NEURO-FUZZY MODELS FOR AIR QUALITY PLANING: THE CASE STUDY OF OZONE IN NORTHERN ITALY.

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Abstract

To design air quality plans, regional authorities need tools to understand both the impact of emission reduction strategies on pollution index and the costs of emission reduction. The problem can be formalized as a multi-objective mathematical program, integrating local pollutant-precursor models and the estimate of emission reduction costs. Both aspects present several complex elements. In particular the source-receptor models, describing transport phenomenon and chemical non linear dynamics, require deterministic modelling system with high computational cost. In this paper a method based on neuro-fuzzy models is proposed to identify local ozone-precursor models on the basis of the simulations of a photochemical modelling system (GAMES). The methodology has been performed for Lombardia region (Northern Italy); this area, characterized by a complex terrain, high urban and industrial emissions and a dense road network, is often affected by severe photochemical pollution episodes during summer.

1 Introduction

Since last decade photochemical smog episodes have become more and more critical over Europe, mainly in Mediterranean regions, where the sun radiation and the stagnating meteorological conditions occurring in summer season play a significant role in chemical transformations of urban and industrial pollutant emissions. The cause-effect chain relations between precursors (typically nitrogen oxides (NO_x) and volatile organic compounds (VOC)) and photochemical pollutants (mainly tropospheric ozone, NO₂, PAN and formaldehyde) are thousands and characterized by different reactive times, resulting complex and non-linear.

This property depends on the specific urban and industrial structure of the area, on the local meteorological conditions, on the contribution of regional and local emissions of photochemical smog precursors, "hot spot" areas occurring especially in Mediterranean areas and the local photochemical regimes [18].

As a consequence of such complexity, the European Union suggests regulatory Agencies to define the problem at regional level in order to better interpret the air pollution situation and to define plans in terms of reductions of the emissions of ozone precursors. Such measures can be selected on the basis of different techniques such as the cost-benefit analysis or the cost-effectiveness analysis ([12] and [19]).

As the estimation of pollution damages often is difficult to be estimate proves unfeasible, the problem can be formalized as a multi-objective optimization ([5], [13], [15] and [8]). This approach presents the difficulty of including the complex non linear dynamics of ozone formation within the optimization problem formulation.

The source-receptor relationship can be simulated by deterministic 3D modelling systems, describing transport and chemical atmospheric phenomena. Such models require so high computing times that they are virtually unserviceable in a multiobjective mathematical program.

To get round the problem, in literature the source-receptor relationship has been described using ozone isopleths [7], [11] or with reduced form models. These last can be divided in turn into simplified photochemical models (for instance, by adopting semi empirical relations calibrated with experimental data, as in [20], or by using statistical regressions on the results of very complex 3D transport-chemical models (long term simulations for Europe domain in [13] and [8], short term simulations for Lombardia domain in [1]). The final multiobjective mathematical problem can then be solved by various techniques, including genetic algorithms, as in [11].

In this paper, a two-objective analysis (air quality and costs) to select effective ozone control plans is formalized.

The nonlinear relation between emission and pollution is described for Lombardia Region (Northern Italy) by neuro-fuzzy models, calibrated on long term simulations of GAMES [21] photochemical modelling system.

2 **Problem formulation**

The ground level ozone control can be formulated as a twoobjective mathematical programming problem including the effectiveness of emission reduction policies and their costs.

The air quality objective is the minimization of the seasonal accumulated ozone dose (AOT60) above the 60 ppb cut-off value for daylight hours over a grid domain. This index measures the population exposure in World Health Organization and EU Directives.

The daily cell exposure can be formalized as follows:

$$AOT60_{i,j}(d) = \sum_{h=1}^{H_d} [O3^h_{i,j}(d) - 60] \quad for \ O3^h_{i,j}(d) > 60ppb$$
(1)

where:

- i, j are the cell position indexes;
- *d* is the daily index during the reference summer season (April-September);
- H_d is the number of daylight hours (during dth day), i.e. when the potential global radiation is >50 $\frac{W}{m^2}$;
- $O3_{i,j}^{h}(d)$ is the mean ozone concentration (ppb) in (i, j) cell for *h*th daylight hour during *d*th day;

 $AOT60_{i,i}(d)$ is in $[ppb \cdot h]$

As photochemical pollution is formed from emissions of nitrogen oxides and of volatile organic compounds in the presence of sunlight, the daily cell exposure is function of meteorological parameters (that cannot be handled) and of emissions (decision variables).

