Environ Monit Assess (2016) 188: 499
DOI 10.1007/s10661-016-5519-5

# Impact assessment of $PM_{10}$ cement plants emissions on urban air quality using the SCIPUFF dispersion model

**Vincenzo Leone · Guido Cervone · Pasquale Iovino**

Received: 14 March 2016 / Accepted: 28 July 2016 / Published online: 2 August 2016


**Abstract** The Second-order Closure Integrated Puff (SCIPUFF) model was used to study the impact on urban air quality caused by two cement plants emissions located near the city of Caserta, Italy, during the entire year of 2015. The simulated and observed $PM_{10}$ concentrations were compared using three monitoring stations located in urban and sub-urban area of Caserta city. Both simulated and observed concentrations are shown to be highest in winter, lower in autumn and spring and lowest in summer. Model results generally follow the pattern of the observed concentrations but have a systematic under-prediction of the concentration values. Measures of the bias, NMSE and RMSE indicate a good correlation between observed and estimated values. The SCIPUFF model data analysis suggest that the cement plants are major sources for the measured $PM_{10}$ values and are responsible for the deterioration of the urban air quality in the city of Caserta.

**Keywords** Air quality · Transport and dispersion modelling · Statistical analysis · SCIPUFF

V. Leone · G. Cervone
GeoInformatics and Earth Observation Laboratory (GEO), Department of Geography and Institute for CyberScience, The Pennsylvania State University, University Park, PA, USA

V. Leone (✉) · P. Iovino
Department of Environmental, Biological and Pharmaceutical Science and Technologies, Second University of Naples, via Vivaldi, 43, 81100 Caserta, Italy
e-mail: vincenzo.leone@unina2.it

V. Leone · P. Iovino
Environmental Technologies, University Spin Off, Second University of Naples, Caserta, Italy

G. Cervone
Research Application Laboratory, National Center for Atmospheric Research, Boulder, CO, USA

## Introduction

The presence of high concentrations of $PM_{10,}$ defined as particulate matter with an aerodynamic diameter smaller than 10 μm, has been shown to cause respiratory problems and increase both mortality and morbidity (Anderson et al. 2012; Stanek et al. 2011). Long-term exposure to high concentrations of particulate matter increases the risk of lung cancer, respiratory diseases and arteriosclerosis, while short term exposure causes the worsening of several forms of respiratory diseases, including bronchitis and asthma, as well as changes in heart rate variability (Lee et al. 2015).

High concentrations of $PM_{10}$ are caused by both naturally occurring and anthropogenic sources, such as transportation and industrial facilities. The greatest potential for the general public to develop health problems caused by the exposure to ambient air pollution occurs in urban areas (Pollice and Lasinio 2010; Iovino et al. 2007, 2009a). The presence of dense industrial facilities next to urban areas usually increases the risk of exposure to low air quality.

**Table 1** Monitoring sites description

| Station | Position (UTM WGS84 33 T) | | z | h | Area | Meteorological | Air quality |
|---|---|---|---|---|---|---|---|
| Code | Lon E (m) | Lat N (m) | (m) | (m) | Type | Data interval | Data interval |
| CE01 | 444,419.73 | 4,547,694.53 | 76 | 10 | Urban | 1 h | 1 h |
| CE02 | 444,961.17 | 4,548,339.04 | 90 | 10 | Urban | 1 h | 1 h |
| CE03 | 452,188.00 | 4,545,219.21 | 52 | 15 | Sub-urban | 1 h | 1 day |

A previous study of air pollution in the city of Caserta correlated the observed $PM_{10}$ concentrations with source emission through $PM_{10}$ chemical investigation and meteorological observations (Iovino et al. 2013).

Numerical air transport and dispersion models are paramount for the simulations of emissions because they take into account non-steady meteorological conditions, atmospheric physics and terrain characteristics (Johansson et al. 2007; Iovino et al. 2009a). A simple definition of dispersion is the spread of pollution as it moves through the atmosphere both vertically and horizontally. Meteorological and topographical conditions largely determine the transportation, dispersion and deposition of air pollutants (Iovino et al. 2009b; Wai and Tanner 2005). Seinfeld and Pandis (1998) reported that there are two principal mechanisms that govern the pollutants dispersion into the atmosphere: the mean airflow that transports the pollutants downwind and the turbulent velocity fluctuations that disperse the pollutants in all directions. Air quality models incorporating parameterization for turbulence, dispersion in the convective boundary layer and terrain interactions of pollutant plume are best suited for the estimation of spatial dispersion of pollutants (Holmes and Morawska 2006).

Dispersion models use mathematical equations, which describe the atmosphere, dispersion, chemical and physical processes within the plume, to calculate concentrations at various locations (Johansson et al. 2007).

In this paper, a dispersion model is used to compute the $PM_{10}$ emissions of two cement plants located near the city of Caserta and their impact on urban air quality. The model was validated using observed $PM_{10}$ concentration at three monitoring stations arranged throughout Caserta urban and sub-urban areas. The SCIPUFF transport and dispersion model was used. The specific objectives of the present study are:

