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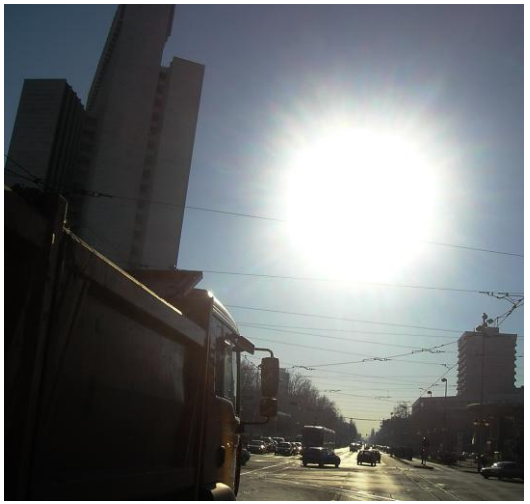


# *European association for the science of air pollution*

## EURASAP GOVERNING BODIES





**CONTENTS**



*Front cover: Savska street, Zagreb, Croatia (photo by B. Rožman)*

## EDITORIAL

Dear EURASAP members,

After a delay, I am happy to present to you the issue 70. I also kindly invite you to be more active in sending your contributions and sharing your knowledge, ideas and opinions in the EURASAP Newsletter.

Those members, whose email address has changed, please help us update our database. Send the new address to the Newsletter Editor (zklaic@gfz.hr).

In the present issue you will find an article of Angelina Todorova who obtained EURASAP travel grant for participation in ACCENT/GLOREAM Workshop on tropospheric chemical transport modelling (26-27 November 2009, Brescia, Italy). The article deals with the use of computer system in the air pollution modelling.

*The Newsletter Editor*



*Scientists' Contributions*

## DEVELOPMENT OF GRID COMPUTING FOR AIR POLLUTION MODELLING IN BULGARIA

***Angelina Todorova***

*Geophysical Institute, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., Bl.3, Sofia 1113, Bulgaria*

**Abstract:** Comprehensive atmospheric composition studies require multi-scale numerical experiments to be carried out, which to clarify to some extend different scale processes interaction, but also to further specify requirements for input data (emissions, boundary conditions, large scale forcing). Model interfaces from synoptic trough meso- to local scale have to be tailored. Shortly speaking, extensive sensitivity studies have to be carried out, tailoring the model set-up and parameters – a possible forerunner of single model ensemble forecasts.

Performing extensive simulations of this kind with up to date highly sophisticated numerical models obviously requires computer resources of the order of magnitude of those provided by the so-called supercomputers. Using supercomputers, however, is rather expensive and far beyond what most of the research groups can afford. Luckily an alternative technology – the grid computing, is recently very intensively developing, which makes it already quite

relevant to formulating and solving problems absolutely unthinkable several years ago.

Some examples of environmental problems which are recently developed as grid applications are given in the present paper.

**Key words**: *air pollution modelling, multi-scale modelling, emergency response, GRID computing*

## INTRODUCTION

### *Why using the GRID?*

Atmospheric composition studies with up to date highly sophisticated numerical models often requires a large number of multy-scale numerical experiments to be carried out. Performing extensive simulations of this kind requires computer resources of the order of magnitude of the so-called supercomputers or shared/distributed memory clusters. Using supercomputers, however, is rather expensive and far beyond what most of the research groups can afford. Luckily an alternative technology – the GRID computing, is recently very intensively developing, which makes formulating and solving problems absolutely unthinkable several years ago already quite relevant.

### *What is a computational GRID?*

A Computational GRID is a computing environment which enables the unification of widely geographically distributed computing resources for shared use (Atanassov et all., 2006, Foster and Kesselmann, 1998). The GRID is a computer system primarily intended for supporting e-Science, but however the technology itself is very adaptable to the whole area of present and future computer usage.

The individual computing resources commonly consist of computer clusters and individual computers which are interconnected by a high speed network over a very wide area. The major goal of the GRID is to enable the clustering and unification of distributed computing and data processing resources, collecting as much computing power as possible usable to applications necessitating high computer strength during the time of peak calculations, like applications from the fields of particle physics, climate analysis, biomedical research, meteorology etc. The GRID is virtually free for all users. The basic elements of the GRID are shown on Fig.1.

