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## Summary report 2003-2005

### **CEREA** **Research and Teaching Center** **in Atmospheric Environment**

Joint Laboratory  
Ecole Nationale des Ponts et Chaussées  
Electricité de France R&D



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## **CEREA**

### **Research and Teaching Center in Atmospheric Environment**

#### **Joint LABORATORY ENPC-EDF R&D**

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## **General presentation**

CEREA was created in 2003 as a research center at Ecole Nationale des Ponts et Chaussées and has become in 2004 a joint laboratory ENPC-EDF R&D, with two locations (ENPC/Champs sur Marne and EDF R&D/Chatou). Its research activities concern the modelling of the atmospheric environment with a special focus on the assessment of environmental impact of transport and energy production (thermal or nuclear). These activities are coupled with the programs of EDF R&D and strongly related to other organizations of the French Ministry for Transport through its Research Directorate.

Other key relationships have been developed for specific applications, with IRSN for radionuclides and with INERIS for impact studies or environmental forecast.

CEREA takes part in the R2D2 network (Research Network for Sustainable Development) promoted by Ile de France region since 2005.

CEREA organizes its modelling activities through four research teams: fluid mechanics and dispersion at local scale, dispersion at regional and continental scales, multiphase modelling, and data assimilation. The data assimilation team is also part of an INRIA project, the CLIME project. A small measurements team is also active in the study of the atmospheric boundary layer, especially for EDF applications.

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## **Research topics**

CEREA develops modelling activities mainly with two numerical models: a comprehensive CFD (Computational Fluid Dynamics) tool, Mercure\_Saturne, for small scale dispersion (urban pollution, industrial risk), and a modelling platform, Polyphemus. Polyphemus includes different models from local scale (Gaussian and puff models) to regional and continental scales (the Chemistry-Transport Model Polair3D). Some appropriate physical parameterizations and multiphase reactive box models are developed and plugged in these three-dimensional models.

The resulting models are compared to measured data and used for impact studies or environmental forecast. In this framework, the research actions devoted to data assimilation (coupling between model outputs and measurements) aim at improving the ability of models to make good forecasts and/or perform inverse modelling of pollutants.

Apart from modelling, the measurements team is implied in several campaigns in order to improve the knowledge of the atmospheric boundary layer

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## Research Groups

### Local scale and fluid mechanics

(Group leader: Bertrand Carissimo)

The research actions are related to the preoccupations of the French Ministry for Transport (urban pollution) and those of EDF (dispersion at an industrial site). They mainly rely on the development of an integrated numerical model, *Mercure\_Saturne* (EDF). This code is based on a general purpose CFD tool, *Code\_Saturne*. In this framework, the team adapts or develops parameterisations suitable for the atmospheric environment (urban canopy parameterisations, transport equation for concentration fluctuations, microphysical cloud scheme, atmospheric radiative scheme, chemistry model, aerosols model...).

2003 has been a transition year for the model *Mercure*. The solver, which was initially based on the numerical kernel *ESTET*, a code based on a structured grid approach, moved toward a new kernel named *Code\_Saturne* based on an unstructured grid approach. The resulting modifications are important, especially for the atmospheric parameterisations that need to be adapted to the new code structure. The unstructured grid has many advantages (it is easier to take into account complex geometries for instance) but also some drawbacks: for example it is more complex to develop parameterisations in the unstructured environment and all the existing post processing facilities has to be replaced by new procedures.

In 2004, two key functionalities have been added to *Mercure*. The first one is the ability to take into account chemical reactions; the second one is the microphysical description of water.

In 2005, in addition to further development of the above functionalities, the transport equation for fluctuations of concentration has been tested. The aerosol modelling already developed for *POLAIR3D* has been adapted for small scales and coupled in *Mercure*. A new activity has also been started in the area of wind energy with the accurate modelling of wind field in complex terrain.

There is finally a strong link of this modelling activity with the measurements team at *CEREA* for the observation of the atmospheric boundary layer with appropriate means (sodar, anemometers, UHF radar, sonic mast).

#### *Cloud scheme for cooling tower plume and fog*

A detailed microphysical parameterization for water has first been developed in *Mercure* (PhD work of Emmanuel Bouzereau, defended in December 2004) for the simulation of cooling tower plumes. This parameterization describes the liquid water content in clouds and in rains. The size distribution of droplets is also predicted.

This parameterization has been extensively validated by a detailed comparison with data from the field campaign around the aerorefrigerant tower of Bugey (in the 1980s). A second application is the simulation of orographic precipitations with data available in the literature. This work was performed with the former version of *Mercure* and the transition to the new unstructured version has been done as an additional task.

