USE OF CHEMICAL TRANSPORT MODELS AND NEURAL NETWORK IN A POLLUTANTS STUDY OVER ROME URBAN AREA

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INTRODUCTION

Air quality problems produced by high levels of ozone (O3) has been of concern for their effects on human health. The city of Rome is a typical Mediterranean metropolitan area experiencing frequently pollution episodes, characterized by high concentrations of ozone, associated with hot sunny days and stagnant conditions. The spatial extension of these phenomena was only detected by monitoring networks data, which are often duty influenced by local emissions. In a recent modelling study conducted by Gariazzo et al (2007) the chemical transport model (FARM) has been applied to study primary and secondary gas/aerosol pollutants concentrations in the urban area of Rome. The comparison of FARM model results against observations has shown that, although the FARM model was able to predict the observed ozone diurnal concentrations at both urban and rural stations, the night-time predictions were sometimes overestimated due to both an incorrect evaluation of the nocturnal vertical exchange coefficients k_z and to missed local NO_x emissions in rural areas.

Among the complex systems it is well known that neural networks can work as universal approximators of non-linear functions and, consequently, can be used in assessing the dynamics of such systems. Usually, they have become a useful tool either where correct phenomenological models are not available or when uncertainty in input and output data complicates the application of deterministic modelling as may happen, for example, in environmental systems. Pioneering works in developing Artificial Neural Net (ANN) applications for short term forecasting in atmospheric systems has been conducted since the early 1990's (e.g., Boznar et al., 1993,). ANN methods have been developed for forecasting daily maximum ozone levels in various urban areas, (Comrie 1997). Gardner and Dorling (1998) produced an overview of applications of ANN in the atmospheric sciences and in 1999 tested the benefits of using a MLP to model NO2 concentrations in London relative to other statistical modelling approaches.

All above environmental applications use the NN model as regression tools. Pelliccioni et al (2003, 2006) recently coupled ANN with air dispersion models to construct a modelling system able to better predict the ground concentrations of primary air pollutants respect to the results obtained using the dispersion model alone.

In this work this methodology is applied for the first time to a secondary pollutant such as ozone. In particular the comprehensive Chemical Transport Model (CTM) (FARM) has been coupled with a Neural Network, to reconstruct pollution episodes occurring in the city of Rome.

METHODOLOGY

The CTM dispersion model, simulation periods and input data.

The dispersion and the chemical evolution of the pollutants are based on the FARM model (Silibello et al., 2005). FARM is a three-dimensional Eulerian model dealing with the transport and the multiphase chemistry of pollutants in the atmosphere. Photochemical reactions are described by means of SAPRC-90 chemical scheme (Carter, 1990).

A nested approach with three domains has been employed, starting from the Italian national domain, down to the urban domain, embedded in a intermediate regional one. Based on typical local atmospheric circulations/synoptical conditions and on the occurrence of pollution episodes, as revealed by observations, three episodes were selected for the modelling study (20-24 June 2005; 25-29 July 2005; 9-13 January 2006).

The meteorological fields on the three domains have been obtained by means of the RAMS (Cotton et al., 2003) prognostic model using ECMWF analysis, at 0.5 degrees and 6 hours resolution, to get initial and boundary conditions. To better reproduce air fluxes within Rome urban area, the wind fields in the inner urban domain were calculated by means of the MINERVE (Aria Techn., 2001) diagnostic mass consistent model. The meteorological subsystem is completed by SURFPRO (ARIANET, 2005), a diagnostic module to produce PBL scaling parameters, dry deposition velocities and turbulent diffusivities fields, on the basis of the meteorological fields and landuse maps.

As for the emissions, special attention has been paid for the urban traffic. Hour-by-hour traffic emission, related to the primary road network of Rome, have been produced by means of a traffic assignment model and by the TREFIC emission model (Nanni et al., 2005). The emission from the largest industrial emission sources was updated using either stack measured data or owner declarations. Emissions for other sectors have been developed starting from the available Lazio regional inventory (APAT 2000), updated to the year of interest using yearly emission trends.

THE NEURAL NETWORK SET UP

As neural net architecture, we used in our study a 3-layer perceptron model. The first input layer contains the input variables of the net. The second layer consists of the neurons of hidden layer (we tested the simulations with 8, 10 and 12 hidden neurons). The third layer consists of the concentration levels to be reproduced at the different urban stations.

In our simulations, we tested different input variables to the net. As experimental variables, we consider the follows as input of NN: the daily hour, the CO, NO2 and O3 concentration predicted by FARM model and measured by monitoring stations, the meteorological and turbulence parameters (as temperature, mixing height, Monin-Obukhov Length, speed velocity pressure and global radiation) at different stations. The total data amount concerns 1208 patterns, representing the seasonal episodes simulated by FARM model.