GRID is a computer system which is a viable solution for supporting e-Science. New possibilities, which are being offered by the enormously enhanced computing power of distributed systems, open up new areas for computation. It is possible to simulate natural (and thought-out) processes and phenomena in greater detail, using much larger spatial and temporal resolution. New scientific methods, and even new scientific fields, specifically multidisciplinary research, are being 'born' and evolved, based on vast sets of data and massive parallel computing.

The GRID is a parallel execution infrastructure, but it is also more complex for programming (and therefore algorithm selection) than Clusters. The GRID Infrastructure is quite more complex than cluster parallelism and it has its disadvantages. Inter-cluster

communication on the GRID is very inefficient, it is often almost impossible to use a huge number of resources which are not grouped in a specific cluster for the execution of a tightly coupled algorithm.

The optimal calculation time is achieved when using a series of independent shared memory or fully serial programs. Therefore the usage of a GRID Infrastructure, on one hand, gives higher computational power, but, on the other hand, necessitates a much stricter and more careful application execution planning.

## THE SEE-GRID-SCI PROJECT

The active development of the GRID technology is strongly supported by the European Commission through projects in the 6th and 7th FP. Some of these projects are intended to build and maintain a sustainable GRID infrastructure in South Eastern Europe (SEE-GRID). The SEE-GRID eInfrastructure for regional eScience (SEE-GRID-SCI: www.see-grid-sci.eu) project, started on May 2008, stimulates widespread eInfrastructure uptake by new user groups extending over the region, that currently do not directly benefit from the available eInfrastructures. It provides advanced capabilities to more researchers, with an emphasis on strategic groups in seismology, meteorology and environmental protection, increasing the computing and storage resources and involving new partner countries in the region. Finally, SEE-GRID-SCI helps to mature and stabilise the National GRID Initiatives in the region, allowing them to join the new era of longer-term sustainable GRID infrastructure in Europe.

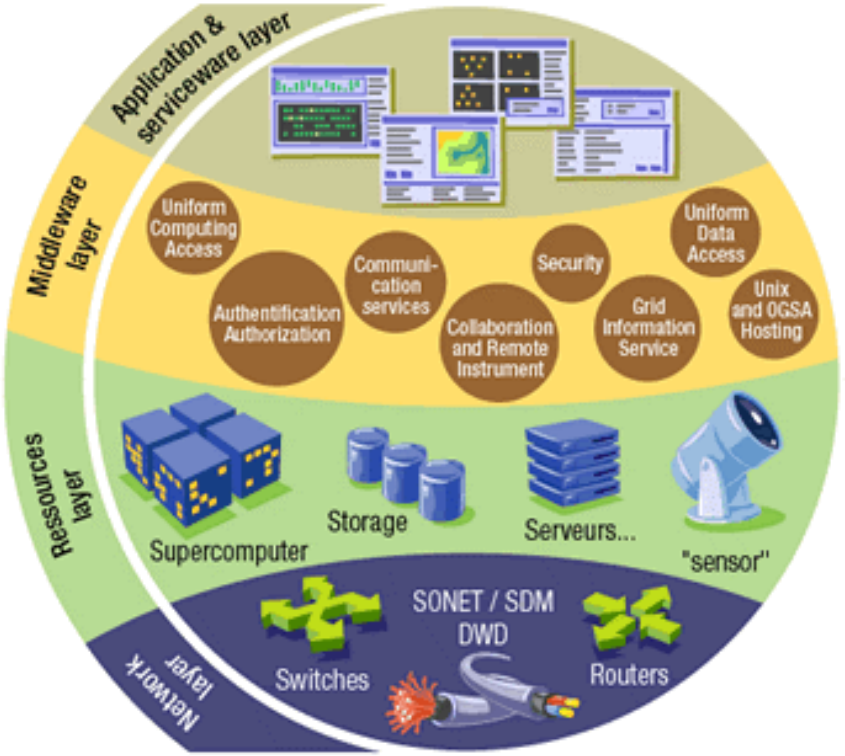



*Figure 1. The components and layers of a GRID structure*

The current SEE-GRID infrastructure consists of 35 GRID clusters with more than 2200 CPUs and 57 TB storage, distributed in 14 countries. A number of applications from diverse end-user

communities are already running on the regional eInfrastructure, as a direct development of two phases of SEE-GRID project and of the various national-level initiatives. Most of these applications are focused on a user community within a single country, with some regional and European collaborations. Within the SEE-GRID-SCI project, applications from three regional Virtual Organizations (VOs) are supported: VO Seismology VO, Meteorology VO and Environmental VO (Karaivanova et all., 2009).

