Air quality modelling at regional scale using WRF/Chem and a GIS based system for emission inventory for the Apulia Region

Umberto RIZZA, Gian Paolo MARRA, Dario CONTE, Mario Marcello MIGLIETTA, Cristina MANGIA, Gianvito QUARTA, Ilenia SCHIPA, Annalisa TANZARELLA

{u.rizza, gp.marra, d.conte, m.miglietta, c.mangia, g.quarta, i.schipa, a.tanzarella}@ isac.cnr.it
ISAC-CNR, S.P Lecce-Monteroni, -73100 Lecce – Italy, tel. +39 0832 298811, fax. +39 0832 298716

Abstract
Air quality simulation and forecasting is a complex problem that involves the knowledge of meteorological factors, chemical processes and emission inventories. In the real atmosphere all of these aspects are coupled in an intricate pattern, with time scales that may be much less than the scales involved only in meteorology. An important feature is the estimation of the emission inventory that must be very accurate. In this context, the emission factors for Apulia Region are used to prepare an emission inventory that will be computed and stored in databases of a GIS. GIS is used as the main component of the system for capturing, storing, checking and manipulating data that are spatially referenced. In particular our GIS approach is based on the use of Open-Sources GIS technologies (GRASS Project and PosrgreSQL with PostGIS extension). A preliminary simulation with the pollutant transport model WRF/Chem in a selected period is shown for SO2 tracer. The utilization of a GIS based system to get the grid-emissions seems to be a promising useful method to investigate air-quality at regional scale.

1. Introduction

In air-pollution applications, due to the elevated number of chemical species involved, it is essential to develop a source emission-inventory, preferably in form of a database. Such database may be used to classify the emissions data given certain criteria that may involve for example the nature of chemical species, the chemical mechanism, the features of geographic area and the industrial activities. In practice the methodology called top-down is considered. This makes use of the global values of emissions generally at province level over yearly basis. These "global values" have to be disaggregated along the numerical grid using statistical algorithms.
The top-down methodology refers to the annual data of concentration of pollutant species of the national inventory of CORINAIR (COordination INformation AIR) (http://www.apat.gov.it/site/it-IT/Servizi_per_l'Ambiente/Inventario_delle_Emissioni_in_Atmosfera_(CORINAIR-IPCC)/), which is part of the CORINE program (Coordinated Information on the Environment in the European Community) (http://dataservice.eea.europa.eu/dataservice/available2.asp?type=findkeyword&theme=Corine), for the purpose of gathering and organization of information on the environmental status and of the natural resources in the European Community. In particular in this work, we have considered the CORINAIR data for the Apulia Region. With this methodology, one can obtain in general the initial-gridded values on the temporal basis of interest of any chemical species. In this procedure of disaggregation the utilization of the Geographic Information System (GIS) may assume a strategic role. In fact, the municipal emission values, represented in raster format, can be associated to a numerical cartographic base and subsequently may be superimposed on a geographic grid of vectorial type (map-overlapping). In this way, it is possible to get the value of emission at each grid-point as the sum of distinct activities called macro-sectors in the

CORINAIR terminology. In this paper, we will describe the coupling of a GIS based pre-processor emission with the model WRF/Chem (G.Grell, S.E.Peckam, R.Schmitz, S.A. McKeen, G.Frost, W.C.Skamarok, B.Ederr, 2005). This will allow the specification of the emission input files within the dispersion model in an efficient, accurate and flexible manner. Efficient because it permits to quickly generate the emissions of the pollutant species, accurate because all of the concentration data are geographically referenced and then, the errors due to incorrect geographic position are strongly reduced, and finally flexible because it allows the user to obtain the input files in an automatic way.
At this preliminary stage only the SO2 emissions will be considered, and the result of the simulations will be showed in chapter 4. Anyway it is evident that such procedure may more useful for photochemical/particulate pollution.

