<u>COST 728/MESOSCALE MODELLING: METHODS AND COUPLED SYSTEMS</u> <u>SESSIONS</u>

NESTED GRID APPLICATION OF A GLOBAL CHEMISTRY MODEL OVER EUROPE

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COUPLING GEOS-CHEM WITH A REGIONAL AIR POLLUTION MODEL FOR GREECE

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COUPLING ATMOSPHERIC CHEMISTRY/AEROSOLS TO REGIONAL CLIMATE MODEL IN HIGH RESOLUTION

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3D URBAN AIR QUALITY SIMULATIONS BY USING CFD AND MESOSCALE AIR QUALITY MODELS: VRML 3D APPLICATION OVER LAS PALMAS (SPAIN)

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AIR POLLUTANTS STUDY OVER ROME URBAN AREA THROUGH COUPLED TRAFFIC ASSIGNMENT AND CHEMICAL TRANSPORT MODELS.

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DIURNAL EVOLUTION OF INNER PARIS COV AND AEROSOL CONCENTRATIONS COUPLING LIDAR AND IN SITU MEASUREMENTS PERFORMED DURING THE LISAIR PROGRAM

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ABSTRACT

This study examines the nested capabilities of the global chemical transport model GEOS-CHEM. The modified version of the model was set up and applied over Europe, by using the one-way nested grid formulation. According to this method, the model runs globally in a coarse grid horizontal resolution, while boundary concentrations are calculated around the domain where the nested grid approach is applied. Then, a new simulation is performed over the nested domain, with a higher resolution, using the boundary conditions produced from the global run. Comparisons between the two model runs and observations showed that CO model concentrations exhibit seasonal variations similar to those of observations, peaking in winter and having low values during summer. As far as the differences between the two model runs are concerned, the high grid resolution run depicts CO concentrations in more detail, while during winter it shows ability to simulate better the higher values.

1. INTRODUCTION

During the last years, several atmospheric chemistry studies have employed the nested grid methodology in an attempt to interpret available observations. The general concept of nesting is that the global chemical composition is modeled at a coarse resolution that represents the main transport features. This composition then serves as boundary conditions for a regional simulation by using the nested approach.

Most of the numerical modeling studies that employ the nested grid methodology concern the regional scale. As far as the global models are concerned, a methodology that is mostly employed is the coupling of a global meteorological or chemistry model to a regional chemistry model (Langmann et al., (2003); Byun et al., 2005). Studies that incorporate a global atmospheric chemistry model with nesting capabilities are not widely developed. Recently Wang et al. (2004) and Li et al (2005) studied the tropospheric chemistry over Asia and N. America respectively, by developing the nested grid formulation of the global chemistry transport model GEOS-CHEM. A common conclusion of most of the studies discussed above is that the comparison with observations normally improves with resolution mainly due to better resolved emissions, especially near urban areas (Tang, 2002). Furthermore, the nested grid model compared to regional models with prescribed constant boundary conditions has the advantage of allowing for accurate and time-varying boundary conditions.

This paper describes the set up, the application and the results of the one-way nested grid formulation of the global chemistry transport model GEOS-CHEM over Europe. A specific objective of the present investigation is to study CO concentrations in order to examine the sensitivity of results to the choice of resolution. Differences between results obtained with the nested grid approach (localized $1^{\circ} x 1^{\circ}$ resolution) and the coarse grid resolution global run (uniform $4^{\circ} x 5^{\circ}$ resolution) are discussed.

2. METHODOLOGY

Technical details as well as first applications of GEOS-CHEM have been described in earlier publications (Bey et al., 2001), and a comprehensive description of the nested approach of the model was presented by Wang et al. (2004) and Li et al. (2005). A short summary of the main model features is presented below.

The global 3-dimensional chemical transport model GEOS-CHEM is driven by assimilated meteorological data with 6-hour resolution (3-hour for surface variables and mixing depths) from the Goddard Earth Observing System of the NASA Global Modeling and Assimilation Office (GMAO). For the purpose of this work we chose to use GEOS-CHEM v7-01-02 (see http://www.as.harvard.edu/chemistry/trop/geos), which includes a simulation of aerosol chemistry (including sulfate-nitrate-ammonium and carbonaceous aerosols) coupled to ozone-NO*x*-hydrocarbon chemistry (Park et al., 2004). This representation of the model has been shown to conserve both tracer mass and mixing ratio. The model has 30 vertical layers specified by sigma surfaces extending up to 0.1 hPa, with an average of nine layers employed to define the surface boundary regime below 2 km.

According to the nested grid approach, first the global model is run as usual over the whole globe, including the nested domain. Results from the coarse global model simulation are used to drive the high resolution model run through boundary conditions defined by the coarse resolution run, but not vice versa (one-way nested approach). The adoption of this approach permits the treatment of the chemistry in the nested area and it preserves the interaction with the coarse global environment. The high-resolution window $(1^{\circ}x1^{\circ})$ is embedded in the global model which has a horizontal resolution of $4^{\circ} \times 5^{\circ}$. The window domain (-20°E to 45° W, 22°N to 74°N) includes all of Europe and a significant portion of the neighbouring countries in the Africa and European Turkey. The vertical resolution is the same in both simulations.

The nested model is applied to an analysis of CO over the period of January to December 2001. CO is a product of incomplete combustion and it is the principal sink of OH, the main tropospheric oxidant, and as such plays a key role in determining the oxidizing capacity of the troposphere. Model results produced by the global and the nested grid simulations are compared to observations collected at 25 stations around Europe by Airbase (<u>http://air-climate.eionet.europa.eu./databases/airbase/index-html</u>). Airbase is the public air quality database system of the EEA and contains information submitted by the participating countries throughout Europe.

3. RESULTS AND DISCUSSION

3.1 Spatial distribution

In Figures 1 CO seasonal spatial distribution at surface produced by the model global simulation and the model nested grid approach application are presented. In both simulations, the model captures the general features of the annual cycle of CO quite well, peaking in winter and reaching a minimum in summer. As far as the differences between the two model runs are concerned, the high resolution run depicts CO concentrations in more detail, while during winter it shows ability to capture the higher values.



Figures 1: CO concentrations spatial distribution over Europe produced by the nested grid simulation during a) winter and c) summer and by the coarse model simulation during b) winter and d) summer

Statistical analysis and comparison (not shown in this paper) between the two different model resolutions at 25 stations over Europe revealed the dominant role of emissions in the corresponding cells of both the coarse and high resolution model. In particular, CO concentrations are lower in the high resolution simulations when the corresponding cell emissions are lower than those of the coarse run. The station altitude could also play a role in this result, but this should be further examined.