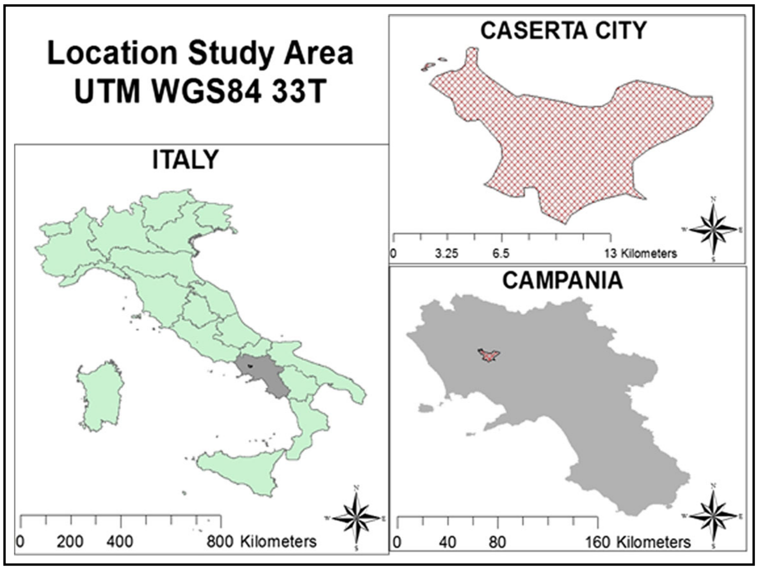


**Fig. 1** Location of the city of Caserta in Italy

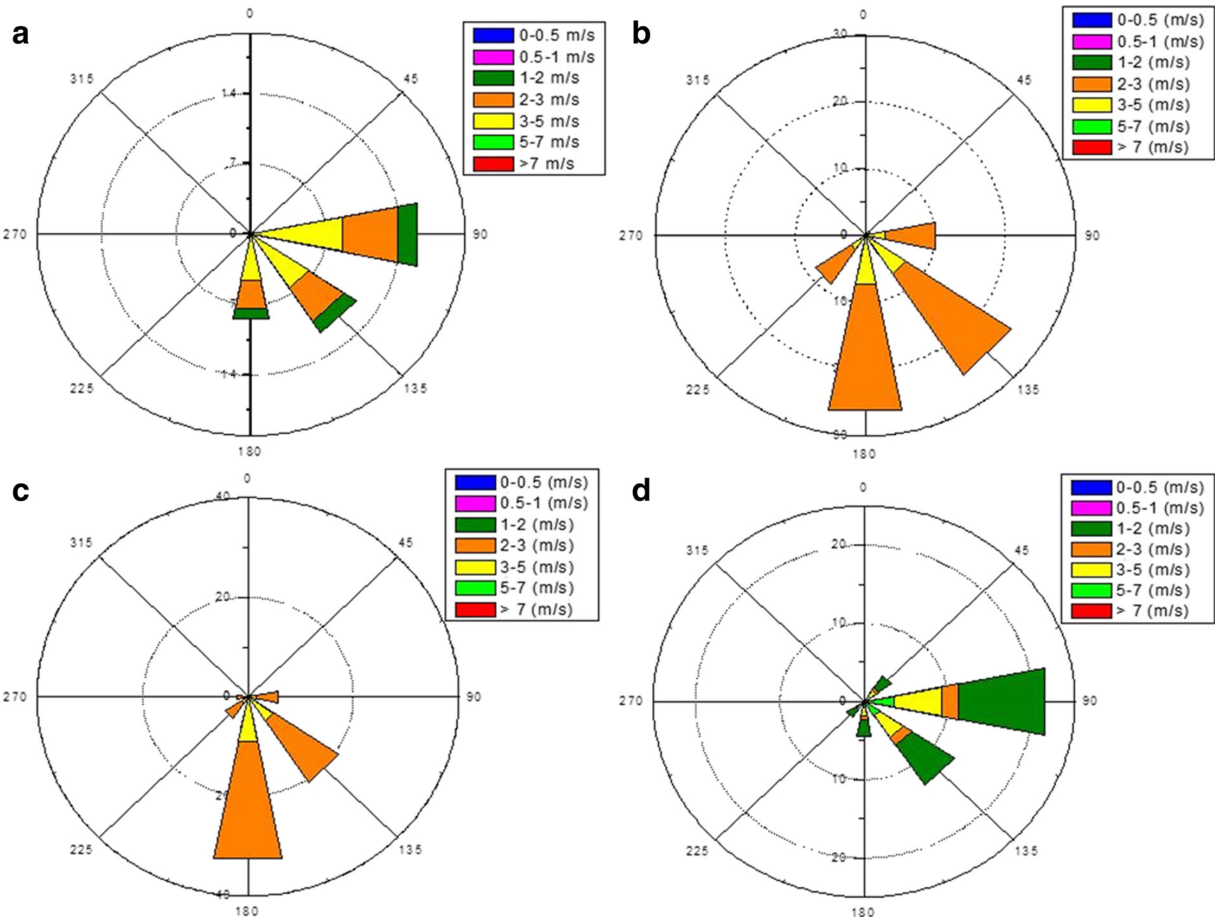


**Fig. 2** Wind direction (% of the time) and velocity (m/s) in the monitoring site CE01. Plot **a** 1 Jan.–31 Mar., **b** 1 Apr.–30 Jun., **c** 1 Jul.–30 Sep. and **d** 1 Oct.–31 Dec.

- Assess the environmental impact of two cement plants on $PM_{10}$ concentrations in the city of Caserta
- Comprehensive evaluation and validation of the SCIPUFF model for prediction of $PM_{10}$ concentrations
- Generation of spatial distribution contours of $PM_{10}$ concentrations

## Material and methods

### Site description

Meteorological and air quality data, such as temperature (°C), pressure (millibar), relative humidity (%), wind direction (degree), wind velocity (m/s), precipitations (mm) and $PM_{10}$ concentrations (μg/m$^3$) have been monitored by three ground stations (called CE01, CE02 and CE03), located within the urban and sub-urban boundaries of the city of Caserta, Italy. Their specific characteristics are reported in Table 1. The data were acquired for the entire year of 2015, on which this study is based.

Caserta is an important industrial centre, with a population of about 79,000 habitants and a territorial area of 56 km$^2$. Caserta is located at the edge of the Campania plain (Fig. 1), along the foot of the Campania Sub Apennine mountain range. The most abundant local rock is limestone, a sedimentary rock largely composed of the minerals calcite and aragonite.

### SCIPUFF model description

SCIPUFF (Second-order Closure Integrated Puff) is a Lagrangian puff dispersion model using Gaussian puffs

