Off-line model integration: EU practices, interfaces and possible strategies for harmonisation

Sandro Finardi[1], **Alessio D'Allura**[1] and **Barbara Fay**[2]
[1]ARIANET, Milano, Italy
[2]German Weather Service, Offenbach, Germany

1 Introduction

A survey of the very many and diverse modelling communities in European countries was performed in COST728 on the basis of partner contributions (Baklanov et al., 2007). Even if the model coverage remains incomplete and somewhat arbitrary the contributions represent a wide spectrum of modelling complexity and effort in 16 European countries and 40 institutions. The majority of the presented systems are based on mesoscale meteorological models (MetMs) available at the national weather services or in weather forecasting consortia (i.e. HIRLAM, COSMO (Lokalmodell), ALADIN) and on international free community models developed by universities (i.e. MM5, WRF, MC2, RAMS). This approach allows the air quality (AQ) modelling community to take advantage and benefit from the development, testing and model validations done for the purpose of weather prediction. At the same time it provides users without large own development capacities or with the need for a standard system to apply model systems supported by a wider community.

The modelling components that deal with transport and transformation of atmospheric pollutants are more diverse than the MetMs, ranging from a simple passive tracer along a trajectory (i.e. CALPUFF) to a complex treatment of reactive gases in an Earth system (i.e. MESSy). The wide spectrum of model applications ranges from diagnostic or climatologic AQ assessments, episode analysis and source apportionment to AQ forecast at regional and urban scale and toxic and radioactive releases emergencies preparedness.

The communication between off-line coupled meteorological and AQ models is a problem of often underestimated importance. The multitude of modelling systems previously introduced give rise to different approaches and methods implemented within interface modules. Tasks covered by interfaces are minimised in coupled systems relying on surface fluxes, turbulence and dispersion parameters (i.e. eddy viscosity) provided by the meteorological driver. Other systems use interface modules implementing surface and boundary layer parameterisations to estimate dispersion parameters. Atmospheric physics parameterisations, and even default or limit values assumed for some key parameters, can have relevant effects on pollutant concentration fields in critical conditions (e.g. low wind and stable conditions). Interface modules can involve the evaluation of emissions of some relevant species that can be strongly influenced by meteorology, like biogenic VOC, windblown dust and sea salt spray. Moreover, mesoscale and urban scale air quality modelling systems are usually nested within larger scale application results, used to initialise and drive AQ fields at domain boundaries. This operation too can have relevant influence on AQ modelled fields, especially evident over complex topography.

1 Off-line coupled models and interfaces

The major components of an integrated meteorological and air quality modelling system are sketched in Figure 1. Since the input data flow connects the meteorological modelling system and the air quality model those two are generally defined as coupled models. Depending on the characteristics of this connection we can distinguish between off-line and on-line coupling. Off-line coupled MetMs and AQ models work separately, there is no feedback from Chemical Transport Models (CTMs) to MetMs and meteorological input to the AQ model is usually limited to averages, either in time or space, of main variables defining the atmospheric status (fields are provided any fixed times, e.g. 1 hour). This specific approach is the traditional way by which those complex system have been developed until now.

The development of these modelling systems is usually focused on the scientific and technical features of emission, atmospheric flow and pollutant dispersion models, while comparatively little attention is devoted to the connection of the different models. Meteorological and air quality models often employ different coordinate systems and computational meshes. In principle, interfaces should simply solve this grid system mismatch to connect MetMs output and AQ models input with minimum possible data handling.

Nonetheless, interface modules are often used to solve other system realisation issues, e.g.:

- some AQ models rely on “standard” meteorological products which usually do not include turbulence, atmospheric stability, mixing height, and dispersion coefficients;
- MetMs cannot provide all the physical variables that are needed by AQ models (e.g deposition velocities) or some meteorological fields may be estimated by parameterisations not compatible with modelling methods implemented in dispersion models;
- sometimes re-computation or “filtering” of dispersion parameters is considered more robust for practical applications;
- the horizontal resolution of the meteorological forecast can be lower than that needed by air quality models, and insufficient to correctly estimate dispersion parameters.

To solve the mentioned problems various tasks are often included within interface modules, as well as: data interpolation, meteorological fields downscaling, boundary layer parameterisations and estimation of dispersion coefficients, evaluation of meteorological driven emissions (e.g. biogenic emission, wind blown dust, sea salt), enhancement of physiographic data.

