

Model evaluation of particulate concentrations and depositions due to a steel plant: intercomparison of ISCST3 and CALPUFF

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1 Introduction

Currently, the high levels of particulate matter, both as total particulate (TSP) and fine particles (PM₁₀), are one of the main air pollution problems in Italian cities. In Brescia, a city in Northern Italy, the national “quality goal” for PM₁₀ (40 µg/m³ for the yearly average) has been exceeded both in 1999 and in 2000, and exceedances of the Regional warning and alarm levels for both TSP and PM₁₀ are common. Often the main contribution to particulate concentrations in urban areas is due to motor traffic, but in the case of Brescia an unusually high concentration of industries, two power plants and an urban waste incinerator, all located within the urban spread of the city, contribute significantly. Since Regional regulations assign responsibility for imposing short-term reduction measures during critical episodes to the Mayor, a reliable model is needed to evaluate the contribution to urban air pollution from the several stacks present.

ISCST3¹ is a widely used and well-tested gaussian model, but the area under study shows geographical and meteorological features that a simple gaussian approach cannot treat, such as the presence of complex terrain and calm winds. The possibility of using the more sophisticated lagrangian puff model CALPUFF² was therefore considered.

In this work, the two models have been compared with the purpose of analyzing the differences between the results for a possible future application to an area of 25X30 Km, including the urban area of Brescia and several neighboring towns. Most of the city and the area to the south are located in the flat land of the Po Valley, but the foothills of the Alps to the north reach elevations of up to 1100 m above sea level.

2 Method of comparison

In the work presented here, the two models have been applied to calculate concentrations and dry depositions of particulate matter emitted by a single point source. In a study by the U.S. EPA³, it was found that, in steady state conditions, without any space or time variations of meteorological regime, ISC3 and CALPUFF produce essentially the same concentrations. In a varying meteorological situation, on the other hand, the two models can differ, partly because of the intrinsic differences between the two approaches, but also because of how they deal with the hour-by-hour evolution of meteorological conditions. In order to emphasize the differences due only to the different modeling approaches, the study has been split into two phases. First, ISCST3 and CALPUFF were run with the same actual meteorological input file (ISC-like); then a more qualitative comparison was made between ISCST3 and the complete CALMET/CALPUFF modeling system, where CALMET⁴ is a diagnostic meteorological model. The source data are those of a steel plant located in the urban area of Brescia: an internal stack diameter of 5.4 m, an outflow velocity of 14.4 m/s, and an emission rate of 1.26 g/s. Stack height has been varied during the simulations.

The modeling domain is common to both models, and two different nested receptor grids were used, with grid spacing of 1 Km (644 gridded receptors) and 0.5 Km (675 receptors), respectively. The larger grid covers the entire area, while the smaller one, centered at the source, was chosen to detail differences near the stack.

2.1 Meteorological input files

Two types of meteorological files have been considered: one with a stationary and spatially uniform wind field, and another, produced by CALMET, with a three-dimensional wind field and a two-dimensional grid of micrometeorological variables. The EPA pre-processor PCRAMMET was used to build the uniform, ISC-like files, using data measured at the Air Force Base of Ghedi. Of the meteorological data obtained from the Air Quality Monitoring Network, only those measured at one of the stations (Mompiano) were considered reliable enough to be used for our purpose. CALMET files were therefore derived from the data of Mompiano and Ghedi. The upper air data were taken at Milan Linate. In order to study the behavior of ISCST3 and CALPUFF in various meteorological conditions, three one-week periods (without rain) were chosen:

- Week A (5-11 January 1998): typical winter situation with fog and many hours of calm winds.
- Week B (4-10 April 1998): spring conditions with moderate winds and a strong perturbation in the last two days.
- Week C (20-26 June 1998): high-pressure summer weather: strong insolation, high relative humidity, gentle winds.

