

## H14-225

## AN INVERSE MODELING METHOD TO IDENTIFY VEHICULAR EMISSIONS IN URBAN COMPLEX AREAS

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**Abstract:** The meteorological model CALMET and the dispersion model CALPUFF were used to predict dispersion of contaminant emitted from industrial, naval and vehicular sources in the Strait of Messina area (Italy). This region is of particular interest in that it relates to the construction of the Messina Bridge, the road infrastructure linking the Italian mainland and Sicily. The modeled domain covers an area of 30x40 Km<sup>2</sup>, with grid spacing of 250 m. The domain includes two cities, i.e. Messina and Reggio Calabria, and other urban complexes located mainly along the shoreline. One of the main problem encountered during the investigation was the lack of data regarding the vehicular emissions. Therefore, an indirect method was utilized, and the data of the urban air quality monitoring stations of the two cities were considered during the procedure. Starting from the Corine Land Cover data base, a hypothetical location of urban areal emissions was derived and the strength of the sources was deduced by the inverse method. The results show a good agreement with measures at receptors. The method seems to give a valid alternative when network traffic data are not available in urban areas.

**Key words:** CALPUFF, Urban dispersion, Inverse method.

## INTRODUCTION

The evaluation of urban air quality represents one of the most important environmental task. This is also due to the increment of vehicular traffic in urban road networks. Most local municipalities have developed networks of air quality monitoring, but often no information is available about vehicular traffic. This lack of data makes the application of dispersion models very complicated. One of the methods to overcome this problem is to develop an origin-destination model, but it requires a preliminary demographic study conducted on the whole urban area. An alternative approach might be the application of an inverse method which furnishes the emissions of the vehicular traffic starting from the air quality data base. In recent years, the inverse method based on the Gaussian solution has been applied by several authors (Jeong, H.-J. et al, 2005; Hogan, W.R. et al., 2005; Lushi, E. and J.M. Stockie, 2010; Stockie, J.M., 2011). Other studies have been conducted using alternative inverse techniques like Kalman filtering, Lagrangian particles and backward integration (see for example Mulholland, M. and J.H. Seinfeld, 1995; Seibert, P. and A. Frank, 2004; Bagtzoglou, A.C. and S.A. Baun, 2005). In the literature, several direct applications of CALPUFF (Scire, J.S. et al, 2000) in urban area are present (see for example Elbir, T., 2004), while in the present work an inverse approach based on the model CALPUFF was developed. In particular, a complex area has been considered, which includes urban complexes, coastal areas and mountains (Figure1). The domain includes the cities of Messina (~250000 inhabitants) and Reggio Calabria (~180000 inhabitants) at the sides of Messina Strait. A five years campaign was conducted to get both meteorological and air quality data base. The model CALMET was used to obtain the meteorological input for CALPUFF. The pollutant considered in the simulation are carbon monoxide (CO), nitrogen oxides (NO<sub>x</sub>), particulate matter (PM10) and benzene (C<sub>6</sub>H<sub>6</sub>).

