to fail [33-35]. They have been also implemented for pollution sources identification [36, 37]. These algorithms are relative fast in terms of computational time.

The present paper deals with the implementation of a back-forward mathematical model for pollutant source spatial localization and identification. Particulate matter was the pollutant agent. The implemented model was calibrated and verified on the basis of the results obtained in specific particulate matter dispersion experiments using a wind tunnel.

The forward problem consists of the determination of contaminant concentration knowing source emission rates and meteorological conditions. A Gaussian plume model was implemented and tested in the small scale scenario.

This Gaussian plume model was then used as “objective function” with a Genetic algorithm to identify pollution source.

BACK-FORWARD MATHEMATICAL MODEL

The implemented back-forward mathematical model is based on Gaussian Plume Dispersion Model and Genetic Algorithms. In the following paragraphs a brief description of Gaussian model, genetic algorithm approach, as well as implemented identification numerical procedure will be given.

Gaussian model

In the present paper, a Gaussian Plume Dispersion Model (GPDM) was used to evaluate PM concentration within control volume. The GPDM is essentially based on solving the concentration equation for each receptor point in the calculation grid. The main advantage of this type of mathematical models is that they have an extremely fast respond. The model’s computational cost mainly depends on the dimensions of the interesting area and the resolution of the computational grid. Moreover, an extremely important phase to take into account in the computational cost is the meteorological data pre-processing and turbulence parameterization. Depending on the complexity of these parameters, the model’s runtime can be extremely reduced that enables its application in real-time decision support software.

These dispersion models vary depending on the mathematics used to develop them. Therefore, all of them require as input data the following parameters:

- Meteorological data: wind speed and direction, atmospheric "stability class" (the amount of atmospheric turbulence), ambient air temperature, height to the bottom of any inversion aloft that may be present, cloud cover and solar radiation;
- Source terms: concentration or quantity of substances in emission or accidental release source terms and temperature of the material;
- Emissions or release parameters: such as source location and height, type of source (i.e., fire, pool or vent stack) and exit velocity, exit temperature and mass flow rate or release rate.
- Terrain elevations at the source location and at the receptor location(s), such as nearby homes, schools, businesses and hospitals.
- The location, height and width of any obstructions (such as buildings or other structures) in the path of the emitted gaseous plume, surface roughness or the use of a more generic parameter "rural" or "city" terrain.

Several assumptions should be done which are critical in the development of a dispersion model. The main assumptions are:

1. The emission rate at the source is constant;
2. Diffusion is negligible in the downwind direction;
3. Horizontal meteorological conditions are homogeneous over the modelled space. For each step: wind speed, wind direction, temperature, mixing height are constant;
4. No wind shear in the horizontal or vertical plane;
5. The pollutants are non-reactive gases or aerosol;
6. The plume is reflected at the surface with no deposition or reaction with the surface;
7. The dispersion in the crosswind and vertical direction take the form of Gaussian distributions.

The sources types may be different: point source, volume source, area source, open pit and flare. Usually, it is possible to implement Gaussian models for more than one source and as assumption it is considered the Superposition principle. The

Gaussian plume adopted in the present work was implemented in MATLAB® and is described as follow.

First of all, an orthogonal Cartesian reference system is assumed with its origin corresponding to base position of the source and the x-axe parallel to the wind direction. The y-axe horizontal and perpendicular to the x-axe while the z-axe in vertical direction corresponding to the height from the ground direction. The concentration C(x, y, z) in any points is described by the following Eq. 1.

$$C(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z U} \cdot e^{\left(-\frac{y^2}{2\sigma_y^2}\right)} \cdot \left[e^{\left(-\frac{(z-L)^2}{2\sigma_z^2}\right)} + e^{\left(-\frac{(z+L)^2}{2\sigma_z^2}\right)} \right] \qquad (1)$$

Where Q is the source emission rate, U is the wind speed at the source height (L), x is the downwind direction, while y and z are the crosswind and vertical directions.

The two Gaussian exponential functions are normalized respect to the maximum value and describe the dispersion degree of the plume in horizontal and vertical direction. The width of the plume is determined by σ_y and σ_z which are defined by atmospheric stability classes [38]. The σ_y and σ_z dispersion coefficients are defined as a function of atmospheric stability class and the distance from the source.