2.2 Phase 1

When a single-station data file, with uniform meteorological fields, is used, CALPUFF and ISCST3 can be compared with very similar input conditions. In this phase of the comparison, the focus was on the differences due only to the two dispersion algorithms, and to the different handling of the meteorological evolution, emphasising CALPUFF non-stationary scheme. Terrain effects were not included. ISCST3 was implemented in the “regulatory default mode” and CALPUFF setup parameters were chosen so as to emulate this mode as closely as possible. By varying the dispersion regime and stack height, a detailed statistical analysis was performed for each of the three weeks, including residual analysis and evaluation of bias, normalized mean square error (NMSE), gross error, linear correlation coefficient, intensity and position of the maxima. For the analysis, the residual was defined as: $R = O_{ISC} - O_{CALPUFF}$, where O stands for the output parameter calculated.

A comparison matrix, for each week and for each grid, was created for first highest hourly concentrations, weekly average concentrations, and total depositions, combining different stack heights (35, 120, 250 m) and dispersion regimes (rural or urban).

2.3 Phase 2

A more qualitative comparison (only intensity and position of the peaks) was made between ISC3 and the complete CALMET/CALPUFF modeling system. In this case, ISCST3 was used with its own terrain adjustment option (COMPLEX 1), while CALPUFF took also advantage of the orography-modified wind field produced by CALMET. In order to emphasize some peculiar features of the puff model, five CALPUFF runs were considered for each week, each corresponding to a different combination of input options, namely the probability density function (*pdf*) for treatment of dispersion in the convective boundary layer, wind calm processing routine, calculation of dispersion coefficients,

and partial penetration of elevated inversion. In this case, unlike phase 1, stack height was kept constant (35 m) and ISCST3 was used only in the urban mode.

3 Results

3.1 Phase 1: CALPUFF with ISC-like input

In general, comparing the results of the two models used with uniform, ISC-like meteorological data, CALPUFF and ISCST3 show rather similar behaviors. Some differences should nevertheless be pointed out. Qualitatively, the spatial distribution of the weekly average concentrations produced by CALPUFF clearly shows the non-stationary nature of this model, which naturally lacks the gaussian plume instantly reaching the limits of the domain shown by ISC. Such a fact is less evident in week C, where several very unstable hours produce short-range high-impact areas for both models. Moreover, the time variation of hourly concentrations at a fixed receptor is smoother for CALPUFF than for ISCST3, because of the inertial effects (contributions to the current hour due to the previous ones) accounted for by CALPUFF.

For a quantitative comparison, a matrix was generated, as described above, containing the values of the statistical parameters calculated for each ISC/CALPUFF simulation. The results for the comparisons of the 1st highest concentrations calculated for week B over the large grid are shown in table 1, where bias, gross error, linear correlation coefficient (r), relative distance of the maxima (d), and the relative percentage deviation ($\Delta\%$) are summarized. In this case and in week C, the bias is always negative, indicating that CALPUFF tends to predict lower peak concentrations. Only in week A the ability of CALPUFF to describe dispersion in calm wind conditions leads to a large positive bias and values of $\Delta\%$ of up to 1074. The residual analysis confirms that the two models produce more similar outputs over the small grid, i.e. near the stack.

Table 1 Summary of the results of the statistical analysis (week B, big grid) for 1st highest hourly concentrations.

Run Conditions (regime/stack height)	d	$\Delta\%$	bias	gross error	r
RURAL / 35 m	0.0	-1.1	-0.39	0.46	0.710
RURAL / 120 m	4.2	-24.1	-0.37	0.46	0.688
RURAL / 250 m	0.0	-28.7	-0.36	0.54	0.675
URBAN / 35 m	0.0	-18.2	-0.40	0.46	0.829
URBAN / 120 m	0.0	-3.0	-0.37	0.41	0.789
URBAN / 250 m	0.0	-2.5	-0.33	0.38	0.783

Weekly average concentrations calculated by ISCST3 in low-impact areas are generally lower than those produced by CALPUFF, as indicated by the always positive bias values. The situation can be reversed in high concentration areas depending on meteorological conditions (see fig. 1a). Intensities and positions of concentration maxima are generally similar, except for three cases in rural regime. During the winter week, several successive hours of calm winds cause CALPUFF to predict a large area of low concentrations that ISC cannot reproduce.