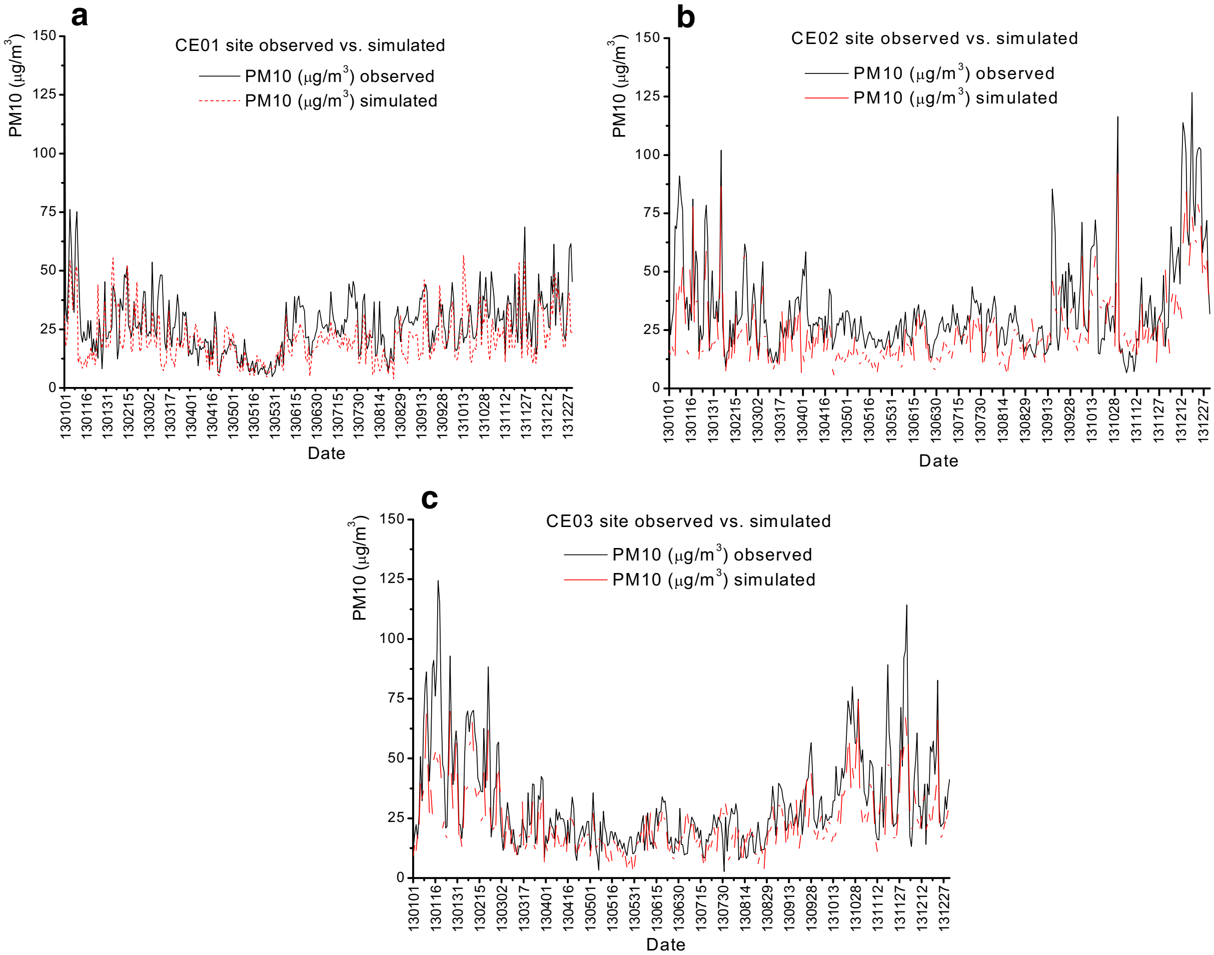


**Fig. 3** Time series comparison of observed versus modelled $PM_{10}$ concentration levels in the monitoring site CE01 (**a**), CE02 (**b**) and CE03 (**c**). *Black line*, observed $PM_{10}$ concentration (μg/m$^3$), *red line*, simulated $PM_{10}$ concentration (μg/m$^3$)

to represent an arbitrary, three-dimensional time-dependent concentration. It can be used to predict expected concentrations of emitted gases, particulates or hazardous releases (Sykes et al. 1999; Holmes and Morawska 2006). SCIPUFF have been developed by Titan's ARAP Group, and it has been recommended as an alternative model by the EPA, which can be used on a case-by-case basis for regulatory applications (Sykes et al. 1999). Daily simulations are performed using the observed meteorological conditions for the entire year of 2015.

## Model configurations input data

The SCIPUFF model has been initialized generating the terrain/land cover file. The simulation grid was as follows: minimum 350,000.00 E, 4,531,100.00 N; maximum 520,000.00 E, 4,752,400.00 N. The grid uses the UTM projection, time zone 33 T, and the datum is WGS-84. Particulate matter ($PM_{10}$) emissions from cement plants have been considered multiple point sources while emissions from urban mobility and other sectors have not been considered in the present study.

Emission sources are two cement plants. There are 90 $PM_{10}$ point sources emissions, and they have been introduced into the multiple point sources. Moreover, we have assumed that the industrial sources emit continuously 24 h/24 h over the whole year. For increased accuracy of the dispersion model, we have divided the time period in four quarters (1 Jan.–31 Mar.; 1 Apr.–30 Jun; 1 Jul.–30 Sep.; 1 Oct.–31 Dec.). The simulations have been carried