The Bulgarian team is responsible for the development of the environmental applications (Syrakov et al. 2009 a,b, Ganev et al. 2009), some of which will be briefly described below.

## SEE-GRID-SCI AIR QUALITY APPLICATIONS – BASIC MODELS

All the air quality applications are based on the US EPA Model-3 system, which was chosen as a modelling tool because it is one of the most widely used models with proved simulation abilities. In the same time, this is a modelling tool of large flexibility with a range of options and possibilities to be used for different applications/purposes. The system consists of three components:

• meteorological model, used as a pre-processor:
  - MM5 - the 5th generation PSU/NCAR Meso-meteorological Model MM5 (Dudhia, 1993, Grell et al., 1994) or,
  - WRF – version 3.0 of the the Weather Research and Forecasting model (wrfmodel.com), employing the ARW dynamical core (Skamarock et al., 2005).

• CMAQ - the Community Multiscale Air Quality System CMAQ (Byun and Schere, 2006; Byun and Ching, 1999);

• SMOKE - the Sparse Matrix Operator Kernel Emissions Modelling System (Coats and Houyoux, 1996; Houyoux and Vukovich, 1999).

## MULTI-SCALE ATMOSPHERIC COMPOSITION MODELING FOR THE BALKANS

### *Application description and main features*

An attempt will be made in this application to develop and promote a modelling system able to interface the scales of the problem from emissions on the urban scale to their transport and transformation on the local and regional scales. The application aims at developing of an integrated, multi-scale Balkan region oriented modelling system, which would be able to:

- Study the atmospheric pollution transport and transformation processes (accounting also for heterogeneous chemistry and the importance of aerosols for air quality and climate) from urban to local to regional (Balkan) scales;
- Track and characterize the main pathways and processes that lead to atmospheric composition formation in different scales;
- Account for the biosphere-atmosphere exchange as a source and receptor of atmospheric chemical species;

- Provide high quality scientifically robust assessments of the air quality and its origin, thus facilitating formulation of pollution mitigation strategies at national and Balkan level.

***Example of evaluation of country-to-country pollution exchange in the Balkans***

Detailed description of integration domains, input data, model set up and nesting procedures can be seen in Ganev et al., 2008, Prodanova et al., 2008.a. It will be only mentioned here that the NCEP Global Analysis Data with 1°x1° resolution was used as meteorological forcing and the MM5 and CMAQ nesting capabilities were used for downscaling to a horizontal resolution of 10 km over the Balkans.

As far as the aim of this simulation is a country-to-country (CtC) study, i.e. to estimate the influence of pollution emissions of each of the three countries (Bulgaria, Romania and Greece) on the pollution levels of the others, four emission scenarios were prepared: basic scenario with all emission sources (scenario All), scenario with Bulgarian emissions set to zero (noBG), scenario with Romanian emissions set to zero (noRO) and scenario with Greek emissions set to zero (noGR). Such a task requires performing of a large number of model runs, which makes it, like all the sensitivity studies of all kinds, a classic example of grid effective application.

When the effects from high ozone levels were studied, one should look not at the ozone concentrations but on some related quantities – ozone indices, like AOT40C - Accumulated over threshold of 40 ppb in the day-time hours during the period from May 1 to July 31 concentrations), or NOD60 - number of days in which the running

