On the importance of brake wear as a source of atmospheric copper concentrations

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Exposure to heavy metals has adverse effects on the human health and biodiversity. To control copper emissions to the environment a good understanding of the sources and sinks is vital. However, this is not yet the case evidenced by a big discrepancy between measured and modelled atmospheric concentrations. In this paper we show that brake wear from vehicles is an important source of atmospheric (particulate) copper concentrations in Europe.
We estimated the copper emission due to brake wear from vehicles to be 2.4 kilo tonnes per year. For comparison, the official database for Europe (without brake wear) totals 2.6 kilo tonnes. For a country like the Netherlands brake pad wear may be the most important source of copper to the atmosphere, responsible for ~80% of the atmospheric copper emissions. Using spatially resolved emission data, copper distributions over Europe were calculated with the LOTOS-EUROS model. Without brake wear the model underestimates observed copper concentrations by a factor 3, in accordance with other model studies. Including the brake wear emissions the bias is largely removed.
Although the estimated brake wear copper emission is associated with a large uncertainty, it significantly improves our understanding of the copper cycle in the atmosphere. It is concluded that especially non-exhaust emissions from road traffic deserve more scientific research to support cost-effective international reduction programs of diffuse emissions from metals to the environment such a copper, zinc, antimony and lead.

Numerical Simulation of an extreme air pollution episode created by coal burning thermal power plants

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Stara Zagora is one of the biggest towns in Bulgaria located in the middle of the country. In the summer of 2004 two very high level SO_2 pollution events happened there, leading to serious discontent among the population. Analogous events happened in 2005, too. An attempt for numerical study of one of these episodes – from 8 to 11 of July 2005 is the subject of the present paper.
The most characteristic feature of the surface concentrations in the city during the period is that sharp SO_2 peaks (about and over the alert threshold of 0.131 ppm) appear in the afternoon hours on a background of low concentration (under 10 ppb). As far as all this happened in summertime and the domestic heating can not be the reason for such pollution, the only sources can be the three thermal power plants disposed at 40 km southeast of the town. The "Maritza-Iztok" TPPs are the main sulphur polluters not only in Bulgaria but in all SE Europe. The total SO_x emission from the TPP is about 700 000 tones per year.
The Models-3 system was applied for simulation and analysis of the episode with a sequential downscaling to a horizontal resolution of 1 km. The main impression from the analysis of time and space variation of the simulated wind fields during the period is that calm and non-oriented winds prevail. There is a very fast change of wind directions in the different points from the region and at different levels. As a whole, the calculated SO_2 concentration fields have a reasonable behavior. The calculated concentrations however, in spite of the numerous runs with different parameters, do not agree well with the measurements. A suitable direction of the wind from TPPs to the town of Stara Zagora is simulated each afternoon. These flows form pollution spots in different places around the town, but not over it. Obviously the meandering of the plume is not simulated precisely enough in this episode with small and none-oriented winds. Several reasons for the ill-simulation are discussed in the study. The good result from these not so successful simulations is that they convinced the relevant authorities in the necessity of organization of operational air quality monitoring system for the region, which is already in a process of development.

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Urban PM10 budget

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One year lasting PM10 components measurements in, around and above Berlin have shown a 15 µg/m³ regional background, a 30% of surface and a further 30% urban background increment to the airborne aerosol concentrations found in the city. This rough estimate has also been found by other surface measurements analyses attributing some 50% of the urban PM10 concentrations to local sources and the remaining 50% to long range transport. The aim of this work is to verify these percentages, to give explanations about their origin and to do a comprehensive process oriented study. Therefore, the Aerosol Chemistry Transport Model REM_Calgrid has been applied in order to simulate the aerosol primary, inorganic and organic components. Its applicability has been proved by comparing observations with simulations. The model has been instrumented with a process analysis tool in order to investigate the contributions of individual physical and chemical processes to the final pollution concentrations. For this reason, an investigation domain comprising Berlin urbanised area has been chosen where aerosol accumulating and diminishing processes have been inspected. The most prominent characteristic of the chosen area is the net difference between the emission-intensive urbanised Berlin area and the mostly rural surrounding domain. Mass exchange rates analyses have shown a predominance of advective processes in dispersing mainly primary aerosols over the whole year from the city toward the surrounding areas, while secondarily built organic and inorganic aerosols exhibit seasonal characteristics. Accumulation due to inflow of sulphate and of organic aerosol components depends on wind direction and on seasons. Primary PM10, including EC and OC, are produced in the city and dispersed via advection toward the surrounding region. The local production to net transport ratio is 1.3 for primary aerosol components. Secondary PM constituents are net accumulated in Berlin via advection as well as via chemical production. Net chemical production is stronger for nitrate than for sulphate over Berlin. Sulphate and secondary organic carbons net accumulation in Berlin is due to advection from the South-East, while all other components show a preferred inflow from the west. The importance of long range transport to the urban aerosol concentrations has been corroborated attributing even more than 50% of total PM10 to non-local processes. Nevertheless, the chemical production from city-related aerosol precursors is not negligible and should be taken into account in any reduction strategy.