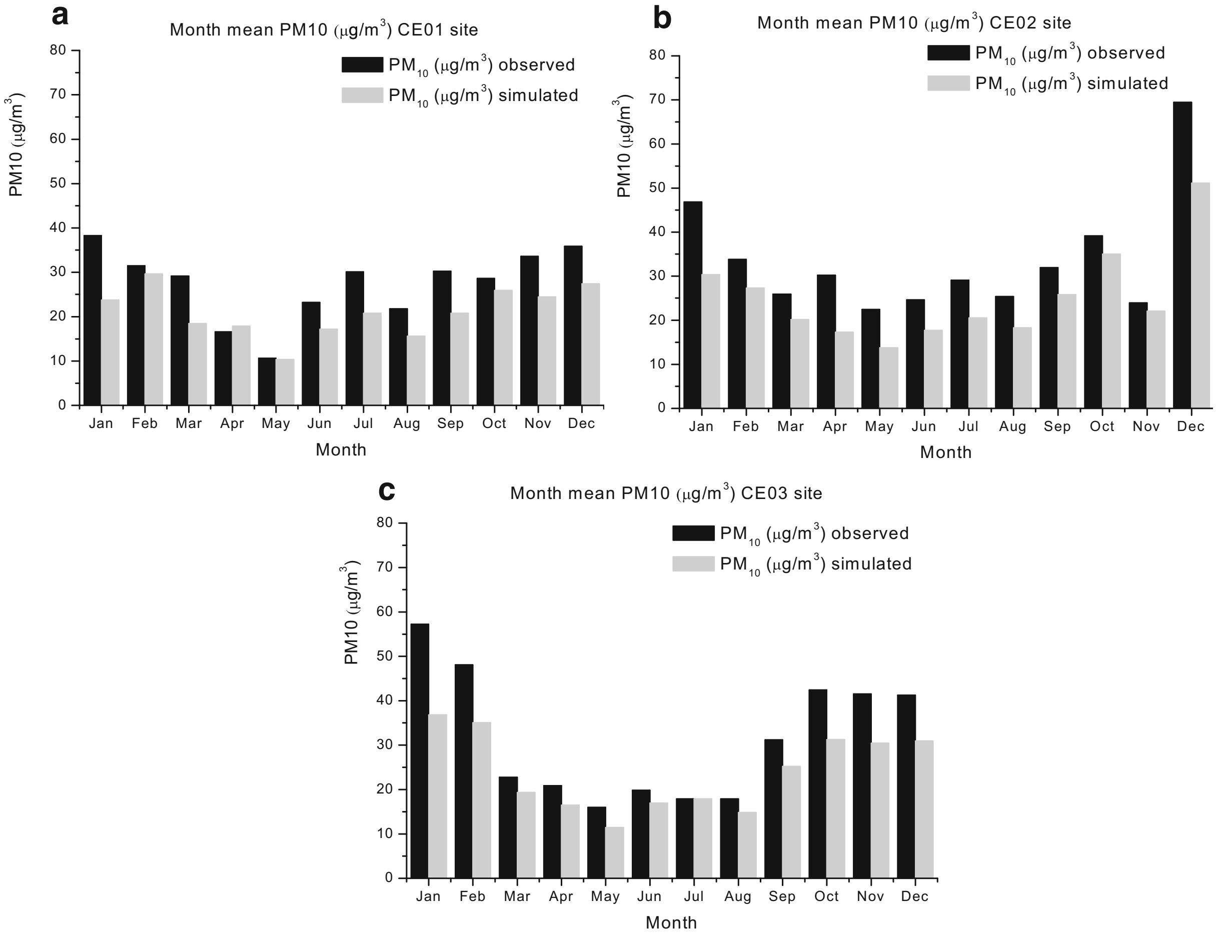


**Fig. 4** Months mean of the $PM_{10}$ concentration (μg/m³) trend for observed concentration (*black*) and for simulated concentration (*grey*) for the monitoring site CE01 (**a**), CE02 (**b**) and CE03 (**c**)

out under the model configurations of urban dispersion coefficients and elevated terrain without considering downwash effects.

In order to validate the $PM_{10}$ dispersion model, three air quality monitoring sites located into urban and sub-urban area of Caserta city, have been used (Table 1).

The $PM_{10}$ emissions rate have been calculated to be 18.29 kg/h according with the emission dates reported in the protection and improvement plans of the air quality of Campania Region, Italy and of the cement plants integrated pollution prevention and control authorizations (IPPC).

## Meteorological conditions

Vertical and surface weather observations, measured hourly in the monitoring site CE01 reported in Table 1, have been used to develop meteorological inputs for SCIPUFF. The meteorological parameters have been measured every hour from 1 January to 31 December and included temperature (°C), pressure (millibar), relative humidity (%), wind direction (degree), wind velocity (m/s) and precipitations (mm). Vertical meteorological profile has been measured every 6 h in the monitoring site CE01 (Table 1). Vertical profile has been established at 2500 m.

Figure 2 shows the wind roses plotted for every quarter. The prevalent wind directions of E (14.0–22.0 % of the time) and SE (10.5–12.0 % of the time) have been observed throughout the 1st and 4th quarters with wind speed of 1.0–5.0 m/s. During the 2nd and 3th quarters, the prevalent wind directions were SE (20.0–22.0 % of the time) and S (25.0–35 % of the time) with a wind speed of 2.0–5.0 m/s.