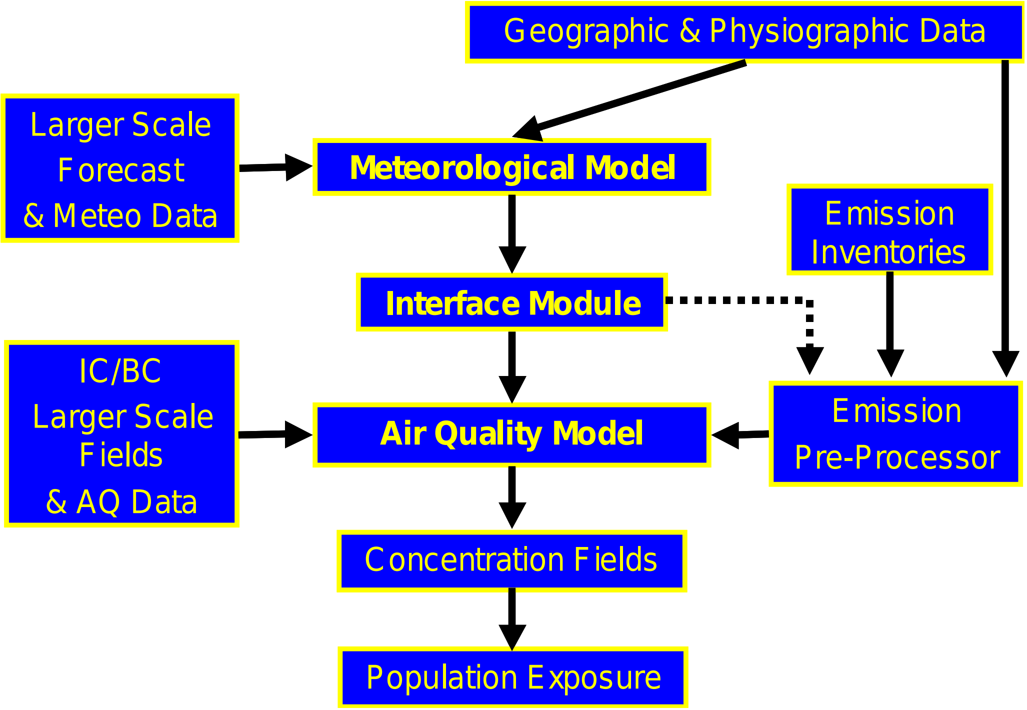

Figure 1. Integrated meteorological and air quality modelling system conceptual scheme.

A multiplicity of off-line coupled modelling system have been developed and are applied all over the world. The most common systems features and interfacing strategies in Europe have been identified, within Cost728/WG2, using: Cost728/732 model inventory (http://www.mi.uni-hamburg.de/index.php?id=539), a questionnaire on interfaces circulated among cost728 participants and previous experiences and knowledge of COST728/WG2 members (Baklanov et al., 2007).
Three main approaches have been identified:

a) joint development of coupled models, with interfaces built on specific models features and needs, this approach is mainly adopted by large institutions and Weather Services developing both MetM and AQ models;
b) use or customisation of US Community modelling systems, e.g. MM5/WRF+CMAQ with MCIP interface module;
c) interfacing of self developed AQ models with EU Weather Services and US Community Meteorological Models through model specific or general purpose interfaces.

The first strategy implies the direct use of physical parameters estimated by MetMs, like e.g. Monin-Obukhov (MO) similarity theory parameters, and limitation of the interface module tasks to the evaluation of missing variables. This approach is particularly attractive when meteorological and air quality models share the same computational grid system and data interpolation can be avoided. It has to be taken into account that changing grid system and topography makes necessary to re-compute the vertical wind component, to guarantee mass conservation, which is essential for dispersion calculations.

The other approaches are mainly based on the development of meteorological processors capable to evaluate surface and boundary layer scaling parameters, mixing height, atmospheric turbulence and dispersion parameters on the basis of the average meteorological variables provided by MetMs and possibly supplementary external data. This approach gives the possibility to interface meteorological and air quality models characterised by relevant differences that can make difficult direct connection, moreover it can allow the introduction of additional high resolution information, like land-use, roughness length, or urbanised parameterisation to be used by computations performed by the interface module. The use of boundary layer and dispersion parameterisations within interface modules or AQ models should take into account the effective resolution of MetM to avoid parameterisation of phenomena explicitly described by modelled meteorological fields, as it can happen when high resolution MetMs results are available.

