An integrated meteo-diffusional modelling system to manage atmospheric pollution in the Tuscany region: a preliminary application in the Livorno industrial area

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Abstract

The Laboratory for Meteorology and Environmental Modelling developed a meteorological and dispersion modelling system to manage atmospheric pollution. The system is conceived as a modelling framework mainly based on the RAMS model meteorological forecasting. RAMS fields are used as input for the CALMET model, which works as a meteo converter to the CALPUFF and CALGRID dispersion models. Thereby, the modelling system is able to cover a wide range of typical pollutant applications, working as it does as two model chains: the RAMS-CALMET-CALPUFF chain to manage inert or slightly reactive pollutants such as particulate matter, and the RAMS-CALMET-CALGRID chain to evaluate photochemical pollution. Furthermore, a RAMS daily forecast archive has been built covering the whole of Tuscany with a 3-D point grid, which allows the system to work both in a diagnostic and in a prognostic mode (that is, by forecasting pollutant concentrations). In the present study a diagnostic preliminary application of the RAMS-CALMET-CALPUFF model chain has been made. The 40x60 Km² study area is located between the two cities of Livorno and Rosignano in Tuscany (Italy), where a large number of strongly emitting industrial sources is located. Starting from RAMS meteo fields, the CALPUFF model has been used in a long-term mode to estimate SO₂ and NOₓ concentrations. The core of the work dealt with the configuration of CALMET and CALPUFF models over a three-month time period, particularly by investigating the more reliable chemical mechanism for CALPUFF. Setting up such a modelling system is the preliminary step to build a supporting tool for Local Authorities in order to integrate meteorological monitoring networks and manage air pollution levels.
1 Introduction

The Laboratory for Meteorology and Environmental Modelling (LaMMA) developed an integrated meteorological and dispersion modelling system to manage mesoscale pollution [1], which is entirely based on the EPA CALMET [2], CALPUFF [3] and CALGRID [4] models. The originality of the LaMMA system is not only the implementation over Tuscany of the EPA modelling system, but particularly the use of the RAMS [5] meteorological model forecast as an input to CALMET, which works as a meteo converter to the CALPUFF and CALGRID dispersion models. Thus, the modelling system is able to cover a wide range of pollutant applications as it works like two model chains: the RAMS-CALMET-CALPUFF one to manage inert or slightly reactive pollutants such as particulate matter, and the RAMS-CALMET-CALGRID one to evaluate photochemical pollution. Furthermore, a RAMS daily forecast archive has been built covering the whole of Tuscany with a 3-D point grid. This archive allows the integrated modelling system to work not only in a diagnostic mode but also in a prognostic one, that is by forecasting pollutant concentrations.

A specific interface has been developed to connect RAMS to CALMET aiming at adapting RAMS meteo fields to use them as an input to the CALPUFF and CALGRID dispersion models. This required the development of a number of specific routines to extract and format data from RAMS archive for the CALMET model, paying particular attention to comply with all CALMET configuration and run parameters. Also, an interface directly connecting RAMS archive to CALGRID has been developed, which is able to completely by-pass CALMET, thereby providing CALGRID with a CALMET-compliant meteorological file, directly generated from the RAMS model.

In the present study a preliminary application of the RAMS-CALMET-CALPUFF model chain in a diagnostic mode has been made. The study area is a 40x60 Km$^2$ coastal area located between the two cities of Livorno and Rosignano in Tuscany, where a large number of strongly emitting industrial sources is located. Starting from RAMS meteo fields, the CALPUFF model has been used in a long-term mode to estimate $\text{SO}_2$ and $\text{NO}_x$ concentrations.

2 Modelling system description

2.1 Overview

The working scheme of the integrated modelling system developed in the present study is shown in Fig. 1. This scheme is made of a meteorological section, including the RAMS and CALMET models, and a dispersion one, focused on the CALPUFF and CALGRID models, which can be applied when both meteorological fields and emission data are provided.