The warm cloud microphysical scheme previously developed for the simulation of cooling tower plumes has then been successfully applied to a first case of fog development and dissipation observed at the Cabauw tower. These first simulations have been performed in one dimension and show that the scheme introduced, that can also predict the droplet distribution, is suitable for both applications. Three dimensional simulations and comparisons with the future campaign *PARISFOG* in the autumn of 2006 are also planned.

#### *Dispersion in urban environment*

These topics are developed through a PhD work (Maya Milliez, to be defended end 2006) that aims at simulating the dispersion in an atmospheric environment with obstacles. A first part has been finished with the simulation of an experiment (the Mock Urban Setting Test (MUST) experiment in the USA). An array of shipping containers (12 rows by 10 columns) was representing an idealized urban quarter. A special unstructured grid has been set up to simulate these 120 buildings with a still reasonable grid of around one million grid cells. The results obtained with *Mercure\_Saturne*

have been compared to the available observational data for several days and good comparison statistics have been obtained.

An original part of this work has been the ability to simulate fluctuations of concentrations through an additional Eulerian transport equation for the variance of concentration which also compares reasonably well with the observations of MUST.

In the course of this work, some tools for handling unstructured meshes have been developed.

The last part of this PhD work is devoted to the simulation of thermal and radiative effects in complex geometries of the urban canopy in order to take into account both the solar and infrared radiations in a complex geometry (buildings and street canyons). It is derived from numerical techniques used for combustion and adapted for atmospheric applications. We have compared the results to simple experiments and existing measurements giving the variation of albedo as a function of solar zenith angle.

#### *Dispersion around industrial site*

In the PhD work of Emmanuel Demael the first objective was to compare Mercure with models which are classically used for these applications (Gaussian plume models). The differences have been quantified and explained, in particular for the behaviour very near the source. The work has then followed with the simulation of two actual industrial sites, including buildings and topography, for which the mesh and simulation domain have been constructed.

One of these sites is in the center of France with moderate topography; the other one is on the coast of Normandy and constructed on the foot of a cliff and therefore in very complex topography. For these industrial sites very detailed wind tunnel measurements are also available and are used for the comparison for both the dynamical fields (wind and turbulence) but also dispersion fields (concentration and fluctuations).

A number of sensitivity studies have already been performed. A rigorous uncertainty analysis on the simulation results is also one of the objectives of the work (to be used for impact studies of actual industrial sites).

#### *Wind potential estimates*

In this area, current studies use very simple linearized models that have shown several limitations. Our goal in this area is first to improve the estimates currently obtained. The very simple models fail in complex terrain and along the coast where local circulations induced by the thermal contrast can develop.

An additional objective of this work is to quantify the effect of "mask" found in very large wind farms when a large set of wind mills modifies the local flow and can reduce the energy potential. This work has started in 2005 and is performed by introducing this masking effect in Mercure by ways of a drag within the flow (PhD work of Laurent Laporte). Results in two dimensions have already been obtained. The classical case of the Askervein hill has also been carried out to check the modelling results.

#### *Small scale reactive dispersion*

A chemical mechanism describing the fastest atmospheric chemical reactions has been coupled to MERCURE, (NO/NO<sub>2</sub> conversion just after emission). This reactive version of MERCURE has been compared to data measured in a Copenhagen street (the Jagtvej Street). This data base has already been used for box models. The results (a common work of S. Lacour, E. Colin and B. Carissimo) prove that the reactive version of MERCURE leads to a better estimation of chemical concentrations when the chemical regime is standard.

Spatial average concentrations in a street canyon were found to be next windward levels. The NO<sub>2</sub> roof fluxes is very sensitive to ozone background concentrations. The MERCURE reactive version is now used to study the efficiency of new building materials proposed to reduce NO<sub>x</sub> pollution near busy streets.

#### *Estimation of pollution induced by tunnels*

A project has been initiated with CETU to estimate the pollution induced by tunnels (Stéphanie Lacour). Flow velocity inside a tunnel fluctuates due the unsteady forces exerted by the vehicular flux. An item of the CETU project was to give an estimate of the effect on outside concentrations related to the unsteadiness boundary condition at the tunnel portal. Periodical boundary conditions at the tunnel exit have been established to take into account heavy duty vehicles passing through

the tunnel portal. These have been used in a MERCURE simulation of the dispersion of pollutant around a tunnel.

The reactive version of MERCURE has also been used in order to describe the impact of a tunnel plume. Comparison between passive and reactive dispersion under various pollution situations were made in order to estimate the impact on the NO<sub>2</sub> concentrations. NO<sub>2</sub> is systematically underestimated in the case of a passive dispersion, especially when ozone concentration is high. The gap between reactive and passive concentrations is less pronounced when ozone concentration is low. Box models were employed to give rough estimates of NO<sub>2</sub> concentrations around tunnel portal. Results have been used in the user's guide of air pollution study for tunnels written by the CETU.

