INTERCOMPARISON, SENSITIVITY AND UNCERTAINTY ANALYSIS BETWEEN DIFFERENT URBAN DISPERSION MODELS APPLIED TO AN AIR QUALITY ACTION PLAN IN TUSCANY, ITALY

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Abstract: The Tuscan Regional Administration funded project MoDiVaSET-2 (MOdellistica DIffusionale per la VAlutazione di Scenari Emissivi in Toscana 2) was established in order to develop a decision support modelling system for implementing the Air Quality Action Plan for the metropolitan area of Florence, Prato and Pistoia. The objective of the work is to build an integrated meteorological and dispersion models for simulating and evaluating different future emission scenarios of PM_{10}, NO_x and NO_2 in the study area. With this purpose, the project included several 1-year long dispersion modelling applications and a detailed evaluation study, including sensitivity, validation and uncertainty analysis. Several dispersion models (ADMS-Urban, CALPUFF, CALINE4, SAFE AIR II and CALGRID) were applied and evaluated against monitoring data; the intercomparison between different models is crucial in order to develop reliable modelling techniques.
The obtained results point out the importance of including the following critical factors: smaller scale effects (monitoring stations are often located in complex environments; this implies a decrease in the effectiveness of validation studies) and secondary pollution (primary PM_{10} levels are only a small part of the total PM_{10} concentrations; much of the urban PM_{10} is actually produced by chemical transformations and other physical mechanisms, for example, resuspension).
In order to understand the weight of these issues, further modelling options (full chemistry and street canyon simulations) were investigated by using CAMx and smaller scale nested models.
All the factors listed above affected the evaluation work. However, this does not alter the validity of the scenario analysis, because it is based on the differences between calculated primary pollutants concentrations.

Key words: *Urban air quality model, model evaluation, uncertainty, validation, scenario analysis.*

1. INTRODUCTION

The work presented in this paper has been carried out in the framework of the MoDiVaSET-2 project (MOdellistica DIffusionale per la VAlutazione di Scenari Emissivi in Toscana 2). The project, funded by the Regional Administration of Tuscany, is aimed at evaluating different emission scenarios (2003-2012) of PM_{10} and NO_2 in the metropolitan area of Florence, Prato and Pistoia.

The objective of the project is to develop an integrated meteorological and dispersion modelling system which can be reliably used by administrators and policy makers in order to understand the weight of the different emission sources (road traffic, industrial sites and domestic heating) and establishing the efficiency of the environmental actions that could be adopted to ensure compliance with the air quality limits in the Air Quality Action plan. With this aim, in addition to the scenario analysis, the project also included several long-term (1-year long) dispersion modelling applications and a detailed evaluation study (sensitivity, validation and uncertainty analysis), which is often neglected in similar applications, despite its importance.

2. DISPERSION MODELLING APPLICATIONS

The simulations were mainly carried out using ADMS-Urban. In order to compare results from different models, simulations were also performed by means of CALGRID (grid source), CALPUFF (point sources), CALINE4 (line sources), and SAFE_AIR_II (point and line sources). All the simulations were realized without considering chemistry mechanisms, except for NO_2, where the NO_x-NO_2 correlation of Derwent and Middleton (1996) was applied. Further modelling options (full chemistry simulation and street canyon) were investigated by using CAMx and the street canyon model included in ADMS-Urban.

The full year 2002 time period was chosen, using a 1-hour time step, thereby all models were applied in a long-term mode. Measurements from six meteorological stations within the study domain (Baciacavallo, Monte Morello, Empoli-Ridolfi, Montale, Firenze-Ximeniano and Peretola Airport) were used as input, while vertical profiles of wind and temperature were retrieved from the RAMS forecasting system archive of CNR-IBIMET/LaMMA (see also Corti et al., 2006). A suitable scaling to the 1×1 km^2 final working resolution was then performed by using the CALMET meteorological model. The results were directly used as input for the CALGRID and CALPUFF simulations, while a further elaboration proved to be necessary for the other models. The domain was divided in 32 sub-domains for the CALINE4 simulations, using a single CALMET point for each sub-domain. 8 of these points were also used as input for the SAFE_AIR_II own meteorological preprocessor. The same methodology was applied to ADMS-Urban, but using only one CALMET point.