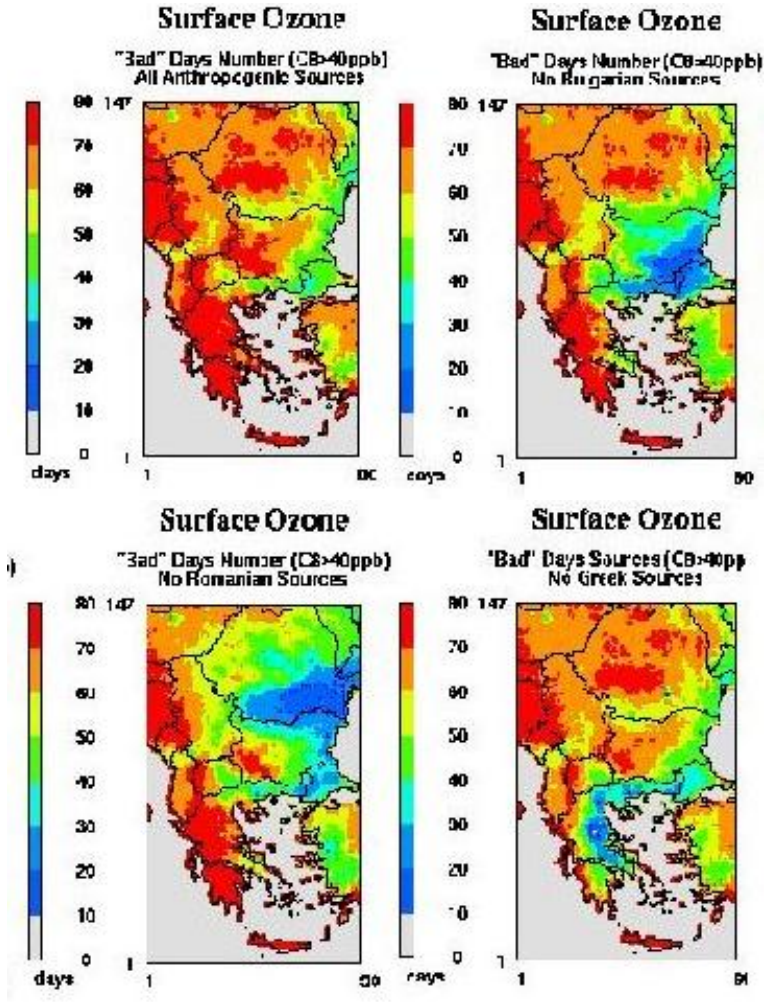



*Figure 2. Number of days with averaged $O_3$ concentration over 40 ppb for May-July 2000*

8-hour average over ozone concentration exceeds at least once the critical value of 60 ppb. If the limit of 60 ppb is exceeded in at least one 8-hour period during a given day, then the day must be classified as "bad".

The calculated NOD60 fields are given in Fig. 2. From the scenario noBG, one can see that switching off Bulgarian sources leads to considerable decrease of this index not only over the territory of the country itself but over the European part of Turkey and the northern Greece. The fact that the NOD60 over Romania is not so much influenced by the elimination of Bulgarian emissions is due to the prevailing NW transport of air masses in the domain. From its side, Romania contribute essentially to the ozone pollution not only in Bulgaria and Moldova but even in Turkey and part of northern Greece, as can be seen from scenario noRo. The last graph in Fig. 2 shows the results of scenario noGR. The exclusion of emissions over the Greek territory decreases the ozone pollution mainly in the country itself. Only European Turkey is influenced to some extent by Greek NOx and VOC pollution.

***Example of local scale simulation – a case of extreme air pollution in the City of Stara Zagora***

The "Maritza-Iztok" TPPs, situated near the city of Stara Zagora, are the main sulphur polluters not only in Bulgaria but in all SE Europe. The total SOx emission from the TPP is about 700 000 tones per year, i.e. about 2000 tones daily. In the summer of 2004 two very high level SO2 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 was described in (Prodanova et al, 2008.b).

As a whole, the calculated SO2 concentration fields have a reasonable behaviour from physical point of view (an example is shown in Fig. 3). At night time, in relatively stable PBL, the pollution released from elevated sources (gases with high temperature and release velocity) keeps aloft, while during the day the fast development of turbulent mixing drains the pollution to the surface at short distance to the stacks, forming well defined plumes with high concentrations.

The calculated concentrations, in spite of the numerous runs with different parameters, do not agree well with the measurements. Wind direction from TPPs to the town of Stara Zagora is simulated each afternoon and the flow forms 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. Here, all difficulties faced when trying to model local scale phenomena in complex conditions emerge. Most probably the main shortcomings come from the MM5 simulations. Several reasons for the ill-simulation can be identified:

- The episode is characterized by weak and unstable winds. The small wind speed makes the use of PBL parameterizations very uncertain.