A methodology to constrain the potential source strength of various soil dust sources contributing to atmospheric PM10 concentrations.

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Crustal material or soil particles typically make up 5-20% of the mass of ambient PM10 samples. In certain regions and/or specific meteorological conditions the contribution may even be higher. Crustal material may originate from distinctly different sources e.g., wind erosion of bare soils, agricultural land management, driving on unpaved roads, resuspension of road dust, road wear, handling of materials and building and construction activities. Despite the importance of crustal material in total PM10 mass, the sources are still poorly understood and not well-represented in emission inventories. This is due to the fact that some sources can be defined as natural sources (e.g., erosion) whilst others like re-suspension are not recognized as primary emission but a re-emission. Separating the source contributions is difficult because the unique tracers for crustal material in PM10 samples (e.g., Si, Ti) do not allow a distinction between the potential sources of this material. To make progress in our understanding of the crustal material source strengths we need a combination of flux measurements, emission estimates, chemical analysis of ambient PM10 samples and atmospheric transport modelling. In this paper we present a methodology to check first order estimates of the various source strengths. Simple and therefore transparent emission functions are combined with activity data or land use maps to make emission grids. The gridded emissions are used as input for the LOTOS-EUROS model to calculate the resulting concentrations. The predicted concentrations will be compared with a small set of observations in various parts of Europe derived from the literature. This will give an indication if the source strengths are in the right order of magnitude to explain observed crustal material contributions to ambient PM10.

On influence of wild-land fires to the european air quality

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This paper considers an influence of wild-land fires on air quality in Europe using spring and summer seasons of 2006 as a prominent example. It discusses the experience of its forecasting by the SILAM modelling system that considers anthropogenic, natural and fire-related emission sources. The fire emission was deducted from the near-real-time MODIS satellite retrievals using two sets of products of the instrument, which were assimilated daily by the emission pre-processor. We analysed several episodes and compared an impact of fires with contribution from anthropogenic sources. For example, exceptionally high concentrations of nearly all pollutants were detected in Central, Eastern and Northern Europe in April and May of 2006. Simulations showed that this episode was formed by contributions of all three main sources: major wild-land fires in Russia, substantial amounts of anthropogenic air pollutants accumulated for a few days over Eastern Europe, and intensive birch flowering in Russia. A synchronization role was played by meteorology. Specific weather conditions promoted formation of the multi-component pollution cloud, which was then transported across most of Central and Northern Europe causing widespread allergic symptoms and other illnesses associated to poor air quality. Several other episodes were more localised. Thus, August of 2006 was particularly difficult in Portugal and Spain, but also in Finland. The model predictions were compared with available information from ground-based monitoring sites and the satellites retrievals. The agreement was fairly good, especially for timing of rise and fall of concentrations, while the quality of absolute levels reproduction appeared to depend on the original fire product.

Forest fires impact on air quality over Portugal using an ensemble of model results

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Smoke has to be considered one of the several disturbing effects of forest fires. Its impacts on air quality and human health can be significant, because large amounts of pollutants, like particulate matter (PM), carbon monoxide (CO), volatile organic compounds (VOC) and nitrogen oxides (NOx), are emitted to the atmosphere. In 2003 Portugal faced the worst fire season ever recorded. There were 4,645 fires burning 8.6% of the Portuguese forest area.

The main purpose of this work is to evaluate the effects of these forest fires emissions on the air quality applying two numerical modelling systems (MM5-CHIMERE and LOTOS-EUROS) to the case study of 2003 summer over Portugal and analysing its joint results based in an ensembling technique.

Emissions from forest fires were estimated using a simple methodology, which include emission factors, burning efficiency, fuel loads and area burned. Specific values for Portugal were selected based on data from the National Forest Inventory, on the characteristics of the consumed forest type and shrubs, and fire data like ignition point and time and area burned. Emission factors were selected according to the most suitable for south European ecosystems, namely for the Portuguese land use types. These estimated forest fire emissions were then incorporated in the emission input data of both modelling systems.

