# Application of the ISCST3 model to an industrial area: comparison between predicted and observed concentrations

M. Andretta[1], B. Leonzio[2], P. Lucialli[3] & S. Righi[2]
[1]*Montecatini Environmental Research Centre, Edison Group, Italy*
[2]*University of Bologna,*
*Interdepartmental Research Centre for Environmental Science, Italy*
[3]*Regional Agency for Prevention and Environment,*
*Department of Ravenna, Italy*

## Abstract

This study assesses the performance of the Industrial Source Complex Short Term (ISCST3) model in the industrial area of Ravenna, located in the North East of Italy. The ISCST3 model is based on a steady-state Gaussian plume algorithm. It has been developed by USEPA for assessing air quality impact from point, area, and volume sources.

In this work, ISCST3 was applied to simulate the air quality for both a short-term (one hour) and a long-term (annual) period.

The model performance has been evaluated by comparing predicted and measured concentrations of $NO_2$, $SO_2$, TPS (Total Suspended Particulate). The software has been tested using the data available from the industrial area of the town and measured by the air quality network of the local Environmental Protection Agency (ARPARER).

The model exhibits better performance for long-term than for short-term periods. Generally, simulation of $NO_2$ and TPS is very good with an accuracy between 30 and 50%. The ISCST3 shows lower performances for $SO_2$. It is interesting to note that the $SO_2$ concentration predictions, both short- and long-term, generally appear overvalued. This result could be due to an overestimation of industrial emission fluxes. A more precise estimation of the emission inventory could allow for a better modelling of the pollutant dispersion.
*Keywords: ISCST3 model, Gaussian model, air quality, air pollution, emission sources.*

WIT Transactions on Ecology and the Environment, Vol 91, © 2006 WIT Press
www.witpress.com, ISSN 1743-3541 (on-line)
doi:10.2495/RISK060181

# 1 Introduction

Both the monitoring and modelling of air pollution is essential to provide a picture of the damage humans are doing to the environment, and to enable pollution problems to be discovered and dealt with. Since the 1970s, local authorities are being encouraged to make assessments of local air quality (a local air quality review), through the monitoring of air pollutant emissions and atmospheric concentrations. In the last years the importance of numerical modelling of atmospheric physical and chemical processes has been increasingly recognised. At present, the European and National legislation stresses out the need of model application as a supplementary assessment method to reporting of monitoring data. The EU Directive 96/62/EC [1], that defines the legislative basis for assessment and management of air quality in European Union Member States, provides for assessment of air quality by measurement, modelling or use of both methods. It defines the means of achieving sustainability of air quality wherever this is good and improvement in polluted locations. In Italy, Directive 96/62/EC has been assimilated by Legislative Decree 351/1999 and Ministerial Decree 60/2002 [2, 3].

The evaluation of model performance is a matter of great interest, and it becomes particularly important when modelling is applied for a prediction exercise. Generally, model performance is evaluated by comparing measured and predicted concentrations. The Ministerial Decree 60/2002 permits the combined use of monitoring measures and predictions through atmospheric dispersion models when the relative error of predictions is minor or equal to the fixed values. In the present study we evaluate the performance of the ISCST3 as relative error, as required by Ministerial Decree 60/2002. We have simulated the air quality of Ravenna for both a short-term (one hour) and a long-term (annual) period. The performance evaluation is made comparing the results of ISCST3 model with hourly and annual observed values. Models have been applied to the main emissions in the industrial area of Ravenna, for the simulation of $SO_2$, $NO_2$ and PTS dispersion.