The deposition maxima calculated by ISCST3 are up to 50% larger than those estimated by CALPUFF. Moreover, in all 18 cases, the linear correlation coefficient is nearly 1 and the bias is always negative (about -0.30). The scatter plot of fig. 1b exemplifies a general situation where the ratio of depositions (ISCST3/CALPUFF) is rather constant (about 1.5) over the entire domain. This is mainly due to the way the concentration values are estimated in the deposition algorithm.

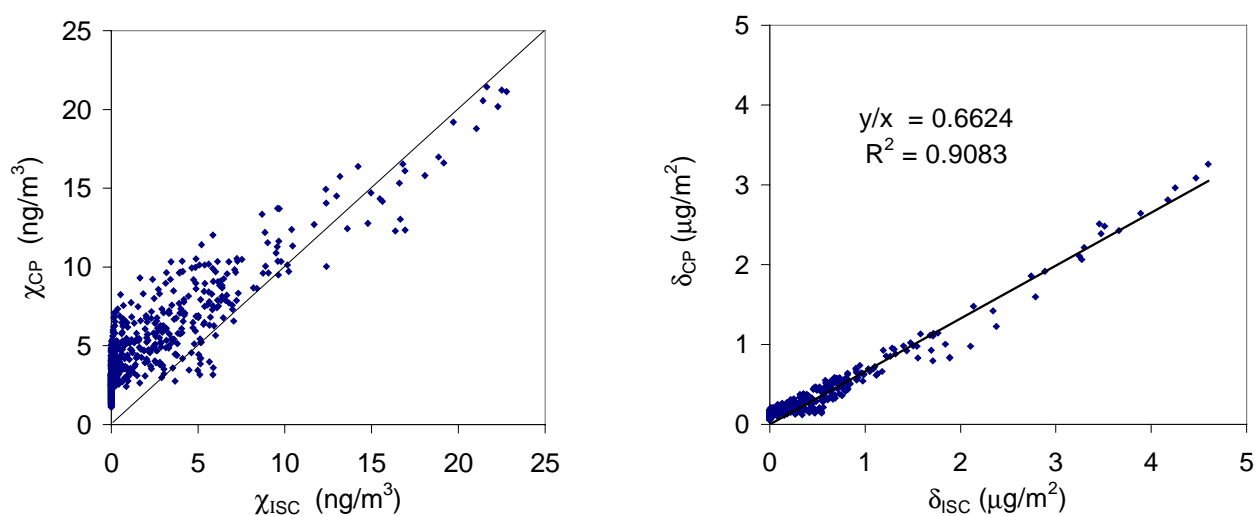


Figure 1 Scatter plot of predicted weekly average concentrations (left - a) and total weekly depositions (right - b) in a run of week A (small grid).

3.2 Phase 2

When the comparison is performed between ISC and the complete CALMET/CALPUFF system, the differences are inevitably more pronounced, both for the spatial distribution and for peak values. This is partly due to the different meteorological inputs and partly to the way dispersion coefficients are calculated. Weekly average and 1st highest hourly concentrations produced by CALPUFF in maximum impact areas are up to 90% lower than those calculated by ISCST3: in particular, the peak values predicted by CALMET/CALPUFF appear to be closer to those given by ISCST3 with rural dispersion regime. A summary of the statistics is given in table 2.

Table 2 Range of values for the relative distance of the maxima and percentage deviation.