3.2 Comparison with observations

In Figures 2 time-series of CO model concentrations are plotted against observations for both the high and coarse grid model simulations at three selected sites over Europe in: Netherlands, Italy and Switzerland. At these sites simulated CO concentrations exhibit seasonal variations similar to those of observations, peaking in late winter and having low values during summer. In figure 2a, it is evident that the model, especially the high resolution run, performs very well compared to the observed values. Figure 2b presents a case, which is typical of several low altitude stations, where the model (at both resolutions) underestimates the observed concentrations. This is possibly due to higher pollution levels at station level, which cannot be resolved by the emissions' spatial distribution, even at this higher resolution. Figure 2c presents a case where the model overestimates the observed concentrations at a high altitude station in Switzerland. This situation possibly arises from the fact that the station is above the boundary layer mixing height hence it receives reduced emissions as opposed to the model's higher values. This explanation is also supported by the fact that the concentrations measured at this station are kept very low throughout the whole year, without significant seasonal variations.

Statistical analysis (not shown in this paper) for 25 rural stations over Europe reveal that on an annual basis, the correlation coefficient between the model and the observations, calculated using daily averages, is good at most of the sites, ranging from 0.4 to 0.7 and from 0.3 to 0.6 for the nested grid and for the coarse global simulations respectively.

4. CONCLUSIONS

In this study the nested capabilities of the global 3-D chemical transport model GEOS-CHEM were examined. Comparisons between the two model runs and observations showed that CO concentrations produced by the model exhibit seasonal variations similar to those of observations, peaking in late winter and having low values during summer. The model, especially the high resolution run, performs very well compared to the observed values, while underestimation or overestimation is present at lower or higher altitudes respectively. As far as the differences between the two model runs are concerned, the high grid resolution run depicts CO concentrations in more detail, while during winter it shows ability to simulate the higher values.

5. ACKNOWLEDGEMENTS

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Abstract

In this study we investigate the influence of several gas phase pollutants over Greece, for various synoptic conditions. For this purpose, a global-to-mesoscale model chain is developed and applied, with a nesting procedure coupling the individual models' simulations. The global to mesoscale model chain used in this study consists of the following Eulerian models: the global chemistry-transport model GEOS-CHEM (Bey et al., 2001) applied in a one way nested procedure (Protonotariou et al., 2007) and the combination of the regional MM5 meteorological and UAM-V chemical dispersion models applied with a spatial resolution 6kmx6km. It was found that the coupling procedure is necessary especially for the primary pollutants, such as SO₂, with large spatial variation. In this extended abstract we only present the influence of large-scale ozone background on near-surface ozone over Greece, for selected synoptic conditions.

1. INTRODUCTION

Photochemical in-situ production is the most important source of ozone in the planetary boundary layer. However, the contributions of other mechanisms such as stratospheric intrusion, lightning, convective mixing and intercontinental transport are also significant. In order to accurately consider all these sources, a chain of global to mesoscale models is inevitable. Recently, the methodology that employs the global models is their coupling to regional atmosphere-chemistry model (Langmann et al., 2003; Byun et al., 2005). This paper presents a tropospheric chemistry study over Greece, coupling a global chemistry transport model to a regional one.

Model results and comparisons with ground based observations at Finokalia in Crete and Aliartos in central Greece for the year 2001 are presented and discussed for ozone. Comparisons for NO_2 and SO_2 have also been performed but are not presented in this study.

2. METHODOLOGY

The global to mesoscale model chain, developed in this study, consists of two Eulerian models: The global chemistry-transport model GEOS-CHEM (Bey et al., 2001), by using the one-way nested grid formulation (Protonotariou et al., 2007) and the combination of the regional atmosphere PSU/NCAR Mesoscale model (MM5) (Grell et al., 1994) and chemistry Urban Airshed Model, UAM-V (SAI, 1999). First, the global model GEOS-CHEM is run with a horizontal resolution of 4° x 5°, over the whole globe. Subsequently, a high resolution 1°x1° GEOS_CHEM run is performed for the nested domain of -20°E to 45°W and of 22°N to 74°N. Then, results from the nested domain are used as boundary conditions to drive the regional atmosphere-chemistry model for the third domain that is centered solely over Greece, with a resolution 6kmx6km. The GEOS-CHEM model with the nesting procedure is applied over the period of January to December 2001 (Protonotariou et al., 2007), while simulations with the regional models are performed for selected days, representing eight different types of synoptic scale atmospheric circulation; South Westerly flow (SW), North Westerly flow (NW), Long Wave trough (LW), Closed Low (CL), Zonal flow, Open Anticyclone (OA), Closed Anticyclone (CA) and High Low (HL). This classification was based on daily distribution of the geopotential height and the wind flow at 850hPa during a 20 year period (1983-2002).

In this procedure, the GEOS-CHEM model provides the lateral boundaries of the country, with hourly mixing ratios of the major longer lived photooxidants and precursor species at a horizontal grid resolution $(1^{\circ}x1^{\circ})$, instead of the default coarse global models resolution $(4^{\circ}x5^{\circ})$. Then, these hourly mixing ratios were assigned to the UAM-V horizontal and vertical boundaries. Because of differences between the chemical mechanisms of the global and the mesoscale chemical models, a matching was necessary, especially with respect to the organic part. GEOS-CHEM organic species were linked to PAR (parafins), OLE (olefins), ISOP (isoprene), HCHO (formaldehyde), ALD2 (acetaldehyde) and ALDx (higher aldehydes). Default boundary values have been used for the CB-IV-TOX species for which no information was available from GEOS-CHEM (e.g. aromatics).

3. **RESULTS AND DISCUSSION**

Initially, we analyze the influence of the large-scale ozone background at the boundaries of the third domain centred over Greece. In particular, the simulated concentrations are presented in relation to the synoptic scale atmospheric circulation, in figure 1. This allows to view the strong variation of ozone both horizontally and vertically and justifies the need for this study. In particular, it was found that the background ozone concentrations as determined by the global model high resolution (nested $1^{\circ}x1^{\circ}$ mode) differs more than

10ppb from South to North and even larger differences are evident between the surface and the higher levels. Furthermore, significant variations of ozone background levels is evident among the various synoptic categories. At lower levels, both HL and OA types of atmospheric circulation are related to higher ozone values, especially for the OA case and during the summer period. This is also justified by the surface measurements at Aliartos and Finokalia station, as shown in figure 2. This difference is also reflected to the regional simulations by UAM model. At higher levels this behaviour is not so clear.

In figure 3 the spatial ozone concentration is presented for the domain over Greece, for two days from the summer period, that correspond to synoptic conditions both related to high ozone production. It is found that the background ozone as determined by the global $1^{\circ}x1^{\circ}$ model affects the results of the higher resolution limited area model increasingly with height. The comparison, with the boundary inflows provided either by the global model or taken constant during the simulation, reveals that the coupling procedure contributes with an amount of more than 5ppbv, to near surface ozone, in the afternoon hours.