Emission data are provided from the “IRSE” regional emission inventory set up by the Tuscany Region Authority [6]. Such an inventory, updated to year 2001, covers all different kinds of emission sources (point, area and line) and pollutant species. The methodology of “proxy” variables is applied to make both the spatial and time emission disaggregation.
2.2 The RAMS archive

The meteorological RAMS model is currently used at the LaMMA laboratory for the regional weather forecasting service. RAMS is worldwide used as one of the most reliable meteorological model as it enables the simulation of mesoscale weather systems, convective and cirrus clouds, precipitating weather systems, soil heat and moisture exchanges, radiation balance, etc. RAMS is based on a non-hydrostatic approach taking into account all the complex terrain features, and provides an accurate representation of lower atmosphere particularly because of the inbuilt accurate simulation of atmospheric turbulence.

Starting from January 1st, 2002, RAMS forecasted fields are daily stored into an archive covering the whole of Tuscany with a 3-D point grid. In particular, a 4x4 Km² horizontal grid resolution with 12 vertical levels is used. Thereby, the archive’s spatial domain is made of 45x55x12 grid points, for a total area of 180x220 Km². Vertical profiles range from a 38-m a.g.l. first height to a 2856-m a.g.l. top height. Meteorological variables are stored both as 3-D and 2-D fields. 3-D meteo fields are: wind speed (three components), air temperature, pressure, moisture and rain precipitation. 2-D meteo fields are: PBL height, friction and convective velocity, solar radiation, etc. The archive is meant to be a supporting...
tool for Local Authorities to, e.g., integrate meteo monitoring networks, locate sites for eolic plants, climatologically characterize areas, etc.

2.3 Connecting RAMS to CALMET

CALMET is a meteorological model including a diagnostic wind field generator containing objective analysis and parametrized treatments of slope flows, kinematic terrain effects, and a divergence minimization procedure. A specific routine has been developed to extract from the RAMS archive all the meteo fields necessary to run CALMET. In terms of CALMET input files, RAMS is used not only as a prognostic model in place of MM5, which is the default prognostic 3-D model to CALMET, but also to provide observation data to CALMET, that is making up both the surface station and the air upper station files. This required the development of a specific interface connecting RAMS to CALMET. This interface is made by a geophysical and a meteorological section, both aimed at “translating” into the “CALMET language” both the geophysical parameters and the meteorological variables contained in the RAMS archive features.

As far as the geophysical section is concerned, aimed at preparing the “GEO.dat” CALMET input file, the CORINE Land Cover classification has been used to provide land use categories for calculating parameters such as roughness length, albedo, Bowen ratio and leaf area index. A 100x100 m² starting resolution for the land use classification is available, as well as for the Digital Elevation Model, which provides the terrain elevations for “GEO.dat”. Two grid options are available: one whose points exactly match those of the RAMS archive, and the other one which is a subset of the RAMS point grid. On the other hand, CALMET vertical layers are always set identical to the RAMS ones.

The meteo “translation” of RAMS variables to CALMET is accomplished by “splitting” RAMS outputs into CALMET meteo input files. These include a surface station file (“SURF.dat”), a number of upper air station file (“UPn.dat”), and the prognostic 3-D meteo file provided by the MM5 model (“MM5.dat”). In particular, RAMS vertical profiles have been used in place of the MM5 model ones to provide the prognostic 3-D gridded wind fields to CALMET. Accordingly, the surface station file and the upper air station files are all made by RAMS meteo data only, by using a number of CALMET “stations”, only limited by the CALMET maximum station number settings.

2.4 The CALPUFF and CALGRID models

CALPUFF is a non-steady state dispersion model that advects Gaussian “puffs” of material emitted from sources by using a Lagrangian law. It includes modules for terrain effects, overwater transport, coastal interaction effects, building downwash, wet and dry removal and deposition, and a simplified chemical transformation mechanism. It is designed for inert or slightly reactive pollutants, either through a short-term or a long-term application mode.

On the other hand, CALGRID is an Eulerian transport and diffusion model including modules for horizontal and vertical advection/diffusion and dry
deposition. It is specifically conceived to manage photochemical pollution, particularly the ozone-related one, featuring a number of modules to fully reproduce all chemical and photochemical reactions by the ozone precursor species, such as NOx and VOCs. Moreover, the application of CALGRID requires all concentration boundary conditions to be provided as external input. CALGRID is a fundamental modelling tool to support Local Authorities in such cases as investigating the possibility of reducing O3 concentrations or re-locating the O3 monitoring stations.

