PERFORMANCE ASSESSMENT OF LONG-TERM PHOTOCHEMICAL MODELLING SYSTEM

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INTRODUCTION

Ozone is considered one of the most significant pollutants with respect to the potential impact to human health and natural ecosystems, both in terms of critical episodes and as long-term exposures. Consequently, in order to assess the comprehensive effects of photochemical pollution, not only ozone peak concentrations need to be examined, but also ozone exposures on "seasonal" scale need to be quantified.

Photochemical air quality models play a central role both in scientific investigation of pollutants behavior in the atmosphere and developing policies to manage air quality. In the past, photochemical models were applied for the duration of one or a few ozone critical events. Recent works (*Hogrefe, C. et al.*, 2001, *Tarasson, L. et al.*, 2001) point out the importance to perform policies analysis on a "climatological" basis rather than focusing on a single critical episode. This allows to better evaluate model performances and also to quantify policy effects with respect to long-term air quality standards.

In this study the methodology applied to evaluate the performance of a long-term modeling system is presented. The results have been evaluated using statistical indexes and model performance indicators, in order to assess the model capability to actually reconstruct temporal and spatial features of pollutant concentrations.

THE PHOTCHEMICAL MODELLING SYSTEM

An integrated modeling system has been designed and implemented, including 3D meteorological pre-processor CALMET (*Scire, J.S. et al.*, 1999), a flexible emission inventory module POEM (*Catenacci, G. et al.*, 1999) and two photochemical transport models, CALGRID (*Yamartino, R.J. et al.*, 1992) and STEM-FCM (*Silibello, C. et al.*, 2001).

The selected simulation domain (240×232 km^2) includes the whole Lombardia Region. It is a complex terrain region located in the Po Valley and it is one of the most industrialized and populated area of Northern Italy. Industries and a close road network are the most relevant sources in the basin. The critical anthropogenic emissions, the frequent stagnating meteorological conditions and the Mediterranean solar radiation regularly cause high ozone level episodes, especially during summer months. Thus, the models have been run for the period May-July 1996 (*Gabusi, V. et al.,* 2002a). Ozone time series from the air quality networks have been analyzed by means of a clustering analysis technique, to evaluate similarity in terms of levels and temporal variability. A reduced set of monitoring stations has been selected (*Gabusi, V. et al.,* 2002b). In addition, the stations have been subdivided into two sets: the stations located in a high emission density area (HEDA) and those located in a low emission density area (LEDA).

MODEL EVALUATION

Model evaluations are carried out for a variety of purposes including management studies, ability of the science to support operational uses of a model, and model development. In this study we are primarily interested in investigating the models' ability to reproduce the observed concentrations for a seasonal simulation. Often, the reliability of models is only determined by a graphical comparison between measured and simulated concentrations at some specific locations, while attention should be also given to the use of proper statistics that are essential in integrated model testing. Consequently, the model evaluation has been conducted taking into account the US EPA recommendations for an acceptable model performance, the new European Directive and other statistical indices and parameters.

The US EPA developed guidelines (*US EPA*, 1991) for a minimum set of statistical measures to be used for model performances evaluation. Due to the insufficient density of monitoring stations in the domain, only the Mean Normalized Bias Average and the Mean Normalized Gross Error have been calculated, as shown in Table 1. The suggested performance criteria for these statistics are ±5÷15% for MNBE and +30÷35% for the MNGE. The correlation coefficient (r), although not explicitly recommended, has often been applied in model evaluation studies, as well as the Root Mean Square Error (RMSE).