Figure 1: Modelled (GEOS-CHEM) hourly O_3 concentrations at the northern (a,b) and southern (c,d) boundary of Greece, at 60m (a,c) and 2km (b,d) height. The colours denote the different types of synoptic scale atmospheric circulation (SW, NW, LW, CL, Zonal, OA, CA and HL).



Figure 2: Measured hourly surface O₃ concentrations at two stations Aliartos (northern Greece) and Finokalia (Crete island). The colours denote the different types of synoptic scale atmospheric circulation (SW, NW, LW, CL, Zonal, OA, CA and HL).



Figure 3: The simulated (MM5-UAM-V) horizontal spatial distribution of ozone concentrations, for two synoptic conditions (HL and OA).

4. CONCLUSIONS

The analysis of ozone background at the boundaries of Greece shows strong variation of ozone both horizontally and vertically and proves the necessity for the coupling procedure.

The comparison, with the boundary inflows provided either by the global model or taken constant during the simulation, reveals that the coupling procedure contributes an amount of more than 5ppbv, to near surface ozone, in the afternoon hours.

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ABSTRACT

Recent studies show considerable effect of atmospheric chemistry and aerosols on climate on regional and local scale. For the purpose of qualifying and quantifying the magnitude of climate forcing due to atmospheric chemistry/aerosols on regional scale, the development of coupling of regional climate model and chemistry/aerosol model has been started recently on the Department of Meteorology and Environment Protection, Faculty of Mathematics and Physics, Charles University in Prague. For this coupling, existing regional climate model and chemistry transport model are used. Climate is calculated using model RegCM while chemistry is solved by model CAMx. Meteorological fields generated by RegCM drive CAMx transport a dry/wet deposition. A preprocessor utility was developed on the department for transforming RegCM provided fields to CAMx input fields and format. As the first step, the distribution of pollutants can be simulated for long period in the model couple. There is critical issue of the emission inventories available. Monthly and yearly one way coupled climate/chemistry/aerosol model runs are scheduled in framework of ongoing projects with further studies of on-line impact implementation in regional climate simulations. At this moment, one way coupling on lower resolution is compared with the high resolution simulation at 10 km nested into the lower resolution run to have better boundary conditions both for meteorology and chemistry. Sensitivity of the model couple to the development of urban and industrialized areas in the central Europe is studied for the EC projects QUANTIFY and CECILIA.

1. INTRODUCTION

There is significant problem for decision making process arising from the weak link between climate change information based on global climate models and impact studies necessarily based on real local conditions. Global Circulation Models (GCMs) can reproduce reasonably well climate features on large scales (global and continental), but their accuracy decreases when proceeding from continental to regional and local scales because of the lack of resolution. This is especially true for surface fields, such as precipitation, surface air temperature and their extremes, which are critically affected by topography and land use. However, in many applications, particularly related to the assessment of climate-change impacts, the information on surface climate change at regional to local scale is fundamental. To bridge the gap between the climate information provided by GCMs and that needed in impact studies, especially when aiming the interactions of climate and air-quality issues, dynamical downscaling, i.e., nesting of a fine scale limited area model (or Regional Climate Model, RCM) within the GCM is the most convenient tool.

In the region of Central and Eastern Europe the need for high resolution studies is particularly important. This region is characterized by the northern flanks of the Alps, the long arc of the Carpathians, and smaller mountain chains and highlands in the Czech Republic, Slovakia, Romania and Bulgaria that significantly affect the local climate conditions. A resolution sufficient to capture the effects of these topographical and associated land-use features is necessary. That is why 10 km resolution has been introduced in the project CECILIA of EC FP6. The main aim of the project dealing with climate change impacts and vulnerability assessment in targeted areas of Central and Eastern Europe is the application of regional climate modelling studies at a resolution of 10 km for local impact studies in key sectors of the region. The project contains studies on hydrology, water quality, and water management (focusing at medium-sized river catchments and the Black Sea coast), agriculture (crop yield, pests and diseases, carbon cycle), and forestry (management, carbon cycle), as well as air quality issues in urban areas (Black Triangle – a polluted region around the common borders of the Czech Republic, Poland and Germany). Climate change impacts on large urban and industrial areas modulated by topographical and land-use effects which can be resolved at the 10 km scale, are investigated by CECILIA.

The concentration of air pollutants depends on both anthropogenic and climate factors. A main issue is the quantity of emissions of primary pollutants as well as of precursors of secondary pollutants. Long range

transport to the target regions will be taken into account by simulation for the whole Europe, driven by RCM with a grid resolution of 50x50 km. These simulations will be used to constrain nested higher resolution runs (10x10 km) for a smaller domain focusing in CEE both for present and future climate. The key species will be ozone, sulphur and nitrogen as well as PM, which have a central role in tropospheric chemistry as well as the strong health impacts. Emphasis will be given to future key species exceedances of the EU limits for the protection of human health, vegetation and ecosystems as well as WHO guidelines. Another risk factor for the human health, which finally goes hand in hand with the issue of air quality through the chemistry of pollutants, are heat waves, and in certain extent even cold waves. The summer of 2003 encompassed one of the most severe heat waves on record in central and western Europe causing both human losses and damage to natural ecosystems. First guess of possible impacts of climate change on mortality and attempt to split the direct effect of heat and cold waves from the effects of air quality will be given on the basis of this study. Climate change may affect exposures to air pollutants by a) affecting weather and thereby local and regional pollution concentrations; b) affecting anthropogenic emissions including adaptive response of increased fuel combustion for fossil fuel-fired power generation; c) affecting natural sources of air pollutant emissions; and d) changing the distribution and types of airborne allergens. In addition, the chemical composition of the atmosphere may in turn have a feedback effect on the local climate. Weather is also associated with energy demands (e.g., for space heating and cooling) that could alter patterns of fossil fuel combustion. In particular, individual responses to extremely hot weather can result in large increases in air conditioner use. In addition, high temperatures cause increased VOC evaporative emissions when people run motor vehicles. The health effects of air pollution are broad and diverse, including dramatic episodes of increased mortality at high concentrations. In humans, the pulmonary deposition and absorption of inhaled chemicals can have direct consequences for health. Nevertheless, public health can also be indirectly affected by deposition of air pollutants in environmental media and uptake by plants and animals, resulting in chemicals entering the food chain or being present in drinking-water and thereby constituting additional sources of human exposure. Furthermore, the direct effects of air pollutants on plants, animals and soil can influence the structure and function of ecosystems, including their self-regulation ability, thereby affecting the quality of life. The most sensitive groups include children, older adults and persons with chronic heart or lung disease.