3 Modelling system preliminary application

3.1 Reference site

The reference site is a 40x60 Km² coastal area located between Livorno and Rosignano in Tuscany, as shown in Fig. 2. While several industrial sources close to Pisa appear in the above domain, main emitting sources are in Livorno and Rosignano industrial areas, which can be definitely numbered among the most polluted areas in the whole Tuscany region. In particular, a great petrol refinery is located in the Livorno industrial area, together with a number of other sources such as one rubbish incinerator, a few cementery plants and other chemical treatment plants. Furthermore, Livorno features a major harbour with a large number of shipyards. As regards Rosignano, this is dramatically dominated by a huge chemical production plant including some 30 emitting chimneys.

3.2 The RAMS-CALMET-CALPUFF model option

One preliminary application of the newly developed modelling system has been made. In particular, according to the working scheme shown in Fig. 1, the RAMS-CALMET-CALPUFF model option has been chosen, in order to estimate SO2 and NOx concentrations over the reference site, these definitely being the major pollutant species affecting air quality in the study area.

Using RAMS archive data, one modelling application has been carried out through two different phases: a preliminary test case, where both CALMET and CALPUFF run in a short-term mode, and a definitive case-study, where the long-term option has been applied. The test case, referring to a 6-days time period from February 23rd to 28th, 2002, is focused on enabling the configuration of both CALMET and CALPUFF models on the case-study to be done. In particular, the CALMET
configuration was achieved by setting every run option and parameter to best fit the initial meteo fields from RAMS. Once CALMET has been set, a number of CALPUFF runs has been made, aiming at investigating more reliable chemical mechanisms to reproduce SO\textsubscript{2} and NO\textsubscript{x} atmospheric transformation. Thereafter, the definitive CALMET and CALPUFF configuration has been used for running the model chain in a long-term mode, particularly over a 3-month time period from February to April, 2002.

3.3 Case-study main parameters

The spatial domain used to run CALMET (Fig. 2) is a 60\times40 Km\textsuperscript{2} area covered by 15\times10 grid cells, with a 4 Km spacing, thereby including 150 RAMS vertical profiles in total. In accordance with RAMS, vertical layers are 12, with a top height equal to 3200 m a.g.l.

As for meteorological data, 25 RAMS-provided surface stations and 25 corresponding upper air stations has been used. As already pointed out, this number is set by the maximum number of stations allowed by the current CALMET version, although a more up-to-date CALMET version could be applied in the future to increase this limit. On the contrary, the MM5-like prognostic 3-D meteo file based on RAMS data was applied over the whole spatial domain.

Main CALMET wind field options refer to the diagnostic wind module, involve no extrapolation of surface wind observations to upper layers, and use of the MM5-like prognostic RAMS meteo file as observations.
As regards CALPUFF run options, a total number of 59 point sources have been taken into account, whose emissions have been disaggregated into hourly-varying rates through the above mentioned “proxy” variables method. The main industrial emitting point sources in the area have been taken into account. SO\textsubscript{2} and NO\textsubscript{x} pollutants were analysed, calculating their concentrations have been calculated by using three different chemical options: the MESOPUFF-II mechanism, the ARM3/RIVAD mechanism, and the option of considering SO\textsubscript{2} and NO\textsubscript{x} as mere inert pollutants. The use of the first two chemical mechanisms caused some more pollutants such as SO\textsubscript{4}, NO\textsubscript{3}, HNO\textsubscript{3} and NO\textsubscript{x} splitted into NO and NO\textsubscript{2} to be analysed too.