The Industrial Source Complex Short Term (ISCST) model is among the most used models for evaluation studies of air quality in the world. The ISCST is a gaussian plume dispersion model which predicts air concentrations downwind from point or area sources using emission rates and meteorological conditions as model inputs. Through Gaussian models, the concentration $C$ (in µg m$^{-3}$) is given by the formula:

$$\frac{C}{Q} = \frac{1}{2\pi\, u\, \sigma_y \sigma_z} e^{-\frac{y^2}{2\sigma_y^2}} \left[ e^{-\frac{(z-H)^2}{2\sigma_z^2}} + e^{-\frac{(z+H)^2}{2\sigma_z^2}} \right] \tag{1}$$

where: $Q$ is the strength of a continuous source (in µg s$^{-1}$) at effective height ($H$) above the ground; $u$ is the wind speed; $\sigma_y$ and $\sigma_z$ are standard deviations of the distribution $C$ in the $y$ and $z$ directions respectively. The coordinate $y$ refers to horizontal direction at right angles to plume axis with *y* equal to zero on the axis. The coordinate *z* is height above ground, which for the time being is assumed to be flat and uniform. The purpose of the last term is to account for reflection of the plume at the ground by assuming an image source at distance h beneath the ground surface.

The ISCST was originally developed in the 1970s [4]. The ISCST2 model was developed by the US EPA between 1989 and 1992 [5], and represented a major restructuring and reprogramming of the model code. The ISCST3 model is the latest version of the regulatory model ISCST and assesses pollutant concentrations from wide variety of sources associated with an industrial complex [6].

# 2 Materials and methods

## 2.1 Study area

The study was conducted in the industrial area of Ravenna, in north-eastern Italy. The site is located in flat, homogeneous terrain. In this area, the dominant action on weather conditions is performed by the sea and the wind-speed regime. In particular the wind rose of Ravenna area shows, during the winter, a prevalence of winds blowing from west-northwest, which allow industrial emissions to deviate from the town; on the contrary, during the summer, the breeze regime, due to the proximity of the sea, starts a strong turbulence, which, while allowing pollutants dilution also causes their partial re-suspension, thus emphasizing the presence of some pollutants (dusts). In the final analysis, the deposition of industrial pollutants may occur mainly during the winter, under dead calm conditions. Over the Ravenna territory, thermal inversions in altitude give rise to frequent and thick fog banks, which often do not dissolve not even during the day, thus persisting for several consecutive days; fogs frequency is equal to 9% of the total number of annual observations [7].

It should be noted that, emissions being equal, fogs cause an increase in concentrations at the ground level.

## 2.2 ISCST3 modelling

ISCST3 is a Gaussian plume model, which accepts a variety of source geometries and emissions schedules in order to compute ambient air concentrations and surface deposition fluxes at specified receptor points. The dispersion model runs omitted particle-phase deposition, plume depletion, and chemical decay in the air. Further details for the ISCST3 can be found in EPA [6]. The input data includes emission, air quality and meteorological data.

In this study, model performance was evaluated by comparing measured and predicted concentrations of $NO_2$ (nitrogen dioxide), $SO_2$ (sulphur dioxide) and PTS (Total Suspended Particulate). The model was applied to simulate the air quality for both a short-term (one hour) and a long-term (annual) period. The model performance is tested by the method required by Ministerial Decree

60/2002 [3]. In order to quantify the agreement between predicted (P) values and observed (O) data the modelling system must be evaluated statistically with the following formula:

$$E(\%) = \frac{C_o - C_p}{C_p} * 100$$

where E(%) is the relative error, $C_O$ is the observed concentration minus the background concentration and $C_P$ is the predicted concentration. The Ministerial Decree 60/2002 permits the combined use of monitoring measures and predictions through atmospheric dispersion models when the relative error of predictions is minor or equal than the values shown in table 1. Note that the permitted relative errors are differentiated for hourly and annual simulations.

Table 1: Maximum relative errors for combined use of monitoring measures and predictions permitted by Italian Ministerial Decree 60/2002.

| SIMULATION | ERROR | |
|---|---|---|
| | $NO_2$ $SO_2$ | PTS |
| Hourly averages | 50% | (a) |
| Annual averages | 30% | 50% |

(a) At present there is no reference value.

This particular study does not consider the performance of the modelling system under extreme episodic conditions which could be the focus of future investigations.

## 2.3 Emission inventory

The emissive scenario taken into account includes nineteen stacks, corresponding to the main industries of the Ravenna chemical pole. In particular, all the emissions exceeding by 10% the highest emission for each single pollutant have been taken into account. Emission rates were assumed constant throughout the year. Specific information on production capacities, stack emission characteristics including stack height, diameter, flue gas temperature and exit gas velocity were drawn from the authorizations on emissions provided to the local Environmental Protection Agency (ARPARER) for the year 2001.