2. MODEL COUPLE

It is now well established that climatically important (so called radiatively active) gases and aerosols can have substantial climatic impact trough their direct and indirect effects on radiation, especially on regional scales (Qian and Giorgi, 2000, Qian et al., 2001, Giorgi et al., 2002). The study of these effects requires coupling of regional climate models with atmospheric chemistry/aerosols to assess the climate forcing to the chemical composition of the atmosphere and its feedback to the radiation, eventually other components of the climate system. For this coupling, existing regional climate model and chemistry transport model are used. At our Department climate is calculated using model RegCM while chemistry is solved by model CAMx, for the projects the attempt is done to develop and to use the couple ALADIN-Climate and CAMx as well.

The model RegCM used here was originally developed by Giorgi et al. (1993a,b) and then has undergone a number of improvements described in Giorgi et al. (1999), and, finally, Pal et al. (2005). The dynamical core of the RegCM is equivalent to the hydrostatic version of the mesoscale model MM5. Surface processes are represented via the Biosphere-Atmosphere Transfer Scheme (BATS) and boundary layer physics is formulated following a non-local vertical diffusion scheme (Giorgi et al. 1993a). Resolvable scale precipitation is represented via the scheme of Pal et al. (2000), which includes a prognostic equation for cloud water and allows for fractional grid box cloudiness, accretion and re-evaporation of falling precipitation. Convective precipitation is represented using the radiation package of the NCAR Community Climate Model, version CCM3 (Giorgi et al. 1999). This scheme describes the effect of different greenhouse gases, cloud water, cloud ice and atmospheric aerosols. Cloud radiation is calculated in terms of cloud fractional cover and cloud water content, and the fraction of cloud ice is diagnosed by the scheme as a function of temperature. For more details on the use of the model see Elguindi at al. (2006).

CAMx is an Eulerian photochemical dispersion model developed by ENVIRON Int. Corp. (Environ, 2006). Currently in version 4.40 CAMx is used for air quality modeling in more than 20 countries by government agencies, academic and research institutions, and private consultants for regulatory assessments and general research. It is available for free in the form of the source code with various supporting programs. CAMx can use environmental input fields from a number of meteorological models (e.g., MM5, RAMS, CALMET) and emission inputs from many emissions processors. CAMx includes the options of two-way grid nesting,

multiple gas phase chemistry mechanism options (CB-IV, SAPRC99), evolving multi-sectional or static twomode particle size treatments, wet deposition of gases and particles, plume-in-grid (PiG) module for sub-grid treatment of selected point sources, Ozone and Particulate Source Apportionment Technology, mass conservative and consistent transport numerics, parallel processing. It allows for integrated "one-atmosphere" assessments of gaseous and particulate air pollution (ozone, PM2.5, PM10, air toxics) over many scales ranging from sub-urban to continental. CAMx simulates the emission, dispersion, chemical reaction, and removal of pollutants in the troposphere by solving the pollutant (eulerian) continuity equation for each chemical species on a system of nested three-dimensional grids. These processes are strongly dependent on the meteorological conditions, therefore CAMx requires meteorological input from a NWP model or RCM for successful run.

3. PRELIMINARY RESULTS

Meteorological fields generated by RegCM drive CAMx transport and dry/wet deposition. A preprocessor utility was developed for transforming RegCM fields to CAMx input fields and formats. Briefly, it takes RegCM's outputs and convert them to fields and formats accepted by CAMx. As the first step, the distribution of pollutants can be simulated for long period in the model couple. There are problems with the emission inventories available, at this stage emissions from EMEP 50 km x 50 km database are interpolated. We are testing VOC speciation technique, biogenic emissions of isopren and monoterpenes calculated as a function of 2m temperature, global radiation and landuse by Guenther et al. (1993,1994). Initial and boundary conditions are set to CAMx's top concentrations (independent of time) (Simpson et al., 2003), in our setting CB-IV chemistry mechanism is used (Gery et al.,1989). We use 23 vertical σ -levels reaching up to 70hPa, with time step of 150 s, at 50 km resolution in preliminary experiments for RegCM configuration, the same horizontal grid for CAMx. Some examples of integration for year 2000 are presented in Fig. 1 for selected species. More interesting comparison of the results with selected time series can be seen in Fig. 2. Underestimation of the ozone concentration by the model, especially during warm season, appears for some stations as well as the overestimation in some other cases.



Figure 1. Average concentration of O₃ (left panel) and NO₂ (right panel) for year 2000 in ppbv.



Figure 2. Comparison of simulated and measured daily average concentration of O_3 for Kosetice station (left panel) and for Montelibretti (right panel) in year 2000 ($\mu g/m^3$).

4. FUTURE OUTLOOKS

At present we are running the experiment in very high resolution of 10 km. The next step will be the inclusion of the radiative agents from CAMx into RegCM radiative transfer scheme to calculate the changes of heating rates. Only the modification of radiative transfer due to atmospheric chemistry/aerosols will be taken into account first, the indirect effect of aerosols will be taken into account later, there are still many uncertainties in understanding of this issue and possibility of inclusion of appropriate processes into the model. The feedback of chemistry/aerosols on climate will be studied in terms of monthly and yearly averages of 2 m temperatures and of the top-of-the-atmosphere (TOA) radiative forcing, the results will provide the estimate of the effect of interactive atmospheric chemistry and aerosols on climate in regional and local scales.

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3D URBAN AIR QUALITY SIMULATIONS BY USING CFD AND MESOSCALE AIR QUALITY MODELS: VRML 3D APPLICATION OVER LAS PALMAS (SPAIN)

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ABSTRACT

The interest on carrying out air quality impact application studies in real complex urban environs has increased substantially during the last years. This contribution presents the results of different experiments carried out in Madrid (Spain) and Las Palmas (Spain) with a CFD model, MICROSYS which includes an adapted version of the microscale model MIMO (University of Karlsruhe, Germany) and the well-known MM5-CMAQ air quality modeling system, which is a representative of the third generation of air quality dispersion models. An adapted version of EMIMO is used for emission data which includes a detailed cellular automata model (CAMO) (Technical University of Madrid (UPM), 2003) to describe in detail the complex urban traffic emissions with a very high spatial (1 m) and temporal resolution (1 s). Different traffic scenarios are used such as normal traffic conditions, decreasing on 30 % the total number of private cars and increasing on 15 % the total number of public buses. The results shows that these tools are providing a considerable level of detail and the results can be used for decision makers on air quality issues. A sophisticated VRML 3D model is also developed to provide the information in real-time over the Internet and with navigation and 3D frames for the user.