Besides the comparative evaluation based on the available monitoring stations that are located preferentially along the coast, far away from the larger fire occurrences, model results showed a significant performance improvement when forest fires are taken into account. PM_{10} and O_3 values can reach differences in the order of 30%, showing the importance and the influence of this type of emissions from local to regional air quality. Both models presented the same kind of behaviour concerning PM_{10}, but for O_3 the pattern is slightly different. LOTOS-EUROS O_3 results are not so sensitive to the inclusion of forest fire emissions. Also, this modelling system has smaller values of RMSE, but lesser correlation coefficients, when compared to CHIMERE results.

Nevertheless, the comparison between model and observed data indicates better agreement when the ensemble results are analysed. This was evident for all the statistical parameters applied for model validation, and in particular for the systematic (BIAS) and root mean square (RMS) errors.

Influence of soil moisture on PM emissions from soils

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Wind erosion and tillage operations are causes of PM emissions from soils. Wind erosion is limited to a certain extent because a susceptible soil surface and a given erosivity of the climate have to coincide. In the Federal State of Brandenburg it is temporally restricted to the spring months and constrained spatially by the acreages of root crops, corn and summer cereals, which amount to about 20 per cent of the agricultural used area. Dust emission resulting from tillage operations affects all soils, even those which are considered to be non-erodible. This is mainly caused by higher contents of silt and clay particles, which support the formation of aggregates or crusts. On the other hand these soils have a higher potential for dust emission when they are disturbed by the impact of tillage tools. On the North European plains dust emission induced by tillage was measured as being four to six times higher than the dust emission by wind erosion events. The main controlling factor for the emitted amount of dust is the soil moisture, or the vertical distribution of moisture in a soil profile at the moment of tillage. Therefore, the relation between soil type, soil moisture and PM emission of twelve soils were investigated with regard to their water content, ranging from 0 to 40 mass per cent.
The results show that soils can emit dust over a certain range of moisture, but already a small increase in soil moisture causes a distinct reduction of dust emission. The results are used to calculate the dust emission potential of all agricultural used land in Brandenburg. A comparison of the contributing parts of wind erosion and tillage operations is presented in monthly time steps for a chosen year.

Modelling and satellite observations of air pollution in the Netherlands and Europe

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In our contribution we will describe an air-pollution forecasting system for Europe and the Netherlands. This system is based on the Dutch Lotos-Euros and the French Chimère models, coupled to ECMWF and HIRLAM operational weather forecasts. The work is part of a collaboration between TNO, RIVM and KNMI. Results will be shown of the comparison between the two models, and the verification/ validation with surface observations and satellite NO2 measurements from the OMI satellite spectrometer on EOS-Aura. An assimilation capability for both surface and satellite observations is currently developed.

Enhancing high-resolution air quality forecasting in Europe and the Iberian Peninsula within a supercomputing framework: the CALIOPE project

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According to recent studies of the European Environmental Agency, air pollution is the environmental factor with the greatest impact on health in Europe and is responsible for the largest burden of environment-related disease. For instance, ozone (particularly in southern Europe and the Mediterranean during summer months) and particulate matter and especially small particles with a diameter less than 2.5 micrometers (PM2.5) are associated with increased mortality, especially from cardiovascular and cardiopulmonary diseases.
One of the topics in which the European Commission has shown a greater concern (Directive 1996/62/EC) is the necessity of developing actions that allow increasing the knowledge on transport and dynamics of pollutants to assure the accomplishment of legislation and to inform the population about the levels of pollutants, especially before 2010, date when the Directive 1999/30/EC (setting the thresholds for particulate matter) comes into effect. The regulation is especially demanding when the threshold levels are exceeded. In this case, it demands a detailed diagnosis of those areas where the exceedances are found and a forecast of the evolution of ground-level concentrations.
In this context, the CALIOPE project has as main objective to establish an air quality forecasting system for Spain coordinated by the Spanish Ministry of the Environment through funded project 441/2006/3-12.1, delivering air-quality related products useful to a wide range of users for reducing the impacts of air pollution on human health. A partnership of four research institutions composes the CALIOPE project: the Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS), the CIEMAT, the Earth Sciences Institute 'Jaume Almera' (IJA-CSIC) and the CEAM Foundation. This consortium will deal with both operational and scientific aspects related to air quality monitoring and forecasting.
CALIOPE activities include the development, implementation and validation of an integrated air quality modelling system with a high resolution (spatial resolution of 12 km for Europe and 4 km for Spain, with nesting to 1 km to the cities of Madrid and Barcelona; and temporal resolution of 1 hour), formed by a set of models taking into account both anthropogenic and natural pollution. These models are the WRF-ARW meteorological model; the HERMES emission model; the CMAQ and CHIMERE chemistry transport model; and DREAM mineral dust model. Integrations are performed thanks to the high-performance computational resources of MareNostrum supercomputer.
The HERMES emission model has been specifically developed as a high-resolution emission model for Spain under a GIS framework. The emission model focuses in the estimation of gas