The AQ models have to be interfaced with pollutant emissions and initial and boundary conditions imposed from larger scale AQ forecast. Pollutant emissions can be influenced by meteorological conditions through different kind of processes of both anthropogenic and natural origin. Air temperature determines the amount of fuel consumption for house heating, the meteorological conditions often influence people behaviours (e.g. car or public transport usage) determining some features of pollutant emissions. Meteorological conditions influence natural emission processes like surface erosion, wind blown dust resuspension or biogenic emissions of Volatile Organic Compounds from vegetation.

Chemical transport models results depend on the initial conditions and on the inflow in the computational domain of background concentrations. The proper nesting of meso and local scale simulations within larger scale forecast results it is generally managed by an interface module that has to match grid and resolution differences and possibly different chemical schemes employed by considered models.

The following sections provide a few examples of the possible effects of the different interfacing issues on the AQ simulation results.

2 Interface module and model nesting effects on air quality simulation

An integrated air quality modelling system similar to those previously sketched has been applied in two different urban environments with the intent to highlight its sensitivity to dispersion processes parameterisations and AQ model initialisation implemented within the interface module. The modelling system used for the following applications is based on the MetM RAMS (Pielke et al., 1992; Cotton et al., 2003) and on the Eulerian chemical transport model FARM (Calori and Silibello, 2004). The cited meteorological and air quality models are connected by the interface module GAP/SurfPRO (Calori et al., 2005; Finardi, 2005). GAP (Grid AdaPtor) is a grid interpolation tool with capability to re-compute vertical velocities, that has been developed to interface FARM with any MetM. SURFPRO (SURFace-atmosphere interface PROcessor) is a meteorological processor based on the Monin-Obukhov similarity theory designed to provide turbulence and dispersion scaling parameters, as well as eddy diffusivities and deposition velocities (Beljaars and Holtslag 1991; Hanna and Chang 1992; Zilitinkevich et al. 2002b).

The cities of Rome and Turin are respectively the first and the fourth largest urbanized areas in Italy, they are exposed to severe air pollution episodes induced by complex air flow pattern and atmospheric boundary layer dynamics, due to both intrinsic complexity of the urban canopy and specific mesoscale flow features (e.g. sea breezes, catabatic flows and stagnation). The nested computational domains for both mentioned systems are depicted in Figure 2. Rome is the largest Italian city, characterised by a widely spread urbanized area, with a total population around 3.5 millions people. The city is often affected by high ozone and PM concentrations, likely to be detected in both summer and winter. During summer, the high insulation favours photochemical activities; while in winter, persistent high pressure systems with very weak pressure gradients determine weak wind conditions and possibly temperature inversion causing, pollutants accumulation in the lower layers of the atmosphere.