As a regional authority can impose a reduction to a certain emission sector, the daily cell emissions is expressed with respect to a reference situation and split in 11 sectors according to the CORINAIR classification [4]. So the cell AOT60 can be described stressing the emission dependance as follows:

$$AOT60_{i,j}(d) = AOT60_{i,j}(N^{s}_{i,j}(d) \cdot r^{N}_{s}, V^{s}_{i,j}(d) \cdot r^{V}_{s}) \quad (2)$$

where:

- $N_{i,j}^{s}(d)$ and $V_{i,j}^{s}(d)$ are respectively the daily cell NO_x and VOC emissions in the reference case for sector s;
- $\Xi(r_s^N, r_s^V)_{s=1,..,11}$ is the decision variable set, namely the percentage of sector precursor emission reductions (respectively for NO_x and VOC).

The formalization of source-receptor function, explaining complex local and regional factors (transport processes, atmospheric chemical non linear behavior, anthropogenic and biogenic emission mixture), is described in the next section.

The air quality objective, minimizing the seasonal domain population ozone exposure (POE), is:

$$min(POE) = m_{\Xi}^{i} n \sum_{\forall i,j} \sum_{d=1}^{D} [p_{i,j}AOT60_{i,j}(d)]$$
(3)

where $p_{i,j}$ is the population density in (i, j)th cell and D is the amount of the summer days.

The second objective of the ozone planning is the minimization of precursor (NO $_x$ and VOC) emission reduction costs:

$$min(Costs) = m_{\Xi} in \sum_{s=1}^{11} (N^s \cdot r_s^N \cdot c_s^N(r_s^N) + V^s \cdot r_s^V \cdot c_s^V(r_s^V))$$

$$\tag{4}$$

with the constraints:

$$0 \le r_s^N \le R_s^N \tag{5}$$

$$0 \le r_s^V \le R_s^V \tag{6}$$

where:

- $c_s^N(r_s^N)$ and $c_s^N(r_s^V)$ are functions giving the unit costs related to NO_x and VOC emission reduction;
- N^s and V^s are the seasonal domain NO_x and VOC emissions in the reference case;
- R_s^N and R_s^V are the maximum feasible reductions allowed by the available technologies.

3 Pollutant-precursor models for Lombardia Region

The precursors-AOT60 relationship (Eq. 2) remains to be described. It could be performed by deterministic 3D modelling systems, but they require so high computing times that they are virtually unserviceable in an operational research procedure. In this section neuro-fuzzy precursor-ozone models, tuned by deterministic 3D modelling system simulations, are suggested and implemented for Lombardia Region (Figure 1).



Figure 1: The simulation domain orography (m a.s.l.).

3.1 GAMES long term simulations

Ground level ozone concentrations and exposure have been simulated implementing the GAMES modelling system consisting of some main modules (Figure 2).



Figure 2: The GAMES modelling system

The photochemical model TCAM [3] is an eulerian threedimensional model. It solves, time by time, by means of adequate numerical algorithms, for each cell and pollutant species, the mass balance equation:

$$\begin{bmatrix} \frac{\partial c_i}{\partial t} \end{bmatrix} = -\left(\frac{\partial (u_x c_i)}{\partial x} + \frac{\partial (u_y c_i)}{\partial y} + \frac{\partial (u_z c_i)}{\partial z}\right) + \frac{\partial}{\partial x} \left(K_x \frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial c_i}{\partial z}\right) + S_i + E_i - D_i$$
(7)

where:

 c_i is the concentration of the *i*-th species;

 u_x, u_y, u_z are the components of mean wind speed;

 K_x, K_y, K_z are the turbulent diffusion coefficients;

 S_i is the chemical production and reduction term;

 E_i is the emission term;

 D_i is the deposition term.

The TCAM implements simplified chemical mechanisms based on both lumped molecule (SAPRC90 and SAPRC97, [2]) and lumped structure approaches (CB4, [10]). The meteorological pre-processor CALMET [14] provides to the TCAM the 3D meteorological fields of wind, temperature and turbulence. The emission data feeding TCAM are provided by the emission processor POEMPM [6], specifically designed to produce present and alternative emission scenarios.