In order to check the influence of every input parameter to MLP, we performed a pre-elaboration using as input variables of net the single one parameters. We obtain the correlations coefficients for the ozone levels given in Table 1.

In this preliminary elaboration, the most important input meteorological variables to the net seems to be the temperature, mixing height, pressure and global radiation.
In our NN simulations, we consider the Monin-Obukhov Length parameters as input variables to taking into account the turbulence conditions.

	NN Input
Hour	0.55
CO Meas	0.51
CO FARM	0.60
NO2 Meas	0.67
NO2 FARM	0.69
O3 FARM	0.85
Temp	0.79
HMIix	0.83
1/L	0.44
U	0.47
Rad Glob	0.64
UR	0.69
Press	0.49

Table 1 Correlation coefficients for the ozone levels

RESULTS AND DISCUSSION

Give the above considerations, in our simulation, we use as input variables of the net the followings 4 variables: the mixing height, the Monin-Obukhov Length, the air temperature and global Radiation and, most important, the Ozone concentration levels predicted by FARM model. The best MLP was obtained with 8 hidden layer. In our simulation we divided the data set in two side. The first set concerns the 60% of the monitoring stations data and was used during the training phase and the remaining 40% has been used for the generalization phase. The results are always all referred to generalisation phase.

The NN weights corrections was performed using two methods: the coniugate gradient and the back propagation algorithms.

During the training phase a good correlation coefficient was obtained (R=0.89), while for the generalization a value of R=0.87 was achieved (table 2).

Table 2. Correlation coefficients R related to application of FARM model and integrated model (FARM-NN) for train and test phase.

	R
FARM	0.71
FARM+NN(Train)	0.89
FARM+NN(Test)	0.87

In the Figure 1 are shown the results coming from the generalization. It is to underline that this NN model present a good reproduction for all ozone range.

The Error distribution between the forecasting and measured levels shows a net improvement respect to the error distribution obtained with FARM model (Figure 2). A decrease of skweness can also be observed respect to the FARM alone.

The error distribution shows an under-prediction of the observed ozone levels (as can be deduced by the negative sign of the mean error value (m) in the Table 3). This behaviour is systematic (as evident by the skewness of the error distribution) and the work of the Neural Net concerns the adjustment of the performance of the air dispersion model.

The mean of error distribution shows an improvement when we use the FARM-NN model (the mean error value is m=0.17) than FARM model alone (m=-2.79).

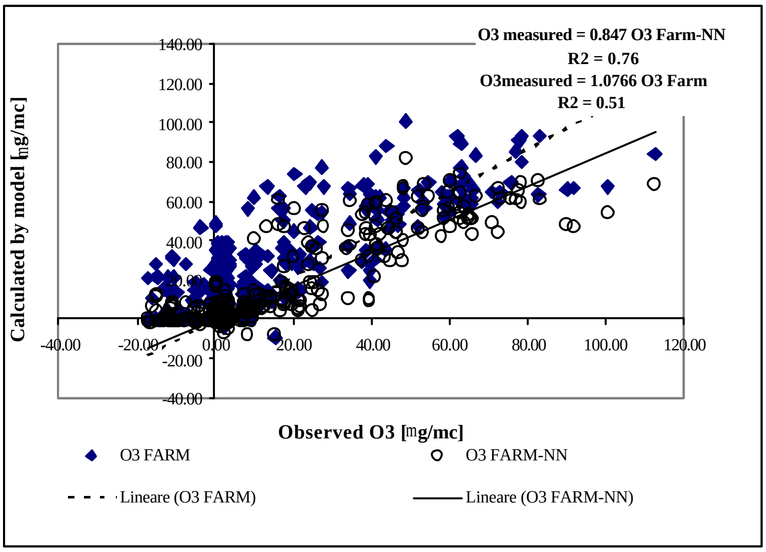

Fig. 1; Ozone predicted and observed at different monitoring station using FARM and FSRM-NN model.

Table 3. Error distribution parameters (mean and standard deviation) between the forecasting and measured levels related to application of FARM model and integrated model (FARM-NN)

	FARM model	Farm-NN model
Mean of Error distribution (m)	-2.79	0.17
Stand Dev. of Error distribution	19.36	7.33

The FARM model reproduce well ozone levels during the day, during the night the model under predict heavily the ozone pollutants levels. While during the day, NN have done no correction of ozone predicted by FARM, during the night (with high stability turbulence) NN model need to modify the ozone given by FARM model.