The study area is 49×40 km^2 sized. For the evaluation study, emissions were retrieved from the Tuscan Regional Emission Source Inventory (IRSE-RT, 2001) according to a hour-by-hour time disaggregation. PM_{10} (primary only), NO_X and SO_X were the chosen pollutant species. Three source categories have been considered: main point sources (stacks of the main industries), main line sources (motorways), and other sources treated as grid area sources. A newer emission source inventory was used in the scenarios analysis (IRSE-RT, 2004), and the grid area sources were further divided in four subcategories: small industries, local road traffic, domestic heating and other sources. Area emissions were provided according to a 1×1 Km^2 spaced cell grid exactly matching the computational one used by the meteorological and dispersion models. A total number of 1960 grid cells was used.

The regional background concentrations were included in the simulations using the monitored concentrations of the peripheral background site of Livorno-Maurogordato; it is acknowledged by the regional administration as the reference regional background site (see PATOS project, Particolato Atmosferico in TOScana).

3. MODEL EVALUATION

The model evaluation was performed in order to evaluate simulation results and compare the different approaches used within the project. The results of the simulations were compared to measured data during year 2002 by the monitoring networks of the three Provinces involved: Florence, Prato and Pistoia. 25 monitoring stations are present in the study area: 14 background, 9 roadside and 2 industrial sites. The evaluation work included: sensitivity study, validation exercise and uncertainty analysis.

The statistical indices used for the sensitivity study and the validation exercise are derived from the BOOT software (Hanna, 1989) and the Model Validation Kit (MVK, Olesen, 1995, 2005). Furthermore, two other indices originally proposed by Poli and Cirillo (1993) were used. The resulting statistical set is similar to that applied by Canepa and Builtjes (2001): mean (MEAN), bias (BIAS), fractional bias (FB), geometric mean bias (MG), standard deviation (SIGMA), fractional standard deviation (FS), linear correlation coefficient (COR), fraction within a factor of 2 (FA2), normalised mean square error (NMSE), geometric variance (VG), weighted normalised mean square error of the normalised ratios (WNNR), and normalised mean square error of the distribution of normalised ratios (NNR).

Chang and Hanna (2004) introduced acceptability criteria for some of the statistical indices provided by the BOOT software, basing on an extensive literature review. They proposed the following criteria for a "good" model: FA2>0.5; -0.3<FB<0.3; NMSE<4.

Sensitivity study of ADMS-Urban results

Hourly and annual mean concentrations of NO_2 have been calculated at each background site for three scenarios plus the base scenario. These are: scenario D1 (parameter changed: constant average emissions data instead of hourly emission values), scenario D2 (parameter changed: minimum Monin-Obukhov length = 50 m instead of 30 m), and scenario D3 (parameter changed: meteorological input data from the Baciacavallo measuring station instead of the CALMET point). Calculated concentrations and the statistical indices described previously have been compared one to another and to the monitored values. Only statistics based on annual mean concentrations are reported in Table 1 for brevity.

Table 1. Statistical indices based on annual mean concentrations of NO_2. Model performances are defined acceptable if FA2>0.5, -0.3<FB<0.3 and NMSE <4 ("acceptability" criteria of Chang and Hanna, 2004).

NO2		MEAN [μgm^{-3}]	FB	SIGMA	FS	COR	FA2	NMSE	WNNR	NNR
Background sites	Measurements	36.67	0.00	8.95	0.00	1.00	1.00	0.00	0.00	0.00
	BASE SCENARIO	20.03	0.52	9.74	-0.08	0.16	0.47	0.46	0.49	0.39
	SCENARIO D1	28.97	0.23	10.93	-0.20	0.38	1.00	0.17	0.17	0.14
	SCENARIO D2	20.86	0.55	8.89	0.01	0.33	0.50	0.47	0.50	0.43
	SCENARIO D3	29.92	0.20	10.57	-0.17	0.39	0.93	0.15	0.15	0.13

Results proved to be particularly sensitive to the meteorological input. In order to find the most reliable meteorological measuring station, further sensitivity study with different meteorological input data (Baciacavallo, Ximeniano and Monte Morello stations) was performed and showed that Baciacavallo site is the most suitable.