## 2.4 Air quality monitoring

In this paper simulations are compared with measurements from several monitoring stations in Ravenna in the year 2001 [8]. The network contains ten permanent multi-component stations. The location of the air quality monitoring stations in the Ravenna Area and the pollutants monitored in 2001 are presented in Fig. 1. The measurements at these stations were conducted by the Regional Agency for Prevention and Environment. Most of these stations were located with the purpose of monitoring ‘‘hot spots’’ in the vicinity of the busiest traffic environments, or major local energy production sources. We have selected the stations of "Sapir", "Germani" and "Marina di Ravenna" (in the following "Marina") for the comparison between predicted values and observed data. The criteria for selecting these stations were that these are located surrounding the chemical pole, i.e., the main source in the Ravenna Area of $NO_2$, $SO_2$ and PTS.

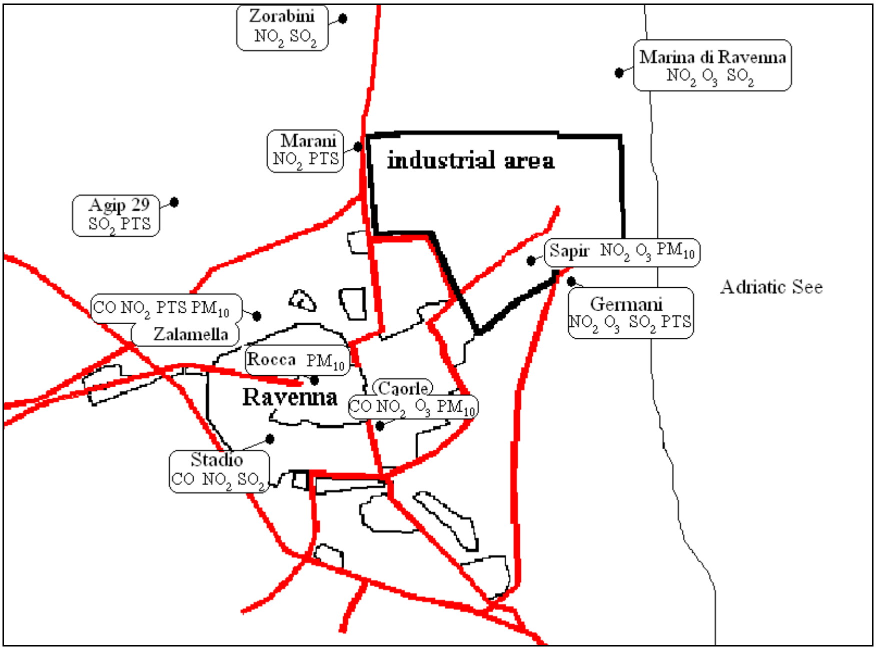


Figure 1: Location of the air quality monitoring stations in the Ravenna Area in 2001. The labels show the name of the station and the pollutants that are measured continuously. The figure also shows the location of the industrial area. All the stations are permanently located.

The ISCST3 model used in this effort will predict only the pollutant concentrations in the air that are due to emissions from the industrial area. Therefore, a procedure had to be developed to subtract the "background" of $NO_2$, $SO_2$ and PTS due to the "non" industrial sources. Only then can one appropriately compare predicted and observed concentrations. Background concentrations were differently estimated for short- and long-term simulations. In the case of short-term simulations, background concentrations were assumed equal to the concentrations measured by the monitoring station located "upwind" to the industrial area and the comparison was made between the measured concentrations by the monitoring station located "downwind" to the industrial area and the predicted values. In the case of long-term simulations, background concentrations were calculated from the total pollutant concentrations knowing that in this Region the industrial contribute to $NO_2$ concentration is 29% of the total, to $SO_2$ concentration is 84% of the total and to PTS concentration is 45%

of the total. The comparison was made between the measured concentrations, after subtracting the "non" industrial contributions, and the predicted values.