2. The Meteorological/Chemistry transport model

Until recently, the chemical processes in air-quality investigations were usually implemented "offline" the meteorological models, as in CALGRID (Yamartino, R. J., J. S. Scire, G. R. Carmichael and Y. S. Chang, 1992), CAMX (http://www.camx.com) and more recently CMAQ (D.W. Byun and S.Ching, 1999). This approach is computationally very appealing as retrospective analysis of air-quality can be done just considering one meteorological simulation. Anyway this separation between meteorology and chemistry may cause loss in important pieces of information for those meteorological processes that have little time-scale (less than one hour) or coarse space-scale (less than few kilometres) resolution. In the last few years various chemical modules have been implemented into the WRF (Weather Research and Forecasting model, http://www.wrf-model.org/index.php) meteorological framework, creating an "online" WRF/Chem model (G.Grell, S.E.Peckam, R.Schmitz, S.A. McKeen, G.Frost, W.C.Skamarok, B.Ederr, 2005.). Transport is done using the same system of coordinates and the same physics parameterization with no interpolation in space or time.

3. The emissions pre-processor

3a. The top-down CORINAIR methodology

To realize the emissions-database we adopt the top-down CORINAIR methodology. This classifies the emission data in function of the chemical species, the temporal interval, the geographic area and the natural/anthropic activities and it uses the global values of emissions (per ton annually) available all over the Italian provinces. By means of an algorithm that we describe later, it is possible to disaggregate this global information both from a spatial or a temporal point of view.
Specifically, for the area of interest, we have considered the CORINAIR data for the the five provinces of Apulia Region (see fig.1a,b). Each of the provincial emission concerns distinct activities according to specific codes SNAP (Selected Nomenclature for sources of Air Pollution – year 1997) (http://reports.eea.europa.eu/EMEPCORINAIR/en/page009.html).

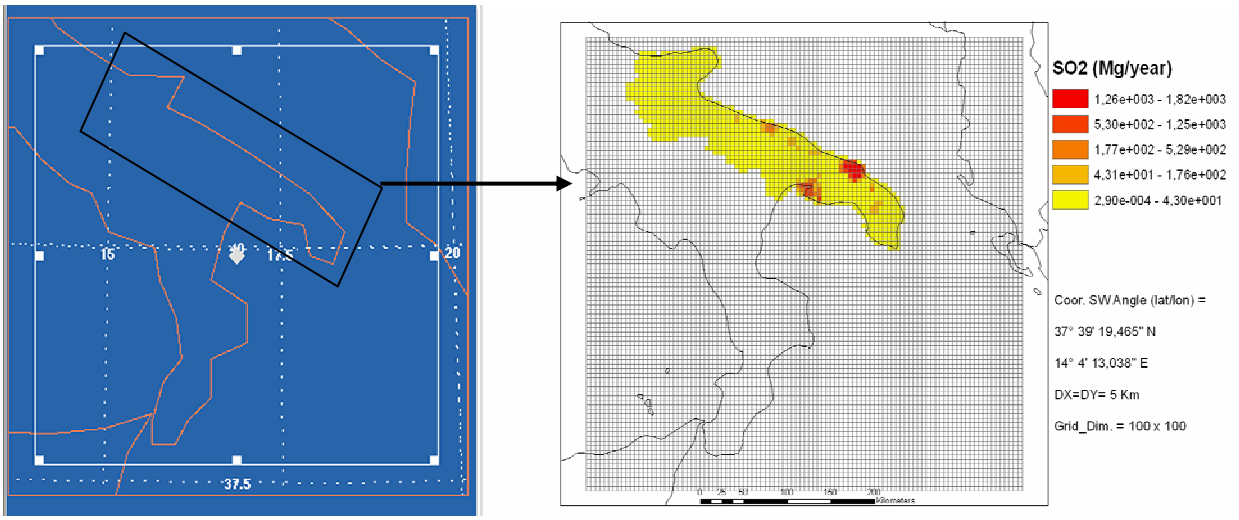

Fig.1: The meteorological/emission domain

As a result, with this technique, we can obtain annual values for the emissions distributed along each municipal area.
The spatial/temporal algorithm is based on equation of the form