Validation exercise

Before beginning the calculation of the various statistical indices, a first simple comparison between the results was done using scattering plots of the calculated annual average concentrations and maximum hourly or daily concentrations. The plots are not reported here for brevity.

Statistics described previously have then been calculated based on annual mean concentrations for each site, first for the background site, then the roadside and all the sites together. Only results about concentrations of NO_2 and PM_{10} are reported in Table 2 for brevity.

The statistical analysis confirms the result obtained in terms of scattering plots. Good performances are obtained for nitrogen and sulphur oxides in the background sites, while performance values for PM_{10} and for the roadside sites are rather low and provided underestimated values. The acceptability criteria proposed by Chang and Hanna (2004) are verified for SO_2, NO_2 and NO_X values in the background sites, although Chang and Hanna's results are referred to research level measurements. The statistical indices were applied also to the maximum and to the time series of the calculated/measured hourly mean concentrations. Results are not reported here for brevity, but they substantially confirm the previous results, even if the calculated values are obviously poorer than for the annual mean concentrations.

As expected, the background sites results provided better performances than the roadside ones; this is due to the fact that the modelling systems used did not consider the small scale effects. These effects are fundamental as far as roadside sites are concerned, often located in complex environments and characterized by high local traffic emissions. This implies that the statistical analysis done for the background sites are the most representative of the model performances. A possible way to investigate the concentrations at the roadside sites would be to include smaller scale nested model, for example street canyon models. In order to demonstrate the feasibility of this approach, the street canyon module of ADMS-Urban was applied with encouraging results to one of the roadside site inside the study area (FI-Mosse). The major obstacle to an extensive use of this approach is the lack of reliable traffic volume data for the entire study area. Results of this study will be presented at the conference.

The PM_{10} results showed a systematic underestimation of the concentrations; this is due to the fact that primary PM_{10} levels are only a small part of the total PM_{10} concentrations; much of the urban PM_{10} is actually produced by chemical transformations. In order to overcome this problem, full chemistry applications were investigated using the CAMx model. The statistical analysis (see Tab. 2) provided poor results for every pollutants (see also uncertainty analysis); the acceptability criteria proposed by Chang and Hanna (2004) are not verified for any pollutant, especially for NO_2 and SO_2. The PM_{10} estimations, although better than in the inert approach, are not satisfactory. The unsatisfactory results are probable due to the lack of reliable input data (speciation of VOC emissions, turbidity, ozone column density, water vapour concentrations) needed for the application of the CAMx's chemistry module.

Table 2. Statistical indices based on annual mean concentrations of NO_2 and PM_{10} for the background, the roadside and all available sites. Comparison between CALGRID-CALPUFF-CALINE4 (CGPL), CALGRID-SAFE AIR (CGSA), ADMS-Urban (ADMS), CAMx models and the monitoring network data (Measures). Model performances are defined acceptable if FA2>0.5, -0.3<FB<0.3 and NMSE <4 ("acceptability" criteria of Chang and Hanna, 2004.