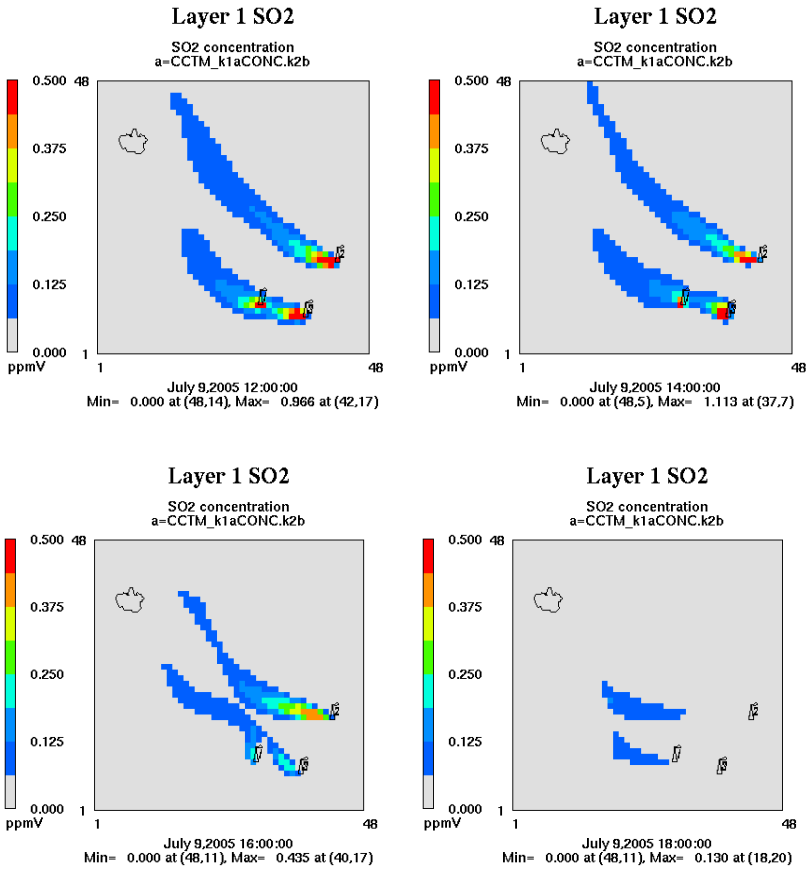



*Figure 3. Evolution of the surface SO2 fields for July 9, 2005*

- The unstable winds can also lead to mis-reproducing of the real variables. The wind direction changes rapidly from almost all directions during a day. As far as the PBL parameterization schemes present stationary state of the PBL, the achievement of which needs some time. When the wind changes its characteristics rapidly there is not enough time for full adaptation and this is an additional source of discrepancies between the simulated and real fields.
- Finally, it is quite possible that the used vertical resolution of MM5 is not enough to accurately reproduce the complex characteristics of the local boundary layer and its evolution.

The applied modeling system is quite complex and needs validation for each region of simulation. Therefore, when important air pollution management decisions are needed, not only *modelling* but measurements of the vertical structure of the atmosphere are crucial at least for short periods.

## MODELING SYSTEM FOR EMERGENCY RESPONCE TO THE RELEASE OF HARMFUL SUBSTANCES IN THE ATMOSPHERE

### *Application description and main features*

Scientific and technical information is critical for helping emergency managers to make sound decisions with regards to response to critical threats. The main features of a dispersion modeling systems that are critical for emergency management needs probably are

adequate, proper and detailed treatment of the underlying surface heterogeneities – topography, land-sea interactions, urban effects. The system should have high enough speed for the "fast decision phase" and at the same time produce accurate enough estimates for the preparedness and recovery phases.

The current application aims at developing of unified Balkan region oriented modeling system for operational response to accidental releases of harmful gases in the atmosphere (as a result of terrorist attack or industrial accident), which would be able to:

- Perform highly accurate and reliable risk analysis and assessment for selected "hot spots";

- At a warning signal from the measuring network, to detect (if not known) the harmful release location and evaluate the nature and the amount of the released harmful gases by using the adjoint functions technique;

Provide the national authorities and the international community with short-term regional scale forecast of the propagation of harmful gases;

- Perform, in an off-line mode, a more detailed and comprehensive analysis of the possible longer-term impacts on the environment and human health in the Balkan region and make the results available to the authorities and the public.

***Example of risk analysis simulations: Instantaneous chlorine release***

The risk analysis in case of accidental harmful gas releases means that a huge number of simulations for near comprehensive set of meteorological conditions have to be performed. The obtained ensemble of outputs will show the spatial distribution of the probability some regulatory threshold value to be exceeded. Knowing this probability distribution may be helpful when short-term emergency response activities (like evacuation, directing medical crews, etc.).

The risk analysis is again a task very suitable for grid computing. The task is in the stage of preparation developing and testing the cluster and grid-mode, so some very preliminary results will be demonstrated.