$$e_{i,c,a,t} = E_{p,i,a} \frac{s_{c,p,a}\gamma_{t_a}}{\Gamma} abl_{i,c,a} \qquad [1]$$

where $e_{i,c,a}$ is the municipality emission of chemical pollutant i^{th} for the activity denoted by a to time t, $E_{p,i,a}$ is the provincial emission of chemical pollutant i^{th} for the activity denoted by a, $S_{c,p,a}$ is the disaggregation factor for the municipality c, for the province p and the activity denoted by a, γ_{ta} is the temporal normalization coefficient, Γ is the normalization coefficient, and finally $abl_{i,c,a}$ is the reduction coefficient of the pollutant i^{th}, for the municipality c and for the activity denoted by a.

3b. The GIS methodology

The municipal level has still not enough resolution for the grid of the simulation domain. This is generally true for grid resolution of the order of few kilometers, so that we have to make a further discretization of the emissions by calculating each emission values for user defined grid points starting from the municipal level. Uppermost, GIS-module produces a PostgreSQL (http://www.postgresql.org/) table that contains municipality administrative boundary map with an empty attribute column, in which we will store municipality emission produced by the spatial/temporal disaggregation. In particular, PostgreSQL geographic data are extracted from a shape file, projected into Lambert Conformal Conic coordinate system and formatted in a textual SQL script file through shp2sql PostGIS (http://postgis.refractions.net/) command, in accord with GeomFromText PostGIS specification. After these operations the emissions are georeferenced, and thus they can be analyzed with the GIS tools. Next we have to superimpose the numerical grid of the simulation domain into the georeferenced emissions. In the GIS context this can be done in two steps. The first is to set up an ensemble of geographical polygons to build a vectorial grid cells. The user must provide, of course, basic geographical information, like: South-West grid angle coordinates, width and height of cells, grid dimension, and so on. As for the municipal map, the vectorial grid is stored into PostgreSQL database as a geographic table with an attribute column that will contain cell emission values. The second step consists in doing a map overlapping GIS operation between the emission municipality map (spatial/temporal disaggregation from CORINAIR) and the vectorial grid cells map. The goal of second step is to obtain the emission value of the cells of vectorial grid. To do this we define the quantity n as the

number of cells into the vectorial grid, and m the number of municipalities of the Apulia region, so we have:

$$G_i = \sum_{j=1}^{m} e_{c_j} \frac{Area(S_{c_j} \cap S_i)}{Area(S_{c_j})} \qquad [2]$$

with $i \in [1, n]$, and where G_i is the emission value of ith cell, S_i is the GIS geographic entity of the ith cell, S_{c_j} is the GIS geographic entity of c_j^{th} municipality with $j \in [1, m]$ and finally e_{c_j} is the emission of c_j^{th} municipality. The last step of the emission pre-processor consists in putting the gridded-emission file inside the WRF/Chem model. This has to be done taking into account that units must be transformed in mol km^{-2} hr^{-1}.

4. Case study

4a. The simulation domain

The meteorological simulation domain covers the southern Italy. The emissions inventory is provided just for the Apulia region (fig.1) following the methodology described above (chapter 3). This region with about 4 million inhabitants is located in the southeast side of Italy, with longitude between 15° and 19° East and latitude between 39° and 42° North. It has two heavy industrialized areas producing about 70% of the total emissions of the whole region (Brindisi and Taranto).