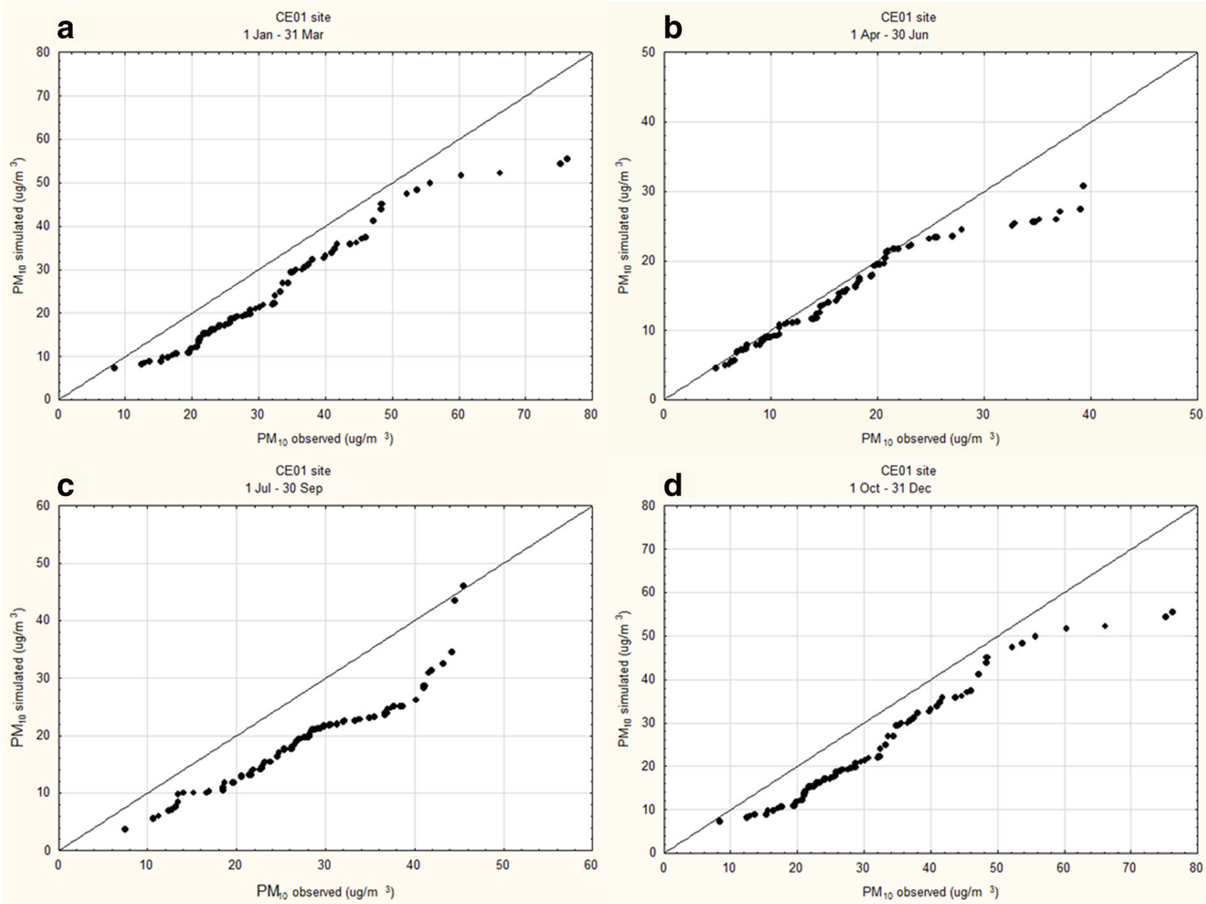


**Fig. 5** Q-Q plot observed versus modelled $PM_{10}$ concentrations ($\mu g/m^3$) for the validation periods at monitoring site CE01. **a** 1 Jan.–31 Mar. **b** 1 Apr.–30 Jun. **c** 1 Jul.–30 Sep. **d** 1 Oct.–31 Dec.

Temperatures in cold weather sometimes reach a minimum of 6.8 °C with maximum at almost 13.3 °C. In summer (June to September), the maximum temperature can go up to 28.0 °C. During the rainy season (July to September), the relative humidity is generally over 80 %.

## Validation parameters

The observed $PM_{10}$ concentrations in the monitored sites (Table 1) have been compared with simulated $PM_{10}$ concentrations, of the SCIPUFF model, in the same sites, for establishing the ability of the model to reproduce the measured concentrations in the city of Caserta.

The model performance and validation was evaluated using the statistical indicator recommended in the US Environmental Protection Agency (EPA) modelling guidance (Beck and Mulkey 1994).

The statistical indicators are as follows: index of agreement (IOA), normalised mean square error (NMSE), root-mean-square error (RMSE), mean normalized bias (MNB), bias reported in Eqs. 1–5 and quantile-quantile (Q-Q) plots (Rötter et al. 2012; Borrego et al. 2008).

$$\mathrm{MNB} = \frac{1}{N}\sum_{i=1}^{N} \frac{(\mathrm{Si{-}Oi})}{\mathrm{Oi}} \times 100 \quad (1)$$

$$\mathrm{IOA} = \frac{\sum\left(\mathrm{Si{-}\overline{Oi}}\right)^2}{\sum\left(\left|\mathrm{Si{-}\overline{Oi}}\right| + \left|\mathrm{Oi{-}\overline{Oi}}\right|\right)^2} \quad (2)$$

$$\mathrm{NMSE} = \frac{\overline{\left(\overline{\mathrm{Oi}}{-}\mathrm{Si}\right)^2}}{\overline{\mathrm{Oi}}\overline{\mathrm{Si}}} \quad (3)$$

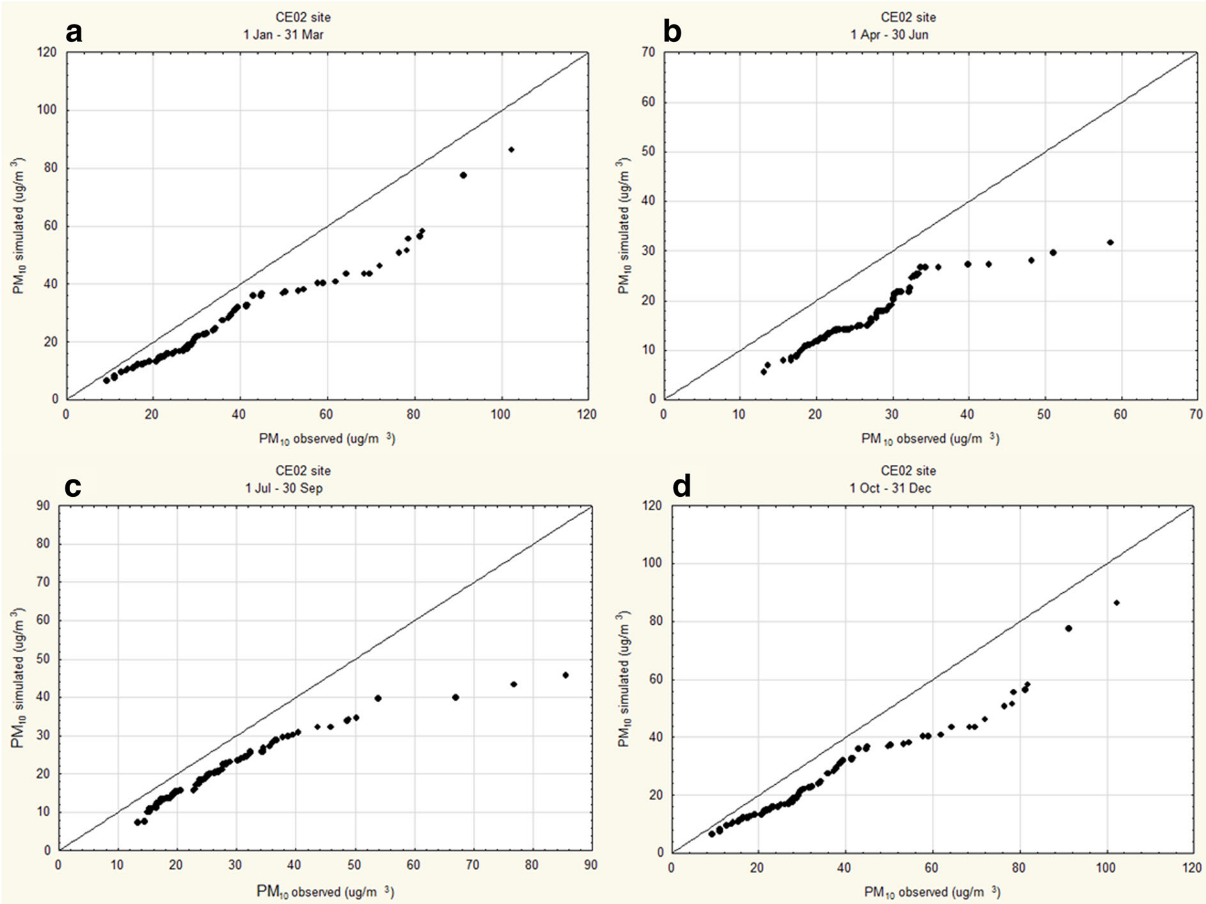


**Fig. 6** Q-Q plot observed versus modelled $PM_{10}$ concentrations (μg/m$^3$) for the validation periods at monitoring site CE02. **a** 1 Jan.–31 Mar. **b** 1 Apr.–30 Jun. **c** 1 Jul.–30 Sep. **d** 1 Oct.–31 Dec.