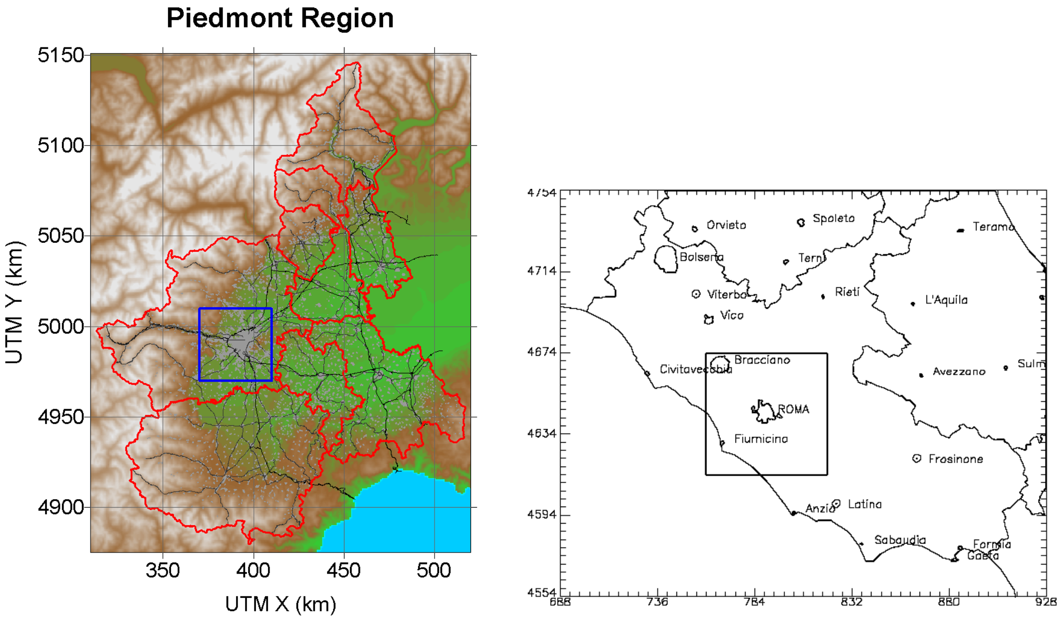

Figura 2 Turin (left) and Rome (right) urban area air quality modelling systems computational domains.

Turin metropolitan area has a resident population of about 1.5 millions people. It represent the core of one of the major industrial areas in northern Italy. The city is located at the western edge of the Po Valley, and it is sited mainly on flat topography between the Western Alps and a range of hills on its east side. Local circulation is strongly influenced by the shelter effect of the Alpine chain, and it is dominated by the superposition of mesoscale (e.g. Po Valley stagnation, mountain/valley breezes and föhn) and urban flow features.

1.1 Dispersion parameterisation effect

The modelling system introduced in the previous section has been applied to analyse a summer air pollution episode in the area of Rome (Gariazzo et al., 2007). The area is exposed to sea breeze circulation during daytime, while very week land breeze, turning to calm conditions within the city of Rome, characterises night time circulation. Surface turbulent fluxes and Eulerian dispersion coefficients (eddy diffusivities) used by the chemical transport model FARM are computed by the interface module SURFPRO. The similarity theory is based on the general assumptions of quasi-stationary and horizontally homogeneous flow, and constant (independent of height) turbulent fluxes within the surface layer (Arya, 1988). These assumptions are generally not fulfilled in urban areas and in complex terrain. The MO theory is nevertheless applied in most models even in these cases, mostly due to lack of other practical formulations (Mahrt 1999). During very weak wind conditions like those observed in Rome at night time the values provided by parameterisations for the eddy diffusivity is very low and usually falls under the minimum K_Z value. Different minimum values for K_Z are used by AQ models, normally ranging from 0.1 to 1. m^2s^{-1}. In SURFPRO different minimum values can be imposed as a function of land use:

$$K_z^{\min} = K_{rur}^{\min} \cdot (1 - f_{urban}) + K_{urb}^{\min} \cdot f_{urban}$$

where f_{urban} indicates the urban land use fraction within each grid cell, $K_{rur}^{\min}$ and $K_{urb}^{\min}$ indicate minimum K_Z for rural and urban area for which values of 0.1 and 1 m^2s^{-1} are those more commonly used. This assumption can be justified due to the urban canopy effect, that has the tendency to maintain neutral or slightly unstable conditions over the city during the night, consequently increasing pollutant dispersion with respect to rural conditions.

Figures 3 and 4 show an example of the modelling system results for O_3 and NO_2 at a urban background (Villa Adda) and rural station (Cavalieri). The reference simulation (black line), with minimum K_Z defined by the previous formula, shows e overestimation of ozone concentrations at the urban station during night time, while nitrogen dioxide concentrations are slightly underestimated. A second simulation has been performed imposing everywhere a minimum K_Z value of 0.1 m^2s^{-1}. The simulation results in Figure 3-4 (grey line) show an enhancement of ozone results at the urban station, and an excessive growth of nightly NO_2 concentrations. As expected, no relevant change affects concentrations at rural location and during daytime. The stronger limitation imposed to vertical mixing by small K_Z value makes rise NO_X concentrations and causes consumption of Ozone (Ozone titration) in VOC-limited photochemical regimes.

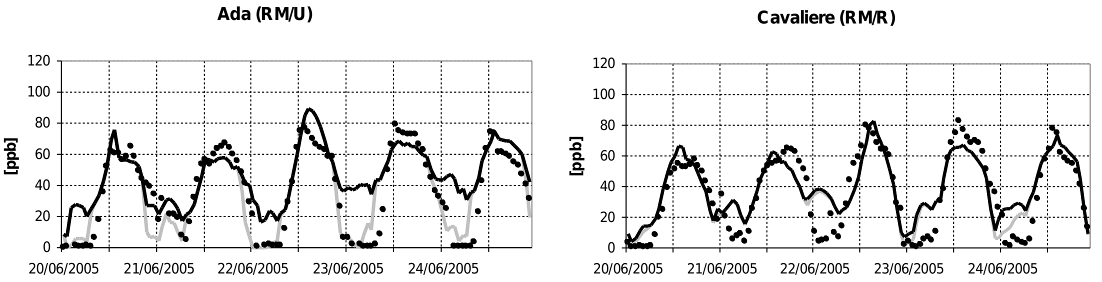

Figura 3 Comparison among O_3 observed (black dots) and computed concentration with K_Z minimum value set to 0.1 m^2s^{-1} (grey line) and 1 m^2s^{-1} (black line) at urban (left side) and rural (right side) stations.