INTRODUCTION

Considerable interest exists on investigations related to detailed air quality exposure doses in highly dense urban environs in large world cities. The advances on the capability of Computational Fluid Dynamics models and Air Quality Modelling Systems during the last decade have been quite substantial. The increase on computer capabilities and on the knowledge of turbulence parameterization and numerical schemes has also been very important during the last ten years. On the other hand, there is a considerable public interest on information related to the "real" pollution they are exposure on when they are walking in the street going to work or even during the period they are driving a car from/to work or other daily activities. At street level the differences in the concentration values at both sides of a street can be important, particularly, for instance, on relation to photochemical production during summer time in Mediterranean regions. In this contribution we have used the CFD model MIMO (U. of Karlsruhe (Germany)) [4] and the mesoscale air quality modelling system MM5-CMAQ-EMIMO (NCEP / EPA / Technical University of Madrid) to produce air quality forecasts with 10 m resolution over the Las Palmas (Canary Islands, Spain). These complex systems could evaluate the impact of several urban strategic emission reduction measures such as reduction of private traffic, increase of public transportation, impact on introduction of new fuel cell vehicles, etc. Also, they could be used for analysis of pollution concentrations at different heights (buildings) and on different areas of urban neighbourhoods. Air dispersion in urban areas is affected by atmospheric flow changes produced by building-street geometry and aerodynamic effects. The traffic flow, emissions and meteorology are playing also an important role. Microscale air pollution simulations are a complex task since the time scales are compared to the spatial scales (micro) for such a type of simulations. Boundary and initial conditions for such a simulation are also critical and essential quantities to influence fundamentally the air dispersion results. Microscale Computational Fluid Dynamical Models (CFDM) are playing an increasing role on air quality impact studies for local applications such as new road and building constructions, emergency toxic dispersion gases at urban and local scale, etc. Microscale air dispersion simulations are applied to predict air-flow and pollution dispersion in urban areas. Different combinations and applications appear in the literature as in Reference by integrating a Lagrangian model and a traffic dynamical model into a commercial CFD code, Star-CD to simulate the traffic-induced flow field and turbulence.

In this contribution we have applied the microscale dispersion model MIMO to simulate the air concentrations at street level in Las Palmas (Canary Islands, Spain). The MIMO CFD code has been adapted and incorporated into a mesoscale air quality modelling system (MM5-CMAQ-EMIMO) to fit into the one-way nesting structure. MM5 is a meteorological mesoscale model developed by Pennsylvania State University (USA) and NCAR (National Centre for Atmospheric Research, USA). The CMAQ model is the

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Community Multiscale Air Quality Modelling System developed by EPA (USA) [1] and EMIMO is the Emission Model [3]. MM5 is a well recognized non-hydrostatic mesoscale meteorological model which uses global meteorological data produced by global models such as GFS model (NCEP, USA) to produce high resolution detailed three dimensional fields of wind, temperature and humidity which are used in our case as input for the photochemical dispersion model CMAQ [2]. In addition of MM5 output data, EMIMO model produces for the specific required spatial resolution, hourly emission data for different inorganic pollutants such as particulate matter, sulphur dioxide, nitrogen oxides, carbon monoxide and total volatile organic compounds VOC's. The VOC's are split according to SMOKE (Sparse Matrix Operator Kernel Emissions) [2,3,4]. The CFD and mesoscale models solve the Navier-Stokes equations by using different numerical techniques to obtain fluxes and concentrations at different scales. Mesoscale air quality models cover a wide range of spatial scales from several thousands of kilometers to 1 km or so. In this contribution we have applied the MM5-CMAQ-EMIMO models over Las Palmas (Canary Islands, Spain) domain to obtain detailed and accurate results of the pollutant concentrations at this spatial resolution and the MIMO CFD model over a 1 km x 1 km domain with several spatial resolutions (2 m - 10 m) and different vertical resolutions. MM5-CMAQ-EMIMO data serves as initial and boundary conditions for MIMO modelling run. The MM5-CMAQ-EMIMO modelling system has been used to provide detailed initial and boundary conditions to a system called MICROSYS which is composed by the MIMO CFD microscale dispersion model and CAMO which is a cellular automata traffic model. The results show that the air quality modelling system offers realistic results although no comparison with eddy-correlation measurement system has been performed in the area. The tool can be used for many air quality impact studies but in particular for traffic emission reduction strategies. The mesoscale air quality modeling system requires the use of an emission model. In our case we are applying the EMIMO model developed in our laboratory. EMIMO is currently operating with the so called Version 2 which includes the CLCL2000 with 44 different landuse types with 100 m spatial resolution. EMIMO 2.0 also uses the CIESIN 30" (CIESIN, 2004), population database and the Digital Chart of the World 1 km land use database to produce adequate emission data per 1 km grid cell per hour and per pollutant. In order to apply the EMIMO CFD model, we need detailed information related to the building structure in the 1 km grid cell. This information is shown in Figure 3 for the total of the Madrid Community (Spain). The height of the buildings is not included in this file and it has been estimated directly for this experiment. A cellular automata traffic model (CAMO) has been developed. CAMO - which has been included into the extended version of EMIMO modelling system - is based on transitional functions defined in a discrete interval t. We have used the Moore neighbourhood with 8 different surrounding cells where each cell – representative of a vehicle – can move on. The whole system focusing on the 1 km x 1 km urban area in Las Palmas downtown is called MICROSYS system. In our application, the MM5-CMAQ-EMIMO (OPANA V4) system runs in forecasting mode under daily basis operational mode. These runs produce air concentrations with 1 km resolution for 72 hours (today, tomorrow and the day after tomorrow). This information is used as boundary and initial condition for running the MICROSYS system. The MIMO adapted version is applied in diagnostic mode one minute every hour to present in the Internet a representative picture and data for such an hour. We have to run MICROSYS 72 times a day for one minute per hour to produce surface maps which can be visualize in the Internet. The model domain cover by MICROSYS corresponds with 7 1x1 km areas in the downtown domain of Las Palmas (Canary Islands, Spain) as selected by environmental authorities. These 7 areas are covered by MICROSYS with one map per hour for the 72 forecasting hours every day. Each 1 km x 1 km model domain has a vertical structure composed 15 layers up to 167 m in height (to be sure to be well over the buildings). See Fig. 1 and 2 for details. The VRML language is applied to produce 3D images with full interaction with the user over the Internet. See Figure 3.3

Conclusions

The MM5-CMAQ-EMIMO modelling system has been used to provide detailed initial and boundary conditions to a system called MICROSYS which is composed by the MIMO CFD microscale dispersion model and CAMO which is a cellular automata traffic model. The results show that the air quality modelling system offers realistic results although no comparison with eddy-correlation measurement system has been performed in the area. The tool can be used for many air quality impact studies but in particular for traffic emission reduction strategies. The need to have air quality forecasts in detail in space and time is becoming more important since the environmental authorities and citizens are requiring air quality information in advance in order to take measures and actions to eventually be protected from pollution episodes but also to have a proper knowledge of the air quality in the areas where they live or they are going to visit.