and particulate matter pollutants, including the ozone precursors and using a high spatial and temporal resolution for Spain. The land has been divided in cells of 1 km^2.
For that the model uses land-use information (CORINE Land Cover Map of high resolution, 100 m, population density, industrial location, etc.). The emission model includes biogenic and anthropogenic (on-road, ship and planes traffic, airports and ports, industrial sectors, power generation, domestic and commercial) and it is essential when providing data to the air quality models on a hourly, daily, monthly and annual basis.
The model qualitative and quantitative evaluation studies performed so far for a reference year (2004) using data from observation networks and satellite information have outlined the good skills of the modelling system concerning the concentrations of gaseous pollutants and aerosols in Spain and Europe. The initial state of the system and the operational forecasts are available at http://www.bsc.es/plantillaA.php?cat_id=399 or http://salam.upc.es/caliope. The improvement of the resolution achieved with CALIOPE project in the whole region may serve as a standard tool, for public and private, state and local forecasters who provide tailored forecasts for their communities, and will allow taking preventive measures to safeguard human health.
The CALIOPE system will contribute to a deeper understanding of atmospheric processes and the dynamics of air pollutants in Europe, the Iberian Peninsula and the urban areas presenting important exceedances of the thresholds set in the regulations for protecting the human health and the ecosystems. Also, it should be highlighted that this system is useful to complement the data obtained in the present networks of air quality measurements managed by regional and local authorities, and in certain experimental measurement campaigns or air quality studies performed both in urban or background areas.

Evaluation of an operational "ensemble prediction system" for ozone concentrations over Belgium using the CTM Chimere

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In the framework of operational air quality forecasts in Belgium, an ensemble prediction system based on the chemical transport model (CTM) Chimere has been implemented. The Chimere model was forced by ECMWF meteorological fields and by the EMEP emission database. The simulation domain covers Western Europe with a spatial resolution of 0.5 degree.
The objective of these ensemble simulations consists of evaluating the impact of uncertainties from emission and meteorological data on the simulated concentrations of pollutants. Such evaluations are important in the operational context, since they contribute to reduce the risk of false alarm and inappropriate broadcast of information to the public. Indeed the forecaster has at its disposal more information to better judge to what extent a change in one or more particular input parameters can influence the modelled pollutant concentrations.
A first assessment of the ensemble prediction system has been performed for ozone forecasts during summertime. Currently, the Chimere model is run considering 13 different scenarios in which some variables influencing pollutant dispersion and ozone chemistry (e.g. temperature, wind velocity, cloud cover) are perturbed. The treatment of all these simulations allows defining a confidence interval around the concentrations simulated by the reference (i.e. without change in input parameters) simulation, which contributes also to improve the accuracy of the ozone forecast. Considering physical aspects, the ensemble prediction system contributes to point out – for each specific situation – the most sensitive input parameters that influences ozone concentrations.

The observations, used to validate the Chimere model are deduced from an advanced interpolation method. This "RIO-algorithm", developed by VITO (Hooyberghs et al., 2006), provides every hour an ozone value which takes into account the representativeness of the location the user is interested in. The ozone maps created with this algorithm have a spatial resolution of 5 km^2.

Preliminary results of MM5/CAMx simulations for winter and summer 2006 in Switzerland

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Quantitative measurements of aerosols performed by aerosol mass spectrometer (AMS) in Switzerland indicate that organics are the major components of the aerosol composition in winter as well as in summer and they are mostly secondary. Additional measurements using ^{14}C as tracer show that biogenic emissions in Zurich contribute about 60 and 27 % to organic carbon (OC) in summer and winter, respectively. Recent measurements suggest that wood burning emissions might contribute significantly to the aerosol concentrations, especially in winter. The contribution of wood burning however, is still difficult to model because of the lack of their emissions in the emission inventory.

In this paper, the application of the MM5/CAMx model system under winter (January-February 2006) and summer (June 2006) conditions over the complex terrain of Switzerland will be discussed. The focus will be on the formation and transport of particulate matter (PM) and the contribution of various sources to the aerosol formation. Three nested domains with 27 km (Europe), 9 km (Switzerland and neighbouring countries) and 3 km (Switzerland) resolution are used. Aerosol components are calculated for particle sizes smaller than 2.5 μm. The model's capability to reproduce the aerosol concentrations is investigated by comparing the model results with the speciated aerosol measurements performed during the same periods.