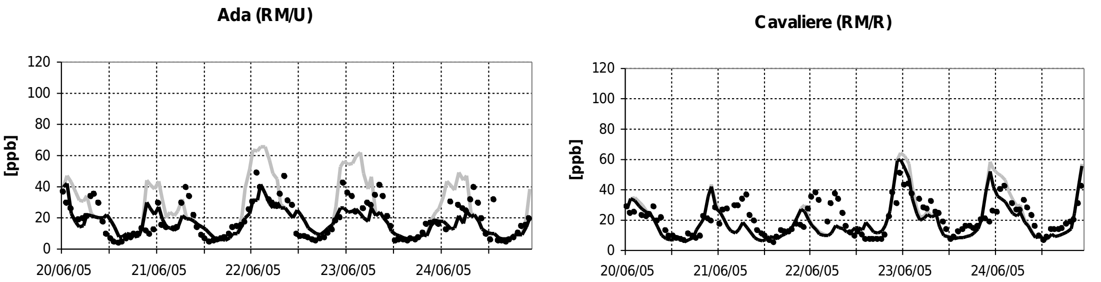

Figura 4 Comparison among NO_2 observed (black dots) and computed concentration with K_Z minimum value set to 0.1 m^2s^{-1} (grey line) and 1 m^2s^{-1} (black line) at urban (left side) and rural (right side) stations.

Further tests and previous experiences in other geographic locations confirmed that minimum K_Z is a relevant (and often neglected) parameter to properly model dispersion during weak wind and very stable conditions. Unfortunately no general value for minimum K_Z can be defined, while proper values depend on season and local climatology.

1.2 Surface fluxes and boundary layer parameterisation effect

In principle the direct interfacing methods consisting in the evaluation of dispersion parameters from meteorological models average fields and turbulent fluxes should be preferred to guarantee the modelling system consistency and to take advantage of the modelling capabilities of new generation MetMs, e.g. higher order turbulence closures, surface layer parameterisations and soil-surface-canopy models. On the other hand this approach can suffer the intrinsic weakness to be influenced by possible meteorological forecast errors or local scale flow features that can have relevant impact on surface fluxes, mixing height value and pollutant dispersion.

A test case to set in evidence the possible effect of different interfacing approaches has been run over Torino area. The simulations concerned a summer fair weather period, when thunderstorm activity occurred over the western Alps. The AQ model has been driven by two different set of turbulent surface fluxes and scaling parameter. The first set has been estimated using the surface fluxes produced by the MetM RAMS, the second one has been computed by SURFPRO interface module according to van Ulden and Holtslag formulation for surface fluxes and MO similarity. Figure 5 shows the relevant differences obtained from the two test simulations for almost all the considered parameters (sensible heat flux, friction velocity, mixing height and vertical diffusivity at the first vertical level) during the first day of simulation. The comparison of computed and observed concentrations (Figure 6) highlights the mismatch of NO_2 concentrations produced by the simulation using RAMS turbulent fluxes. The sensible heat flux has been largely underestimated, producing a very limited PBL growth with relevant effects on local NO_X concentrations but limited influence on Ozone. Further analysis pointed out as a localized convective precipitation event has been mispredicted by RAMS, affecting part of Torino city with a strong precipitation event that did not occur. The high uncertainty of storms location and intensity forecast it is not surprising, due to the geographical complexity of the region and seasonal (July) thunderstorm phenomena frequency.