Figure 2. Definition of the architecture where the MICROSYS system is applied with 10 m spqatialm resolution over Las Palmas (Canary Islands, Spain).



Figure 3. VRML images produced by full interaction between the user and the Internet interface. The user can navigate through the streets and visualize the different air concentrations at different times and for different pollutants.

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AIR POLLUTANTS STUDY OVER ROME URBAN AREA THROUGH COUPLED TRAFFIC ASSIGNMENT AND CHEMICAL TRANSPORT MODELS.

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ABSTRACT

The city of Rome is often characterized by high ozone and PM episodes in both summer and winter seasons. In this study, the chemical transport model FARM has been applied to study primary and secondary gas/aerosol pollutants concentrations in the urban area of Rome during selected episodes. A nested approach with three domains has been employed, starting from the national to the urban domain. Special attention has been paid for the urban traffic. Hour-by-hour traffic data, related to more than 9000 links making up the 700 Km of the primary road network of Rome, have been produced by a traffic assignment model based on source-destination approach for the selected episodes, and then used to estimate emissions. Results have revealed that the models system, in the selected seasonal episodes, is able to reproduce the observed ozone concentrations at both urban and rural stations. Underpredictions are observed for PM_{10} ground concentrations.

1. INTRODUCTION

Air quality problems produced by high levels of ozone (O_3) and particulate matter (PM) have been of concern for their effects on human health. The latter are critical especially in large metropolitan areas where transport emissions are relevant causing a greater exposure of population with consequent health problems. The city of Rome is a typical Mediterranean metropolitan area experiencing frequently pollution episodes, characterized by high concentrations of ozone and particulate matter, 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. Although the usefulness of modeling techniques to support air pollution study is well known, a modeling study aimed to simulate emission and dispersion of primary and secondary pollutants was never conducted in the city of Rome. Only Leuzzi *et al.* (2004) carried out preliminary simulations for CO dispersion around the city of Rome.

In this work a comprehensive chemical transport model is applied for the first time in the city of Rome to reconstruct pollution episodes occurring in this area, with the aim of getting information on spatial extension of these phenomena.

2. METHODOLOGY

2.1Field campaigns description

A meteorological field campaign has been conducted from June 2005 to June 2006 to get information on the typical meteorological conditions of the studied area and to feed the meteorological models with real data. Surface and upper air meteorological measurements were carried out at different locations placed in Rome downtown, its surrounding and rural areas. The criteria pollutants concentration, routinely collected by the ARPA monitoring network, were used for model results evaluation. Intensive field campaigns were also conducted to collect further VOC and PM measurements.

2.2 The modeling system

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). The Model-3/CMAQ Aero-3 module (Binkowski, 1999), based on the modal approach, is employed for particulate matter. In this approach particle size distributions are represented as the superposition of three lognormal sub-distributions or modes.

2.3 Domains and episodes selection

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. The inner domain consists of 61x61 cells at 1 Km resolution which encompasses the urban area of Rome and its surrounding areas. The intermediate regional domain contains 66x58 cells at 4 Km resolution covering the whole Lazio region. Finally the nation

wide domain consist of 62x62 cells at 16 Km resolution. Based on typical local atmospheric circulations/synoptical conditions and on the occurrence of pollution episodes, as revealed by observations, two episodes were selected for the modelling study. The first, occurring in summer (20-24 June 2005), is related with typical summer Mediterranean conditions characterized by high insulation and sea-land breeze effects. High ozone peaks are detected in this periods. The second period (9-13 January 2006) is a typical pollution episode detectable in winter. PM_{10} peaks are revealed by observation, mainly produced by stagnant meteorological conditions with consequent pollutants accumulation.

2.4 Meteorological inputs

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. Data assimilation techniques were applied to improve the description of the local atmospheric recirculation characteristics, using meteorological data collected in the field campaigns. 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 using 16 surface stations data and three SODAR/radiosounding vertical profiles as well as the wind vertical profiles produced by RAMS in the boundaries of the urban domain. 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.

2.5 Emission inventory

A proper emission inventory has been developed starting from the Lazio regional inventory (APAT 2000). Diffuse emissions at province level (SNAP 3) were available for the year 2000. To update it at the year of interest (2005), national trends on yearly emissions were used. The emission of greatest industrial emission sources was updated using either stack measured data or owner declarations. According to the emission inventory, traffic is one of the main responsible for pollutants emissions. While proxy-disaggregated data from APAT inventory were used to define emissions produced by provincial and state roads, as well from urban areas other than Rome located in the regional domain, emissions from traffic in the urban area of Rome were directly estimated from vehicles flows. For this study a new model for the within-day Dynamic Traffic Assignment (DTA) on road networks was used, addressing explicitly the simulation of queue spillovers, where a user equilibrium is expressed as a fixed point problem in terms of arc flow temporal profiles. The traffic assignment model system architecture is based on a calculation engine (Gentile *et al.*, 2005). The system consists of two models developing the following software modules:

- Off line: it allows to make an assignment or a Origin-Destination (OD) matrix correction/evaluation on the basis of collected data, and to simulate different scenarios as defined by users;
- On line: it allows to represent traffic flows configuration on the network on the basis of a graph, OD matrices (eventually output of the off line model) and of real time traffic data.

Based on the hourly urban traffic flows calculated by DTA model system for each selected episode, the correspondent traffic emissions were then calculated by means of TREFIC emission model (Nanni *et al.*, 2005), based upon the COPERT III methodology integrated with more detailed emission factors for particulate emissions from brakes and tire wear (IIASA, 2001). More than 9000 links making up the 700 Km of the primary road network of Rome were included in this traffic emission estimation. Natural PM emissions from both sea (as sea salt) and soil (as soil erosion by means of wind) were also calculated using SURF*PRO* model according to the methodologies described by Zhang *et al.* (2005) and Vautard *et al.* (2005).

The developed emission inventory has been then spatially and temporally disaggregated using proxy variables and activity specialized temporal profiles. VOC and aerosol emissions were also speciated into respectively SAPRC-90 chemical compounds and aero-3 fractional components, according to source activity speciation profiles.

2.6 Initial and boundary conditions

The initial and boundary conditions used for the regional domain are based on simulations carried out at national level in the MINNI project (Zanini *et al.*, 2004) for the year 1999. These results were used to produce national maps of monthly climatological values to be used as initial and boundary conditions.

3. RESULTS AND DISCUSSIONS

3.1 Ground level ozone (O₃)

In the June episode all the considered stations reach an ozone peak of about 80 ppb. Figure 1 shows the highest ozone concentration map predicted during the simulated periods.