NO_2		MEAN [μgm^{-3}]	FB	SIGMA	FS	COR	FA2	NMSE	WNNR	NNR
Background sites	Measures	34.22	0.00	8.96	0.00	1.00	1.00	0.00	0.00	0.00
	ADMS	27.93	0.20	10.39	-0.15	0.42	0.87	0.16	0.16	0.13
	CGPL	33.34	0.03	5.53	0.47	0.39	0.93	0.06	0.06	0.05
	CGSA	26.10	0.27	3.91	0.79	0.44	0.93	0.15	0.16	0.11
	CAMx	65.85	-0.63	44.84	-1.33	0.35	0.13	0.55	0.41	0.44
Roadside sites	Measures	56.31	0.00	12.70	0.00	1.00	1.00	0.00	0.00	0.00
	ADMS	32.77	0.53	13.25	-0.04	0.16	0.67	0.49	0.52	0.43
	CGPL	29.62	0.62	6.79	0.61	0.27	0.56	0.57	0.57	0.43
	CGSA	23.77	0.81	4.88	0.89	0.52	0.22	0.97	0.97	0.76
	CAMx	62.95	-0.11	46.37	-1.14	0.49	0.78	0.10	0.08	0.09
Overall statistics	Measures	43.70	0.00	16.06	0.00	1.00	1.00	0.00	0.00	0.00
	ADMS	30.14	0.37	12.57	0.24	0.40	0.83	0.34	0.37	0.25
	CGPL	32.91	0.28	6.09	0.90	0.06	0.88	0.28	0.30	0.15
	CGSA	26.07	0.51	4.14	1.18	0.18	0.75	0.50	0.52	0.27
	CAMx	66.40	-0.41	44.74	-0.94	0.18	0.42	0.31	0.19	0.27
PM_{10}		MEAN [μgm^{-3}]	FB	SIGMA	FS	COR	FA2	NMSE	WNNR	NNR
Background sites	Measures	42.06	0.00	6.42	0.00	1.00	1.00	0.00	0.00	0.00
	ADMS	16.42	0.88	1.24	1.35	-0.28	0.00	1.02	1.02	0.91
	CGPL	17.02	0.85	0.57	1.67	-0.03	0.11	0.93	0.93	0.84
	CGSA	16.45	0.88	0.40	1.77	-0.11	0.11	1.01	1.01	0.91
	CAMx	22.40	0.61	6.95	-0.08	-0.22	0.67	0.53	0.53	0.44
Roadside sites	Measures	40.55	0.00	10.03	0.00	1.00	1.00	0.00	0.00	0.00
	ADMS	18.92	0.73	1.81	1.39	-0.61	0.33	0.77	0.77	0.54
	CGPL	17.06	0.82	0.58	1.78	0.49	0.33	0.94	0.94	0.71
	CGSA	16.52	0.84	0.54	1.79	0.55	0.33	1.00	1.00	0.76
	CAMx	25.47	0.48	7.56	0.07	0.03	0.73	0.35	0.35	0.27
Overall statistics	Measures	41.46	0.00	8.09	0.00	1.00	1.00	0.00	0.00	0.00
	ADMS	17.42	0.82	1.93	1.23	-0.43	0.13	0.91	0.91	0.74
	CGPL	17.04	0.84	0.58	1.73	0.22	0.20	0.93	0.93	0.78
	CGSA	16.48	0.86	0.46	1.78	0.27	0.20	1.01	1.01	0.85
	CAMx	30.07	0.30	5.92	0.52	0.45	0.83	0.16	0.16	0.10

Uncertainty analysis

Uncertainty analysis methods can be classified in two categories. The widely used approach can be referred to as "bottom-up", and it attempts to quantify the single error sources, and then to calculate the overall error by means of statistical techniques such as error propagation analysis, sensitivity analysis, sampling methods and Monte Carlo methods. This approach is the most applied in literature, although the error quantification is often arbitrary. For this reason, Colvile et al. (2002) introduced an alternative approach, referred to as “top-down”, which does not consider the single error sources, but the overall error is quantified by means of a high number of measures sufficiently representative of the phenomenon. This latter technique was used in this work: the uncertainty is quantified by means of the estimation of the model precision, calculated after removing the bias, and normalised using the appropriate limit value for the considered pollutant. Eventually the precision is calculated using the logarithmic mean square deviation of the modelled values with respect to the measured ones.

It was not easy to perform an uncertainty analysis, given the systematic underestimation resulting from the models applications. This is confirmed by the calculation of the “accuracy” as recommended by the European legislation 1999/30/EC and 2000/69/EC (relative maximum error, RME), which gives not acceptable results. More useful, in this case, is the methodology proposed by Colvile et al. (2002), because it allows the removal of the systematic underestimation effect (caused by smaller scale effects and secondary pollution). The calculated “precision” values are reported in Table 3.

Table 3. Model precision calculated following the European legislation and Colvile, R.N et al. (2002) methodology.