The improvement of error distribution demonstrate that NN is able to reproduce the nocturnal ozone peak in the Rome urban area.

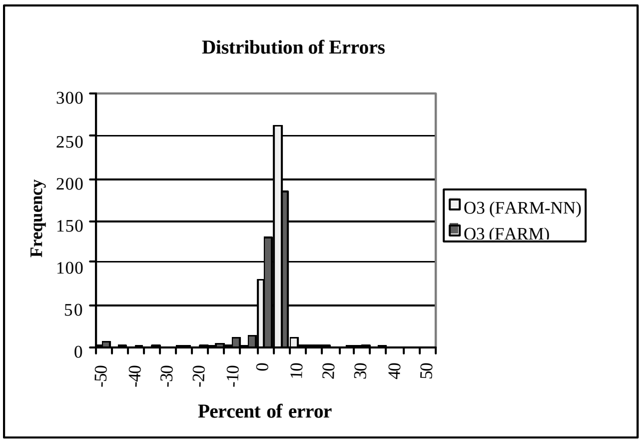

Figure 2. Distribution of error between Ozone predicted and observed at different monitoring station using FARM and FSRM-NN model.

CONCLUSIONS

We have applied for a complex urban situations a mixed models composed by a deterministic model and a NN network. The mixed model, validated using an urban Rome field campaign, shows good results.

An improving of the model performance is observed, decreasing the mean error between the calculated values and the measured ones. Both during the training than generalization phases a good correlation coefficient was obtained.
The use of integrated model seems to suggest the direction to follow for improve the performances of deterministic models in complex area as urban one.

The Ozone concentrations levels predicted by dispersion model could carry on the same trend with the atmospheric stability.

REFERENCES

APAT Agency for Environmental Protection and Technical Services, 2000. http://www.sinanet.apat.it/it/sinanet/bdemi/

Aria Technologies, 2001. Minerve Wind Field Models version 7.0, General Design Manual. ARIA Tech. Report, May 2001

ARIANET (2005) SURFPRO (SURrface-atmosphere interFace PROcessor) User's guide.

Boznar M, Lesjak M, Mlakar P., (1993). A Neural Network based method for the short-term predictions of ambient SO2 concentrations in highly polluted industrial areas of complex terrain. Atmos. Environ., 27B (2), 221-230.

Carter, W.P.L, 1990. A detailed mechanism for the gas-phase atmospheric reactions of organic compounds. Atmospheric Environment, 24A, 481-518.

Comrie R.S, (1997). Comparing neural network and regression models for ozone forecasting. Journal of the Air and Waste Management Association 47, 653-663.

Cotton, W.R., Pielke, R. A., Walko, R. L., Liston, G. E., Tremback, C. J., Jiang, H., McAnelly, R.L., Harrington, J. Y., Nicholls, M. E., Carrio, G.G., McFadden, J. P., 2003. RAMS 2001: Current status and future directions. Meteorol. Atmos. Phys., 82, 5-29.

Gariazzo, C., Silibello, C., Finardi, S., Radice, P., Piersanti, A., Calori, G., Cecinato, A., Perrino, C., Nussio, F., Cagnoli, M., Pelliccioni, A., Gobbi, G. P., Di Filippo, P., 2007: "Air pollutants study over Rome urban area through couplet traffic assignment and chemical transport models"; 6th International Conference on Urban Air Quality, Cyprus, 27-29 March 2007

Nanni., A., Radice, P., Piersanti, A., 2005. TRaffic Emission Factor Improved Calculation (TREFIC). User manual - Version 4.0, ARIANET R2005.02, Milan, Italy.

Pelliccioni, A., Gariazzo, C., Tirabassi, T., 2003: "Coupling of neural network and dispersion models: a novel methodology for air pollution models"; Int. J. of Environment and Pollution – Vol. 20, Nos. 1-6, 2003

Pelliccioni, A., Tirabassi, T., Bellantone, S., Gariazzo, C., 2006: "Deterministic models and Neural Nets: a successful methodology for the air dispersion models"; IEEE World Congress on Computational Intelligence- WCCI 2006, Vancouver, BC, Canada July 16-21 2006.

Silibello, C., Calori, G., Brusasca, G., Giudici, A., Angelino, E., Fossati, E., Peroni, E., Buganza, E., Degiarde, E., 2005. Modelling of PM10 concentrations over Milan urban area: validation and sensitivity analysis of different aerosol modules. In: Proceedings of 5th International Conference on Urban Air Quality, Valencia, Spain, 29-31 March 2005.