Table 1. Statistical formulation of applied US-EPA indexes

MNBE	**r**
$\frac{1}{N}\sum_{t=1}^{N}\frac{C_{\mathrm{mod}}(x,t)-C_{obs}(x,t)}{C_{obs}(x,t)}$	$\frac{\sum_{t=1}^{N}\left(C_{\mathrm{mod}}(x,t)-\overline{C}_{\mathrm{mod}}(x,t)\right)\cdot\left(C_{obs}(x,t)-\overline{C}_{obs}(x,t)\right)}{\sqrt{\sum_{t=1}^{N}\left(C_{\mathrm{mod}}(x,t)-\overline{C}_{\mathrm{mod}}(x,t)\right)^2}\cdot\sqrt{\sum_{t=1}^{N}\left(C_{obs}(x,t)-\overline{C}_{obs}(x,t)\right)^2}}$
MNGE	***RMSE***
$\frac{1}{N}\sum_{t=1}^{N}\frac{\left\|C_{\mathrm{mod}}(x,t)-C_{obs}(x,t)\right\|}{C_{obs}(x,t)}$	$\sqrt{\frac{1}{N}\sum_{t=1}^{N}\left(C_{\mathrm{mod}}(x,t)-C_{obs}(x,t)\right)^2}$

N is the number of data, $C_{mod}(x,t)$ and $C_{obs}(x,t)$ are respectively the predicted and the observed concentrations at position x for time t, $\overline{C}_{\mathrm{mod}}(x,t)$ and $\overline{C}_{abs}(x,t)$ are the mean values.

The EC 2002/3 Directive in force for air ambient quality provides reference techniques for ozone modeling by defining the uncertainty levels for modeling simulation. The Directive considers two parameters, the 1 hour averages (daytime) and the 8 hours daily maximum. The uncertainty for modeling and objective estimation is defined as the maximum deviation of the measured and calculated concentration levels over the period for calculating the appropriate threshold, without taking into account the timing of the events. The threshold is, for both indexes, equal to 50%.

RESULTS

In this exercise our issues concerned both the models' ability to predict the temporal evolution of pollutants and the investigation of the behavior of two different photochemical models.

1-hourly and 8-hourly daily maximum ozone concentrations have been used for evaluating the model performances. These concentrations are more appropriate for comparison with observations than the hourly ozone values as shown e.g. in (*Hogrefe, C. et al.*, 2000, *Schmidt, H. et al.*, 2001, *US EPA*, 1991). Observed and predicted concentrations are paired in space but not necessarily in time. Following US EPA predicted values at monitoring stations have been derived by a bilinear interpolation of the predicted values at the nearest four grid cells. No ozone threshold values have been used in computing statistics.

EPA and traditional Statistics

The statistics reported in Tables 2 and 3 show a satisfying performance for both models. MNBE indexes show that both CALGRID and STEM overestimate on average the measured concentrations for the LEDA stations, while slightly underestimate at HEDA ones. HEDA stations share the same behavior, highlighting a perfectible reconstruction of the photochemical process. Differently, LEDA stations show a large variety of behaviors depending on a non-optimal prediction of ozone spatial distribution. The data are well correlated, which indicate a good reconstruction of the ozone daily trend. With the exception of RMSE, all LEDA indexes are better than HEDA ones. This is for RMSE is an absolute (non-normalized) error. Consequently, it is greater in a high emission area, where the ozone concentrations are greater. The 1-hourly daily maxima indexes are similar to those related to the 8-hourly maxima concentration. This means that both the peak concentrations and the daily shapes are satisfactorily computed. No systematic errors afflict the models, as all statistics are better for the group average concentrations than for the single monitor location.

