UNCERTAINTY AND VALIDATION OF URBAN SCALE MODELLING SYSTEMS APPLIED TO SCENARIO ANALYSIS IN TUSCANY, ITALY

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INTRODUCTION

The work presented in this paper has been carried out in the framework of the MoDiVaSET project (MOdellistica DIffusionale per la VAlutazione di Scenari Emissivi in Toscana). The project, funded by the Regional Administration of Tuscany, is aimed at developing modelling techniques for simulating atmospheric dispersion of PM_{10}, NO_x and SO_x 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 used by administrators and policy makers in order to evaluate different future emission scenarios. With this aim, the project also included several long-term (1-year long) dispersion modelling applications and a detailed evaluation study, which is often neglected in similar applications, despite its importance.

The study area is 49×40 km^2 sized. Emissions were retrieved from the Tuscan Regional Emission Source Inventory (*IRSE-RT, 2001*); three source categories have been initially considered: main point sources (87 industrial stacks), main line sources (A1 and A11 motorways) and all remaining ones (treated as 1×1 km^2 grid area sources).

AIR QUALITY MODELLING

Dispersion models

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). Further modelling options (full chemistry simulation, street canyon, ...) are being investigated by using CAMx, OSPM and other models.

The full 2002-year time period according to a 1-hour time step was chosen, 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, A. 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.

Modelling applications results

The contribution to air quality played by main point sources (87 industrial stacks) located in the study area were firstly taken in to account. Emission data were provided by the IRSE regional inventory according to a hour-by-hour time disaggregation (*IRSE-RT*, 2001). PM_{10} (primary only), NO_x and SO_x were the chosen pollutant species. The CALPUFF, SAFE AIR and ADMS-Urban dispersion models were applied to estimate pollutant concentrations from point sources. The considered main line sources are the A1 and A11 motorways. The models applied to this type of sources were CALINE4, SAFE AIR and ADMS-Urban. 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 CALGRID and ADMS-Urban dispersion models were applied to estimate pollutant concentrations from grid area sources. Concentration maps are not reported here for brevity.

VALIDATION AND UNCERTAINTY

Sensitivity analysis of ADMS-Urban results

Concentrations of NOx, SOx and PM10 have been calculated at each site for three scenarios plus the base scenario. These are: scenario 1 (parameter changed: constant average emissions data instead of hourly emission values), scenario 2 (parameter changed: minimum Monin-Obukhov length = 50 m instead of 30 m), and scenario 3 (parameter changed: meteorological input data from the Baciacavallo measuring station instead of the CALMET point). Calculated concentrations have been compared one to another and to the monitored concentrations during 2002. The tables are not reported here for brevity. Results proved to be particularly sensitive to the meteorological input.

Validation versus monitoring data

Model evaluation was then 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 provided by the monitoring networks of the three Provinces involved: Florence, Prato and Pistoia. 25 monitoring stations are present in the study area (see Fig. 1). The evaluation work included: simple intercomparison of the models, separately for each source type; detailed validation exercises using advanced statistical techniques; uncertainty analysis.

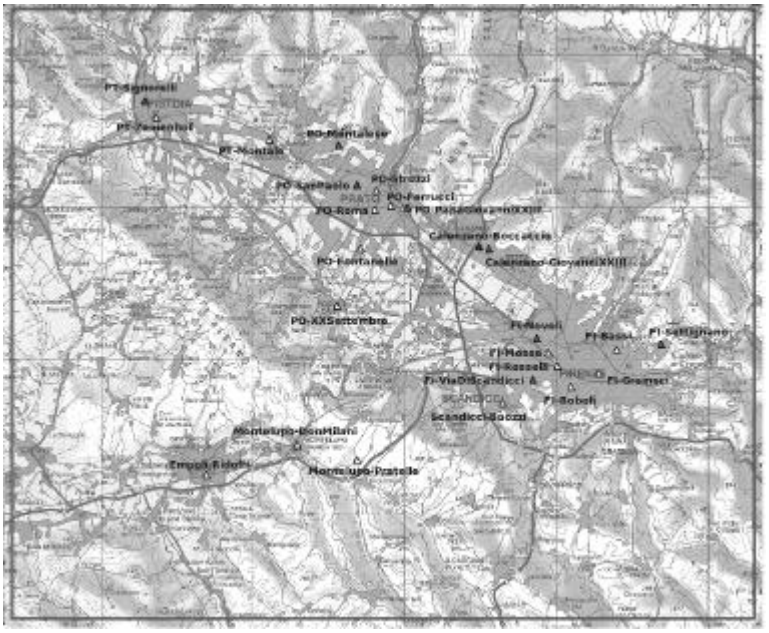

Fig. 1; Monitoring stations in the MoDiVaSET domain.

The statistical indices used for the validation exercise are derived from the BOOT software (*Hanna, S.R.*, 1989) and the Model Validation Kit (MVK, *Olesen, H.R.*, 1995, 2005). Furthermore, two other indices originally proposed by *Poli, A.A. and M.C. Cirillo* (1993) were used. The resulting statistical set is similar to that applied by *Canepa, E. and P.J.H. Builtjes* (2001) for the validation of the SAFE AIR code in complex terrain. These statistical indices are: mean (MEAN), bias (BIAS), fractional bias (FB), standard deviation (SIGMA), fractional standard deviation (FS), linear correlation coefficient (COR), fraction within a factor of 2 (FA2), normalised mean square error (NMSE), weighted normalised mean square error of the normalised ratios (WNNR), and normalised mean square error of the distribution of normalised ratios (NNR).