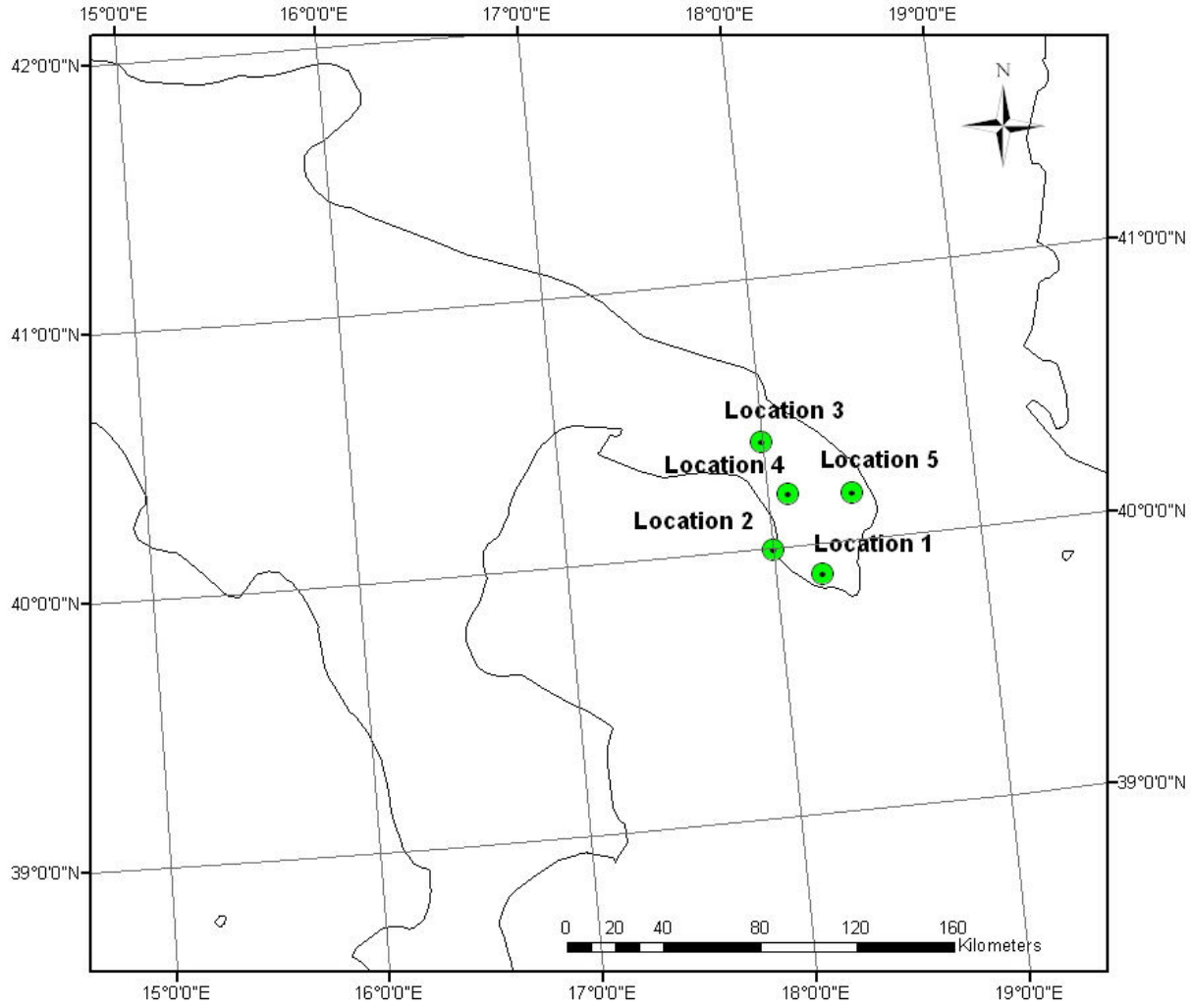

Fig.2: locations of the virtual monitoring points

The simulated period is 21-24 July 2006. We run the model WRF/Chem turning off the chemistry packages for Ozone and Aerosols and just considering SO2 as a tracer contaminant. The model was initialised and driven using NCEP final analysis updating fields every six hours at 1 degree resolution. The main grid had a mesh of 100x100 points with 5 km grid spacing, and 31-vertical levels in the terrain following hydrostatic pressure coordinate system.

4b. Results and discussion

In order to test the functionality of the coupling between the emission inventory database and the WRF/Chem model a multi-day simulation in the period 21-24 July 2006 has been performed. The output of the model WRF/Chem is in the netCDF (http://www.unidata.ucar.edu/software/netcdf) universal format. It is provided with a collection of post-processing utilities for analyzing the output results. In particular we have extracted the concentration of the SO2 tracer in some selected points (virtual monitoring stations) of the modelling domain as depicted on Table I.

	lat	lon	city
Location 1	39.89	18.23	Ugento
Location 2	40.00	18.00	Gallipoli
Location 3	40.40	18.00	Campi Salentina
Location 4	40.20	18.10	Nardò
Location 5	40.18	18.41	Otranto

Table I: location of the five virtual monitoring stations

The evolution of SO2 concentration is showed in the following fig.3.