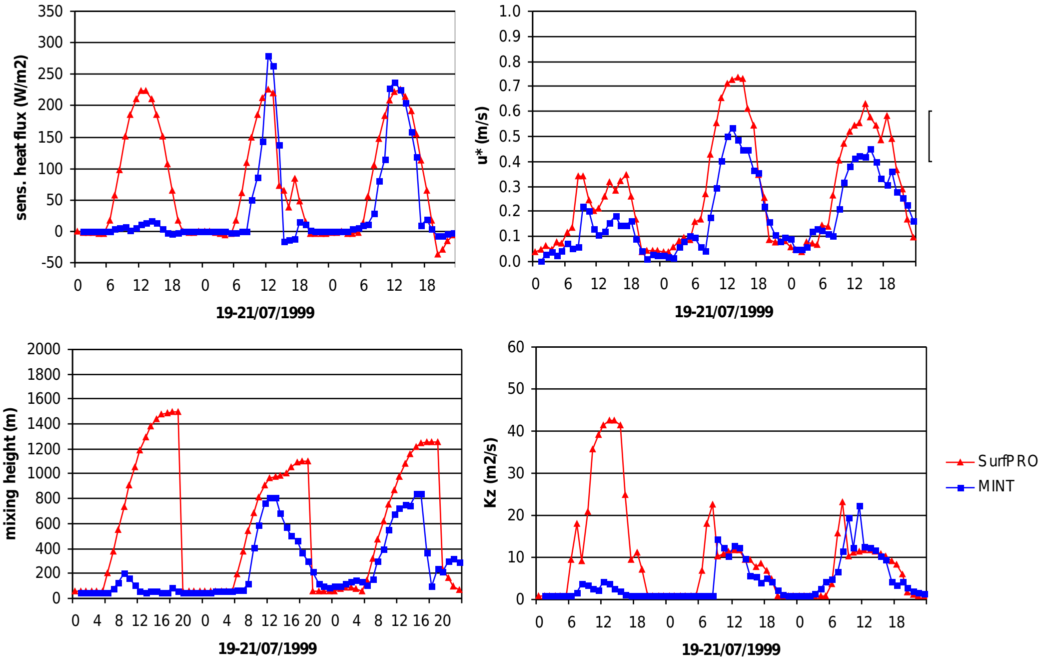

Figure 5. Comparison of sensible heat flux (top left), u_* (top right), mixing height (bottom left) and K_Z (bottom right) computed by RAMS (blue line) and SURFPRO (red line) during a summer thunderstorm episode in Torino.

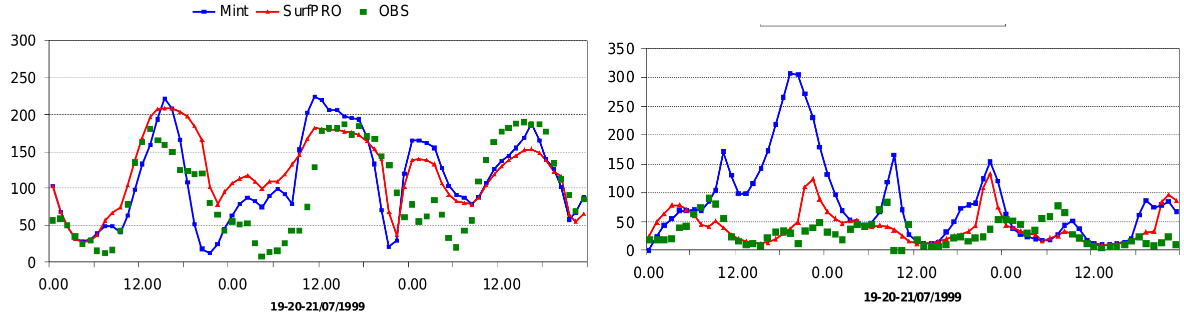

Figure 6. Comparison of O_3 (left), NO_2 (right) concentrations computed using RAMS (blue line) and SURFPRO (red line) turbulent fluxes and scaling parameters.

During adverse meteorological events the use of an interface module to model dispersion parameters can have the advantage to reduce forecast error effects on predicted concentrations. Anyway, further analysis showed that the discussed results were strongly dependent on the radiation scheme used by RAMS model. Running the model with Harrington instead Chen scheme (Cotton et al., 2003), the NO_X overestimation could be reduced due to the larger values of surface radiation obtained.

1.3 Air quality initialisation at regional and urban scale effect

During the evaluation of the air quality forecasting system for Torino metropolitan area (Finardi et al., 2007) it clearly emerged the effect on model results of AQ initial and boundary conditions. To define these data the modelling system relies on CHIMERE continental forecasts provided by *Prev'Air* European Scale Air Quality Service (http://www.prevair.org). This large scale air quality forecast was initially used to define both initial and boundary conditions. In principle local observations could be used to build more realistic initial concentration fields, but they are not yet available at the forecast simulation start time.