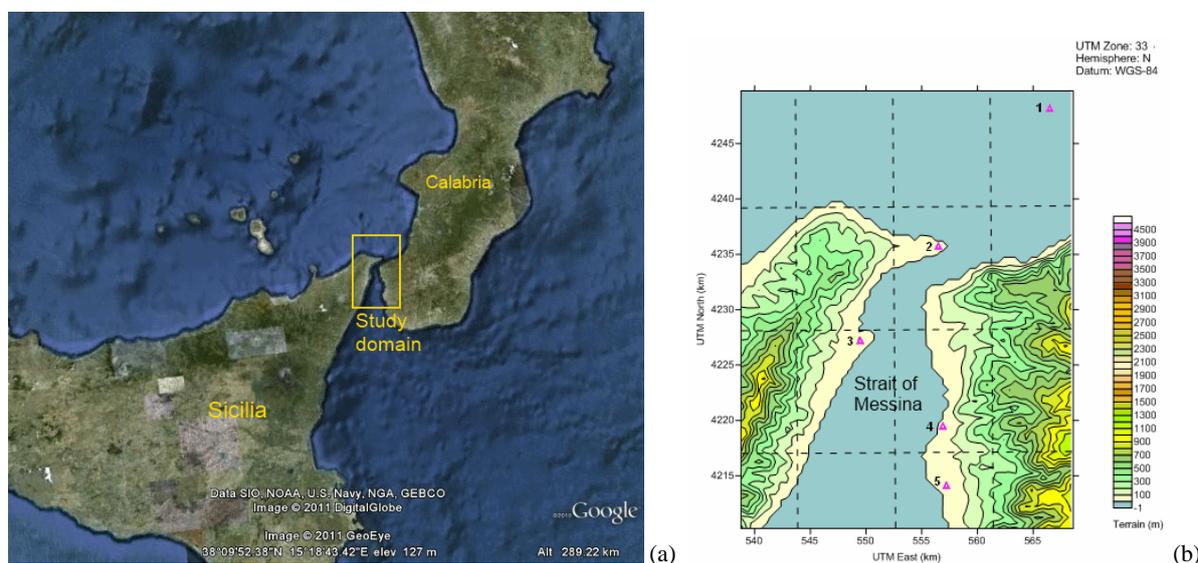


Figure 1. (a) The location of the study domain (yellow rectangle) (b) The topography of the study domain with the position of the meteorological stations used for the simulation. (1) NCAR grid point; (2) Punta Faro; (3) Messina; (4) Reggio Calabria; (5) Strait Airport.

## THE STUDY DOMAIN AND THE INPUT DATA

The domain was chosen on the basis of the topography, the meteorology and the location of the main pollutant sources. Figure 1 shows the studied area together with the positions of the meteorological stations used to give the input data to CALMET. The selected stations ensured the temporal continuity during the considered time period for the simulation. The pollutant sources related to the incinerator (triangle 1), the ship traffic (lines) and the ship stationing at harbors (triangles 2-6)

are reported in Figure 2a. The strengths of the known pollutant sources are listed in Table 1, with the exception of the ship traffic, which was negligible.

Due to lack of information about the vehicular traffic, in order to evaluate the strengths of the pollutant sources, an inverse modeling method was developed. By this approach the emissions are derived from the pollutant concentrations measured at the air quality monitoring stations. The shapes and the locations of the vehicular emissions (assumed as areal) were deduced from the Corine Land Cover. In particular, both continuous and discontinuous urban fabric areas were taken into consideration. The estimation of the vehicular emissions was realized by referring to the year 2009, during which more data were present.

Since only three air quality stations were available, only three distinct emission rates were calculated (details on the necessity of this constraint will be given below). Figure 2b shows the three vehicular areal sources and the corresponding monitoring stations. For each areal source, four strengths were considered, one for every pollutant species analysed. Not all the pollutant were monitored at the air quality stations, the available ones are listed in Table 2. In the case of the absence of the data in one of the monitoring stations, the emission was assumed equal to that calculated for the adjacent area.

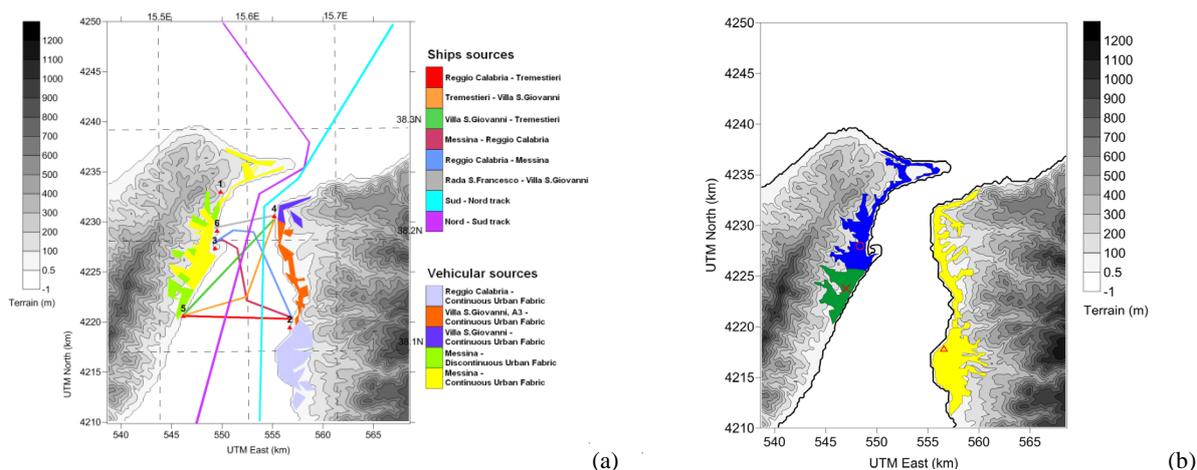


Figure 2. Location of the pollutant sources. (a) Incinerator (triangle 1), ship traffic (lines), ship stationing (triangles 2-6) and urban zones as deduced from Corine Land Cover (colored areas). (b) Vehicular areal sources and the corresponding air quality monitoring stations: Boccetta (circle), Minissale (cross) and Castello (triangle).