Table 2. EPA statistics for daily maxima of 1-h ozone prediction

	MNBE		**MNGE**		**r**		**RMSE**	
	CALGRID	STEM	CALGRID	STEM	CALGRID	STEM	CALGRID	STEM
Gambara	0.528	0.596	0.542	0.604	0.427	0.558	28.226	33.633
Ispra	0.219	0.223	0.287	0.269	0.572	0.697	19.876	19.326
Parma	0.240	0.221	0.279	0.261	0.479	0.693	22.625	22.176
Re_Masse	0.417	0.403	0.435	0.419	0.467	0.581	30.722	29.663
Varenna	-0.087	-0.116	0.255	0.266	0.551	0.585	30.620	32.070
LEDA	**0.204**	**0.190**	**0.237**	**0.230**	**0.616**	**0.780**	**16.990**	**17.870**
Legn_Sma	0.055	-0.028	0.280	0.244	0.386	0.648	27.556	24.613
Limbiate	-0.077	-0.122	0.244	0.228	0.428	0.704	27.191	23.176
Mi_Juva	0.008	-0.059	0.327	0.306	0.471	0.622	28.493	27.732
Vimercat	-0.025	-0.084	0.269	0.242	0.438	0.713	25.377	22.560
HEDA	**-0.031**	**-0.090**	**0.245**	**0.230**	**0.455**	**0.749**	**24.594**	**21.026**

Table 3. EPA statistics for daily maxima of 8-h ozone prediction

	MNBE		**MNGE**		**r**		**RMSE**	
	CALGRID	STEM	CALGRID	STEM	CALGRID	STEM	CALGRID	STEM
Gambara	0.642	0.681	0.644	0.681	0.647	0.646	30.490	34.248
Ispra	0.277	0.280	0.329	0.312	0.583	0.730	20.049	19.095
Parma	0.254	0.203	0.287	0.246	0.626	0.707	21.398	19.831
Re_Masse	0.498	0.440	0.506	0.452	0.535	0.617	30.910	28.241
Varenna	-0.072	-0.123	0.221	0.219	0.679	0.673	23.480	24.847
LEDA	**0.297**	**0.240**	**0.317**	**0.270**	**0.737**	**0.784**	**19.240**	**18.106**
Legn_Sma	0.130	0.002	0.288	0.228	0.516	0.671	21.927	19.907
Limbiate	-0.043	-0.137	0.235	0.265	0.490	0.675	22.014	21.760
Mi_Juva	0.113	-0.021	0.358	0.309	0.559	0.640	21.976	22.041
Vimercat	0.007	-0.055	0.245	0.223	0.586	0.737	19.161	16.791
HEDA	**0.021**	**-0.090**	**0.221**	**0.220**	**0.609**	**0.759**	**18.304**	**16.655**

EU Directive statistics

In order to evaluate the model uncertainty, according to the EU directive, we computed the number of the exceedances of the threshold of 50%, for both statistical parameters. The percentage values are presented in Table 4. A feature common to both models is the difficult to correctly predict the ozone concentrations for the station in the Southern part of the domain (Gambara, Parma end Reggio). This probably descends from an inadequate reconstruction of the boundary concentration in the SE part of the domain (as shown also by EPA statistics).