An alternative approach, based on a short-range version of Polair3D, has been developed for impact studies of roads and tunnels. A classification of pollution has been proposed in order to distinguish the "background" component and the "local" component. Some strategies have been proposed in order to simulate the long-term impact of such infrastructures. Artificial measurements were elaborated with a gaussian model that simulates the dispersion around a tunnel portal with noisy and variable series of meteorological/emission inputs. The yearly concentrations and its variability are computed from these results at different locations around the pollutant source. It is shown that a large amount of simulations is required to discriminate pollution levels on an annual basis at the different locations.

#### *Estimation of pollution near a road in an urban area*

Impact studies for roads focus on the effects of traffic but few data are available for emissions from road works. A road repairing has occurred in 2002 near a traffic air quality monitoring station in northern France (Dunkerque). Data on vehicle flows and work schedule and devices have been put together with atmospheric data (concentrations and meteorological parameters) collected by the local monitoring network in order to build a database. In collaboration with LCPC, some quantitative elements about the atmospheric pollution related to conventional species around a road work place were extracted from this database. Non-parametric regressions were used to select the data suitable for linking air concentrations to emission. A dispersion model was used to find out the maximal impact on concentrations measured at sensor. Road works contributions are found weak and are discussed in terms of representativeness and reliability. A project is being built to analyse the impact of the new management scheme on this site after works and to better explain the links between traffic and concentration, in particular during nights.

#### *Indoor Air Quality*

In 2004 a collaboration with CSTB has been led for indoor air quality modelling. A simple box model has been developed in order to describe the indoor/outdoor transfer, indoor chemical reactions and deposition. The model outputs have been compared to data measured in a flat (in the Paris suburb). The results validate the model and indoor deposition velocities have been proposed.

### **Multiphase modelling**

(Group leader: Karine Kata-Sartelet)

The activity of the group is focused on the development and the validation of two multiphase models that are coupled to the three dimensional host models Polair3D and Mercure\_Saturne. The two multiphase models mostly differ in the discretization of the size distribution of aerosols: log-normal distribution for MAM (Modal Aerosol Model) and size-resolved distribution for SIREAM (Size Resolved Aerosol Model).

#### *PAM project*

The main part of the model development has been performed in the framework of the PAM project (Multiphase Air Pollution), funded by the French research program Primequal/Predit (2001-2006) and led by Bruno Sportisse. Apart the modelling activities at CERE, the PAM project has taken part in the LISAIR Campaign at Paris (led by Partick Chazette, LSCE).

The development of the models MAM (Karine Sartelet) and SIREAM (Edouard Debry and Bruno Sportisse) has first focused on the General Dynamics Equation (GDE) for aerosols, which describes

the time evolution of the aerosol distribution in a box under nucleation, condensation/evaporation and brownian coagulation. The aerosol size distribution is made of four log-normal modes in MAM and of a specified number of sections in SIREAM, with diameters typically ranging from 0.01 $\mu\text{m}$  to 10 $\mu\text{m}$ . The assumption of internal mixing is made (to each size corresponds a unique chemical composition). The species are inorganic (on the basis of the thermodynamic models ISORROPIA or EQSAM: sodium, ammonium, sulfate, nitrate and chloride), organic (primary organic aerosols and parameterized representation of Secondary Organic Aerosols with two-product formulations), inert (mineral dust and Black Carbon) and water. Parameterizations are used to model binary nucleation (sulfuric acid and water) and ternary nucleation (sulfuric acid, ammonia and water).

Many appropriate algorithms have been developed and/or used for the numerical simulation of the GDE, ranging from stochastic mass flux methods to lagrangian methods, collocation or variational formulations (Edouard Debry and Bruno Sportisse). Specific mode merging and splitting have been developed in MAM to force modes to be of distinct size ranges throughout the simulations (Karine Sartelet and Bastien Albriet). New algorithms have been proposed for the redistribution of aerosol lagrangian bins on a fixed grid (Edouard Debry, Marilyne Tombette, and Bruno Sportisse).