Table 1. Strengths of the continuous emissions produced by the incinerator and the stationing ships.

$\text{g s}^{-1}$	Incinerator	Reggio Calabria	Messina	Tremestieri	Rada S. Francesco	Villa S. Giovanni
CO	2.30 E-01	6.50 E-02	3.80 E-02	1.40 E-01	2.20 E-01	3.40 E-01
NO <sub>x</sub>	2.04 E-01	5.85 E-02	3.42 E-02	1.26 E-01	1.98 E-01	3.06E-001
PM <sub>10</sub>	1.60 E-01	3.60 E-02	2.10 E-02	8.00 E-02	1.20 E-01	1.90 E-01
C <sub>6</sub> H <sub>6</sub>	-	5.67 E-04	3.20 E-04	1.20 E-03	1.90 E-03	3.00 E-03

Table 2. List of the pollutant species monitored at the three air quality stations. The cross indicates the available measures.

	Boccetta	Minissale	Castello
CO	X	X	X
NO <sub>x</sub>	-	-	X
PM <sub>10</sub>	X	X	-
C <sub>6</sub> H <sub>6</sub>	X	-	X

## METEOROLOGICAL ANALYSIS

In order to have better understanding of the meteorological circulation typically observed in the studied domain, an analysis was conducted by using five years of observations taken at the Messina meteorological station. Some summary results for the year 2009 are reported in Figure 3. The wind is clearly channeled along the strait axis (Cf. Figure 1), with prevailing provenience from the north sectors (Figure 3a). The influence of synoptic moderate winds ( $4\text{--}5 \text{ ms}^{-1}$ ) together with sea breeze events is well-visible in the histogram of Figure 3b. A similar behavior was observed for the other years considered in the analysis (not shown).

The numerical model CALMET was used to calculate the meteorological input for the dispersion model CALPUFF. The computational domain consists of  $121 \times 161$  horizontal grid points with a constant grid size of  $250 \times 250 \text{ m}^2$ . The vertical grid has 11 unevenly spaced levels, i.e.,  $z=20 \text{ m}$ ,  $z=40 \text{ m}$ ,  $z=60 \text{ m}$ ,  $z=100 \text{ m}$ ,  $z=150 \text{ m}$ ,  $z=210 \text{ m}$ ,  $z=300 \text{ m}$ ,  $z=500 \text{ m}$ ,  $z=1000 \text{ m}$ ,  $z=1600 \text{ m}$  and  $z=2500 \text{ m}$  above the ground level. The simulation was performed for the years 2000, 2006, 2007, 2008 and

2009. The surface input data were taken from the meteorological stations Punta Faro, Messina, Reggio Calabria and Strait Airport (Figure 1b). The upper air data observation was derived from the NCAR reanalysis data base. Figure 4 shows an example of a typical summer day, when the sea breeze interacts with a northerly synoptic wind.

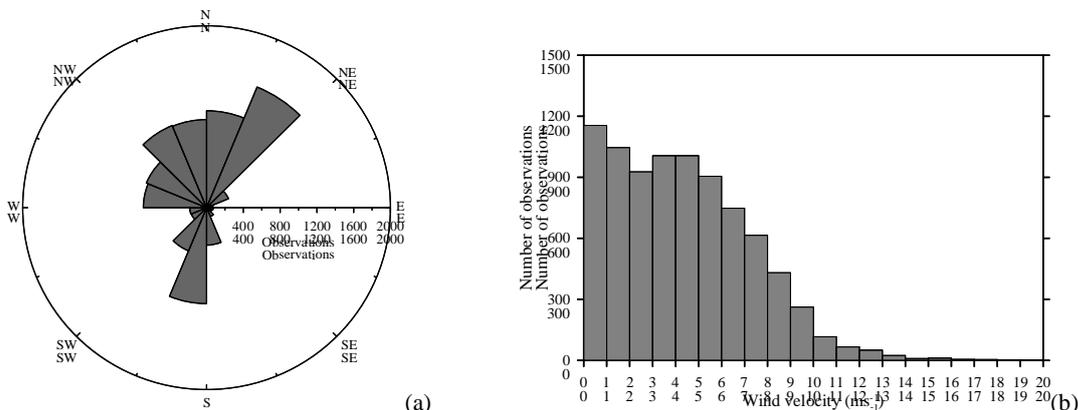


Figure 3. (a) Wind rose and (b) number of observations of the horizontal wind velocity taken at Messina during 2009.