The modelling system has been performed over the whole of Lombardia Region, a densely inhabited and industrialized area located in the Po Valley (Northern Italy) which is regularly affected by high ozone levels during summer months. The area is characterized by a VOC-limited atmospheric chemistry in the plain, suggesting that pollution control measures should first aim at a reduction of VOC emissions, while the mountain region follows the NO_x -limited photochemical regime, claiming for NO_x emission reductions [17].

The domain (240 x 232 km2) has been horizontally subdivided into 60 x 58 cells, with a resolution of $4x4 \text{ km}^2$ each. Vertical domain extends up to 3900m a.s.l., subdivided into 11 layers of growing thickness.

Simulations have been performed for 1996 summer season (from April to September), assuming initial and boundary conditions from a nesting procedure of the European scale EMEP Lagrangian Photo-oxidant Model ([4]).

Implementing the actual meteorology, emission and border conditions of that period, the base case simulation has been performed, supplying pollutant hourly concentration fields. The comparison with the actual values measured during the simulation period meets US EPA recommendations and recent European Directive on modelling validation [9]. The computation of such a simulation takes few days and this explains why GAMES cannot be directly used by an optimization procedure that would processing hundreds of model runs.

Keeping the meteorology and border conditions of simulation period as constant and arbitrarily reducing ozone precursor emissions of a certain ratio, seven alternative scenarios (reducing or increasing NO_x or/and VOC emissions) have been performed and collected for the calibration of simplified sourcereceptor models described in the following section.

3.2 Neuro-fuzzy source-receptor models

Simplified source-receptor models have been set up by means of neuro-fuzzy architecture. In neuro-fuzzy systems, neural networks are used to tune the membership functions of the fuzzy system and to automatically extract fuzzy rules from numerical data ([16]). In this work, a four-layer neuro-fuzzy network has been considered. The nodes of the first layer represent the crisp inputs. The activation functions of the second layer nodes act as membership functions. Each neuron of the third layer acts as a rule node so that this layer provides the fuzzy rule base. The output of this layer determines the activation level at the output memberships. As ordinary neural nets, the neuro-fuzzy one learns from a training data set, tuning membership functions and rules.

One neuro-fuzzy model has been identified for each domain cell. The input data are the cell maximum daily temperature and the daily VOC and NO_x emissions estimated for an area around the cell within an radius of 4 to 10 km. The output data are the daily AOT60 estimation performed by the GAMES system. The neuro-fuzzy models, running in simulation mode, estimate the daily cell exposure from which the AOT60 seasonal values are provided according to Equation 2.

The tuning and validation data series are selected processing the eight performed GAMES simulations. Each simulation covers the 1996 summer season, namely 183 days, so the available data correspond to 183x8 days. The validation set has been yielded selecting, from the simulation pattern, groups of data that are representative of different emission scenarios and meteorological conditions, for a total amount of a entire season, i.e. 183 samples. The identification pattern includes the remaining 183x7 samples.

4 Neuro-fuzzy model performances

The performances of the simplefied source-receptor models, evaluated on validation data set, are assessed in terms of correlation between neuro-fuzzy models and GAMES results. Figures 3, 4 and 5 show neuro-fuzzy models vs. GAMES simulations, for three cell groups, respectively below 200m a.s.l., between 200m a.s.l. and 700m a.s.l. and above 700m a.s.l.



Figure 3: GAMES versus neuro-fuzzy AOT60 estimation for validation data set (cells below 200m a.s.l.).

The trend lines and correlations of the scatter diagrams show that the neuro-fuzzy models perform high capability to reproduce the nonlinear source-receptor relationship with some remarks for the three elevation levers. In the plain, corresponding to the most pollutant emitting part of the domain, the neurofuzzy model underestimate the exposure about 5-10% (Figure 6).

The foothill area is better described and the error is limited to about $\pm 4\%$ in the worst cases. The Alps region AOT60 are overestimate by the the simplified pollutant-precursor models.

As the three area are characterized by different ozone accumulation processes and photochemical regimes, these results indicate that the neuro-fuzzy models

- perform good AOT60 estimation for all emissions, transport and photochemical conditions;
- have high capability in describing Milan ozone plume attracted by the breezes towards the foothill;



Figure 4: GAMES versus neuro-fuzzy AOT60 estimation for validation data set (cells between 200m a.s.l. and 700m a.s.l.).



Figure 5: GAMES versus neuro-fuzzy AOT60 estimation for validation data set (cells above 700m a.s.l.).