#### *Hybrid approaches for condensation/evaporation*

Condensation/evaporation is a key process for the aerosol composition and distribution. Gaseous species may condense onto existing aerosols, or species in the aerosol phase may evaporate. This mass transfer between the aerosol and the gaseous phases depends on the difference of concentrations of gaseous species far from aerosols and the concentrations of gaseous species at the surface of aerosols (which are assumed to be at local thermodynamic equilibrium with the aerosol internal composition). Mass transfer can be computed dynamically, or by assuming thermodynamic equilibrium between the gaseous species far from aerosols and the internal aerosol composition. As dynamical mass transfer requires a lot of computing time compared to thermodynamic equilibrium and as the assumption of thermodynamic equilibrium may not be accurate for large aerosols, a hybrid approach has also been developed: thermodynamic equilibrium is assumed for small size aerosols and dynamic mass transfer is computed for large aerosols (Edouard Debry and Bruno Sportisse).

#### *Aqueous-phase chemistry and heterogeneous reactions*

Further developments have concerned the aqueous phase of aerosols by adapting the cloud model VSRM (Variable Size-Resolved Model, Carnegie Mellon University; Kathleen Fahey, Marilyne Tombette and Bruno Sportisse). This work is a follow-up of works devoted to the numerical modelling of aqueous-phase chemistry (Rafik Djouad and Bruno Sportisse). Inorganic heterogeneous reactions at the surface of aerosols have also been studied (Marilyne Tombette). They may have a significant impact on gaseous photochemistry and particles, especially for nitrate.

#### *3D parameterizations for aerosol modelling*

To couple the 3D chemistry transport model Polair3D to the multiphase models SIREAM and MAM, other processes have been taken into account, such as dry deposition, below-cloud scavenging, the influence of the acidity of clouds for below-cloud scavenging, in-cloud scavenging and the treatment of emissions (Kathleen Fahey and Karine Sartelet). Sea-salt emissions have been parameterized with specific approaches (Karine Sartelet). The aerosol water content, which is used to compute the aerosol wet diameters, has been parameterized using an updated Gerber scheme (Edouard Debry). Specific works have been devoted to the parameterization of in-cloud and below-cloud scavenging for gases (Bruno Sportisse).

#### *Validation at regional/continental scales*

The 3D chemistry transport model Polair3D, coupled to SIREAM, has been validated by comparison to data at continental scale over Europe (Kathleen Fahey, Edouard Debry, Karine Kata-Sartelet, Yelva Roustan, Marilyne Tombette), over Asia (Karine Kata-Sartelet) in the framework of the MICS project, at regional scale over Greater Paris (Marilyne Tombette), over Marseille in the framework of the ESCOMPTE campaign (Mohammad Taghavi, Karine Kata-Sartelet) and over Lille (Rémy Lagache). Polair3D-MAM has been validated by comparison to data at regional scale over Tokyo (Karine Kata-Sartelet).

Studies to assess the sensitivity of aerosol concentrations to different physical processes (coagulation, mass transfer, sea-salt emissions, aqueous chemistry and heterogeneous reactions)

were performed over Asia in the framework of the MICS project, over Europe and at the regional scale over Paris.

#### *The MICS project*

At continental scale over Asia, Polair3D-SIREAM participated, thanks to a collaboration with CRIEPI (Central Research Institute of Electric Power Industry), to the phase 2 of MICS (Model InterComparison Study) Asia. Eight teams participated to MICS Asia phase II, which aimed at having a common understanding of model performance and uncertainties in Asia. The study focused on transport and deposition of sulfur, nitrogen compounds, ozone and aerosols in East Asia for March, July, December 2001 and March 2002. A comprehensive sensitivity analysis has also been performed (Karine Sartelet).

#### *Local scale*

At local scale, Polair3D-MAM is used to simulate aerosol formation and dispersion in the vicinity of roads (Bastien Albriet, Stéphanie Lacour, and Karine Kata-Sartelet). Traffic emission leads to high concentrations of sulphuric acid and to high nucleation events (ultra-fine particles of diameter around 1nm composed of H<sub>2</sub>SO<sub>4</sub>-NH<sub>3</sub>-H<sub>2</sub>O). Several measurement campaigns have put in evidence the rapid growth of the aerosol diameter close to a traffic source. Polair3D-MAM is used to try to reproduce the quick growth of these ultra-fine particles, and to identify the mechanism(s) responsible for this growth, e.g. condensation, coagulation, heterogeneous reactions of organic/inorganic species. MAM is also coupled to the model MERCURE-SATURNE for a more detailed study.

#### *Resuspension*

In the framework of a project with CEA (Commissariat à l'Energie Atomique), models of aerosol resuspension have been studied (Stéphanie Lacour). This preliminary work leads to a synthesis of available models, parametrisations and measured data to be used by the IAEA (International Atomic Energy Agency) for its Handbooks. The work continues with the development of a model of deposition and resuspension at small scales.

#### *Aircraft soot*

A joint project with ONERA has been retained by the French Research Program Primequal/Predit devoted to the measurement and the modelling of aircraft soot. CEREAs is involved in the modelling part of the project, which should begin in late 2006.