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\mathrm{Si}-\overline{\mathrm{Oi}}\right)^2} \quad (4)$$

$$\mathrm{Bias} = \frac{1}{N}\times\sum_{i=1}^{N}(\mathrm{Si}-\mathrm{Oi}) \quad (5)$$

Where, $N$ represents the number of data, Si and Oi are the predicted and observed concentrations, respectively, $\overline{\mathrm{Si}}$ and $\overline{\mathrm{Oi}}$ are the mean values of the predicted and observed concentrations, respectively and σSi and σOi are the standard deviations of the predictions and observations.

The MNB has been calculated from the difference between the modelled and observed values, normalised by the observed value (퀵퀳) and have been reported as a percentage.

IOA varies from 0.0 to 1.0. In a perfect model, the bias is equal to zero. Positive or negative value indicates that the model is under predicting or over predicting, respectively. The NMSE affirm the scatter in the entire data set, and smaller values of NMSE indicate better model performance. RMSE value should be near to zero for a good precision.

## Observed $PM_{10}$ concentrations

Three observed concentrations of $PM_{10}$ have been used to assess the results from SCIPUFF. They are relative to different locations of the city of Caserta: sites CE01 and CE02, in urban area and site CE03 in sub-urban area (see Table 1).

The $PM_{10}$ concentrations at CE01 and CE02 sites have been collected at 1 h interval from January 1 to

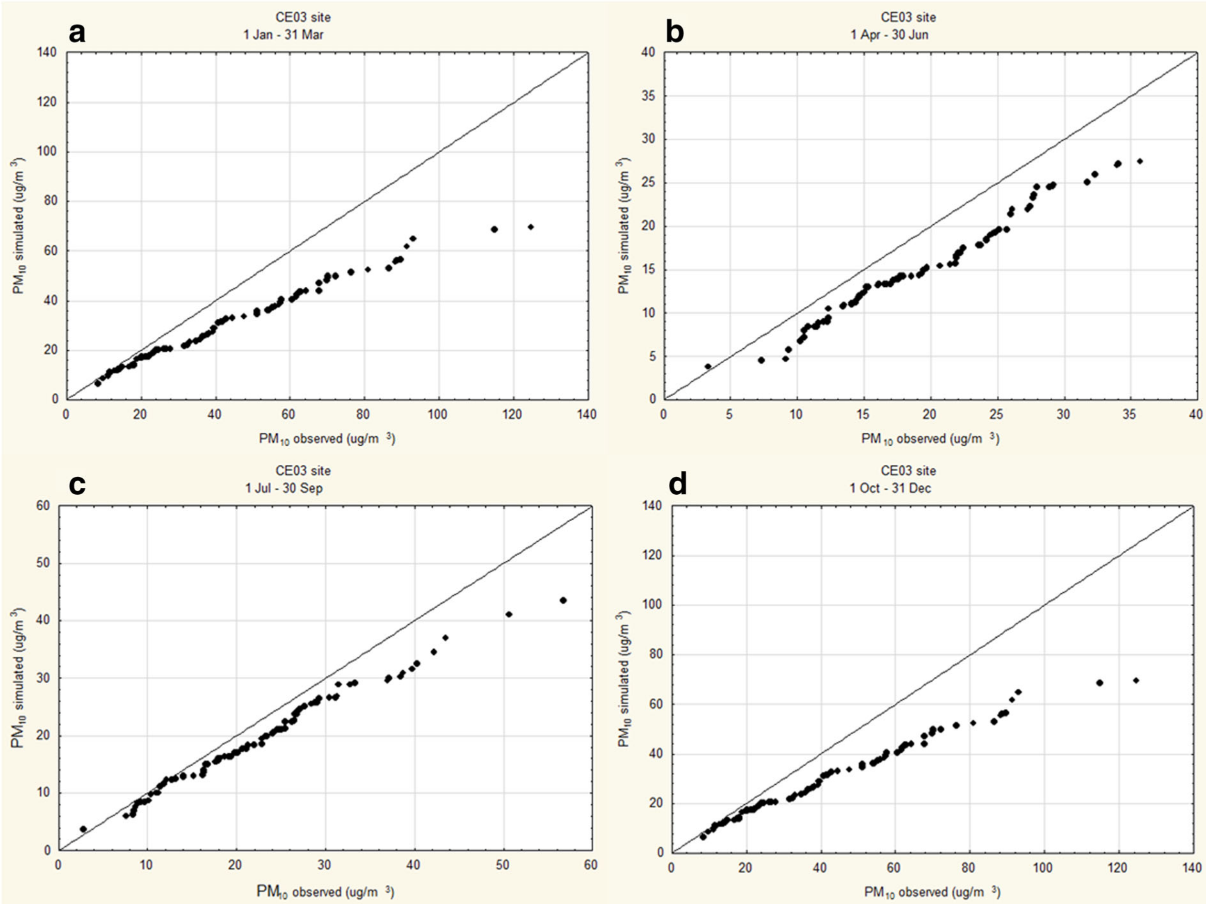


**Fig. 7** Q-Q plot observed versus modelled $PM_{10}$ concentrations (μg/m$^3$) for the validation periods at monitoring site CE03. **a** 1 Jan.–31 Mar. **b** 1 Apr.–30 Jun. **c** 1 Jul.–30 Sep. **d** 1 Oct.–31 Dec.