Figure 6: Neuro-fuzzy model AOT60 estimation error (%) for validation period

• are biased by VOC emissions: the VOC-limited region (the plain) is characterized by AOT60 underestimation, on the contrary the AOT60 computed for Alps area (NO_x-limited) are overestimate.

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References

- S. Barazzetta, G. Corani, and G. Guariso. A neural emission-receptor model for ozone reduction planning. In *Proc. iEMSs 2002*, volume 2, pages 130–135, 2002.
- [2] W. P. L. Carter, D. Luo, and I. L. Malkina. Environmental chamber studies for development of an updated photochemical mechanism for VOC reactivity assessment. Final report, California Air Resources Board, Sacramento (CA), 1997.
- [3] E. Decanini and M. Volta. Flexible modelling system for air pollution simulation and control in Northern Italy. In *Proc. EUROTRAC-II Symposium*, 2002.
- [4] EMEP/CORINAIR. Atmospheric Emission Inventory Guidebook, second edition. Technical report, European Environment Agency, 1999.
- [5] G. Finzi and G. Guariso. Optimal air pollution control strategies: a case study. *Ecological Modelling*, 64:221– 239, 1992.
- [6] G. Finzi, M. Volta, C. Carnevale, and C. Ragni. PO-EMPM: an emission model for size and chemical description of particulate matter. In *Proc. EUROTRAC-II Symposium*, 2002.
- [7] R. C. Flagen and J. H. Seinfeld. *Fundamentals of Air Pollution Engineering*. Prentice-Hall Inc., 1988.
- [8] R. Friedrich and S. Reis. *Tropospheric ozone abatement*. Springer-Verlag, 2000.
- [9] V. Gabusi, C. Pertot, G. Pirovano, and M. Volta. Evaluating seasonal model simulations of ozone in Northern Italy. In Proc. 26th NATO/CCMS International technical meeting on Air Pollution Modelling and its Application, 2003.
- [10] M. W. Gery, G. Z. Whitten, and J. P. Killus. Development and testing of the CBM-IV for urban and regional modeling. Technical Report EPA/600/3-88/012, U.S. Environmental Protection Agency, research Triangle Park, NC., 1988.

- [11] D. H. Loughlin. Genetic algorithm-based optimization in the development of tropospheric ozone control strategies. PhD thesis, Graduate Faculty of North Carolina State University, 1998.
- [12] R. Schleiniger. Comprehensive cost-effectiveness analysis of measures to reduce nitrogen emissions in Switzerland. *Ecological Economics*, 30:147–159, 1999.
- [13] W. Schöpp, M. Amann, J. Cofala, C. Heyes, and Z. Klimont. Integrated assessment of european air pollution emission control strategies. *Environmental Modelling and Software*, 14:1–9., 1999.
- [14] J. S. Scire, E. M. Insley, and R. J. Yamartino. Model formulation and User's Guide for the CALMET meteorological model. Technical Report A025-1, California Air Resources Board, Sacramento, CA, 1990.
- [15] J. Shih, G. J. McRae, and A. G. Russell. An optimization model for photochemical air pollution control. *Eur. J. Operational Research*, 106(1):1–14, 1998.
- [16] J. Shing and R. Jang. ANFIS: Adaptive-Network-based Fuzzy Inference System. *IEEE trans. on System, Man* and Cybernetics, 23:665–683, 1993.
- [17] C. Silibello, M. Volta, G. Calori, G. Pirovano, and G. Brusasca. The use of indicator concept to evaluate ozone-NO_x-VOC sensitivity during an ozone episode over Northern Italy. In *Proc. 9th Int. Conf. Automation and Decision Making*, pages 509–518, 2000.
- [18] S. Sillman. The relation between ozone, NOx and hydrocarbons in urban and polluted rural environments. *Atmospheric Environment*, 33:1821–1845, 1999.
- [19] D. G. Streets, Y. S. Chang, M. Tompkins, Y. S. Ghim, and L. D. Carter. Efficient regional ozone control strategies for eastern United States. *Journal of Environmental Management*, 61:345–365, 2001.
- [20] A. Venkatram, P. Karamchandani, P. Pai, and R. Goldstein. The development and application of a simplified ozone modeling system (SOMS). *Atmospheric Environment*, 28:3665–3678, 1994.
- [21] M. Volta and G. Finzi. GAMES, a new Gas Aerosol Modelling Evaluation System. In Proc. 4th International Conference on Urban Air Quality, 2003.