### **Modelling at regional and continental scales**

(Group leader: Vivien Mallet)

The team focuses on air quality modelling from regional to continental scales. The applications are photochemistry (ozone), heavy metals (like mercury or lead) and radionuclides. The activities range from process studies to forecast and impact studies.

These activities now rely on a new and comprehensive modelling system, the Polyphemus platform, which hosts the Chemistry-Transport Model of CEREAs, Polair3D.

Many joint projects with other teams have been initiated with this modelling system, from forecast of radionuclides (with IRSN, France) or photochemistry (INERIS, France, or Meteo-Chile) to impact studies (with EDF Polska; with the University of Stuttgart, IER, for Cost-Benefit analysis in the framework of the European project NEEDS).

#### *Development of the Polyphemus platform*

A new modelling system has been developed, through the work of Vivien Mallet and Denis Quélo: the Polyphemus (<http://www.enpc.fr/cerea/polyphemus/>) platform, a multi-function and multi-scale modular system for atmospheric modelling.

The new approach with Polyphemus is to split the modelling system into 4 distinct levels:

- Physical parameterizations and preprocessing with the object-oriented AtmoData library (potentially shared with any team involved in atmospheric modelling, whatever the model is);
- High-level drivers of models seen as black boxes (for data assimilation, for coupling, for Monte Carlo simulations, for ensemble runs);
- Numerical models as such (for instance Polair3D but also gaussian and puff models);
- Postprocessing facilities, for instance for statistics and model-to-data comparisons, through the Python library AtmoPy.

One advantage of this structure is the possibility to have a multi-modelling approach through the available parameterizations. This system has been used for numerous applications (listed below), implying a growing number of teams in joint projects.

#### *Air quality ensemble forecast*

Due to the wide range of uncertainties, a promising approach for air quality forecast is related to ensemble techniques. The PhD work of Vivien Mallet (defended in December 2005) has focused on the assessment of the a priori uncertainties in the outputs of a Chemistry-Transport Model through Monte-Carlo methods and a multi-modelling approach in the Polyphemus platform. The next step is to improve the forecast through an appropriate combination of the available models (up to 50 configurations with the Polyphemus platform). This work is also connected to data assimilation activities.

Moreover, the coupling to the Prev'air platform of INERIS has been achieved (Hervé Njomgang, Christelle Bordas and Vivien Mallet) and the computation of an extensive set of model-to data statistics has been initiated (Christelle Bordas and Vivien Mallet). The Polyphemus platform begins an operational test from July 1<sup>st</sup>, 2006, on the Prev'air platform for photochemical forecast.

#### *Mercury and heavy metals*

These works have been done in the framework of the PhD thesis of Yelva Roustan (defended in December 2005).

The development of the mercury model has been completed with two available models (a simple one based on the so-called Petersen formulation and a model based on a gas/phase-aqueous/phase chemical mechanism). Model-to-data comparisons have been performed for year 2001 over Europe. Moreover, an innovative sensitivity analysis has been developed (see section devoted to Data Assimilation) and inverse modelling with respect to boundary conditions has been performed. Another model version has been developed with the coupling to the gas-phase mechanism RACM, which has shown that only a slight impact was obtained on observed concentrations (total gaseous mercury). Meanwhile oxidized gaseous species, and therefore deposition fluxes, may be significantly affected.

For lead and cadmium, two advanced approaches have been considered. The first one consists in representing the aerosol size distribution with several diameters rather than with a simple mass mean diameter. The second one is to add lead and cadmium as "inert" heavy metals in the size resolved aerosol module of Polair3D (SIREAM). An intercomparison and model-to-data comparisons have been performed.

#### *Air Quality Modelling over Lille*

CEREA has taken part in a research project supported by the PREDIT program in order to assess the health impact of the Lille Urban Mobility Plan for year 2015 (R.Lagache and D.Quélo). An integrated modelling chain has been built by coupling a traffic model (EMME2), an emission model, Polyphemus for the reactive dispersion (photochemistry and Particulate Matter) and indicators of health impacts. The dispersion model has been validated over year 1998 by model-to-observation comparisons with good results.



### *Impact studies at continental scale*

A work has assessed the sensitivity of ozone concentrations with respect to emissions (Vivien Mallet and Bruno Sportisse). The sensitivity study concerned the temporal, spatial and chemical features of NO<sub>x</sub> and COVs emissions.

CEREA is also implied in the European project NEEDS, devoted to Cost-Benefit Analysis. The objective is to compute transfer matrices to be used for Cost-Benefit Analysis. The project has begun (Yelva Roustan) and should allow joint works with EMEP/West and IER Stuttgart. A follow-up of NEEDS (HEIMTSA) has been retained in FP6 and should begin in early 2007.