A number of researchers have used various curve fitting to approximate the behaviour if σ_y and σ_z as a function of distance from the source and Pasquill's turbulence types (atmospheric stability classes) [39-41]. The simplest is the approach developed by Caraway [42]. Caraway supposed that the dispersion coefficients can be defined as described in Eq. 2 and Eq. 3.

$$\sigma_y = 465.11628 \left(\frac{x}{1000}\right) \tan\vartheta \qquad (2)$$

$$\vartheta = 0.017453293 \left(c - d \log\left(\frac{x}{1000}\right)\right) \qquad (3)$$

$$\sigma_z = a \left(\frac{x}{1000}\right)^b \qquad (4)$$

where x is the downwind distance in meters from the source, while a and b are the pre-exponential and exponential coefficients for σ_z (see Eq. 4) and c and d are coefficients of σ_y according to Eq. 2 and Eq. 3.

In order to use the Gaussian Plume Dispersion Model in a confined environment such as the test chamber of a wind tunnel, an adaption of the horizontal and vertical dispersion coefficients was necessary. In the present study, the adaption of the two coefficients was carried out using a Genetic Algorithm approach [43].

An experimental data set was used as a target in the coefficients searching procedure. A Genetic Algorithm was used to minimise the errors between simulated and experimental PM concentrations for all sensors. Starting from an initial population composed by individuals with a, b, c and d constants as genes, a genetic evolution sequence (ranking, reproduction, mutation, reinsertion and ranking, …) was used to obtain adapted constants (see Fig. 1).

With reference to Eq. 2, Eq. 3 and Eq. 4, Table 1 shows original and modified pre-exponential and exponential coefficients obtained by adaption procedure.

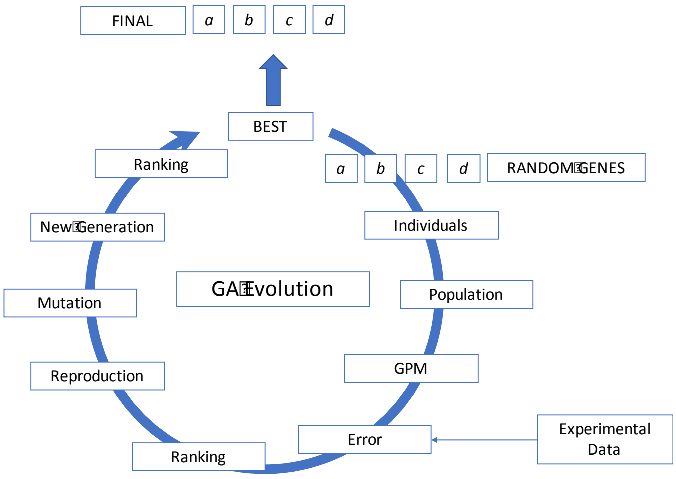


Figure 1. Genetic Algorithm coefficients adaption procedure

Table 1: Original and modified pre-exponential and exponential coefficients used for atmospheric stability class "Very Stable".

	Coefficients			
	a	*b*	*c*	*d*
Original Values	15.209	0.81558	4.1667	0.36191
Modified Values	33.5226	0.9346	6.4464	0.0

Genetic algorithm

In the present paper, a Genetic Algorithm approach was used. Genetic Algorithms (GAs) are search and optimization algorithms based on the natural mechanics of selection and genetics. These algorithms are computationally simple yet powerful in their search for improvements. Furthermore, they are not fundamentally limited by restrictive assumptions about the search space as continuity, existence of derivatives, unimodality, etc. Simplicity of operation and power of effect are two of the main attractions of GAs. They are different from the traditional optimization and search procedure in several ways.

First of all, they search from a population of points and not from a single point.

Secondly, they use payoff information based upon an objective function, rather than derivatives or others auxiliary knowledge.

Thirdly, they use probabilistic transition rules, not deterministic rules, to guide the search. However, the use of probability does not suggest that the methods are some simple random search.

GAs use randomized operators as a tool to guide a search towards regions of the solution space with likely improvement. Lastly, they are able to depart from local optima, maintaining at the same time a high rate of convergence towards the global optimum. Taken together, these differences contribute to a GAs' robustness and resulting advantage over other more commonly used optimization techniques.

The Identification procedure

A genetic approach was used in order to identify pollutants source. The identification procedure consisted to find three main different variables to characterize the pollutant source: the source height (L), the source mass flow rate (Q), and the spatial coordinates (x and y). This procedure was implemented in MATLAB®. A spatial grid corresponding to the test chamber of the experimental set-up (see next paragraph) was implemented, the coordinate x corresponds to the same wind direction, while y to the orthogonal direction. The Gaussian plume equation (Eq. 1) was used as objective function. The tests were performed by varying U and finding the global optimum in terms of the variables cited before. They were very fast (some minutes) given that the simplicity of the Gaussian plume model and the powerfulness of the genetic algorithm too.