December 31 using fixed monitoring stations of the Regional Environmental Protection Agency (ARPA Campania). Details on data recorded at the monitoring stations are online (www.arpacampania.it). For the CE03 site, the determination of $PM_{10}$ in daily samples was performed gravimetrically. Glass fibre filters, 47 mm diameter (Whatman, Germany), were used to collect aerosol. These filters were preheated at 300 °C for 3 h before use to lower their water and organic matter blank values. $PM_{10}$ was collected using a high-volume sampler (TCR Tecora Skypost) with a size selective inlet (LVS $PM_{10}$) and a flow of 2.3 m$^3$/h. The filters were weighed twice before and after sampling using a microbalance with 0.01 mg sensitivity to obtain $PM_{10}$ concentration. The specific procedure has been reported in previous paper (Iovino et al. 2013).

## Results

### SCIPUFF results validation

Figure 3 shows the yearly time-ßseries for both the observed and modelled daily average $PM_{10}$ concentrations for the three measurement stations CE01 (plot a), CE02 (plot b) and CE03 (plot c). The predicted temporal variations of $PM_{10}$ concentrations show a good agreement with the measured observations. It can be observed that the model results generally follow the trend of the measurements, including extreme episodes of high $PM_{10}$ concentrations during the winter (December, January and February) which were correctly simulated by the model. The model tends to underestimate both the maximum and minimum observed $PM_{10}$ concentrations values, as shown in the figures.

**Table 2** Statistical model evaluation parameters of the predicted and measured $PM_{10}$ concentrations at the station CE01, CE02 and CE03

| | 1 Jan.–31 Mar. | 1 Apr.–30 Jun. | 1 Jul.–30 Sep. | 1 Oct.–31 Dec. |
|---|---|---|---|---|
| Model point CE01 | | | | |
| Mean (μg/m$^3$) (observed) | 33.05 | 16.76 | 27.34 | 32.70 |
| Mean (μg/m$^3$) (simulated) | 23.76 | 16.23 | 21.50 | 19.26 |
| Max (μg/m$^3$) (observed) | 221.50 | 39.17 | 45.46 | 68.70 |
| Max (μg/m$^3$) (simulated) | 55.52 | 30.90 | 46.12 | 56.66 |
| *N* | 90 | 91 | 92 | 92 |
| RMSE (μg/m$^3$) | 14.40 | 5.91 | 11.62 | 12.62 |
| MNB (%) | −16.86 | −2.95 | −27.68 | −16.89 |
| IOA | 0.996 | 0.997 | 0.995 | 0.996 |
| NMSE | 0.08 | 0.01 | 0.13 | 0.05 |
| Bias | −9.23 | −1.67 | −8.30 | −6.74 |
| Model point CE02 | | | | |
| Mean (μg/m$^3$) (observed) | 35.57 | 25.74 | 28.78 | 44.42 |
| Mean (μg/m$^3$) (simulated) | 25.90 | 16.23 | 21.50 | 36.23 |
| Max (μg/m$^3$) (observed) | 102.03 | 58.53 | 85.37 | 126.75 |
| Max (μg/m$^3$) (simulated) | 86.57 | 31.67 | 45.89 | 91.83 |
| *N* | 90 | 91 | 92 | 92 |
| RMSE (μg/m$^3$) | 15.25 | 12.09 | 12.30 | 18.31 |
| MNB (%) | −24.15 | −35.19 | −19.56 | 0.49 |
| IOA | 0.996 | 0.994 | 0.996 | 0.997 |
| NMSE | 0.10 | 0.22 | 0.09 | 0.04 |
| Bias | −9.68 | −9.52 | −7.28 | −8.19 |
| Model point CE03 | | | | |
| Mean (μg/m$^3$) (observed) | 42.52 | 18.89 | 22.24 | 41.77 |
| Mean (μg/m$^3$) (simulated) | 30.23 | 14.95 | 19.26 | 30.88 |
| Max (μg/m$^3$) (observed) | 124.53 | 35.64 | 56.63 | 114.28 |
| Max (μg/m$^3$) (simulated) | 69.74 | 27.51 | 43.67 | 74.08 |
| *N* | 90 | 91 | 92 | 92 |
| RMSE (μg/m$^3$) | 19.13 | 6.70 | 8.90 | 15.90 |
| MNB (%) | −21.44 | −13.99 | 4.70 | −21.18 |
| IOA | 0.997 | 0.996 | 0.996 | 0.997 |
| NMSE | 0.12 | 0.06 | 0.02 | 0.09 |
| Bias | −12.29 | −3.94 | −2.99 | −10.89 |

Figures 4a–c show a detailed histogram of the observed and simulated $PM_{10}$ monthly mean concentrations for the three monitoring sites CE01 (plot a), CE02 (plot b) and CE03 (plot c). It can be seen that in all cases, the model results underestimated the monitored concentrations. This result can be explained because the cement factories are assumed to be the only source of emissions. The simulations do not consider emissions from vehicular traffic and from domestic fuel use contributions. It is expected that the difference between simulated and observed concentrations is precisely due to the absence of these additional sources.

## Evaluation of observed and simulated concentrations using Q-Q plots

Figures 5, 6, and 7, show the Q-Q plots of the data for each quarter of the year, respectively.

