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Implementation of an Integrated Stationary – Non Steady State Gaussian Modeling System to Simulate Contaminants Dispersion into the Atmosphere

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Contaminants and odor emissions are some of the major environmental problems that several industrial sites have to face. Particularly, complaints exhibited by the population living near plants characterized by both unpleasant odor emissions and hazardous contaminants dispersion (e.g. waste treatment and disposal plants, wastewater treatment plants, chemical industries, food industries, livestock activities, rendering plants, tanneries, etc.) are becoming more and more frequent, leading to the establishment of either legal suits (in the case of existing plants) or constraints with respect to the construction of new plants. Taking note of the importance of this feature, it is essential to provide industrial sites with easy-to-use software capable of evaluating the effects on the neighborhood of their atmospheric issuances. Therefore, the aim of this work has been the implementation of an integrated stationary – non steady state Gaussian modeling system (based on AERMOD and CALPUFF algorithms) which is able to simulate the dispersion of both contaminants and odors into an open field choosing automatically the most correct algorithm to be used. Its robustness and reliability has been tested using both AERMOD and CALPUFF simulations. The good agreement among the obtained results makes this software particularly suitable for an easy evaluation of the effects of a generic issuance onto the nearby environment without requiring a deep knowledge of the dispersion modeling system by the users.

1. Introduction

It is well known that, in the last twenty years, the impact of air pollution on human health and environment has received an increasing attention from both public organizations and industries (Copelli et al., 2012; Rada et al., 2014). Particularly, more and more severe regulations concerning the releases of hazardous air pollutants (HAPs), volatile organic compounds (VOCs) and dusts of very different sizes into the atmosphere have arisen, leading to a pressing need for complete and reliable simulations of the dispersion dynamics. Such simulations are often tricky to be carried out by inexperienced users, even when dedicated software with user-friendly interfaces (e.g., commercial versions of AERMOD and CALPUFF) are employed, because of a series of features to be taken into account: the presence of a complex domain on which the diffusion equations need to be integrated (the topography of the area interested by the dispersion), the modeling of both dry and wet deposition, the effects of gravitational settling, temperature and wind velocity.
In particular, simulating the behavior of a generic pollutant released to the atmosphere means to determine its concentration field at any point in space and at any time after the issuance. There are essentially two

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ways to simulate the dispersion of a pollutant into the atmosphere: assuming an Eulerian point of view (in which fixed coordinates in space are employed) or a Lagrangian point of view (in which the coordinates move with the particles). Nevertheless, all dispersion models use mathematical equations, describing the atmosphere, dispersion and chemical-physical processes occurring within a plume (continuous emission) or a puff (discontinuous emission), to calculate contaminants concentrations at various locations.

In this regard, lots of dispersion modeling systems have been proposed. Looking at the methodology on which all these models are based, it is possible to classify them into four categories (Busini et al., 2012; Capelli et al., 2013; Holmes and Morawska, 2006; Torti et al., 2013): 1) box models; 2) Gaussian models; 3) Lagrangian models; 4) Computational Fluid Dynamic models.

Focusing on Gaussian models, they are widely used in atmospheric dispersion modeling, in particular for regulatory purposes, and are often ‘‘nested’’ within Lagrangian and Eulerian models. Such methods are based on a Gaussian distribution of the plume, in both vertical and horizontal directions, under steady and unsteady state conditions. Considering a plume (continuous emission), its normal distribution is modified at huge distances from the source due to the effects of turbulent reflection from the surface of the earth and at the boundary layer (when the mixing height is low). The width of the plume is determined by σ_y and σ_z, which are defined either by stability classes (Pasquill, 1961) or travel time from the source.

It should be noted that, among all these different methods currently available, the United States Environmental Protection Agency (US-EPA) recommends CALPUFF model for the evaluation of long-range transport of pollutants (generally between 50 and 200 km), while in the near field (i.e., within 50 km from the source), US-EPA identifies as a reference the application of the stationary Gaussian model AERMOD (US-EPA, 2005).