The AQ forecasting system results have been compared with observations over a 7 months period: from June 2006 to January 2007. The predicted concentration data have been divided in two time series obtained selecting the first (last) 24 hours of each daily forecast cycle, that covers 48 hours. Comparing the two time series with observations (Figure 7) it turns out that the +48 simulation obtains generally higher concentrations and better compares with observations with respect to +24. This behaviour was common to all pollutants but ozone, that was instead overestimated in the +24 simulation. The comparison of initial and +24 concentration fields showed that this difference was due to the influence of initial conditions on the first day of simulation. The resolution difference from CHIMERE (50 km) to FARM background domain (4 km) didn’t allow to obtain a proper initialisation. On CHIMERE topography Torino is located on the western Alps slope, at about 800m. This feature clearly favour ozone overestimation and other pollutants underestimation, due to the city location outside of the Po valley plane.

This shortcoming identified induced to change the way to initialise AQ fields using previous day the forecasting system results (+24 fields) and to prepare a simple AQ analysis tool, to be able to correct initial fields with local observations when they will be available. A resolution match problem is present, even if less evident, within the boundary conditions too. The final set up of the system is therefore programmed to move to 3 nested domains, introducing a larger background computational mesh enhancing background pollution simulation and reducing the effects of boundary conditions on the AQ forecast, as it was originally experimented in the EC FP5 project FUMAPEX (Finardi et al., 2007).

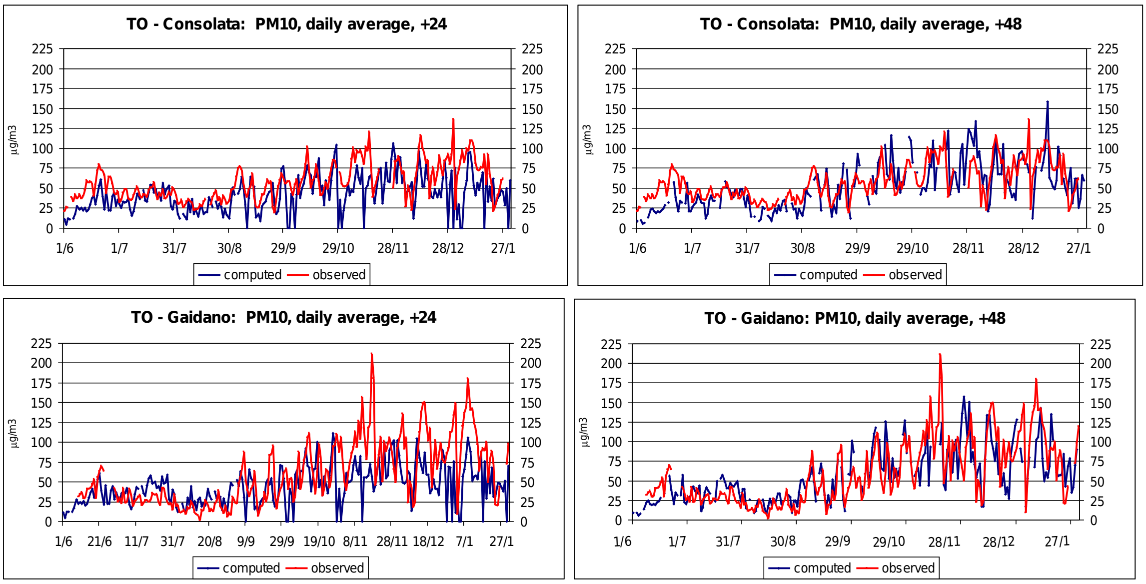

Figure 7. Comparison of computed (blue line) and observed (red line) PM10 daily average concentrations at two Torino city urban background stations (Consolata and Gaidano). Left and right panels refer respectively to the first (0:+24) and second (+24:+48) day of forecast. The comparison refer to June 2006 – January 2007 time period.