EXPERIMENTAL SET-UP

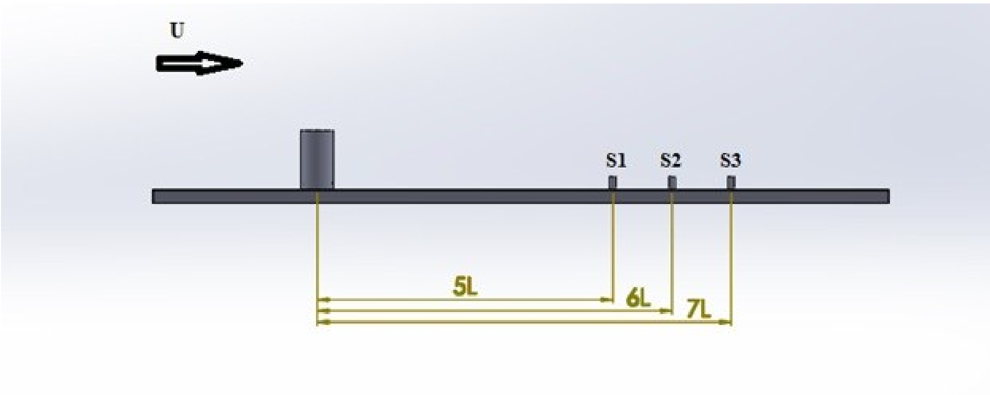
A specific experimental set-up was implemented in the test chamber of a wind tunnel to calibrate the mathematical models and to verify methodology accuracy. The implemented experimental set-up is a wood case [44-45] that fits exactly the bottom of a wind tunnel test chamber (see [46] for more details). This plane acts as set-up reference ground. One PM_{10} emitter [44] (main characteristics are reported in Table 2) was positioned on the ground as well as a grid of PM_{10} sensors. The latter consists of three Aerocet-531S Mass Particle Counters (see Table 3 for main characteristics), while a PM_{10} emitter is essentially a small chimney with controlled mass flow rate and velocity [47]. The emitter of PM_{10} was characterized in terms of PM_{10} mass flow rate and plume initial velocity. PM emission system characterization and validation procedures are reported in [44]. Main characteristics of Aerocet-531S are reported in Table 3, while sensors and emitter disposition are shown in Fig. 2 and Fig. 3. The sensors were located at different distances from the emitter; this distance was chosen multiple of the height of the emitter itself (5L, 6L, 7L). As it is possible to observe in the Fig. 2 all elements were downwind.

Table 2 - PM_{10} emitter main characteristics.

Description	Value
Height (L)	90 mm
Diameter	20 mm
Outlet velocity	0.6 m/s
PM_{10} mass flow rate	10 – 20 μg/s
U	2,3,4 and 5 m/s

Table 3 - Aerocet-531S Mass Particle Counters main characteristics.

Specifications	Value
Particle counter sizes	0.3 μm, 0.5 μm, 1 μm, 5 μm, 10 μm
Mass ranges	PM1, PM2.5, PM4, PM7, PM10, TSP
Concentration range	0 – 100,000,000 particle/m^3
Accuracy	± 10% to calibration aerosol
Sensitivity	High 0.3 μm, Low = 0.5 □m
Flow rate	2.83 10^{-3} m^3/min
Sample time	60 s
Light source	Laser Diode, 90 mW, 780 nm



(a)

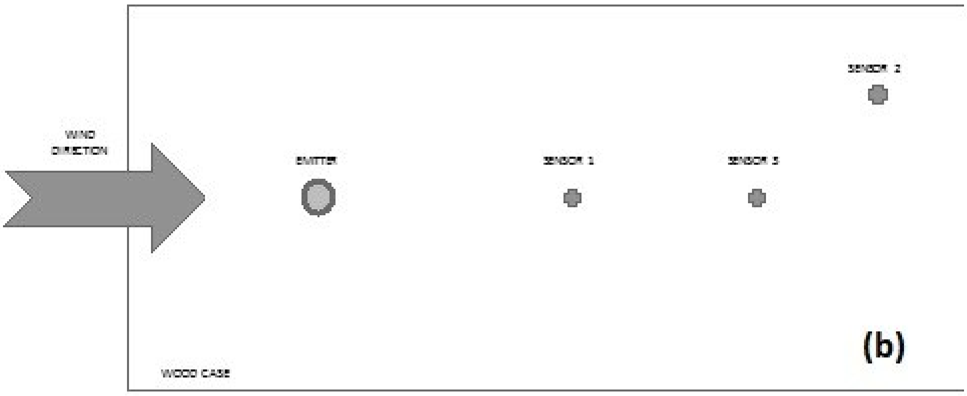


Figure 2 - Experimental set-up scheme in two different views (a-b).