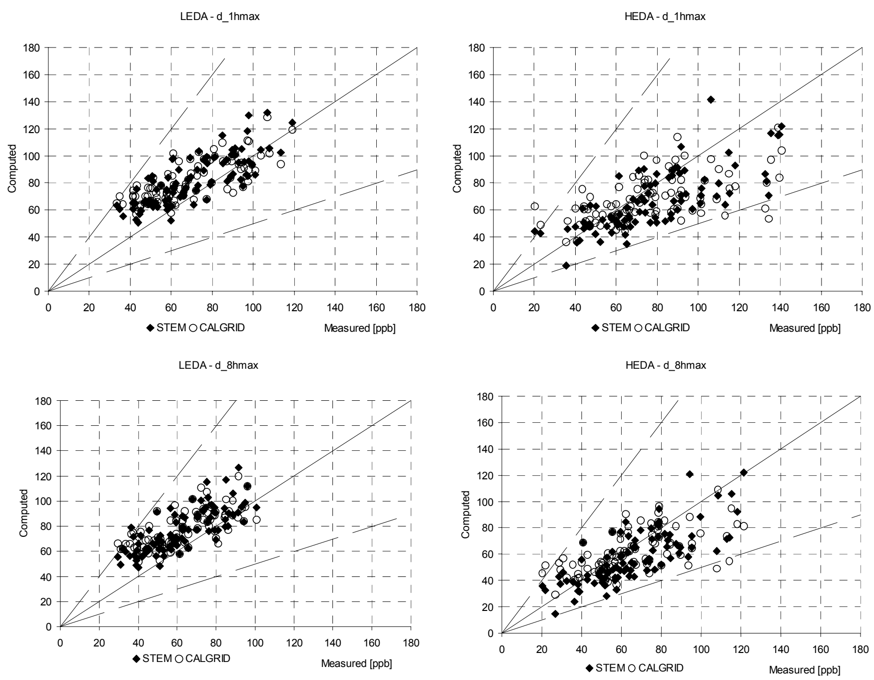

Figure 1. Scatter plots of the observed versus modeled ozone peak concentrations

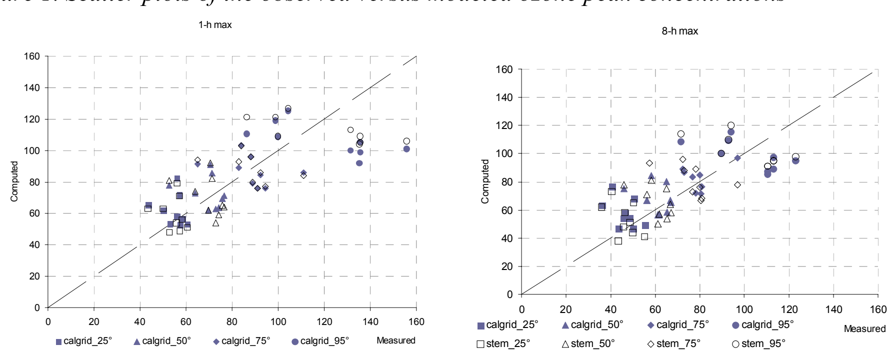

Figure 2. Scatter plots of observed versus modeled ozone peak concentrations at various percentiles

Graphical evaluation

To gain further insight into the sensitivity of the models to predict different parameters, the daily peak ozone values are plotted against the measured values for the two sets of sampling points (Figure 1). Generally there is a good agreement between observed and predicted data, with an over prediction for the LEDA stations and an under prediction of the highest concentrations (> 100 ppb) for the HEDA ones. Calculated values of the 1-h and 8-h ozone peak for the 25th, 50th, 75th, and 95th percentiles, at each location, are shown in Figure 2. It can be seen that the wider spreading is present for the 95th percentile, reflecting the underestimation of higher peak ozone values.

Table 4. EU Directive statistics for ozone prediction

	1-h		**8-h**			**1-h**		**8-h**	
	CALGRID	STEM	CALGRID	STEM		CALGRID	STEM	CALGRID	STEM
Gambara	49.847	54.128	52.439	60.976	Legn_Sma	31.721	31.721	15.730	7.865
Ispra	31.369	37.081	18.478	18.478	Limbiate	25.743	25.743	8.989	6.742
Parma	23.179	19.077	13.924	7.595	Mi_Juva	40.533	40.993	14.130	16.304
Re_Masse	35.983	32.653	42.857	42.857	Vimercat	31.727	29.364	8.696	5.435
Varenna	17.017	17.332	6.250	5.000					
LEDA	**26.268**	**23.279**	**18.478**	**17.391**	**HEDA**	**29.348**	**27.627**	**8.696**	**5.435**

CONCLUSIONS

The results of a long-term simulation of photochemical pollution over Lombardia Region (Northern Italy), carried out with two different modeling systems, have been evaluated using statistical indexes and model performance indicators. Both CALGRID and STEM-FCM systems are able to reproduce the overall temporal and spatial behaviors of measured ozone concentrations, with similar levels of performance and meeting the EPA and UE requirements in most cases. The photochemical process needs to be improved in urban area, as well as the reconstruction of ozone spatial distribution or transportation in rural ones. The unsatisfying models' performances in the Southern domain are probably due to boundary conditions that cannot be accurately prescribed.

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