Figure 3: Time frames of gridded 10-m a.g.l. wind fields calculated in the study area by CALMET starting from the RAMS archive data (23/02/2002).
3.4 Application results: RAMS-CALMET models

In Fig. 3 is presented a sample graphical output of the RAMS-CALMET short-term test case application over the Pisa-Livorno-Rosignano study area. In particular, the time sequence of gridded wind fields at 10m a.g.l. on February 23rd, 2002 is plotted. Winds always appear to be stronger overwater than overland, where kinematic terrain effects apply. On the other hand, wind strength and orientation are dramatically affected by daytime, from early morning (h. 06) to afternoon and evening (hs. 17 and 21). This proves the diurnal land-breeze and sea-breeze phenomena to be correctly reproduced by meteorological models. In particular, late morning (h. 12) seems to be the time of the day when wind orientation changes from land-sea to sea-land, together with a substantial strength increase. Moreover, a different behaviour occurs in the wind field from one land area to the other, particularly in the h. 21 situation if the southern Rosignano area is compared with the northern Livorno and Pisa area. In this case a vortex circulation occurs, starting from the Rosignano area, where strong winds flow from sea to land, with an intermediate channelling along the valley at the back of the Livorno basin, up to the Livorno and Pisa area, where winds appears to be dramatically decreased and oriented from land to sea.

3.5 Application results: CALPUFF model

Once that both CALMET and CALPUFF have been set up in the test case, they have been run over the three-month case-study time period from February to April 2002. An hourly time step has been used for this long-term application, which caused, particularly for the CALPUFF case, a dramatically long computational time for each run. Three mechanisms have been used for simulating NOx and SOx chemical reactions in the study area: the MESOPUFF-II mechanism, taking into account species such as NOx, HNO3, NO3-, SO2, SO4, the ARM3/RIVAD mechanism, introducing a splitting of NOx to NO and NO2 despite MESOPUFF-II, and the option of considering SO2 and NOx as mere inert pollutants.

Figs. 4, 5 and 6 show the three-month averaged SO2 and NOx concentrations estimated by CALPUFF in the study area. In particular, in Fig. 4 SO2 concentrations are shown in the inert pollutant case, whereas in Figs. 5 and 6 outputs of NOx concentrations from the inert case option and the MESOPUFF-II chemical mechanism are compared.
Figure 4: CALPUFF long-term application in the study area: 3-month SO$_2$ averaged concentrations ($\mu$g/m$^3$) in the inert case (Feb. to Apr. 2002).

Figure 5: CALPUFF long-term application in the study area: 3-month NO$_x$ averaged concentrations ($\mu$g/m$^3$) in the inert case (Feb. to Apr. 2002).
Figure 6: CALPUFF long-term application in the study area: 3-month NO\textsubscript{x} averaged concentrations (\mu g/m\textsuperscript{3}) in the MESOPUFF-modelled case (Feb.-Apr. ‘02).

Estimated SO\textsubscript{2} concentrations do not seem to appreciably vary when SO\textsubscript{2} is considered either as a mere inert pollutant or taking into account chemical mechanisms. In both cases SO\textsubscript{4} concentrations appear to be very low. This could be accounted for by the fact that in the 3-month time period no appreciable precipitation occurred in the study area, thereby preventing any significant wet removal and deposition processes, which would cause SO\textsubscript{2} concentrations vary from the inert to the reactive case.

On the contrary, as regards NO\textsubscript{x} dispersion, there is a strong difference between the inert pollutant approach and the other two mechanisms (MESOPUFF-II and ARM3/RIVAD). In fact in the inert case NO\textsubscript{x} concentrations are higher and more localized, whereas the use of both chemical mechanisms causes a decrease in NO\textsubscript{x} concentrations attended by an increase in HNO\textsubscript{3} and NO\textsubscript{3} concentrations.

Conclusions

The integrated modelling system developed at LaMMA is meant to work as a supporting tool for Local Authorities to, e.g., integrate meteorological monitoring networks, manage air pollution levels, provide results in view of adopting policies of emission reduction, etc. Possible uses include: long-term (one-year long) evaluation of concentrations due to industrial sources, in-depth analyses of single sources, time-varying contribution to pollution, etc. Furthermore, the RAMS meteo information basis allows the system to work both in a diagnostic mode and in a prognostic one, thereby allowing the forecast of pollutant concentrations.

Potentiality of this modelling system, initially geared to the Livorno and Rosignano industrial areas in the CALPUFF option, will be enhanced when more case-studies will be taken into account. In particular, the configuration of the
RAMS-CALMET-CALGRID model option over the whole Tuscany region will be carried out in the next months, aiming at providing a first regional-scale scenario of ozone-related pollution concentration levels.

References