The monthly averaged concentrations will be demonstrated as an example of the risk assessment function of the system. The simulations are made for the case of accidental release of chlorine in the "VEREJA-HIM" factory in Jambol. The accidental scenario is of an instantaneous release of 25 t of chlorine near the earth surface in 4 o'clock AM. The simulations were made by series of nesting procedures, downscaling to a horizontal resolution of 1 km. Fig. 4 presents the evolution of the averaged for January surface concentrations of atomic Cl.

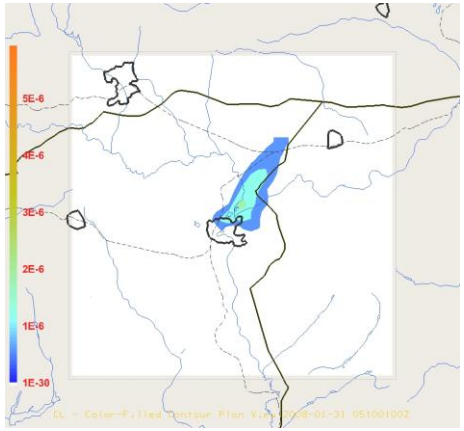
These very preliminary results are a very good illustration of the practical value of the risk analysis simulations – it can be easily seen that during the first 3 hours after the accidental chlorine release

the monthly averaged concentrations along a fraction of one of the main roads is even higher than in the city, hence this road might not be useful for evacuating the people.

## CONCLUSIONS

The examples presented herein show that air pollution modeling tasks are very suitable for grid computing. The grid computing appears to be a very promising and up-to-date technology to be applied for the purpose. It makes it possible to formulate and solve problems that were absolutely unthinkable several years ago. The newly available computer resources allow the simulation of processes and phenomena in greater detail, using much larger spatial and temporal resolution. Multi-scale numerical experiments can be carried out, sensitivity analysis can be performed, ensembles of outputs can be retrieved. The examples given in the current paper demonstrate that a good proficiency in grid computing is already gained by the Bulgarian AQ modeling community.

**Acknowledgements.** The present work is supported by the projects SEE-GRID-SCI - contract № FP7 –RI-211338, NATO SfP N 981393, as well as by the Bulgarian National Science Fund (grants № Д002-161/2008 and Д002-115/2008). Deep gratitude is due to US EPA, US NCEP and EMEP for providing free-of-charge data and software. Special thanks to the Netherlands Organization for Applied Scientific research (TNO) for providing us with the high-resolution European anthropogenic emission inventory.

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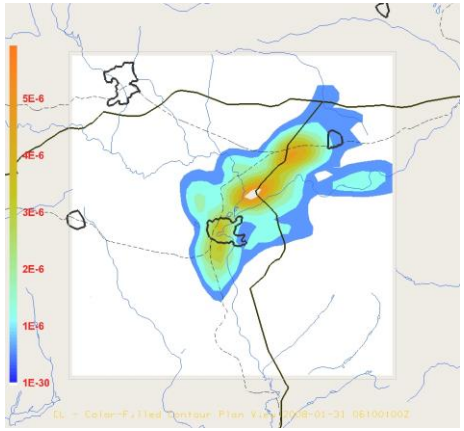


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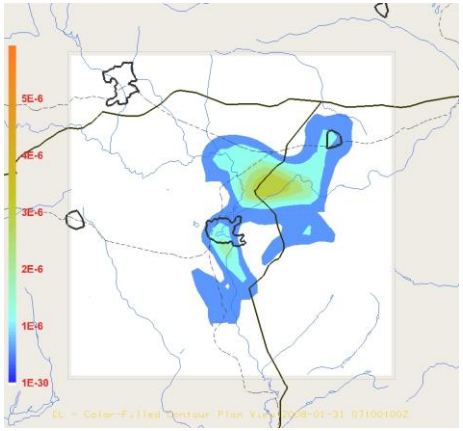
*Figure 4. Evolution of monthly averaged surface Cl concentration [ppmV] from accidental release of 50 t chlorine at 04:00 h, January.*

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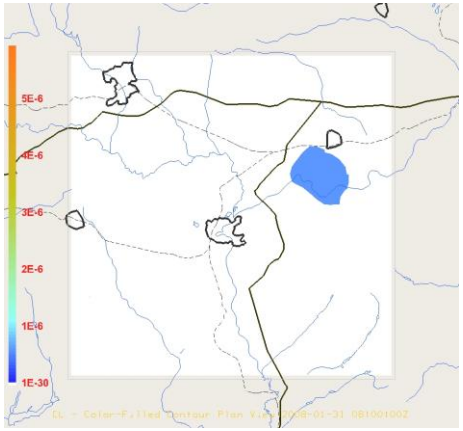