Local to regional dilution and transformation processes of the emissions from road transport

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INTRODUCTION

The objective of the present work is to study in detail the dilution processes and chemical transformations of the generated by road transport from the local scale to the scale of the global models and on deriving some conclusions about the key parameters, which quantify the local dilution and transformation processes impact on larger scale pollution characteristics.

BRIEF DESCRIPTION OF THE NUMERICAL EXPERIMENT SET UP

The US EPA Models-3 system was chosen as a modelling tool. The simulations were consecutively carried out in 3 nested domains. The innermost domain (D3), treated with a resolution of 10 km includes a region with very intensive road transport – the city of London and its "footprint". The CMAQ "Integrated Process Rate Analysis" utility is used to differentiate the contribution of different dynamic and chemical processes which form the pollution characteristics in the region of interest.

Two sets of emission data were used in the present study: 1.) the EMEP data was used for all the countries except the UK; 2.) For the UK data from the National Atmospheric Emissions Inventory, with a 1 km resolution was used. The biogenic VOC emissions were also accounted for. The meteorological background input was taken from US NCEP Global Analyses data.

The simulations in D3 were carried out for January and August 2002-2006 for the following emission scenarios: 1.) All the emissions (detailed inventory); 2.) Emissions from the road transport excluded (detailed inventory); 3.) All the emissions, averaged over D3; 4.) Emissions averaged over D3, but emissions (averaged) from the road transport excluded. The combined analysis of these scenarios made it possible to clarify the role of different dynamic and chemical processes which determine the pollution from road transport pattern and time evolution. Some conclusions about the role of the road traffic emission inventories spatial resolution on the simulated fields and the local to regional scale interaction were made.

CONCLUSIONS

The numerical experiments performed produced a huge volume of information, which have to be carefully analyzed and generalized so that some final conclusions, concerning not only clarification of local scale processes of dilution and chemical transformation but also how to account for them in large scale CTMs could be made. The conclusions that can be made at this stage of the studies are:

1.) The effect of the road transport emissions is well displayed in both the concentration and process analysis fields;

2.) The contributions of different processes have very complex spatial/temporal behavior and variability;

3.) Even horizontally/temporally averaged process contributions may be sensitive to emission resolution.

Influence of transatlantic NO_2- and O_3-transport on air quality in Europe

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A series of model calculations has been carried out to assess the influence of NO_2- and O_3-transport from outside Europe on European air quality. For a better representation of boundary concentrations, the EUROS-model has been nested into the global chemical transport model TM4. Originally, climatological boundary concentrations have been used in EUROS.

Sensitivity studies carried out with EUROS nested into TM4 showed that transatlantic NO_2-transport affects NO_2-concentrations in Western Europe only during some events of increased NO_2-transport over the Atlantic Ocean. However, its contribution to annual mean NO_2-concentrations is small. In contrast, transatlantic O_3-transport has a very high impact on European O_3-concentrations. Additionally, transatlantic O_3-transport influences the NO/NO_2-concentration ratio in Western Europe significantly, leading to higher NO_2-concentrations in areas with high NO_x-emissions such as the Benelux. Hence, it can be anticipated that higher O_3-background concentrations in the Northern Hemisphere will not only lead to higher O_3-concentrations in Western Europe but also to increased NO_2-concentrations in certain areas, leading probably to problems in meeting EU-regulations concerning NO_2-concentration levels.

Modelling air quality in the Lake Baikal region

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We studied the air quality for the summer periods of 2003 and 2004 in the Lake Baikal region in Russia using the AURORA model. The area is centred around the city of Irkutsk and Lake Baikal itself. The region is characterised by so-called complex terrain, consisting of steep and densely forested hill slopes surrounding the lake, which presents a challenge with respect to the correct simulation of atmospheric dynamics and turbulence. The air quality focus here is on the dispersion of industrial emissions, which are the dominant source of air pollution in this area, and for which suitable emission and concentration data were made available.

AURORA is a state-of-the-art CTM developed at VITO using nested grids to model regional and urban air quality. The model input consists of terrain and remote sensing data (digital elevation model, land use, vegetation cover) that are integrated in a GIS system. Meteorological input data are provided by a separate meteorological model (ARPS). The emission input data are resulting from the combination of down-scaled emissions of EDGAR (2000) in combination with a more detailed local emission inventory. TM4 model output is used to provide lateral boundary conditions.