Particularly, CALPUFF (Shire et al., 2000) is a multi-layer non-steady state puff dispersion model designed to model the dispersion of gases and particles using space and time varying meteorology basing on similarity equations, turbulence, emission strengths, transformation and removal. It is able to model point, line, volume and area sources using an integrated puff formulation incorporating the effects of plume rise, partial penetration, stack and building effects. Nevertheless, due to some intrinsic limitations, CALPUFF is not recommended either for performing calculation on timescales shorter than 1 h or for modeling dispersions that are heavily influenced by turbulence, such as in an urban environment (US-EPA, 2005; Brode and Anderson, 2008). AERMOD (US-EPA, 2009) is a near field steady state Gaussian plume model based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources over both simple and complex terrain. In the stable boundary layer the distribution is assumed to be Gaussian in both the horizontal and vertical directions. AERMOD is able to model buoyant plumes and incorporates a treatment of lofting, whereby the plume remains near the top of the boundary layer before mixing with the convective boundary layer (CBL).

Looking at practical features, the use of CALPUFF in the near field is better if there are weather and/or geographic conditions such as to make inappropriate a simulation with AERMOD (Brode and Anderson, 2008; Dresser and Huizer, 2011). These conditions, which can be defined as “non-stationary”, are very common if the wind regime involves high frequencies of wind calm and the presence of both land-sea discontinuities (originated by the presence of coastlines) and complex terrain morphologies that require an accurate reconstruction of the wind field.

In this work, an integrated stationary – non steady state Gaussian modeling system based on AERMOD and CALPUFF algorithms has been implemented in order to: 1) automatically switch between AERMOD and CALPUFF algorithms basing on the pros and cons evidenced above; 2) support inexperienced users in both pre and post processing.

This software has been then used to simulate the near field (4 km) dispersion into the atmosphere of a point issuance containing a mixture of different odorous compounds coming from the cleaning air system of a hypothetical wastewater treatment plant (pumping station and primary settling). The topography taken into account is particularly complex because it involves the presence of both quite high hills and sea. Moreover, wind circulation is characterized by strong oscillations during the day (both in terms of magnitude and direction) thus implying a continuous change in the stability class. In order to perform such a simulation, the CALPUFF algorithm has been selected and, then, obtained results have been compared with those ones coming from a real CALPUFF simulation. The good agreement which has been achieved confirms the reliability of the developed modeling system that can therefore be used for an easy but reliable evaluation of the dynamics of a generic dispersion process.

2. Overview of the software

DISPSIM is an integrated stationary – non steady state Gaussian modeling system developed in order to provide an easy evaluation of the effects of a generic issuance of contaminants and odors into an open

field. As the Gaussian dispersion models on which DISPSIM is based, that is AERMOD and CALPUFF, it is able to treat both complex morphologies and terrain conditions (both urban and open-country), dry and wet deposition, different source types (point, line, volume and area sources), non-steady state emissions and meteorological conditions, vertical wind share, plume rise, building downwash and, finally, overwater and coastal interaction effects.
DISPSIM is particularly user-friendly because it automatically selects the most appropriate dispersion algorithm choosing in between: a near field steady state Gaussian plume model (that is, an "AERMOD-like" model) and a multi-layer, multi-species non steady state puff dispersion model (that is, a "CALPUFF-like" model). This aspect is particularly useful because it makes the software very versatile and easy to use even for inexperienced users who do not posses a deep knowledge of the fluid dynamics influencing the dispersion of contaminants and odors into the atmosphere (and, therefore, they would not be able to choose in between different dispersion models implemented into a software). The criteria implemented for the automatic switch are: a) source emission type (continuous or not); b) presence of wind calm (wind velocity under 0.2 m s^{-1}); c) presence of complex terrain; d) environment (urban, coastal, …); e) timescale simulation; f) field extension.
As AERMOD and CALPUFF, DISPSIM is constituted by three different calculation modules: a pre-processing module, a dispersion module and a post-processing module. The first one, called METSIM, is a meteorological and geophysical model that develops a hourly wind and temperature three dimensional field to be used to calculate stability classes employed by the simulation module. It is derived from an integration of AERMET (the pre-processing module of AERMOD used to compute certain boundary layer parameters used to estimate profiles of wind, turbulence and temperature) and CALMET (the diagnostic 3-dimensional meteorological model that pre-processes data for CALPUFF; US-EPA, 2014).METSIM is also able to retrieve digital terrain elevation data (DTED) from NASA database (NASA, 2000) with a resolution of about 50x50 m (Beauducel, 2013). Moreover, it is possible to import ArcGIS shapefiles or GeoTIFF (georeferenced raster maps) representing Corine land cover and area description, respectively, with the aim of defining urban and open-country terrain conditions (Mathworks, 2010). Sources and specific receptors location is loaded from an ASCII file, a Google Earth kml file (Google, 2014) or through a graphical user interface (GUI) which allows picking points on the previously loaded maps.
DISPSIM is the core of the software and it permits to perform the effective calculation of the 3-D concentration field by implementing both AERMOD and CALPUFF algorithms (US-EPA, 2014).
DISPpost builds different maps showing average contaminants (or odors) concentrations, peak concentrations, the n-th percentile concentrations (computed using a low-demand memory consuming algorithm), and threshold limit value overcoming frequencies (and so on) during a pre-determined period of time (generally, 1-year). Moreover, DISPpost allows to evaluate the time distribution of the overcoming frequencies at the receptors during the day or the seasons in order to evaluate the critical period for the nuisance (e.g. nighttime for inhabitants, during the day for schools, summertime for vacationers, etc..).
The major difference with respect to AERMOD and CALPUFF software is that all these modules are not separated but fully integrated each other.
The parallel computing and the highly structured matrix algorithm capable of processing the different concentration layers is more effective in the AERMOD-like simulations, in which each time step is independent from the others. This makes the simulation very short time consuming.