Chang, J.C. and S.R. 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.

A first simple comparison between the results was done using the calculated annual average concentrations. as reported in Table 1, for some of the monitoring stations.

Table 1. Comparison between NO_2, PM_{10} and SO_2 annual mean concentrations calculated by CALGRID-CALPUFF-CALINE4 (CGPL), CALGRID-SAFE AIR (CGSA) and ADMS-Urban (ADMS), and annual mean concentrations measured by the monitoring stations (Meas); [µg/m^3]

Station (NO_2)	CGPL	CGSA	ADMS	Meas
FI – Bassi	30.3	26.1	18.8	37.8
FI – Boboli	26.6	26.1	20.3	30.7
FI_Montelupo – Pratelle	11.1	8.2	4.2	28.6
PT – Montale	20.9	15.2	10.6	32.2
Station (PM_{10})	CGPL	CGSA	ADMS	Meas
FI – Bassi	3.6	3.2	2.4	42.6
FI – Boboli	2.9	2.4	2.7	37.6
FI_Scandicci – Buozzi	3.1	2.3	2.6	42.7
PT – Montale	1.7	1.2	1.1	53.6
Station (SO_2)	CGPL	CGSA	ADMS	Meas
FI – Bassi	2.4	1.9	1.3	3.8
FI – Boboli	2.1	1.4	1.5	2.9
FI_Empoli – Ridolfi	1.0	0.8	1.3	4.8
PT – Montale	0.8	0.5	0.4	3.1

The statistical indices described previously were then applied to the calculated/measured annual mean concentrations. Unfortunately, the low number of measuring points reduced the significance of the statistical analysis. Results are reported in Table 2.

The statistical analysis confirms the previous results. Good performances are obtained for nitrogen and sulphur oxides, while performance values for PM_{10} are rather low. The acceptability criteria proposed by *Chang, J.C. and S.R. Hanna* (2004) are not completely verified (although SO_2 and NO_2 values are quite close), but it should be noted that in this case

we are using concentrations paired in space. Further, Chang and Hanna's results are referred to research level measures, while in this case routinely monitored data are used.

Table 2. Statistical indices calculated for NO_2, PM_{10}, and SO_2 annual mean concentrations

NO_2	mean	bias	fb	sigm	fs	cor	fa2	nmse	wnnr	nne
Meas	46.12	0.00	0.00	16.61	0.00	1.00	1.00	0.00	0.00	0.00
CGPL	24.58	21.54	0.61	7.60	0.74	0.25	0.60	0.65	0.66	0.41
CGSA	18.85	27.27	0.84	8.04	0.70	0.30	0.27	1.12	1.12	0.79
ADMS	20.34	25.78	0.78	10.95	0.41	0.62	0.53	0.89	0.90	0.81
PM_{10}	mean	bias	fb	sigm	fs	cor	fa2	nmse	wnnr	nne
Meas	41.51	0.00	0.00	8.58	0.00	1.00	1.00	0.00	0.00	0.00
CGPL	2.70	38.82	1.76	0.75	1.68	0.11	0.00	14.11	14.11	12.96
CGSA	2.17	39.34	1.80	0.83	1.65	0.10	0.00	17.98	17.98	16.60
ADMS	2.65	38.87	1.76	1.54	1.39	-0.28	0.00	14.51	14.51	12.48
SO_2	mean	bias	fb	sigm	fs	cor	fa2	nmse	wnnr	nne
Meas	3.07	0.00	0.00	0.35	0.00	1.00	1.00	0.00	0.00	0.00
CGPL	1.98	1.09	0.43	0.84	-0.84	-0.16	0.67	0.35	0.38	0.35
CGSA	1.41	1.66	0.74	0.66	-0.62	-0.09	0.50	0.77	0.77	0.72
ADMS	1.37	1.71	0.77	0.52	-0.40	-0.37	0.50	0.82	0.82	0.73

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, R.N. 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), which gives not acceptable results (not reported for brevity; again, for a complete overview see *Carpentieri, M.*, 2006). More useful, in this case, is the methodology proposed by *Colvile, R.N. et al.* (2002), because it allows the removal of the systematic underestimation effect (caused by other factors, see Conclusion).

The calculated "precision" values are reported in Table 3.

Table 3. Model precision calculated following the methodology by Colvile, R.N. et al. *(2002)*

	NO2	PM10	SO2
CGPL	41 %	34 %	54 %
CGSA	37 %	37 %	61 %
ADMS	51 %	78 %	73 %

CONCLUSION

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

- Regional background concentrations: looking at the results a systematic bias between calculated and measured concentration proved to exist; the models systematically underestimated pollution levels; however, this did not affect the analysis of future scenarios (starting from the hypothesis that background concentrations do not change).
- 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; otherwise, a detailed study on the representativeness of the monitoring sites appears to be necessary.
- 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. Modelling results can be trusted on the basis of the evaluation work, despite the critical factors listed above.

REFERENCES

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.

Carpentieri, M., 2006: Modelling air quality in urban areas, PhD thesis, Università degli Studi di Firenze, Italy.

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 Conference, 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.

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.