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*Figure 4. Cont.*

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***Jobs and PhD Positions***

**PhD position available starting early 2010 at King's College London**

PhD position available starting early 2010 to be part of the project 'ClearFLo'. The student, to be based at King's College London, will focus on the meteorological dimension of the project. The NERC funded ClearFlo project is concerned with the relations between air quality, human health and meteorology in urban areas. ClearfLo aims to provide integrated measurements of the meteorology, composition and particulate loading of London's urban atmosphere, made at street level and at elevated sites, implemented by modelling, to improve predictive capability for air quality. New measurement capabilities in London will be established, including long-term measurements and intensive observation periods. Analysis and modelling of the measurements will be used to establish key processes.

The PhD student research will focus on the micrometeorology and boundary layer meteorology of London. A wide range of new instruments will be installed at sites in and near London including: eddy covariance towers, large aperture scintillometry, and ceilometers. The student will develop their own research thesis within the scope of the larger project; possibilities include the influence of surface characteristics and flux partitioning on boundary layer development.

The student will join a dynamic, international group of PhD students and post-docs working on urban atmosphere research at King's College London http://www.kcl.ac.uk/schools/sspp/geography/people/acad/grimmond/; http://geography.kcl.ac.uk/micromet/index.htm as well as having close collaboration with colleagues at the University of Reading and a number of other UK universities and research institutes involved in the ClearFLo project.

Student: Strong interest in measurement, data analysis, micrometeorology and/or boundary layer meteorology with experience in one or more of these aspects, and keen to learn about the other areas. Background in meteorology, physics, engineering, physical geography or other relevant areas will be considered. A strong undergraduate and master's degree are essential.

Requirements: student must be eligible for NERC funding (i.e. a UK citizen or resident in the UK for longer than 3 years while not participating in education). Please check the NERC website if you are uncertain about your eligibility.

Application: Please send an email with the following: CV, statement demonstrating appropriate skills and interest (1 page), example of previous research (e.g. Master's thesis, published papers), names of two referees. Indicate when you would be available to start a PhD. Please email: Prof Sue Grimmond (sue.grimmond@kcl.ac.uk)

Closing date: December 7th in the first instance. Applications will be accepted until the position has been filled.

For EU/UK citizens: additional opportunities exist on a project concerned with urban energy, water and carbon exchanges (please

follow the application instructions above but clearly indicate that this is for position 2).

Note for non UK citizens (and UK citizens), there are additional PhD opportunities. KCL funding deadline is 1 February 2010 (note you will need to complete an online PhD application http://www.kcl.ac.uk/schools/sspp/geography/phd/apply.html and funding application http://www.kcl.ac.uk/graduate/funding/funding1011.

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**Research Assistant/Associate in**
**Observing and Modelling Urban Surface – Atmosphere Exchanges**
**Fixed term contact – 18-21 months**
**Geography Department, King's College London**

The post holder will participate in two research projects that involve observations in London (including: eddy covariance, scinitillometry, ceilometer techniques). There will be an opportunity to develop (and/or participate) in research associated with the wide spectrum of activities that are occurring in relation to these projects and the post holders interests. The scope of activities currently occurring can be seen at http://geography.kcl.ac.uk/micromet/index.htm.

We are looking for someone who is experienced with instrumentation setup and operations; highly numerate with science or engineering research experience and programming ability (Fortran, MatLab and/or R). Excellent English (written and spoken) is essential. Experience in one or more of: measuring land-surface atmospheric exchanges, modelling land-surface atmospheric exchanges, atmospheric science, urban climatology, and/or hydrology will be advantageous.

The appointment will be made at the Grade 5-6 scale, £27,946 - £33,917 per annum inclusive of London Allowance, depending on qualifications and experience.

For informal enquires please contact Prof. Sue Grimmond on Sue.Grimmond@kcl.ac.uk or W: http://www.kcl.ac.uk/ip/suegrimmond/index.htm).

Further details and application packs are available on the College's website at www.kcl.ac.uk/jobs, or alternatively by emailing Human Resources at cass-recruitment@kcl.ac.uk. Please quote reference number G5/DAR/270/09 in all correspondence.