Figure 3 - Picture of the experimental set up.

DESIGN OF EXPERIMENT

In order to test the accuracy of the implemented methodology a specific design of experiment was implemented. In more details, several pollutant dispersion tests were carried out as a function of pollutant mass flow rate and wind velocity. There were 10 possible configurations in terms of U and $\dot{m}_{PM10}$. For each configuration the test was reproduced 5 times for a total of 50 test. In each test there was first calculated the background C_{PM10} in order to consider only the aerosol emitter contribution. The results were treated by one-way and two-way analysis of Variance (ANOVA). Anova demonstrated that each test did not present a great variance in terms of C_{PM10} in all sensors so it was consider only the average. Moreover the two-way analysis, considering U and $\dot{m}_{PM10}$ as factors, demonstrated that these factors are significant for all C_{PM10} in all sensors.

RESULTS AND DISCUSSION

As far as the experimental results it is concerned, different tests were carried out using the described experimental set-up. In Figures 5, 6 and 7 it is possible to see S1, S2 and S3 C_{PM10} at varying U and Q. In this figures it is possible to see that C_{PM10} in Sensor 1 Sensor 2 and Sensor 3 grows when the emitted PM mass flow rate increases and decreases when the air velocity increases. These results also show how the C_{PM10} varies proportionally with Q in all three sensors. The slope of this variation is almost the same for S1 and S3 while in S2, where there are the highest C_{PM10} concentration values, the slope is greater. Moreover the distance in terms of C_{PM10} tends to decrease with the increase of U in all sensors.

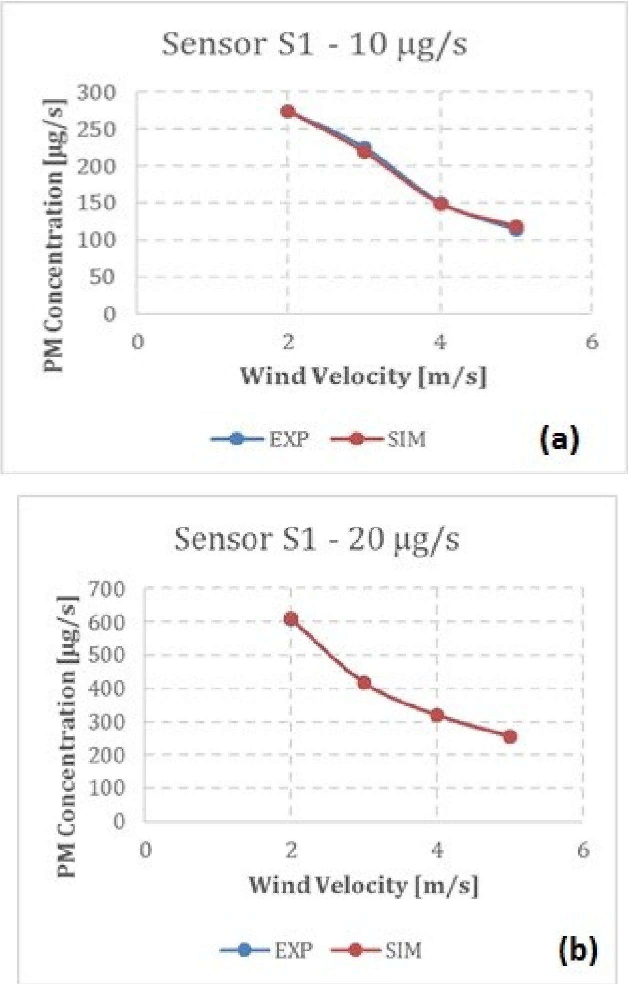
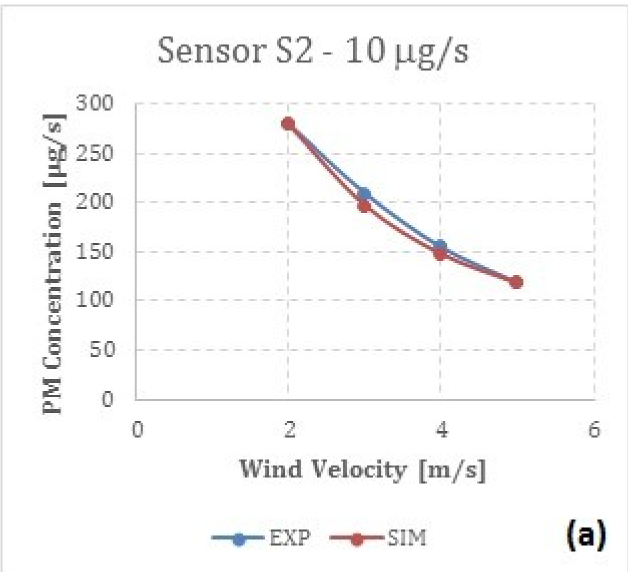


Figure 5 – Comparison between Experimental data and Gaussian model simulation results for sensor S1 with Q= 10 µg/s (a) and Q = 20 µg/s (b).