The aerosol distribution in Europe derived with the Community Multiscale Air Quality (CMAQ) model: Comparison to near surface in situ and sunphotometer measurements

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The aerosol distribution in Europe was simulated with the Community Multiscale Air Quality (CMAQ) model system for the years 2000 and 2001. The results were compared with daily averages of PM10 measurements taken in the framework of EMEP and with aerosol optical depth (AOD) values measured within Aeronet. The modelled total aerosol mass is typically about 30 - 60 % lower than the corresponding measurements. However a comparison of the chemical composition of the aerosol revealed a considerably better agreement between the modelled and the measured aerosol components for ammonium, nitrate and sulfate, which are on average only 15-20 % underestimated. Sligthly worse agreement was determined for sea salt, that was only available at two sites. The largest discrepancies result from the aerosol mass which was not chemically specified by the measurements. The agreement between measurements and model is better in winter than in summer. The modelled organic aerosol mass is higher in summer than in winter but it is significantly underestimated by the model. This could be the main reason for the discrepancies between measurements and model results. The probability distribution function of the PM10 measurements follows a log-normal distribution at most sites. The model is only able to reproduce this distribution function at non-coastal low altitude stations.
The AOD derived from the model results is 20 - 70 % lower than the values observed within Aeronet. This is mainly attributed to the missing aerosol mass in the model. The day-to-day variability of the AOD and the log-normal distribution functions are quite well reproduced by the model. The seasonality on the other hand is underestimated by the model results because better agreement is achieved in winter.

A model inter-comparison study focussing on episodes with elevated PM10 concentrations

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Five three-dimensional chemical transport models of different complexity were applied to Central Europe to assess the ability of models to reproduce PM10 concentrations under highly-polluted conditions. The participating models were: The French CHIMERE model, the Dutch LOTOS-EUROS model, as well as the REM-CALGRID, the EURAD and the LM-MUSCAT models from Germany. In the selected 80-day period, observed PM10 daily mean concentrations reached values well above 50 $\mu g/m^3$ on many days in large parts of Northern Germany. This model evaluation shows that there is an increasing underestimation of primary and secondary species with increasing observed PM10. The high PM levels were observed at cold temperatures under stagnant weather conditions, that are difficult to simulate with either prognostic or diagnostic, interpolation-based meteorological models supporting the assumption that uncertainties in PM emissions and composition or incomplete process sub-descriptions can each separately account for only a portion of the underestimation of high PM. Uncertainties for key boundary layer parameters, which differ by a factor-of-two or more between the models, represent additional and important sources of error – both direct sources of error through the transporting meteorological fields and indirect sources of error through the physico-chemical modules which rely on those key boundary layer parameters.

Model Evaluation Experiences in the US and Europe

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Both in the US, and in Europe several studies and workshops have been held recently on the aspect of model evaluation. Examples in Europe are the studies in Eurotrac on O3 and aerosols, the studies in the framework of City-Delta and Euro-Delta and the review in the frameweork of the unified EMEP-model
(Loon,van M. et al, 2004)
A protocol on model validation has been discussed at the workshop on model benchmarking in Thessaloniki in 2006 (Moussiopoulos and Isaksen, 2006), and presented at the last ACCENT/GLOREAM workshop in Paris (Builtjes, 2006).
In the framework of COST 728 there are ongoing activities on the development of model evaluation methodologies (Schlünzen, K.H. et al, 2007).
Recently, in the US a Workshop on the Evaluation of Regional-Scale Air Quality Modeling Systems was
held at Research Triangle Park in aug. 2007.
Results of that workshop will be presented, and in the discussion will be compared with the experience in Europe.
The idea/proposal is to held in 2008 a workshop to bring together modellers in Europe to review the current practices , and subsequently organise a joint EU-US workshop in 2009.

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The new Danish Centre of Energy, Environment and Health (CEEH) - basic ideas and framework

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The objective of the Centre of Energy, Environment and Health (CEEH) is to provide advanced research of energy production and related environmental/health issues and thereby integrate groups from these areas. The main goals are to study the future production of energy in Denmark and consequences of different scenarios with respect to environmental and human health aspects, and to optimize the type of energy production and consumption not only with respect to direct costs related to the production, but also with respect to economy from environmental and health viewpoints.