	<i>1st highest hourly concentrations</i>		<i>Weekly average concentrations</i>	
	d	Δ%	d	Δ%
Week A	1.6 to 4.3	-64.8 to -42.7	1.1 to 2.7	-91.9 to -70.1
Week B	2.5 to 3.9	-83.1 to -76.9	0.7 to 0.7	-85.2 to -81.7
Week C	0.0 to 0.7	-67.0 to -24.2	0.5 to 0.7	-44.9 to -22.3

The most obvious differences in the spatial distribution can be found in the runs of week B, where the wind field constructed by CALMET produces a channeling effect into the valley that opens to the north of Brescia, as shown in the contour maps of fig. 2. Naturally, this effect is totally missing in ISC. Of the various input options considered, the one that yields the highest peak values is the use of Pasquill-Gifford and McElroy-Pooler dispersion coefficients; similar results are obtained when using both partial penetration of an elevated inversion and the pdf option, together with the dispersion coefficients calculated from the micrometeorological variables produced by CALMET. In general, switching the pdf option on yields higher maximum concentrations. As in phase 1, week C is the one in which the two models show fewer differences.

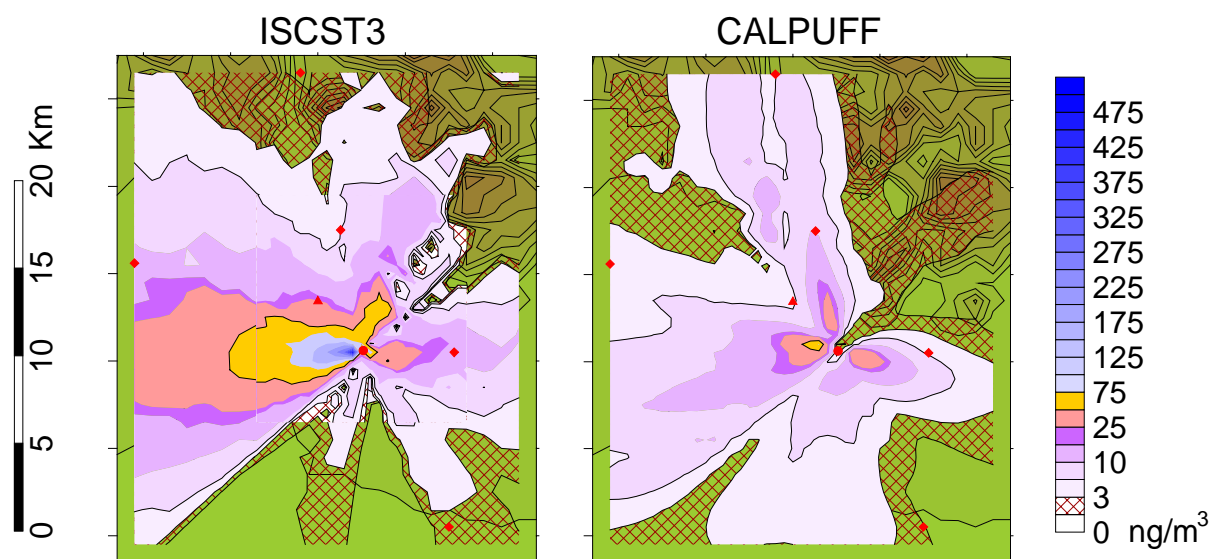


Figure 2 Contour plots of weekly average concentrations (week B) calculated by ISCST3 and CALPUFF (with pdf option).

Conclusions

When the two models are compared using the same meteorological input, the results are very similar. The main differences are observed in regime of calm winds especially when these conditions persist over several hours. In all cases, however, the non-stationary nature of CALPUFF is obvious, particularly farther away from the source. Deposition maps show the same behavior as the corresponding concentration maps, but the values predicted by ISCST3 are consistently higher, by a nearly constant factor of 1.5, than those obtained from CALPUFF. The values of the bias are typically lower over the small grid, showing a better agreement between the two models close to the stack.

From the comparison performed between ISC and the complete CALMET/CALPUFF modeling system, it appears that, for the situation under study, the best choice of input options might be the one yielding higher concentration values, closer to those calculated by ISCST3 in peak areas.

It must be emphasized that the availability of quality meteorological data for the area under study is of critical importance for a reliable performance of CALMET/CALPUFF.

References

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