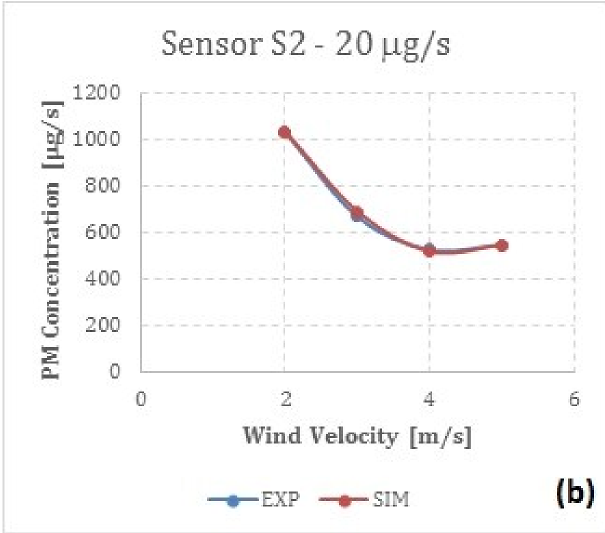


Figure 6 – Comparison between Experimental data and Gaussian model simulation results for sensor S2 with Q= 10 µg/s (a) and Q = 20 µg/s (b).

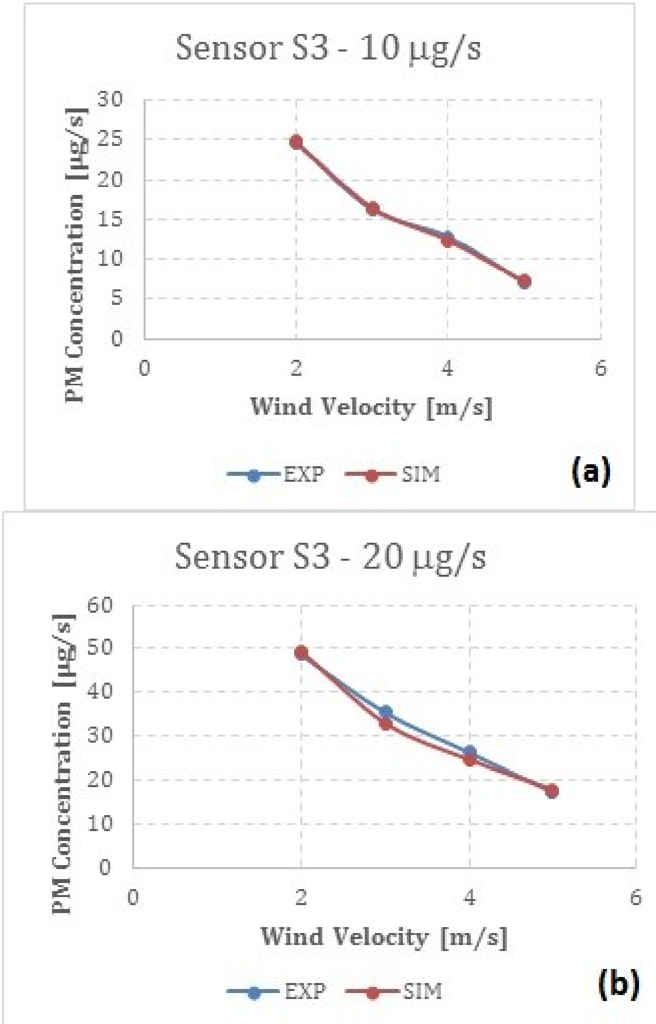


Figure 7 – Comparison between Experimental data and Gaussian model simulation results for sensor S1 with Q= 10 µg/s (a) and Q = 20 µg/s (b).

Table 4 shows the errors obtained between Gaussian results and experimental data. The best configuration in terms of error was obtained with U = 5 [m/s] for all sensors. The errors were in all cases quite low (the maximum was reached at S3 with U= 3 [m/s] and Q= 20 [μg/s]). The steady condition of Gaussian plume equation better fits with higher wind velocity that produces less turbulent unsteady phenomena.