The closing date for receipt of applications is 4 January 2010

Equality of opportunity is College policy.

**Full-time Positions for Atmospheric Scientists and Engineers, Sonoma Technology, Inc.**

Sonoma Technology, Inc. (STI) is looking for scientists and engineers to work with our integrated teams of atmospheric scientists, software and environmental engineers, analysts, editors, and technology specialists to provide solutions tailored to meet each of our client's unique needs. We are currently hiring scientists and engineers for our growing Atmospheric Modeling and Emissions team. The work performed by this team includes developing and assessing emission inventories; model development and evaluation; and the application of meteorological models (e.g., MM5 and WRF); and air quality models (e.g., CMAQ, CAMx, and AERMOD) to meet the research, regulatory, and litigation needs of our clients. Positions ranging from entry-level to senior-level are available. A degree in the Physical or Environmental Sciences or Engineering and experience in meteorological, emissions, or air quality modeling are required. Please visit www.sonomatech.com/careeropps.cfm for specific information about our career opportunities.

Situated in Petaluma, California, just 40 miles north of the Golden Gate Bridge, STI's main office is located in the heart of picturesque Sonoma County. Petaluma offers the excitement and culture of the San Francisco Bay Area and the charm and natural beauty of the North Bay (Marin, Sonoma, and Napa Counties). Selected by the North Bay Business Journal as one of the Best Places to Work for the fourth consecutive year, STI is an employee-owned company that has been providing innovative science- and technology-based solutions for our clients' air quality and meteorological needs for 28 years.

We believe that our most valuable resource is our team. We offer a casual but professional work environment, flexibility, a competitive benefits package, and an opportunity to address intellectually challenging environmental issues. We organize a variety of inclusive activities throughout the year and enjoy a balanced and supportive culture. Sonoma Technology, Inc. is an equal opportunity employer. For more information about STI, visit www.sonomatech.com.

## *Future events*

**INTERNATIONAL EVENT ON GREENING EDUCATION**
**Karlsruhe, Germany, October 27-29, 2010**

A three-day International Event on Greening Education will be held from **27th to 29th of October 2010** in the "green" city of Karlsruhe , Germany . This event will take academia, education and environmental policy makers, senior members of academic institutions, representatives of government and non-governmental organisations and international development agencies, teachers and school administrators, sustainable development and environmental management professionals and other stakeholders through the need for greening education and then discuss effective initiatives that can be taken to translate "education for sustainability" in to actions.

Further to the knowledge sharing on greening education including topics such as ecologizing curriculum (incorporating sustainability), greening of courses and creating low carbon education institutions; the upcoming event also provides an excellent networking

opportunity with academia, sustainable development practitioners and other stakeholders in Europe and beyond. An excursion (optional) on Saturday the 30th of October, 2010 is planned which will also provide an additional and informal networking opportunity.

For further information, please see the event details http://www.etechgermany.com/IGEE2010.pdf .

Organizing Committee
International Greening Education Event
Etech Education for Sustainability Initiative
Dürkheimer Str. 24
76187 Karlsruhe, Germany
Tel.: 0049-721- 476 89 16
Fax.: 0049-721- 476 89 53
Email: mail@etechgermany.com

**THE SIXTH INTERNATIONAL SYMPOSIUM ON NON-CO2 GREENHOUSE GASES (NCGG-6), SCIENCE, POLICY AND INTEGRATION, Amsterdam, November 2 – 4, 2011**

Abstracts should be received by **February 1st, 2011**. Notice on acceptance of proposals will be given by May 1st, 2011. Authors of selected papers will be asked to prepare a digital copy not later than September 1st, 2011.

Michela Maione
ACCENT Executive Secretary
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## *Past events*

**INTERNATIONAL SPECIALTY CONFERENCE: LEAPFROGGING OPPORTUNITIES FOR AIR QUALITY IMPROVEMENT**
**Xi'an, Shaanxi Province, China, May 10-14, 2010**

Information at: http://www.dri.edu/leapfrogging-opportunities-for-air-quality-improvement

**EUROPEAN ASSOCIATION FOR THE SCIENCE OF AIR POLLUTION**
**MEMBERSHIP FORM 2010**

Please fill out the details below and return to:
*Carlos Borrego*
*IDAD - Instituto do Ambiente e Desenvolvimento*
*Campus Universitário*
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*E-mail: eurasap@ua.pt*

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