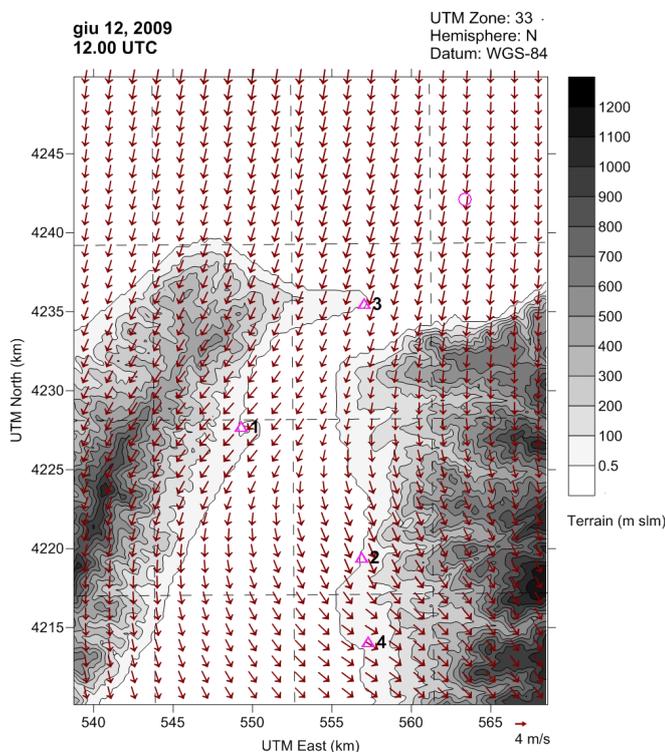


Figure 4. Wind field calculated at 10 m above the ground level by CALMET at 12 UTC of 12 June 2009.

### THE INVERSE METHOD

Since vehicular emissions were not known, an inverse method was used. This technique is based on the consideration that, when the meteorological field and the emission are both stationary, the concentration field can be calculated by the classical Gaussian solution. In the case of  $N$  sources, the latter can be expressed as:

$$c_i = \sum_{j=1, N} \alpha_{ij} q_j \tag{1}$$

in which  $c_i$  indicates the concentration at the  $i$ -th receptor,  $\alpha_{ij}$  is a function dependent on the position of the receptor downwind to the source, on the wind intensity and on the diffusion coefficients.  $q_j$  indicates the unknown rate of the  $j$ -th source. The summation can be used due to the linearity of the diffusion equation which is solved by the Gaussian function. The matrix  $\alpha_{ij}$  can be determined by assigning a unit value to the strength of the  $j$ -th source and by calculating the concentration at the  $i$ -th receptor using the model CALPUFF. By applying this procedure to all the elements  $\alpha_{ij}$ , the linear system (1) can be solved by substituting to  $c_i$  the values measured at the  $i$ -th receptor ( $i$ -th monitoring station). In this way, the unknown vector  $q_j$  is obtained. As stated above, such a procedure should be applied only in stationary conditions. In the

real cases it is not possible to reach a perfect steady state. Anyway, during periods of strong and persistent winds, the pollutant flows throughout the domain without accumulation effects. In this way a diurnal emission cycle can be obtained and it can be extended also to the other days, under the assumption of sources independent of the meteorology. In order to take into account the different traffic flows during the week, the ferial cycle can be distinguished from the holiday and pre-holiday ones.

Equation (1) requires a number of monitoring stations equal to the unknown sources. Anyway, additional sources can be added by hypothesizing that they have the same intensity. The determination of the typical diurnal cycles can give rise to relevant errors due to the seasonal variations of the traffic flows. In the present simulation an alternative approach was used. At each hour the source rates are adjusted as a function of the error calculated with respect to the measured concentration. In this way, after the simulation, we can get the diurnal cycles for all the days of the year and, as a consequence, the mean error calculated respect to measurements was significantly lower. The corrective factor applied to the source strength is proportional to the ratio between the measured and the calculated concentration values performed at the same receptor.

## RESULTS

The model CALPUFF was used to simulate the dispersion during the same period considered for the meteorological simulation. The output of CALMET was utilized as input data for CALPUFF. The rates of the pollutant sources were derived at each hour by using the approach described in the previous section.