Once obtained these results, the genetic algorithm was implemented to identify the source location according the procedure showed in paragraph 2.3. Fig. 8, 9 and 10 show the parameters individuation at varying the U while in Table 5 relative errors are showed. The model performed very well especially in the individuation of the spatial coordinate following wind direction (error varied from 0,78% to 4,32 % with an average value of 2,35%). The error of the other spatial coordinate varied from 9,22 % to 35,78% with an average value of 17,58. The error of height varied from 0,47% to 9,39% with an average value of 5,16 %. The error of the mass flow rate varied from 2,85% to 10,49% with an average value of 5,92%.

Table 4 – Relative errors between Experimental and Gaussian results for each sensor in all possible configurations.

	Error (%)					
U	Sensor S1		Sensor S2		Sensor S3	
	Q = 10 [μg/s]	Q = 20 [μg/s]	Q = 10 [μg/s]	Q = 20 [μg/s]	Q = 10 [μg/s]	Q = 20 [μg/s]
2 [m/s]	0,10 %	0,51 %	0,33 %	0,40 %	0,41 %	1,65 %
3 [m/s]	2,62 %	0,07 %	5,82 %	3,35 %	1,41 %	**6,79 %**
4 [m/s]	1,09 %	0,09 %	4,40 %	1,28 %	3,49 %	5,98 %
5 [m/s]	4,23 %	**0,02%**	0,24 %	0,31 %	1,55 %	4,08 %

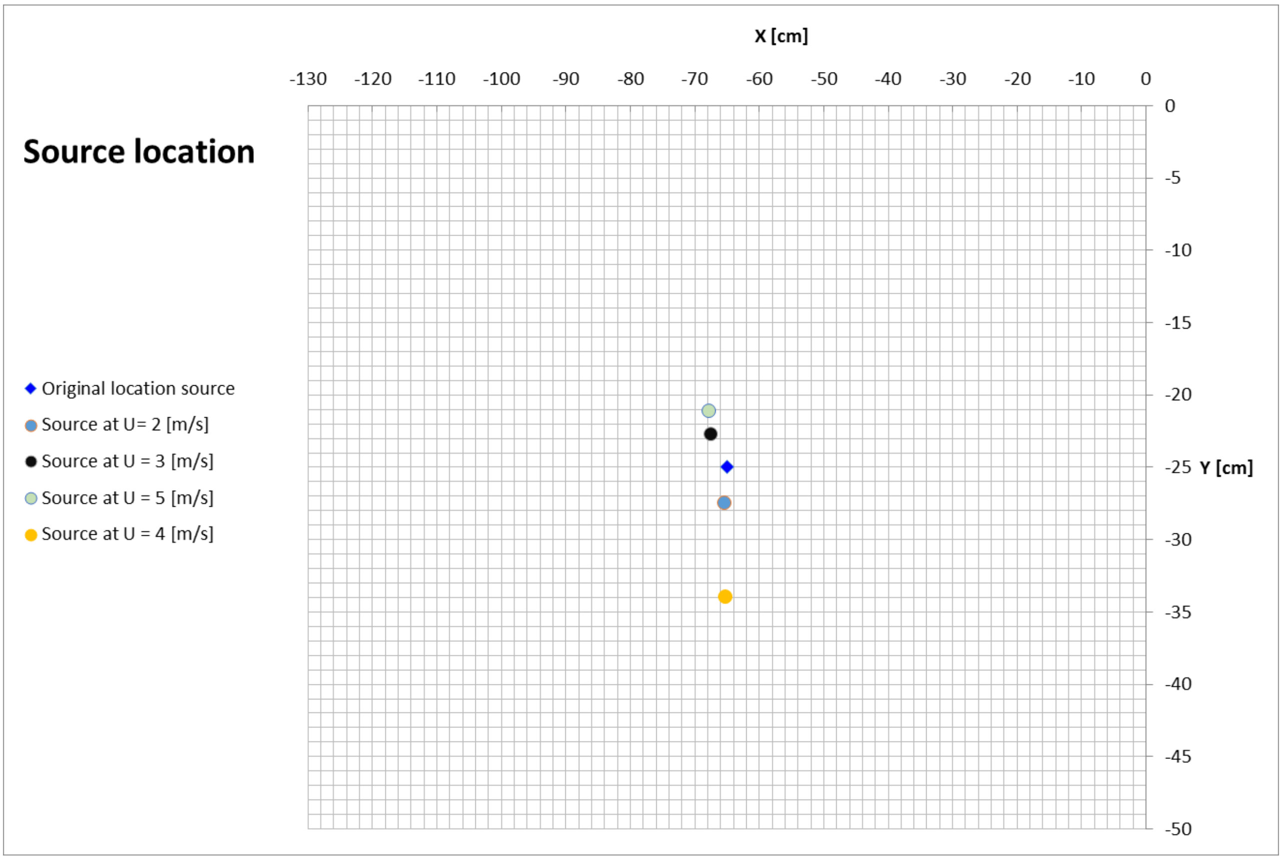


Figure 8 – Spatial coordinates of source location at varying of U.