Moreover, Polyphemus is used by EDF Polska and by the consortium of associated Polish Universities. The objective is to assess air quality in Poska and the related transboundary fluxes.

### *Dispersion of radionuclides*

An important application of Polyphemus is the forecast of the dispersion of radionuclides. This work is done in a joint project with the Emergency Center of IRSN scales. Polyphemus is the support of the future operational forecast system at IRSN (autumn 2006) for the regional scale.

An extensive work (Denis Quélo and Bruno Sportisse) has been devoted in 2005 and 2006 to the simulation of the Chernobyl accident. A sensitivity analysis has been performed with respect to the parameterizations (including MM5 meteorological parameterizations) in order to investigate the sensitivity of wet and dry scavenging (key processes for this kind of simulations). Other applications have concerned the simulations of the ETEX exercise and of the Algeciras accident (Monika Krysta and Marc Bocquet).

### *Escompte*

Mohammad Taghavi has taken part in the model intercomparison study ESCOMPTE, with a focus on ozone modelling for Intensive Observation Periods 2a and 2b (21-26 June 2001).

For the Thermal Mission of EDF Branch Energy, a dedicated study has been realized in order to estimate the impact of Martigues Power plant on particulate matter over the Marseille-Berre area. This work is a follow-up of a study devoted to ozone.

### *Multi-media modelling*

Impact of air quality pollutants on human health is a new field of application of our modelling system focused on thermal power plant impact. In this domain, a work (PhD thesis of Solen Quéguiner) has begun by coupling the outputs of Polair3D for lead and cadmium (air concentration and ground deposition) with the ground transfer model OURSON developed at LNHE Department of EDF R&D. This OURSON model allows to follow pollution in the ecosystems, the cultures and hydrological network in order to estimate doses for human beings.

This work now focuses on the development of a model devoted to Persistent Organic Pollutants (POP) in Polyphemus/Polair3D.

### *Hemispheric modelling*

In order to simulate long-lived species (such as mercury) and to take into account the impact of other anthropogenic sources of emissions in the northern hemisphere, the development of a prototype hemispheric version of Polair3D has been initiated (Denis Wendum). This is based on particularly simple modifications of the limited area model.

### *Plume-In-Grid models*

Polyphemus now hosts two Gaussian models (stationary model and puff model), that are currently developed and used for the local scale (Irène Korsakissok, Hadjira Schmitt-Foudhil, Vivien Mallet), and should be the basis of plume-in-grid abilities in Polyphemus. These works are applied to risk modelling in joint projects with DGA and INERIS for biological tracers and aerosols.

## **Inverse modelling / Data assimilation**

(Group leader: Marc Bocquet)

This group is also part of an INRIA/ENPC project, CLIME, devoted to data assimilation and modelling systems for environmental applications. This project has been approved by the project committee of INRIA in December 2003.

A subsequent action of CLIME, the ADOQUA (Data Assimilation for Air Quality) cooperative action from INRIA, has been accepted. ADOQUA promotes scientific exchange between three projects CLIME (INRIA/ENPC), ASPI (INRIA) and IDOPT (INRIA).

### *Inverse modelling of emissions for passive tracers [2003-]*

The dispersion of a passive tracer is described by a linear advection-diffusion equation. The objective is then to retrieve the emissions on the basis of observational data and a numerical model for the dispersion. Thanks to the linear nature of the underlying equations, this can be performed with adjoint solutions called retroplumes.

If the source is a point-wise source, the simplex method can be used. The problem is more complicated for diffuse emissions. A geometric interpretation of the retroplumes has been proposed by Jean-Pierre Issartel and applied to the retrieval of arsenic emissions in Chile (joint project with Laura Gallardo Klenner, CMM Chile) [Issartel].

Moreover, some new approaches have been proposed for inverse modelling of passive tracers, using the maximum entropy principle. A key advantage (among others) is the way the a priori knowledge is taken into account. They can be applied to accidental releases (for instance to the ETEX campaign) [Bocquet]. This approach also includes variational techniques such as 4D-Var PSAS. In this latter case, it was shown to be equivalent to a projection onto the basis of retroplumes.

Another work is devoted to the assessment of the influence of grid resolution in the framework of inverse problems with entropy regularization [Bocquet]. The singular points near sources are then explained. The existence of an optimal resolution has been proved and an indicator of the inverse modelling procedure has been proposed. The method is now being tested on real data (ETEX-1).