3 Summary and discussion

The Working Group 2 of COST728 started a survey of the very many and diverse coupled meteorological and air quality modelling systems developed and applied European countries. Our attention has been focused on off-line coupled modelling systems, which are by far the more numerous, even if the number of on-line coupled systems recorded is larger than expected. The important role of interface modules has been discussed and more common approaches followed in their development have been briefly described on the basis of COST728 inquiry and known modelling systems analysis. In principle the direct interfacing methods consisting in the evaluation of dispersion parameters from meteorological models average fields and turbulent fluxes should be preferred to guarantee the modelling system consistency. On the other hand interface/processors allowing the user to reconstruct missing variables and dispersion parameters, to increase space resolution and possibly to enhance meteorological fields for lower atmospheric layers and for the urban atmosphere, are widely used by the air quality community. The influence of different interface modules on integrated air quality modelling system results has been shown through application examples taken from the authors experiences.
In the diverse landscape of European modelling, model harmonisation remains an important issue despite earlier efforts, e.g. COST710 (1994-1998) which are continued in the regular Harmonisation conferences. Modular modelling, flexible IO strategies and adaptable interfaces following agreed guidelines for off-line and on-line integrated modelling, which are applied by all including the large consortia and community models, would greatly facilitate model improvement and applicability for European users. The large variety of modelling systems can be considered a scientific richness but creates problems of model result inter-comparison and underlines difficulties in model development collaboration in Europe.

4 References

Arya, S. P. S. (1988) Introduction to Micrometeorology. Academic Press, Inc., San Diego, Caliofornia 92101. pp. 307.

Baklanov, A., Fay, B., Kaminski, J. (2007) Overview of existing integrated (off-line and on-line) mesoscale systems in Europe, COST Action 728, Deliverable 2.1 Report.

Beljaars, A. C. M., and Holtslag, A. A. M. (1991) Flux parametrisation over land surfaces for atmospheric models. J. Appl. Meteorol., 30, 327-341.

Calori G., Clemente M., De Maria R., Finardi S., Lollobrigida F. and Tinarelli G. (2005) Air quality integrated modelling in Turin urban area. Environmental Modelling and Software., in press.

Calori G. and Silibello C. (2004) FARM (Flexible Air quality Regional Model) Model formulation and user manual. ARIANET Report, Milan, Italy, 59 pp.

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. and McFadden, J.P. (2003) RAMS 2001: Current Status and Future Directions. Meteorol. Atmos. Phys., 82, 5-29.

Finardi, S., De Maria, R., D'Allura, A., Calori, G., Cascone, C. and Lollobrigida, F., 2007: A Deterministic Air Quality Forecasting System For Torino Urban Area, Italy. Environmental Modelling and Software, in press.

Finardi S. (Editor), Baklanov, A., Clappier, A., Fay, B., Joffre, S., Karppinen, A., Ødegård, V., Slørdal, L. H., Sofiev, M., Sokhi, R. S., and Stein A., (2005): Improved interfaces and meteorological pre-processors for urban air pollution models. Deliverable 5.2-3 of the EC FUMAPEX project, Milan, Italy, 55 pp.

Gariazzo, C., Silibello, C., Finardi, S., Radice, P., Piersanti, A., Calori, G., Cecinato, A., Perrino, C., Nussio, F., Pelliccioni, A., Gobbi, G.P. and Di Filippo, P. (2007) A gas/aerosol air pollutants study over the urban area of Rome using a comprehensive chemical transport model, Atmospheric Environment 41 (2007) 7286–7303.

Hanna, S.R. and Chang J. C. (1992) Boundary-layer parameterizations for applied dispersion modeling over urban areas. Boundary-Layer Meteorol., 58, 229-259.

Mahrt, L. (1999) Stratified atmospheric boundary layers. Boundary-Layer Meteorol., 90, 375-396.

Pielke R.A., Cotton W.R., Walko R.L., Tremback C.J., Lyons W.A., Grasso L.D., Nicholls M.E., Moran M.D., Wesley D.A., Lee T.J. and Copeland J.H. (1992) A Comprehensive Meteorological Modeling System - RAMS, Meteorol. Atmos. Phys. 49, 69-91.

Slørdal, L.H., S. Finardi, E. Batchvarova, R.S. Sokhi, E. Fragkou, A. D'Allura (2004). Limitations of air pollution episodes forecast due to boundary-layer parameterisations implemented in mesoscale meteorological models. Proceedings of the 27th NATO/CCMS ITM on Air Pollution Modelling and its Application, October 25-29, 2004, Banff, Canada.

Zilitinkevich, S.S., Perov, V. L. and King, J. C. (2002b) Near-surface turbulent fluxes in stable stratification: Calculation techniques for use in general-circulation models. Q. J. R. Meteorol. Soc., 128, 1571-1587.