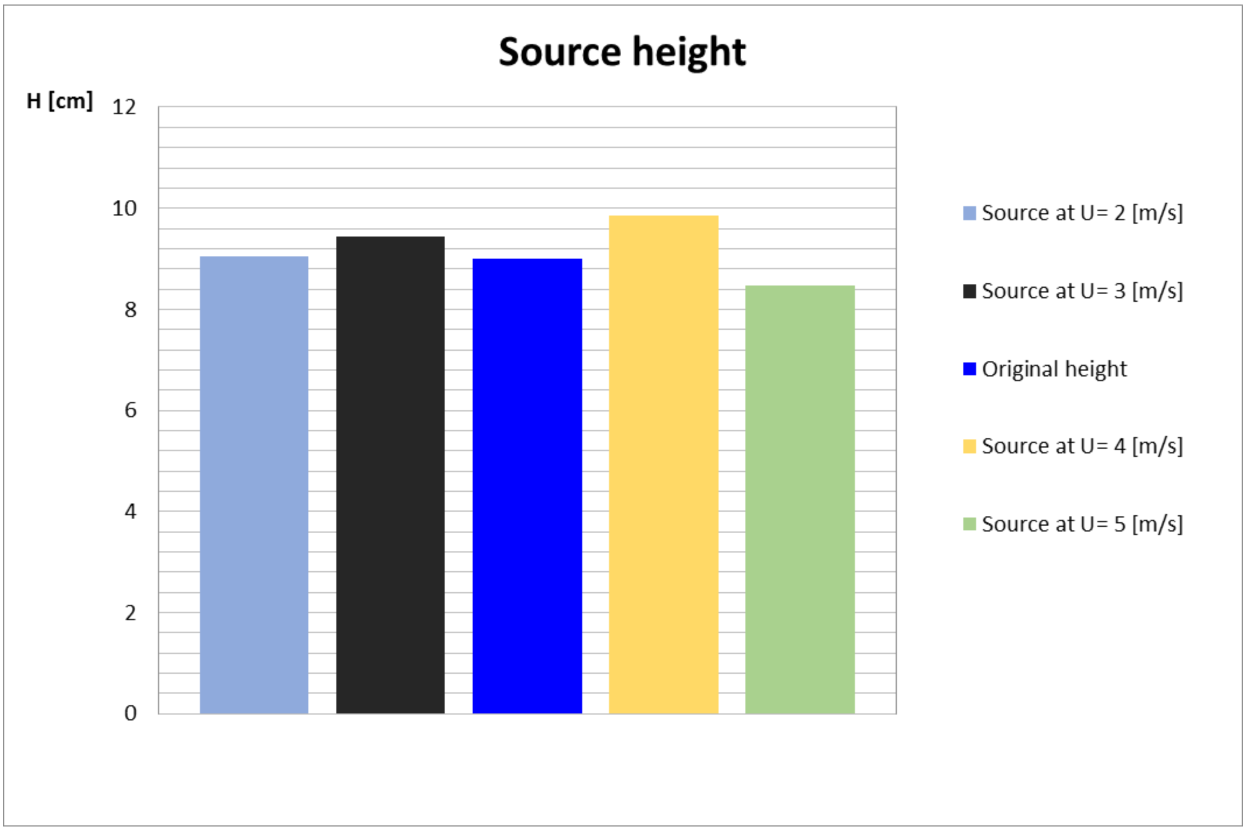


Figure 9 – Source height individuation at varying of U.