	RME			Colvile et al. (2002) precision		
	NO_2	PM_{10}	SO_2	NO_2	PM_{10}	SO_2
ADMS	42%	70%	73%	25%	22%	54%
CGPL	72%	68%	134%	26%	18%	52%
CGSA	45%	68%	101%	26%	18%	51%
CAMx	283%	67%	272%	29%	36%	78%

4. SCENARIOS ANALYSIS

On the basis of the model evaluation, ADMS-Urban seemed to be the most reliable modelling system for the present scenarios analysis. In addition to good performances, ADMS-Urban assured easy use, short computational, pre-processing and post-processing time, and the opportunity of analyzing small scale effects by means his street canyon module. For all these reasons AMDS-Urban was selected in order to realize the scenario analysis.
Two scenarios were investigated:

- Base scenario or actual scenario: referred to the Tuscan Regional Emission Source Inventory 2003
- Future scenario or “business as usual” scenario: referred to 2012 year on the basis of the anticipatory statistical modification of the Tuscan Regional Emission Source Inventory 2003.

NO_2, NO_X and primary PM_{10} concentrations were analyzed, considering the necessity of the Air Quality Action Plan. Annual, maximum hourly and maximum daily average concentrations maps were calculated for every pollutant and for every different emission source of the two scenarios: main point sources (POINT), main line sources (LINE), small industries (IND), local road traffic (ROAD), domestic heating (HEAT) and other sources (OTHER). In order to investigate the variation of the concentrations between the two scenarios, also percentage variation maps were carried out (see Fig. 1). These maps show a global reduction of the concentrations in all the study area; the reduction is evident specially in correspondence of the highways.

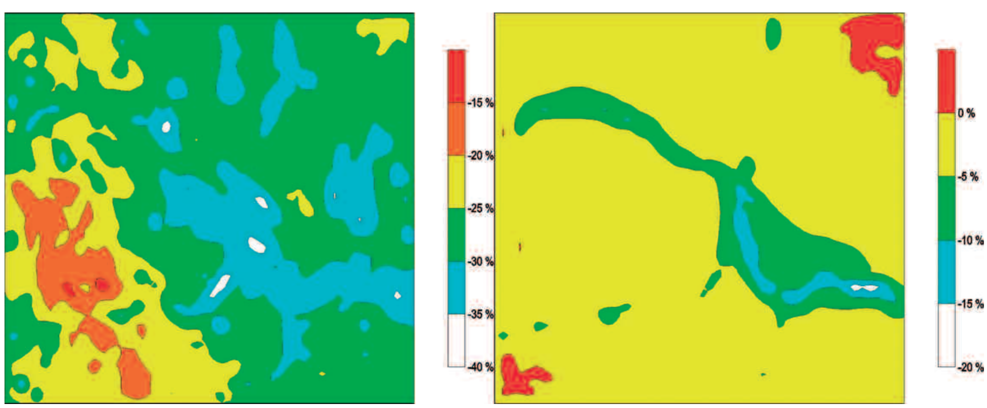

Figure 1. NO_2 (left) and primary PM_{10} (right) concentration percentage variation maps.

In order to evaluate the importance of the different emission sources in terms of pollutant concentrations, the maximum (representative of the local effect), the mean (representative of the global effects) and the minimum percentage contribution relative to the total concentrations of the study area cells were calculated for the two scenarios (see Fig. 2). The percentage contributions are nearly unchanged for the two scenarios (base and future).