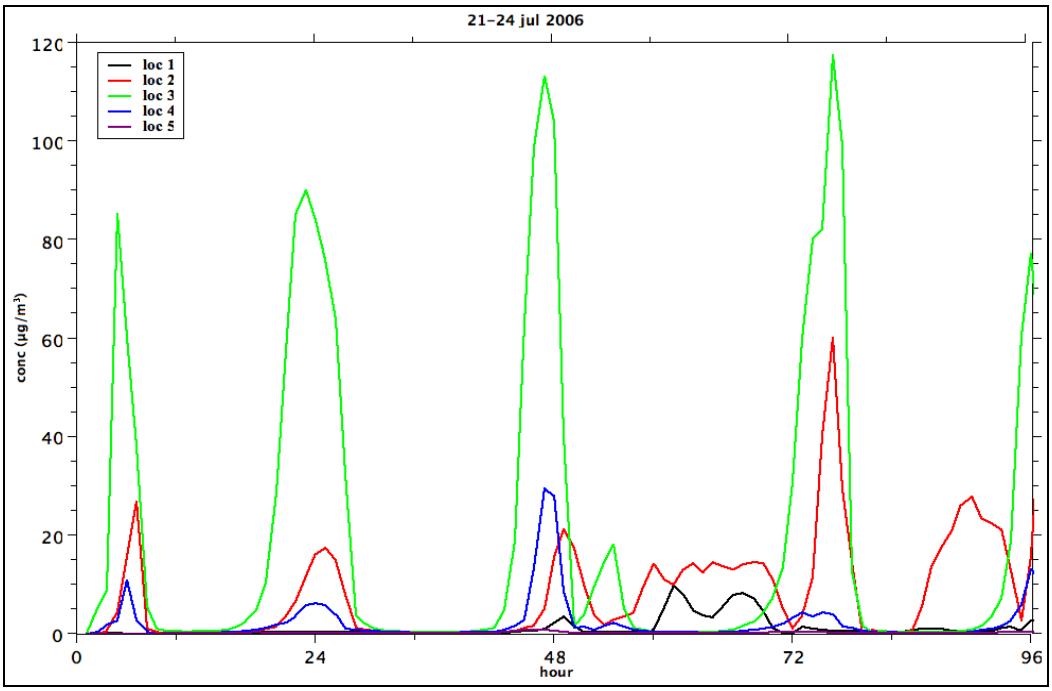

Fig.3: the ground level concentration of SO2 tracer at the five selected locations

Being SO2 a primary pollutant its concentration at ground level is roughly related to the wind direction/speed patterns. The simulation show high levels of SO2 in the proximity of the city of Campi Salentina, which is located 25 km south of the industrial site of Brindisi. During the 96-h simulation the prevalent winds is from north.

5. Conclusions

In the control strategies of air-quality at regional scale numerical modelling assumes a strategic role since it is impossible to measure all the involved chemical quantities and their mutual interactions in large domains. In this context the two decisive points concern: (i) the specification of the numerical algorithms necessary to solve the set of differential equations and (ii) an accurate description of the emissions within the simulated domain.

In this work we have proposed an approach that describes these two points in a modern fashion, that is the WRF/Chem model for the first point and GIS technologies for the second. The WRF/Chem model represents the state of the art in the air-pollution modelling being based on an online coupling between the meteorology and the chemistry. The GIS technology, which is based on the concept of georeference, is a very powerful tool in elaborating the emission scenarioes and we believe it will be used heavily in the future for air-quality evaluations. The next step of the present work will concern the inclusion of the chemical mechanisms to simulate Ozone and Aerosols and the comparison with measured data.

6. References

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