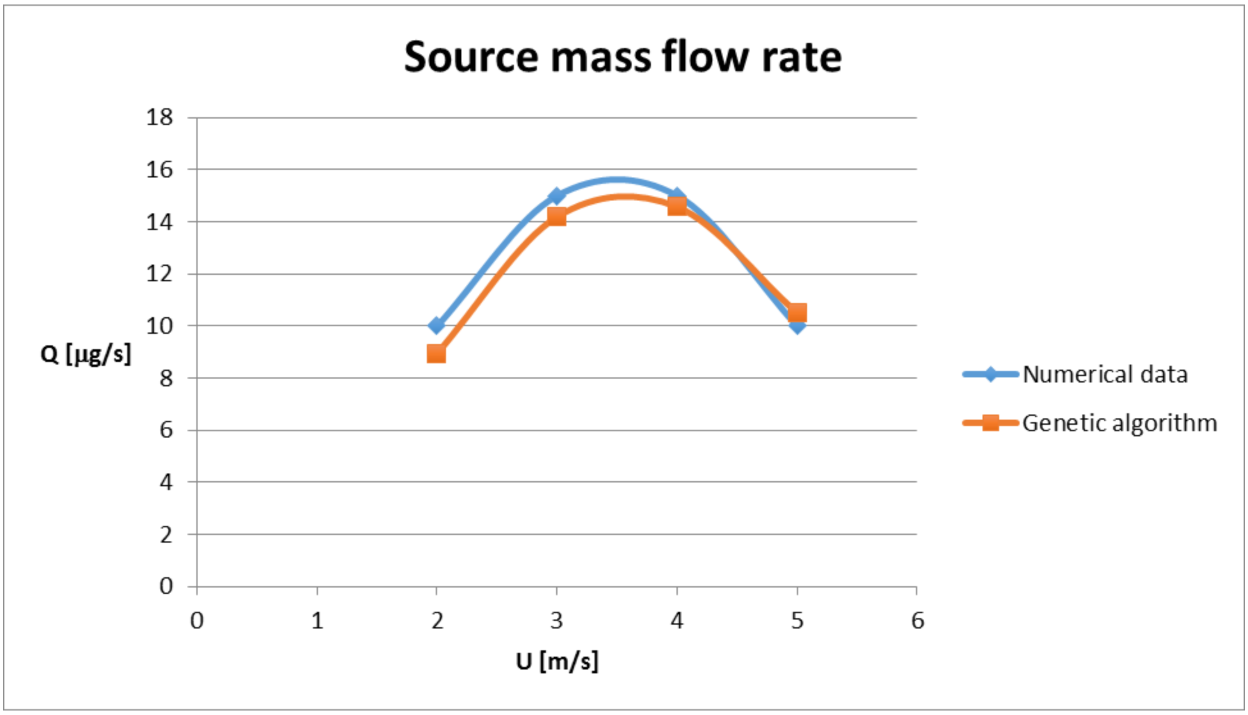


Figure 10 – Source mass flow rate comparison at varying of U.

Table 5 – Individuation parameters and relative errors at varying of U.

Spatial cordinates[cm]	U= 2[m/s]	U= 3[m/s]	U= 4[m/s]	U= 5[m/s]
Xs	-65,50	-67,49	-65,30	-67,86
Ys	-27,44	-22,69	-33,94	-21,11
L	9,04	9,44	9,84	8,48
Mass flow rate [μg/s]	8,95	14,19	14,57	10,49
Error (%)				
Spatial cordinates	**U= 2[m/s]**	**U= 3[m/s]**	**U= 4[m/s]**	**U= 5[m/s]**
Xs	0,78 %	3,84 %	0,46 %	4,32 %
Ys	9,76 %	9,22 %	35,78 %	15,57 %
L	0,47 %	5,00 %	9,39 %	5,78 %
Mass flow rate	10,49 %	5,38 %	2,85 %	4,96 %

CONCLUSIONS

This paper focuses on the implementation of a back forward model to analyze pollutants dispersion in a controlled environment such as a small scale wind tunnel. The model was used to identify PM10 emission sources according different parameters: height, pollutant emission rate and spatial location coordinates. The forward problem was solved by a Gaussian plume model and the results obtained were compared and tested with experimental data. The relative error of Gaussian model tested in different configurations varied from 0,02% to 6,79% with an average value of 2,09 %. Its performances were quite robust at varying of wind velocity and pollutant emission rate. This model was then used as objective function with a genetic algorithm to identify the pollution source. The results of the back forward model reveled good performances especially in the individuation of the spatial coordinate following wind direction (error varied from 0,78% to 4,32 % with an average value of 2,35%) and the height of the source (average value of 5,16 %). This model was quite fast in terms of computational time too and its near-real time nature makes it a good tool for regulatory purpose. The limitations of this model refer especially to the opportunity to extend it to real scale phenomena. It would be determinant to face a deeper analysis of meteorological variables in order to find solution when turbulence conditions occur and to solve limitations due to the presences of obstacles that may consistently deviate the pollutants flow.

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