A key element of the CEEH will be to expand, evaluate and apply integrated models for the whole impact pathways, including integrated energy system, emissions, atmospheric chemistry/transport, human exposure, human health models as well as cost models. The main research areas include:

- Modelling and research in atmospheric transport, dispersion, chemistry and faith of pollutants due to energy production and consumption. Both primary and secondary particles as well as chemical gas-phase constituents will be considered. Knowledge of the regional and local environmental burden related to emissions of pollutants and accidental risks from power production is needed for estimation of environmental and health costs.
- Physiological and statistical studies of the impact of atmospheric pollutants on the human body and on health in general. Based on the atmospheric burden these studies will be used to quantify the relative importance and costs of different types and amounts of emissions (as well as other types of environmental impacts).

The grant for CEEH covers a 5-year period from 2007-2011, and the basic model system to be applied in the Centre is the EVA model system (External Valuation of Air pollution) developed at NERI/AU.

Contribution of atmospheric processes to photochemical pollution by using a process analysis tool in the north-eastern and central Iberian Peninsula

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The Mediterranean and specifically the Iberian Peninsula (IP) undergo frequent photochemical pollution episodes during summertime, in which O_3 and PM10 exceedances of the European air quality targets are commonly registered (Jiménez et al., 2006). Atmospheric modelling combined with different experimental techniques allow identifying the main causes of these episodes. Nevertheless, the air quality models usually provide the net concentration of pollutants, without the capabilities of understanding and isolating the atmospheric processes involved, which would provide a fundamental explanation of the reasons for a model's predictions and show the relative importance of each process (Jeffries and Tonnesen, 1994). Even the sensitivity analysis does not adequately quantify the importance and interactions of modelled processes. Currently, this feature has become feasible thanks to the process analysis tool implemented in some Eulerian grid models, such as CMAQ (Gipson, 1999). Therefore, this work quantifies the contribution of different atmospheric processes to O_3 net concentration in the north-eastern and central IP, where major urban areas of Spain are located: Barcelona and Madrid, by using the process analysis tool available in the CMAQv4.6 model.
The WRF-ARW/HERMES/CMAQ modelling system was applied with a high spatial (1 km^2, 32 vertical layers covering the troposphere) and temporal (1 hr) resolution to the study areas, for the 17-18 June, 2004; a typical summertime photochemical episode in these regions (Jorba et al., 2004). The integrated process analysis tool provided the hourly contributions of gas-phase chemistry, advection and convection, horizontal and vertical diffusion, clouds chemistry, and wet and dry deposition to net O_3 concentration for each cell of both domains.
The maximum chemical production rates of O_3 occur in the urban plumes around 1400 UTC, accounting in the first vertical layer (0-33 m ag) for +50/75 $\mu g\ m^{-3}$. The urban areas and main roads, as main sources of NO_x emissions, act as O_3 sinks, quenching up to -200 $\mu g\ m^{-3}$ per hour during the traffic circulation peaks. The O_3 concentration gradient generated in these areas, larger during daytime, increases the diffusion processes contribution to ground-level O_3 (up to 200 $\mu g\ m^{-3}\ h^{-1}$ fluxes, mainly from upper vertical layers). The advection and convection processes displace the largest amount of O_3, up to 2000 $\mu g\ m^{-3}\ h^{-1}$.
Despite of the similar contribution of the chemical production to net O_3 in both domains, the final concentrations and the ground-level O_3 distribution differ, mainly due to the influence of the mesoscale transport phenomena affected by local orography. While in the north-eastern IP the breezes and mountain-valley winds regime involves the accumulation and recirculation of pollutants aloft, in the central IP the main flows are dominated by thermal phenomena that transports pollutants within the convective recirculation cell.
The process analysis confirms the results of previous experimental and modelling studies carried out in these areas (Millan et al., 1991; Baldasano et al., 1994; Pérez et al., 2004; Jiménez et al., 2006) and provides quantitative information about the origin of O_3 peaks, with a high resolution that allows designing strategies to control this photochemical pollutant levels.

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Application and inter-comparison of atmospheric chemistry mechanisms and advection schemes within the online-coupled regional meteorology chemistry model MCCM

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Since the huge number of chemical species and reactions involved in the degradation of organic compounds does not permit an explicit treatment of these reactions, the use of condensed mechanisms in regional models is necessary. Such mechanisms are for example the RADM2 (Stockwell et al., 1990) or the RACM (Stockwell et al., 1997) mechanism, which are widely applied in regional air chemistry models. With increased knowledge about biogenic VOC's chemistry, updates of the description of organic chemistry may be necessary. Geiger et al. (2003) introduced a new mechanism based on RACM with improved isoprene and biogenic VOC chemistry.
To understand the behavior of the three mechanisms for the application within regional air chemistry models, two case studies were performed for the three mechanisms: A box-model-inter-comparison and a cross-validation of the simulations with the three-dimensional online-coupled regional air chemistry model MCCM (Grell et al. 2000).
The steady increase in computational power opened the possibilities to performe high resolution air quality simulations along with development of detailed emission inventories. The resulting chemical trace species concentrations demand superior numerical schemes to conserve these local gradients on different scales. Numerical advection schemes for the trace species transport have been developed and implemented into MCCM on the basis of the flux limiting advection schemes of Bott (1989, 92) in order to account for the conservation of steep gradients, monotony and positive definiteness and their impact to high resolution air quality simulations have been studied.