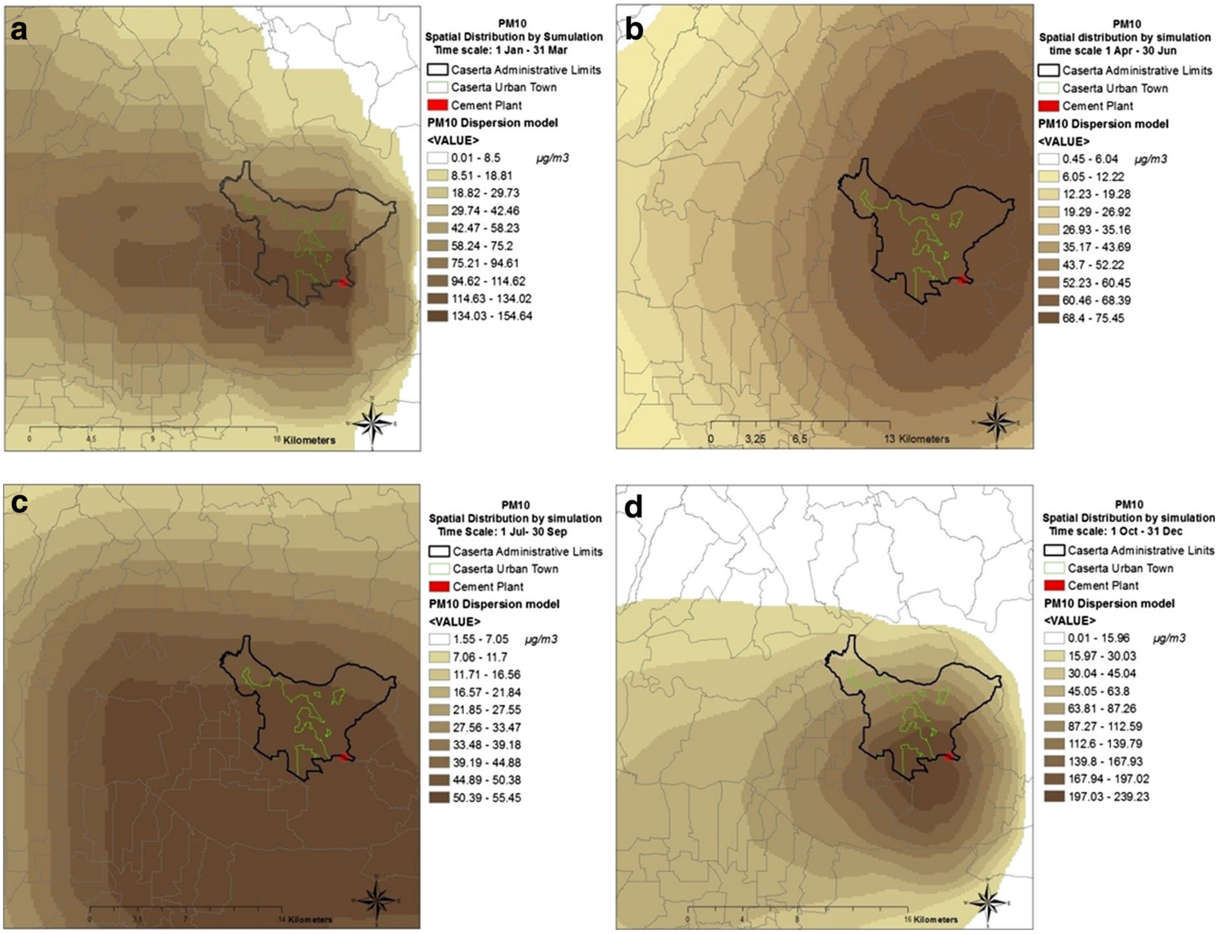


**Fig. 8** SCIPUFF models. Predicted surface $PM_{10}$ concentration (μg/m$^3$) field during 1 Jan.–31 Mar. (**a**), 1 Apr.–30 Jun. (**b**), 1 Jul.–30 Sep. (**c**) and 1 Oct.–31 Dec. (**d**)

The points in the Q-Q plot are positioned along the diagonal (1:1 line) if the two distributions are similar (Perry et al. 2005). As shown in the figures, the simulated and observed $PM_{10}$ concentrations are positioned along the diagonal, but the model are under-predicts the observed values, as it has also been reported by the statistical parameters (Table 2).

Figures 5, 6, and 7 show the Q-Q plot for daily averaged observed and estimated $PM_{10}$ concentrations for the 1st quarter (plot a), 2nd quarter (plot b), 3rd quarter (plot c) and 4th quarter (plot d) and for each of the three monitoring sites (CE01, CE02 and CE03). The plots show the tendency of the model to under-predict the observed concentration distributions.

The results of the statistical analysis have been reported in Table 2. All indicators should take values approximately equal to zero for a perfect modelling, as reported in the "Validation parameters" section. Measures of the bias, NMSE and RMSE indicate a good relationship between observed and estimated values. The RMSE values ranged between 5.91 and 19.13. MNB and bias parameters for all monitored sites have showed negative values (under-prediction concentration) except for some points in the monitored site CE02 (1 Oct.–31 Dec.) and CE03 site (1 Jun.–30 Sep.), that have a positive value (over-prediction of concentration) with values of 0.49 and 4.70, respectively. The NMSE and IOA are also used to evaluate model performance. The EPA guide reports that performance of the model can be acceptable if NMSE is <0.5 and IOA index is >0.5. NMSE values ranged between 0.01–0.13 in the CE01 station, 0.04–0.22 in the CE02 station and 0.02–0.12 in the CE03 station, indicating a good correlation between modelled and observed values.

The IOA is a measure of the aptitude of the model in forecasting variations about the observed mean. The IOA values have been high and ranged from 0.994 to 0.997 for all monitored sites, and they represent very good predictions. The SCIPUFF dispersion model results for each quarter are reported in Figs. 8a–d. The results show that throughout the year, the cement plants are responsible for a portion of the observed concentrations monitored in the city of Caserta. Wind velocity and direction are the main factors which cause the emissions of $PM_{10}$ from the cement factories to disperse along the territory of Caserta.

## Conclusion

The SCIPUFF model was used to study the impact on air quality ($PM_{10}$) caused by emissions at two cement plants located near the city of Caserta, Italy, during the entire year of 2015. Daily SCIPUFF simulations were performed using observed meteorological parameters, and the results were compared with measured concentration values at the three sites. Different statistical measures were used to assess the similarity between observed and simulated values. Results show a statistically significant agreement between SCIPUFF simulated and observed concentration values but point to a systematic under-prediction of the model. This under-prediction is caused by simulating the cement factories as the only sources of pollutants and by not taking into account additional sources like vehicular traffic, domestic fuel use and others.

The $PM_{10}$ concentrations are highest during winter, lower in autumn and spring and lowest during summer both for the observed and simulated concentration values. The statistical parameters and the Q-Q plots results show a statistical significance between simulated and observed concentrations. The model performance was found to be acceptable according to US EPA standards.

The results suggest that the cement plants are major emission sources of $PM_{10}$ pollution and are responsible for the air quality deterioration in the city of Caserta. The ability to accurately model and predict the ambient concentration of particulate matter (PM) is essential for effective air quality management and policies development.

**Acknowledgments** This work has been supported by the grant from P.O.R. Campania FSE 2007-2013–Project "TEMASAV" Technologies and environmental monitoring for the sustainability of wide areas. This research was also partially supported by the Office of Naval Research (ONR) award #N00014-14-1-0208 (PSU #171570).

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