### *Short-range inverse modelling [2003-2006]*

CEREA is implied in a joint project with IRSN devoted to Inverse Modelling of an Accidental Release in the atmosphere (MIRA). A preliminary work has been led in 2004-2005 with twin experiments [Quélo, Sportisse]. Some experiments have been carried out in order to invert parameters related to the emission of a point source or physical parameters for turbulent dispersion (PhD work of Monika Krysta). A variational approach has been applied to a puff model with a set of data obtained in the wind tunnel of École Centrale de Lyon (with a reduced representation of the Bugey power plant). The evaluation of the monitoring network has also been carried out with cross validation techniques [Krysta, Bocquet and Sportisse].

### *Inverse modelling of radionuclides at regional scale [2004-2006]*

First experiments in inverse modelling of radionuclides at regional scale have been investigated using both synthetic and real data. This is a test application for the Maximum Entropy on the Mean [MEM] techniques, with a physics involving removal processes. New objective functions specifically designed for localised sources have been derived analytically and tested numerically on two hypothetical accidents in Europe. The methods are then applied to the Algeciras radioactivity release incident. The temporal inversion leads to satisfying results while a reasonable 3D reconstruction is proven to be impossible with the available data [Krysta, Bocquet].

### *Inverse modelling of ozone precursors using variational assimilation [2004-2005]*

The use of 4D-Var techniques requires the development of the adjoint model of Polair3D [Quélo]. An application is the inverse modelling of NO<sub>x</sub> emissions at regional scale.

The emissions fluxes represent one of the main uncertainties in Chemistry-Transport Models. These uncertainties are mainly related to the time distribution. A work has been performed over the Lille region (May 1998) on the basis of observational data for ozone and NO<sub>x</sub>. The control parameters are hourly coefficients applied to emissions of NO<sub>x</sub>. The forecast of ozone and NO<sub>x</sub> with the

improved emission fluxes is significantly improved for the learning week and for the next two weeks after the learning period [Quélo, Mallet and Sportisse].

#### *Sensitivity analysis of mercury over Europe [2004-2006]*

Elemental mercury is a long-lived species (with a timescale of one year). It is therefore relevant to perform a sensitivity analysis with respect to lateral boundary conditions for a simulation at continental scale. Adjoint methods have been used in order to quantify the sensitivity of observational data of mercury over Europe with respect to emissions, initial conditions and boundary conditions. The technique was applied to both a simplified chemistry based on the Petersen scheme, and a more complex chemistry scheme developed by Yelva Roustan in his PhD thesis [Roustan, Bocquet].

#### *Inverse modelling of mercury over Europe [2004-2006]*

The tools which have been developed for the sensitivity analysis may also be used to perform the inverse modelling of mercury. It was used to invert some of the boundary conditions, in particular the northern border, sensitive to the mercury depletion event. Also it is shown that with the present EMEP network, not enough data are available to invert emissions parameters [Roustan, Bocquet].

#### *Comparison of sequential and variational methods in Air Quality [2006-]*

German Torrès has achieved his postdoctoral fellowship devoted to air quality forecast over Berlin (in collaboration with GMD First, Berlin). A Reduced Rank Square Root Filter and an Ensemble Kalman Filter have been developed and some preliminary applications to an academic case have been performed.

A work in progress is to implement both variational (4D var) and sequential (EnKF) data assimilation techniques in the Polyphemus system using the CTM Polair3D, and compare the merits of both approaches. A secondary aim is to study the impact of non-linearities in air quality data assimilation (main topic of ADOQUA) [Wu, Mallet, Bocquet, Sportisse].

#### *Ensemble methods for air quality forecast [2004-]*

Ensemble methods for air quality forecast [Mallet, Sportisse] which explores learning strategies for a better forecast is the natural outcome of Vivien Mallet' Phd Thesis.

The main idea is to combine members of ensemble forecasts in some optimal sense. A weight is associated to each member of the ensemble so that the weighted linear combination of model outputs may be closer to observations. Weights are forecast on the basis of past observations and past model forecasts. They may minimize the variance of the error over a learning period (superensemble), or they may be estimated with machine learning algorithms which provide an advanced mathematical framework. Significant error decrease, compared to the best model in the ensemble, is found.

#### *Network design for atmospheric dispersion [2006-]*

A research project in network design for air quality has started in January 2006 with the PhD work of Rachid Abida under the supervision of Marc Bocquet (ENPC/IRSN support). In parallel Nikki Vercauteren, and then Olivia Coindreau, will help IRSN define its future aerosol station network for the evaluation of an accidental radionuclides release in France [Vercauteren, Bocquet]. A similar project is also led in a joint project with DGA (2006-). The objective is to apply network design approaches at local and regional scales over a battle field [Korssakissok, Mallet and Sportisse].