The highest peaks are observed in E-NE side stations (Ada and Cavaliere) showing higher concentration than west one (up to 80 ppb at Guido site). This effect is mainly due to the sea-breeze, that, blowing from west (sea) to east (land), transports ozone produced over the city toward the N-E side of Rome.

The January simulation results, conversely, demonstrate the model ability to predict much lower ozone concentrations as a consequence of the lower photochemical activity.



Figure 1. Highest ozone ground concentration maps in the urban domain during the June and January episodes.

3.2 Aerosol

 PM_{10} model results exhibit underestimations of observed concentrations, particularly in the summer episode. Investigation on model reproduction of PM composition revealed that both organic matter and soil components were responsible for the PM underestimation. In particular during the June episode a Saharan dust advection phenomena was not accounted by the climatological boundary conditions used in this study. Figure 2 shows the average PM_{10} concentration maps during the June 2005 and January 2006 episodes. The maps exhibit the typical seasonal behavior of this pollutant, with higher concentrations in winter and lower in summer. The summer average concentration around the city of Rome is about 10-12 μ g/m³ with peaks of 14-16 µg/m³ spatially limited at specific locations. The city of Rome shows similar values. Clearly evident is also the effect on the pollutant concentrations of the road ring (GRA) around Rome. At summertime the breeze effect transports the pollutant, as for the other compounds, to the north-east part of the territory. Both coastland and inland parts of it are also affected by PM_{10} with concentrations up to 12 $\mu g/m^3$. The winter map shows a large area with an average PM_{10} concentration of 20 µg/m³ covering the city of Rome, its surroundings and the south-east part of it up to the coastline. This effect is produced by a high pressure system characterized by persistent north-northeast wind conditions with low wind speed and often calm conditions. So pollutants emitted/produced in the city of Rome are transported to south-southeast. The other parts of the domain are also affected by not negligible average concentrations with values up to $14 \,\mu g/m^3$. Highest PM₁₀ concentration maps produced for each episodes (not shown) exhibit large areas with values up to 40 μ g/m³ manly detected at nighttime when PBL heights are lower and consequently higher concentrations are reached.



Figure 2. Average PM10 ground concentration maps in the urban domain during the June and January episodes.

4. CONCLUSIONS

A gas/aerosol air pollutants study has been conducted in the urban area of Rome carrying out an integrated approach based on the application of a traffic assignment and a comprehensive chemical transport models.

Overall, the model performed well in predicting O_3 concentrations over the modeling domain showing a good reproduction of daily peak values and the time at which they occurred. The model was also found to be able to predict the seasonal magnitude of O_3 concentrations. The O_3 concentration maps provided by the model, revealed that peaks values at summertime are located in the East-Northeast region of the studied area as a consequence of the breeze effects developing in this season.

Predictions of PM_{10} concentrations have shown the model tendency to significantly underpredict the observed values, especially when considerably contributions of trans-national transported aerosol, like in the Saharan episodes, are in progress. The climatological boundary conditions have demonstrated their inability to take into account these PM continental transported phenomena. PM_{10} concentration maps confirmed that the urban area of Rome is strongly affected by high concentrations, with maximum values up to 40 μ g/m³, particularly in the winter season. Large areas of high concentrations have also been detected in both East-Northeast and South-Southwest zones, depending on the seasonal meteorological conditions.

Further improvements of model results should be addressed to an inclusion of continental scale model results into the regional boundary conditions.

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DIURNAL EVOLUTION OF INNER PARIS COV AND AEROSOL CONCENTRATIONS COUPLING LIDAR AND IN SITU MEASUREMENTS PERFORMED DURING THE LISAIR PROGRAM

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ABSTRACT

Mixing ratios of about thirty volatile organic compounds (VOC) and carbon monoxide were continuously measured by gas chromatography during a 20-day campaign in May 2005 in the center of Paris (France) close to the city hall. Simultaneous in situ aerosol measurements have been performed in terms of black carbon concentration, size number distribution and mass concentration. In addition, LIDAR measurements were performed in order to get information on the vertical distribution of aerosols, their optical properties, and the diurnal variation of the planetary boundary layer height. Ambient concentrations of hydrocarbons from C_2 to C_{12} resulting from the mixing of mobile and stationary emissions are presented and discussed on the basis of the short term and diurnal variability. Variability is studied in order to determine some relatively specific tracers linked to the source origins. Remote sensing and in-situ fixed and mobile measurements are examined for the May 18th, showing consistent results between derived boundary layer dynamics and concentrations.

1. INTRODUCTION

Urban pollution monitoring in Paris is usually performed by in situ surface measurements (e.g. AIRPARIF air quality network, http://www.airparif.asso.fr/) since aerosols and gases in Paris planetary boundary layer (PBL) are mainly produced by local sources driven by automobile traffic. Indeed, traffic is now clearly recognized as one of the most important source of pollutants and megacities emerge as an important research topic in atmospheric chemistry and climate change (Menut et al., 2000; Chazette et al., 2005). For some meteorological conditions however, Paris is influenced by air masses transported from big cities (London) or important to understand the vertical repartition of pollutants in the air column and evaluate their transfer at the surface, especially during the day and night transitions.

Moreover, the current European legislation concerns particles whose diameter is less than 10 μ m (PM10). Nevertheless, smaller particles (PM 2.5) may reach bronchioles and pulmonary alveolus and are known to be more harmful for the respiratory tract. As shown on aerosol size and mass distributions during the Etude et Simulation de la QUalité de l'air en region Ile-de-France (ESQUIF) campaign (Chazette et al., 2005), it is necessary to characterize the aerosol in Paris on widespread size and mass distributions, which is possible when using different aerosol measurement instruments.

The LIdar pour la Surveillance de l'AIR (LISAIR) program has been devoted to this concern. The instrumental approach is quite original in Paris since it is based on the synergy between in situ gas and aerosol measurements and remote sensing instruments (lidar and sunphotometer). The scientific objectives of the campaign are

- To better understand the vertical repartition of particles in the urban environment
- To evaluate pollutant transfer at the surface during the day-night transition
- To characterize gas and aerosol concentration diurnal variation in the planetary boundary layer
- To characterize gas and aerosol horizontal distribution
- To define a long-term strategy of lidar/in-situ measurements in order to predict urban aerosol pollution and help emission reduction strategy

2. INSTRUMENTAL SET-UP

Different experimental approaches were used during the LISAIR campaign including fixed and mobile stations. The campaign took place close to the city hall of Paris, France, from May 9th to 29th 2005. Instruments are located along the east wall of the city hall, 5 m away from the façade, either in a ground based Mobile Aerosol Station (MAS) dedicated to the measurement of atmospheric gas and aerosols, either outside for the EZ LIDAR®/LAUV (Easy Lidar/Lidar Aérosol UltraViolet). During some specific days, the EZ LIDAR®/LAUV lidar has been taken onboard a car in order to study the three-dimensional repartition of particle pollutants in and around Paris. Volatile Organic Compounds (VOC) measurements have also been performed at different hours (5 a.m., 8 a.m., 4 p.m. local time) and at different public parks on a sunny day (May 18th) in order to have a map of background VOC concentrations inside Paris. Air is sampled in steel

cylinders which are then analyzed by gas chromatography at the laboratory. Table 1 shows the MAS instruments and the measured parameters during LISAIR campaign.