### 2.5 Micro-meteorology

We have selected the hourly meteorological data for the location of Ravenna, that have been pre-processed using the CALMET to be used in this study, as they contain relevant derived meteorological parameters, such as, e.g., the Monin–Obukhov length and the mixing height. Pre-processed meteorological data input of ISCST3 substitutes a 1.00 m/s wind speed and the previous direction for the calm hour [9]. According to the criteria suggested by the United States Environmental Protection Agency, these data have been converted into a suitable format for the ISCST model. The 8760 records indicated: wind origin (in degrees as against the NORTH); wind speed (m/s); ambient air temperature (°K); Pasquill-Gifford stability class (1 to 6); height of the mixing layer in rural areas (m). As to simulations, three stability classes have been considered: A (representative of the atmospheric instability), D (representative of the atmosphere neutrality conditions) and F+G (representative of the atmosphere stable conditions).

Table 2: The model performance evaluation for short-term simulations of $NO_2$ concentrations (hourly averages).

| Station | Stability class | Values ($\mu g/m^3$) | | |
|---|---|---|---|---|
| | | Observed | Predicted | E (%) |
| Sapir | A | 47 | 32 | 47 |
| Sapir | D | 9 | 13 | -32 |
| Sapir | F+G | 58 | 49 | 19 |
| Germani | A | 9 | 6 | 47 |
| Germani | D | 19 | 14 | 33 |
| Germani | F+G | 54 | 61 | -11 |
| Marina | A | 30 | 15 | 98 |
| Marina | D | 14 | 9 | 50 |
| Marina | F+G | 14 | 9 | 52 |

## 3 Results and discussion

First of all, two important considerations for evaluating the comparison of predicted and measured air concentrations are: (1) having a little number of dates for short-term simulations is a small sample size, and (2) one can expect the ISCST3 to perform better for longer averaging times as compared to shorter averaging times. Short-term simulations make Gaussian models much more sensitive to the assumption of steady state, homogeneous wind flow. It would be fair to conclude that the paired comparisons of predicted and observed 1-h air concentrations are severe tests of model performance.

The final results of the model performance evaluation for short-term simulations have been presented in Tables 2–4. The results for $NO_2$ are presented in Table 2, those for $SO_2$ in Table 3, and those for PTS in Table 4. For all three pollutants, the results have been presented for each stability class; these can be used for evaluating the class-to-class variation of the results.

Table 3: The model performance evaluation for short-term simulations of $SO_2$ concentrations (hourly averages).

| Station | Stability class | Values ($\mu g/m^3$) | | |
|---|---|---|---|---|
| | | Observed | Predicted | E (%) |
| Sapir | A | 0.5 | 2.9 | -83 |
| Sapir | D | 1.3 | 2.2 | -41 |
| Sapir | F+G | 0.3 | 9.0 | -97 |
| Germani | A | 5.0 | 4.2 | 18 |
| Germani | D | 0.25 | 5.6 | -95 |
| Germani | F+G | 0.07 | 5.0 | -99 |
| Marina | A | 1.0 | 4.3 | -77 |
| Marina | D | 0.6 | 16 | -90 |
| Marina | F+G | 2.5 | 5.8 | -57 |

Table 4: The model performance evaluation for short-term simulations of PTS concentrations (hourly averages).

| Station | Stability class | Values ($\mu g/m^3$) | | |
|---|---|---|---|---|
| | | Observed | Predicted | E (%) |
| Germani | A | 13 | 15 | -13 |
| Germani | D | 8.5 | 11 | -24 |
| Germani | F+G | 12 | 22 | -45 |

As mentioned above, for regulatory purposes, it is important that the model performances agree with the relative errors reported in Table 1. In particular, for short-term simulations the relative error must be less than 50%. In the case of $NO_2$ and PTS the model performances are quite good; generally, the relative error stays under 50%. On the other hand, the $SO_2$ predicted vales are overestimated in many cases and the model performances must be considered poor.

The final results of the model performance evaluation for long-term simulations are presented in Table 5.