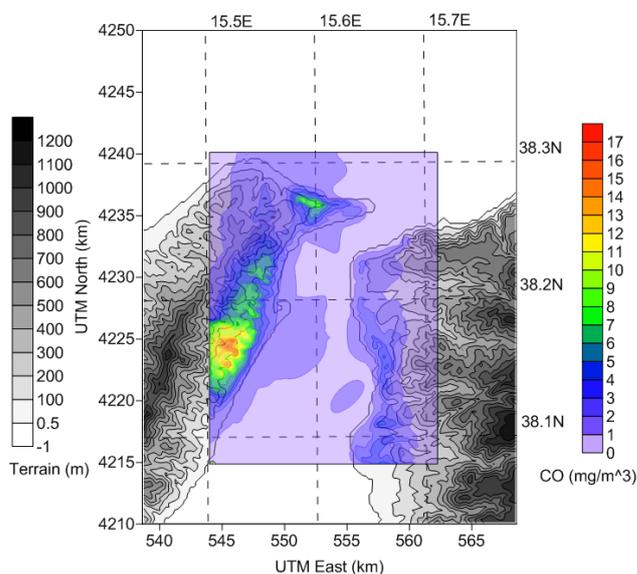


Figure 5. Concentration of CO for the year 2009, calculated as the maxima of the 8-hours averages.

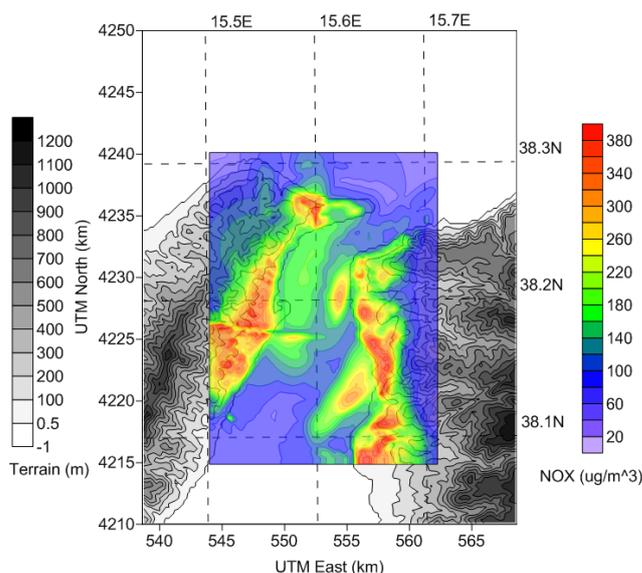


Figure 6. Concentration of NO<sub>x</sub> for the year 2009, calculated as the maxima of the hourly averages.

In Figures 5 and 6 two examples of the concentration fields calculated by CALPUFF are showed. In particular, Figure 5 shows the maximum values of the 8-hours average concentration of CO referred to the year 2009. It is observed that most of the concentrations values are below the legal limit ( $10 \text{ mg m}^{-3}$ ), while some overcoming are present within the center of Messina. Figure 6 depicts the map of the maximum values of the hourly average concentration of  $\text{NO}_x$  for the year 2009. Several nodes in the urban areas show concentration values greater than the legal limit of  $\text{NO}_2$ , this should be due to the presence of other mono-nitrogen oxides.

A preliminary validation of the method was conducted by calculating the metrics Fractional Bias (FB) and Index of Agreement (IA) (Willmott, C.J., 1981). The values calculated at the Bocchetta monitoring station for the pollutants with available measurements are listed in Table 3. Since the errors were calculated in the same station used to set the source strengths, the metrics are very good. Nevertheless, since the metrics take into account also of unsteady effects (when the assumptions of the method do not hold), the results demonstrate that the proposed technique can be extended also to period when some accumulation phenomena occur.

Table 3. Fractional Bias (FB) and Index of Agreement (IA) for the pollutants CO, PM10 and  $\text{C}_6\text{H}_6$  calculated during year 2009 at Bocchetta.

	CO	PM10	$\text{C}_6\text{H}_6$
FB ( $-2 < \text{FB} < 2$ )	-2.1E-03	-2.8E-03	-3.4E-03
IA ( $0 < \text{IA} < 1$ )	0.972	0.970	0.975

## CONCLUSIONS

An inverse method based on the model CALPUFF has been developed and applied to a domain which includes cities, coastal areas and complex topography. An extensive campaign was conducted for 5 years to get input and validation data base. The preliminary results allow to understand the importance of the various pollutant sources which are present in the study domain (i.e. ship stationing, ship traffic, incinerator and vehicular traffic). The metrics calculated at an air quality station are very satisfactory and prove the applicability of the methods also in unsteady conditions. In conclusion, the proposed method seems to furnish a valid tool to evaluate pollutant dispersion for the cases in which emission data from vehicular traffic are not available.

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