Instruments	Measured variables/ retrieved parameters
EZ LIDAR®/LAUV	Aerosol extinction coefficient profile
Lidar LESAA ®	Aerosol extinction coefficient profile
Aethalometer	Black carbon concentration
VAISALA® station	Temperature, pressure, relative humidity
Scatterometer	Aerosol scattering coefficient at 880 nm and 920 nm
TEOM ®	PM10 mass concentration
Nephelometer TSI®	Scattering and backscattering coefficients at 450, 550, 700 nm
Sonic anenometer	Wind direction and intensity
Actinometer	NO2 photolysis rate
Particle counter KC18®	Size distribution 5 classes (>0.1 >0.15 >0.20 >0.30 >0.50 µm)
ELPI ®	Size distribution in 12 classes from 0.03 to 10 µm
CPC	Total number concentration (0.007 à 3 µm)
Filters	Aerosol chemical composition in term of ionic and carbon concentrations
Chromatographs	CO, C2-C6 hydrocarbons, C5-C12 hydrocarbons
Analysers	Ozone, NO _x

Table 1: instruments and associated retrieved geophysical parameters

3. RESULTS AND DISCUSSION

Meteorological conditions during the campaign are very variable with several cloudy and rainy episodes. Mean temperature is around 12°C before May 24th, then slowly increases with maxima of 30°C between May 27th and May 29th. In the PBL, wind direction is generally north-south with eastern winds between May 18th and May 27th. Wind speed is rather weak, not exceeding 5 m/s, with a mean value of 1.2 m/s: surface gas and aerosols concentrations are expected to be rather influenced by the dynamics of the PBL and the traffic sources than by horizontal dispersion. This is examined in the following using the remote sensing and in-situ LISAIR measurements.

- 1) The accurate height of the PBL has been retrieved within an algorithm enabling the detection of vertical variations of particle concentrations derived from lidar signals. The curvature radius of vertical extinction profile is indeed zero at the top of the considered layer (Menut et al., 1999). Calculations of first and second derivatives are performed through a sliding window (Raut et al., 2007).
- 2) In order to identify possible pollution indicators from different sources, we use a principal component statistical analysis on both the set of light (C2-C5) hydrocarbons measurements and the set of heavy (C6-C12) ones. In the latter case, the first principal component explains 79% of the variability in the standardized values. The evolution of C6-C12 hydrocarbons is thus driven by the same processes during the campaign. In the following, benzene (whose concentrations are regulated and should not exceed 5 µg/m³ in 2010 in annual average) has been chosen to represent the group of octane, hexane, heptane, nonane, toluene, ethylbenzene, xylenes and 224TMP (224 trimethylpentane) in Paris. Vardoulakis et al. (2002) showed similar behavior for these compounds and found a similar ratio of toluene/benzene close to 3.5. For the light hydrocarbons, the first three principal components are needed to explain 76% of the total variability (46%, 19% and 11% respectively). We will focus on isopentane and acetylene which are typical tracers of evaporation and combustion respectively.

Figure 1 shows the lidar-derived PBL top height on May 18^{th} along with the diurnal variation of CO, benzene, isopentane and acetylene. May 18^{th} is a clear day, with a mean temperature of ~ 12° C, slowly increasing from a minimum of 7°C in the early morning to a maximum value of 17°C at 5 p.m. GMT. Low winds (varying from 0.6 to 1.5 m/s with mean value of 1m/s) are blowing mainly from SW (NE around 3 a.m. GMT) bringing traffic pollution from Quai de Gesvres, a main traffic road near the City Hall. During the night, pollutants are trapped in the nocturnal inversion layer. Then for each compound, morning high concentrations between 7 a.m. and 8 a.m. GMT (9 a.m. and 10 a.m. local time) reflect the weekday beginning high traffic emissions combined with the low nocturnal inversion layer that traps pollutant close to the ground level. With the erosion of the nocturnal layer by the sun and the subsequent development of the urban boundary layer due to increasing heating onto the surface, all concentrations are decreasing to a floor value from 9 a.m. to 2 p.m. GMT. The vehicle flow data varies weakly of around 15% around Hotel de Ville from 7 a.m to around 7 p.m. GMT. Since the PBL height is fairly constant between 4 p.m. and 7 p.m. GMT,

concentration increase is due to the accumulation of pollutants emitted by cars in the PBL. The sudden decrease (-44 to -58%) between 7 p.m. and 9 p.m. is partly related to decrease in the traffic (-30%). On evening surface becomes colder than the surrounding atmosphere, the urban boundary layer erodes and leads to the formation of the lower nocturnal layer. Lowering of the PBL and late evening traffic then explain the concentration peak between 10 and 11 p.m. GMT.

Similar behavior has been observed from the aerosol number and mass concentrations. On Figure 2, total mass and black carbon concentrations as well as different diameter class number concentrations are reported. A peak is observed in the morning followed by a decrease and a slow accumulation during the day, then a sharp decrease between 7 p.m. and 9 p.m. GMT before the late evening peak. Aerosol size number concentration for diameter < 1.6 μ m is highly correlated with total mass concentration (linear regression coefficient of 0.91), which is not the case for the particles whose diameter is greater than 1.6 μ m. The accumulation mode contributes most to the mass concentration. Note that this mode has been shown to be the main contributor to the aerosol extinction properties (Randriamiarisoa et al., 2005).



Figure 1: Diurnal variation of the PBL height, and normalized concentrations of carbon monoxide (CO), acetylene (C_2H_2), isopentane (iC_5H_{12}) and benzene (C_6H_6).



Figure 2: Diurnal variation of the PBL height, and normalized concentrations of Black Carbon (BC), PM10, aerosol for diameter less than $1.6 \,\mu m (D < 2 \,\mu m)$ and aerosol for diameter more than $1.6 \,\mu m (D > 2 \,\mu m)$.

4. CONCLUSION

In this paper, results of LISAIR campaign are analysed in terms of short term and diurnal variability. Pollutant concentrations close to the City Hall of Paris are mainly governed by the dynamics of the PBL and the traffic emission sources. Principal component analysis shows that heavy hydrocarbons can be represented by a single variable. 3D mesoscale modelling will be further used to explain the results and to evaluate the performances of the emission inventory.

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