3. Case-study

DISPSIM has been used for assessing the atmospheric issuance of odors coming from a hypothetical air cleaning plant located in the south of Italy. The site is located near the coast (east) at sea level (Figure 1a). In the neighborhood, there are: three towns (E, S-SE and S-W), an industrial complex (N), cultivated lands (Figure 1b) and a beach (highly frequented by the population) (S-E). One of the two towns (S-W) is located on a hill. The characteristics of the issuance are summarized in Table 1.
The area here considered for the simulation is constituted by a square of 4.0 km of side (near field), centered on the location of the odors issuance. For the post-processing purposes, the area thus defined has been unbundled into a Cartesian orthogonal grid consisting of a square mesh of 50 m of side for a total of 6,561 points per horizontal layer. Moreover, 8 specific receptors, that describe the position of 5 residential buildings, a school and two aggregation points (beach), have been located around the plant (see Figure 1).
1-year of hourly-averaged meteorological data (lacking data: 0.3%) have been adopted for evaluate the odor nuisance of the plant.

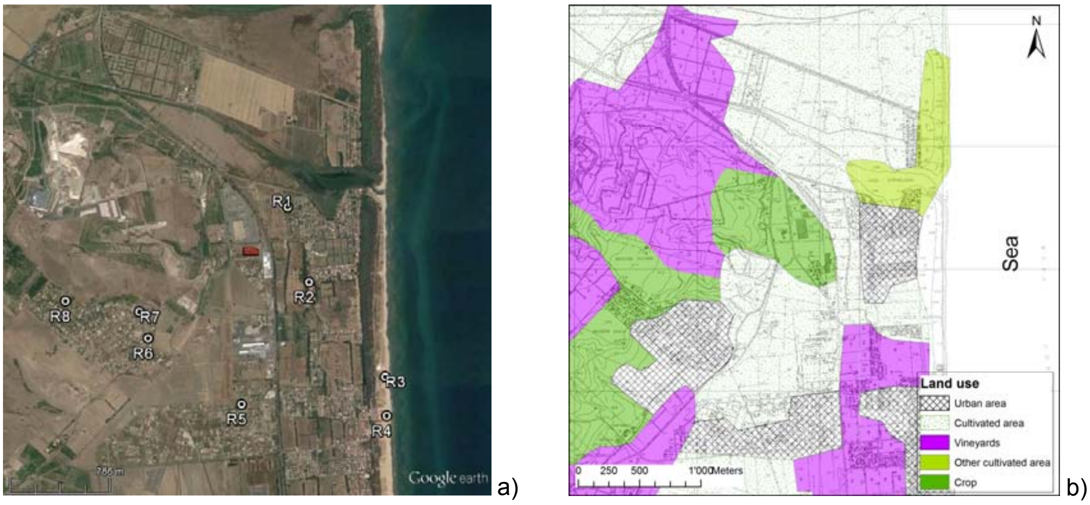

Figure 1: Description of the area surrounding the plant. Aerial view showing the source and eight receptors locations (a); land use overlapped on the technical map (b).

Table 1: Characteristics of the hypothetical issuance treated in the case study.