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Transport and chemical transformations influenced by shallow cumulus over land

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The distribution and evolution of reactive species in a boundary layer characterized by the presence of shallow cumulus over land is studied by means of two large-eddy simulation models: the NCAR and WUR codes. The study focuses on two physical processes that can influence the chemistry: the enhancement of the vertical transport by the buoyant convection associated with cloud formation and the perturbation of the photolysis rates below, in and above the clouds.
It will be shown that the dilution of the reactant mixing ratio caused by the deepening of the atmospheric boundary layer is an important process and that it can decrease reactant mixing ratios by 10 to 50 percent compared to very similar conditions but with no cloud formation. Additionally, clouds transport chemical species to higher elevations in the boundary layer compared to the case with no clouds which influences the reactant mixing ratios of the nocturnal residual layers following the collapse of the daytime boundary layer. Estimates of the rate of reactant transport based on the calculation of the integrated flux divergence range from to -0.2 ppb/hr to -1 ppb/hr, indicating a net loss of sub-cloud layer air transported into the cloud layer. A comparison of this flux to a parameterized mass flux shows good agreement in mid-cloud, but at cloud base the parameterization underestimates the mass flux.
Scattering of radiation by cloud drops perturbs photolysis rates. It is found that these perturbed photolysis rates substantially (10-40 %) affect mixing ratios locally (spatially and temporally), but have little effect on mixing ratios averaged over space and time. We find that the ultraviolet radiance perturbation becomes more important for chemical transformations that react with a similar order time scale as the turbulent transport in clouds. Finally, the detailed intercomparison of the LES results shows very good agreement between the two codes when considering the evolution of the reactant mean, flux and co-variance vertical profiles.

Simulations of large fire plumes dispersion with CHIMERE: three major case studies

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The pollutant injection of large fires, of various origins, may have an important impact on air quality and health, as well as on radiation and atmospheric composition. There are large uncertainties inherent to simulating the plume of such large fires and the dispersion of pollutants contained in the plume. The amount of material released, its chemical content, the size of aerosol particles and the injection height are usually very uncertain. Furthermore, long-range transport of the plume undergoes differential advection and may occur as thin sheets, not captured by the too coarse vertical resolution of models.

We review the ability of CHIMERE to simulate large fire plumes, at European scale, for three major cases: (i) the 2003 Portuguese forest fires, (ii) the extreme Buncefield oil depot fire that occurred on 11/12/2005, and the Summer 2007 greek forest fires. Each case is discussed separately and tested against satellite imagery. The simulation of each fire case then allows discussion and interpretation. This presentation contains results from 3 published articles and one study in progress.

Parameterisation of vertical rain rate profiles for the meteorological driver of LOTOS and RCG

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To obtain an improved 3D analysis of precipitation, data of a Micro Rain Radar which is operating at observatory Lindenberg (German Weather Service) was applied. The focus was put on the vertical profile of precipitation which is amongst others affected by evaporation processes. Through wet deposition pollutants are removed from the atmosphere by precipitation events. As aerosol particles are regenerated following complete evaporation of raindrops an interesting matter is to what extent the evaporation of raindrops in the troposphere impacts the wet deposition process and therewith linked processes.
The diagnostic meteorological analysis system TRAMPER (Tropospheric Realtime Applied Meteorological Procedures for Environmental Research) is the meteorological driver of the Chemical Transport Models REM-CALGRID and LOTOS. The herein calculated scavenging coefficient is proportional to the rain rate. For setting the scavenging coefficient in REM-CALGRID and LOTUS, TRAMPER delivers the ground based rain rate. Vertically the rain rate is assumed to be constant. Evaporation processes that would lead to a downwards decreasing rain rate are not taken into account.
Pursuing the motivation above using Neuro-Fuzzy Models a statistical relation between the rain rate in different heights and other meteorological parameters such as precipitation at ground level, temperature, relative humidity etc. was generated with the intension to derive the ability to interpret numerical analysis respectively.