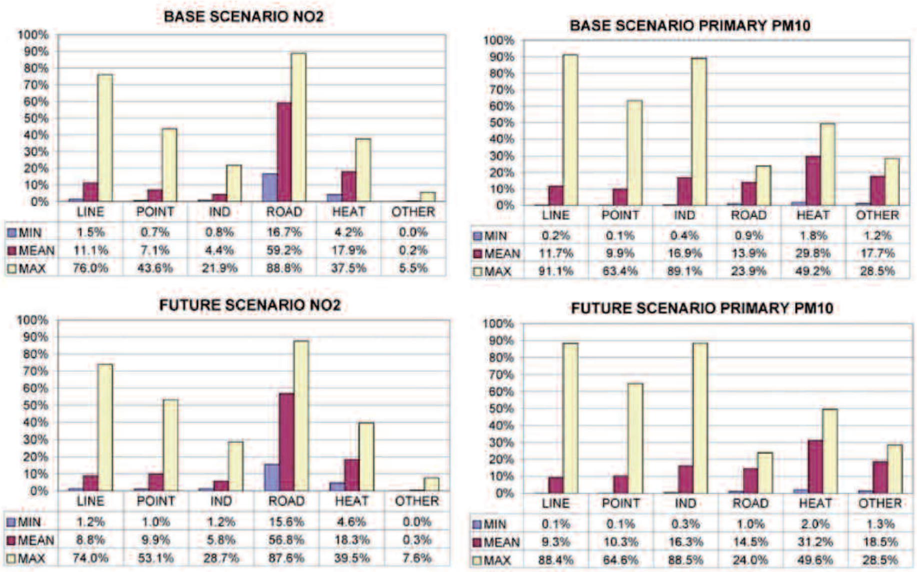

Figure 2. Maximum, mean and minimum percentage contribution to total concentration of NO_2 (left) and PM_{10} (right).

5. CONCLUSIONS

The obtained results point out the importance of including the following critical factors:

1. Smaller scale effects: monitoring stations are often located in complex environments; this implies a decrease in the effectiveness of validation studies; a possible solution would be to include small scale effects (e.g. street canyon modelling) in order to increase the resolution of the models. It is necessary to have reliable traffic volume data of the entire study area.
2. Secondary pollution: primary PM_{10} levels are only a small part of the total PM_{10} concentrations; besides high regional background levels, much of the urban PM_{10} is actually produced by chemical transformations and other physical mechanisms (for example, resuspension).

All these issues strongly affected the evaluation work. However, this does not alter the validity of the scenario analysis, because it is based on the differences between calculated primary pollutants concentrations deriving from the considered emissions. Despite the critical factors listed above, modeling results can be trusted on the basis of the evaluation work and provide indispensable information to the choice of efficient environmental actions that must be adopted in the Air Quality Action Plan of Tuscany.

REFERENCES

Derwent, R.G. and D.R. Middleton, 1996: An empirical function for the ratio NO_2:NO_X. *Clean Air,* **26**, 57-60.

Canepa, E. and P.J.H. Builtjes, 2001: Methodology of model testing and application to dispersion simulation above complex terrain. *International Journal of Environment and Pollution,* **16** (1-6), 101-115.

Chang, J.C. and S.R. Hanna, 2004: Air quality model performance evaluation. *Meteorology and Atmospheric Physics,* **87** (1-3), 167-196.

Colvile, R.N., N.K. Woodfield, D.J. Carruthers, B.E.A. Fisher, A. Rickard, S. Neville and A. Hughes, 2002: Uncertainty in dispersion modelling and urban air quality mapping. *Environmental Science and Policy,* **5** (3), 207-220.

Corti, A., C. Busillo, F. Calastrini, M. Carpentieri, P. Giambini and G. Gualtieri, 2006: Modelling emission scenarios in Tuscany: the MoDiVaSET project, 15th IUAPPA Regional Conf., 6-8 September, 2006, Lille, France.

Hanna, S.R.,1989: Confidence limits for air quality model evaluations as estimated by bootstrap and jackknife resampling methods. *Atmospheric Environment,* **23** (6), 1385-1398.

IRSE-RT, 2001: Inventario Regionale delle Sorgenti Emissive, Regione Toscana, Dipartimento Politiche Territoriali e Ambientali, Firenze, Italy.

IRSE-RT, 2004: Inventario Regionale delle Sorgenti Emissive – aggiornamento 2003, Regione Toscana, Dipartimento Politiche Territoriali e Ambientali, Firenze, Italy.

Olesen, H.R., 1995: Datasets and protocol for model validation. *International Journal of Environment and Pollution,* **5** (4-6), 693-701.

Olesen, H.R., 2005: User's Guide to the Model Validation Kit. Initiative on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes.

Poli, A.A., and M.C. Cirillo, 1993: On the use of the normalized mean-square error in evaluating dispersion model performance. *Atmospheric Environment part A-General Topics,* **27** (15), 2427-2434.