Description	Unit of measurement	Value
Source type	-	Point
Type of efflux	-	Vertical without deflection
	-	Continuous
Volumetric flow rate	$Nm^3\ h^{-1}$	20,000
Outlet temperature	°C	30
Source height (above the ground)	m	10
Source diameter	m	0.75
Odor background concentration	$OU\ Nm^{-3}$	0
Odor concentration	$OU\ Nm^{-3}$	4,000
Peak-to-mean value for odor	-	2.3

4. Results and discussion

Figure 2a shows the mean odor concentration registered in the area. The eastern zones are the most exposed because of both its closeness to the source and meteorological conditions (e.g. receptor R2 mean concentration: 0.16 OU Nm^{-3}); on the contrary the hilly urban area (receptors R6, R7 and, especially, R8) and the southern village (receptor R5) avoid the odor nuisance thanks to their overhead position (only receptor R6 and R7 are at 0.05 OU Nm^{-3}) and the distance from the source. Therefore it follows that two of the three towns do not have particular issues.

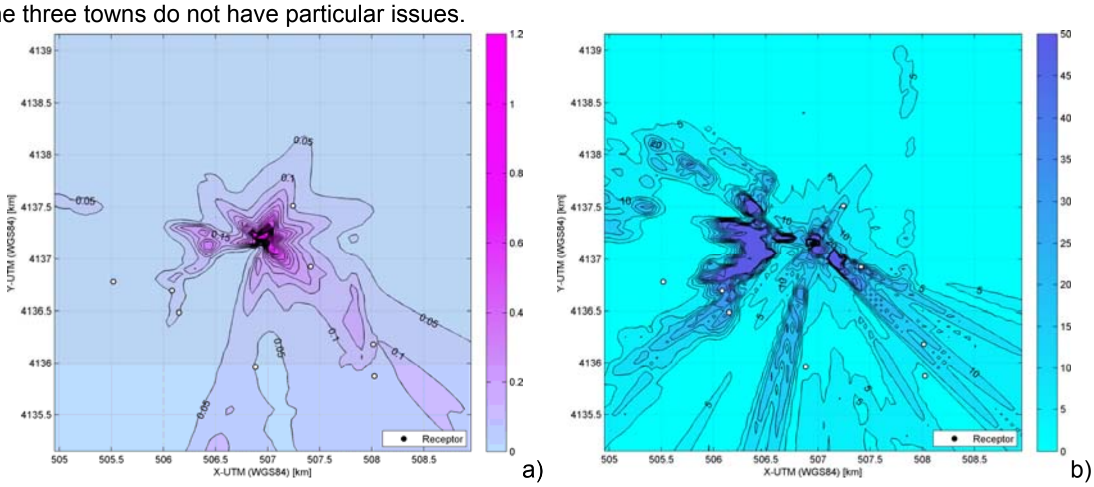

Figure 2: DISPSIM results: mean (a) and maximum (b) odor concentrations (OU Nm^{-3}) in the studied area.

Considering peak concentrations (Figure 2b), the most exposed sites (up to 50 OU Nm^{-3}) are the urban area near receptor R2 and the western cultivated area located within 1,000 m from the source.
The 98th percentile concentration map (Figure 3a), considered also by some Italian local guidelines (Regione Lombardia, 2014) for odor nuisance assessment, confirms critical conditions for the nearby receptors placed in the eastern part of the area (R2, in particular, with 2.3 OU Nm^{-3}). South-eastern shoreline (the most interested by bathing and tourism; receptors R3 and R4) is affected by 98th percentile concentrations higher than 1.5 OU Nm^{-3}. Orography confirm to positively influence the odor conditions, as demonstrated by the receptors R6, R7 and R8 placed on the hill located in the S-W with respect to the source. The school (receptor R5) has a 98th percentile odor concentration below 1 OU Nm^{-3}.