Table 5: The model performance evaluation for long-term simulations (annual averages).

| Pollutant | Station | Values ($\mu g/m^3$) | | |
|---|---|---|---|---|
| | | Observed | Predicted | E (%) |
| $NO_2$ | Sapir | 30 | 24 | 26 |
| $NO_2$ | Germani | 38 | 29 | 30 |
| $NO_2$ | Marina | 61 | 45 | 34 |
| $SO_2$ | Sapir | 3.0 | 7.2 | -58 |
| $SO_2$ | Germani | 3.0 | 6.4 | -53 |
| $SO_2$ | Marina | 2.0 | 5.6 | -64 |
| PTS | Germani | 28 | 31 | -11 |

In the case of long-term simulations, the relative error must be less than 30% for $NO_2$ and $SO_2$ concentration predictions and less than 50% for PTS. The statistical measures indicate the good performance of ISCST3 model for the predictions of $NO_2$ and TPS. The model performances for $SO_2$ concentration predictions are less satisfactory.

The integration of input data with more detailed information on granulometric distribution and density of the particles and a more precise estimation of the TPS inventory could allow for a better modelling of the particulate dispersion.

At last, it is interesting to note that the $SO_2$ concentration predictions, both short- and long-term, generally appear overvalued. This result could be due to an overestimation of industrial emission fluxes. As a matter of fact, we have used the "authorised emissions" instead of "real emissions". This artefact would result in a substantial model overprediction, as the emission data are used as input in the model computations. Clearly, in this case the difference between the model predictions and the data would be caused by the experimental arrangement.

## 4 Conclusions

In this work, the ISCST3 model was applied to simulate the air quality for both a short-term (one hour) and a long-term (annual) period.

A general conclusion from this study is that the ISCST3 model can be a useful and fairly accurate tool of assessment in predicting $NO_2$, $SO_2$ and TPS concentrations in the Ravenna Area. Considering the average results, the results show improved performance for the long-term simulations, compared with the short-term simulations, irrespective of pollutants. This result is also to be expected, as the first ones are less influenced by the simplifications of the dispersion model.

A more precise estimation of the emission inventory could allow for a better modelling of the pollutant dispersion.

The study shall be useful in estimating the impact of future developmental activities and general growth projections with a stated level of confidence.

## References

[1] Council Directive 96/62/EC on ambient air quality assessment and management, Official Journal L296, 21/11/1996, p.0055–0063, European Commission, Brussels, 1996.

[2] Legislative Decree n° 351 of 4 August 1999 implementing EU Council Directive 96/62/CE laying down ambient air quality assessment and management. Italian Republic's official journal n° 241 of 13 October 1999, Italian Parliament, Rome, 1999.

[3] Ministerial Decree n° 60 of 2 April 2002 on pollutants in ambient air. Italian Republic's official journal n° 87 of 13 April 2002, Environment and Territory Ministry, Rome, 2002.

[4] Bowers, J.F., Bjorklund, J.R. & Cheney, C.S., Industrial Source Complex (ISC) Dispersion Model User's Guide. Volume I, EPA-450/4-79-030, U.S.

Environmental Protection Agency, Research Triangle Park, North Carolina 27711, 1979.

[5] Environmental Protection Agency, User's Guide for the Industrial Source Complex (ISC2) Dispersion Models - Volume I. EPA-450/4-92-008a, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina 27711, 1992.

[6] Environment Protection Agency, User's Guide for Industrial Source Complex (ISC3) Dispersion Model – Volume I. EPA-454/B-95-003a, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina 27711, 1995.

[7] Provincia di Ravenna, Settore Ambiente e Suolo, *Workshop tecnico su attività di controllo dell'inquinamento atmosferico - 3 maggio 1996* Quaderni dell'Ambiente, 1997.

[8] Environmental Protection Agency of Emilia-Romagna Region, Contributo all'elaborazione di piani e programmi ambientali: dati di qualità dell'aria. Report, 2001.

[9] U.S. Environmental Protection Agency, *Guideline on Air Quality Models (Revised) –Appendix W of CFR Part 51*, pp. 41837-41894, 1996.