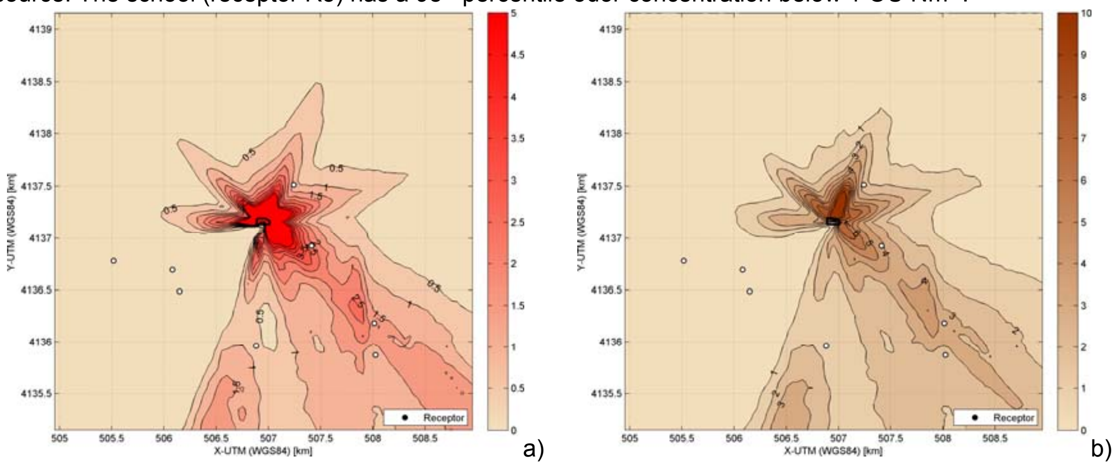

Figure 3: DISPSIM results: 98th percentile (a) concentrations (OU Nm^{-3}) and frequency (as percentage of the total occurrences) of the overcoming 1 OU Nm^{-3} detection threshold value (b).

Figure 3b shows the map of the 1 OU Nm^{-3} overcoming frequency in the studied area during the 1-year simulation. It can be noticed that some of the south-eastern urban areas are afflicted for more than 175 h y^{-1} by odor concentrations greater than 1 OU Nm^{-3}. Considering that 1 OU Nm^{-3} is the odor detection threshold statistically perceived by half of the population (DEFRA, 2010), the issue can represent a trouble for both the inhabitants and the tourism development in the area.
In order to evaluate such situation, DISPpost feature of "time distribution" analysis was applied on receptors R3 (bathing establishment; Figure 4a) and R5 (school; Figure 4b). Such receptors are located in typical "discontinuous use" areas. In fact, the bathing establishment is used only in summertime (typically between May and September) while the school is used in the morning-early afternoon (typically, between 8 am and 4 pm).

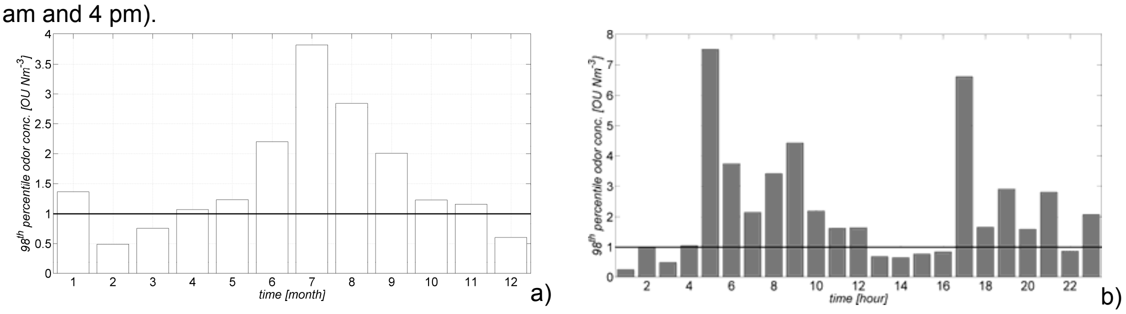

Figure 4: DISPpost "time distribution" analysis tool: 98th percentile concentrations (OU Nm^{-3}) of: a) monthly values (excluding night-time simulations) at receptor R3 (bathing establishment) and b) daily values at receptor R5 (school). The horizontal solid lines show the odor detection threshold.

The monthly 98th percentile concentrations at receptor R3 shows a periodic behavior of odor concentration which affects negatively the bathing establishment during its activity (odor concentration always above 1.5 OU Nm^{-3} in summertime, with a peak of 3.8 OU Nm^{-3} in July): the odor source could be a problem for tourism development if not adequately treated. For what concern daily distribution at receptor R5, maximum concentrations are most frequent in the morning (up to 7.4 OU Nm^{-3} at 5 am) and in the late afternoon (6.6 OU Nm^{-3} at 5 pm) as a consequence of the breezes, with negative effects for the students.

5. Conclusions

In this work, a nimble - integrated stationary–non steady state Gaussian model to simulate contaminants dispersion into the atmosphere has been proposed (DISPSIM) and used to simulate the effects of an odors issuance. The easiness of treating data, such as digital elevation data as well as receptors, source locations and data time-analysis, combined to the integration of pre-post processing with the dispersion model helps to reduce computation time (a complete 1-year simulation on a 4.0 x 4.0 km area takes only 5 minutes). Such features elect DISPSIM as a tool for quick air pollution and odor assessment or, alternatively, a tool for air treatment plant design.

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