#### *Reduced models and propagation of uncertainties [2002-2004]*

The use of data assimilation methods for large-dimensional systems such as those involved in Chemistry-Transport models may require the search for reduced models. Many approaches have been developed and benchmarked: among them, one can cite a singular perturbation technique based on multiscale reduction, reduced Monte-Carlo techniques (DEMM), expansion in chaos polynomial, High Dimensional Model Representation (HDMR) or Proper Orthogonal Decomposition [Boutahar, Sportisse].

## **Meteorological Measurements**

(Group leader: Eric Dupont)

This activity has been existing at EDF-R&D for many years and has been integrated in CEREА at the beginning of 2005. The observational actions are related to the needs of EDF in the fields of atmospheric dispersion at an industrial or urban site, and wind energy resource assessment, in close link with the "local scale and fluid mechanics" activity. The field campaigns are devoted primarily to the tests of instruments, especially wind profilers (sodar, UHF radar), and to the constitution of data bases for numerical simulations in the fields mentioned above. This activity stands on 2,5 people.

A key point is the growing partnership with the IPSL observational site (SIRTA)

### *Sodars intercomparison*

2005 has been dominated by a campaign of intercomparison for sodars. The goal was to evaluate the quality of measurements and the acoustic disturbance of several commercialised sodars, to select an instrument for wind and turbulence measurements both on the French Nuclear Power Plants, and on wind energy production sites. The campaign site was located in Beauce region. It is very flat and opened, and thus well adapted to intercomparisons. Four sodars have been compared during 2 months to a 80 m height mast instrumented with cup and sonic anemometers, and to a reference sodar which has been extensively evaluated in the past. The analysis of the data is currently on the way, in terms of statistical differences on wind and standard deviation of the vertical velocity. This analyses also aims at investigating if sodars can improve the characterisation of wind and turbulence conditions on a wind energy production site, especially by avoiding the vertical extrapolation (generally with a power law) used to derive the wind at hub height.

### *Tests of a UHF radar and derivation of turbulent parameters*

A Degréane UHF radar has been extensively tested for several years in collaboration with the Centre de Recherches Atmosphériques at Lannemezan plateau. It is well known that ground clutter and problem of commutation between emission and reception prevent UHF radar from giving good quality measurements in the first two hundred meters of the atmosphere. During 2005, a campaign has been initiated in order to test some important modifications performed by Degréane on the emitted pulse and on the receiver. The data of this campaign have shown that the comparison between the first level of UHF radar (85 m) and a sonic anemometer are now very similar to those obtained from a comparison between our reference sodar and the same sonic anemometer. Moreover, the use of the spectral width of the meteorological peak allows to determine some turbulent parameters as the dissipation rate of kinetic energy. The comparison of the spectral width on the vertical beam with the standard deviation of vertical velocity measured by a sonic anemometer shows a good agreement during daytime, but large differences during night time.

### *Campaign for acoustic propagation*

A campaign of simultaneous meteorological and acoustic measurements has been organised by EDF-R&D and LCPC (Laboratoire Central des Ponts et Chaussées). CEREА was in charge of wind and temperature measurements on a 60 m height mast. These measurements are currently analysed by another department of EDF-R&D and will lead to a detailed study of the influence of meteorological parameters in the surface layer on the acoustic propagation.

### *Collaboration with IPSL (Institut Pierre Simon Laplace)*

In the framework of a collaboration with the IPSL Institute, the meteorological instruments are going to be installed in the course of 2006 on the experimental site of IPSL (SIRTA, located about 25 km south-west of Paris Ecole Polytechnique). SIRTA gathers a lot of teledetection instruments (lidars and radars) and is included in international networks of experimental sites devoted to research on aerosols and clouds. CEREА will bring instruments for wind and turbulence measurements: UHF radar, sodar, sonic anemometers. A comparison during a long time period between these measurements and the Mercure\_Saturne code is planned in order to study the ability of this code to simulate correctly the meteorological heterogeneities induced by the land use (buildings, trees).

A joint project with IPSL has been retained by Ile de France region (SESAME program) to strengthen the instrumental set up and thus to create on SIRTa an experimental platform for research on meteorology and air quality in this region.

Moreover, CEREa is involved with IPSL and Météo-France in two joint projects which have been submitted to French research programs. The first one is dedicated to the observation and numerical simulation of turbulent, radiative, dynamical, and microphysical processes involved in the life cycle of fog. The second one includes both studies of fog and of turbulent structures in relation with turbulent fluxes in the stable boundary layer.

*Campaign for wind resource assessment in complex terrain*

A 6 months campaign of wind and turbulent measurements on a future wind energy production site is planned for 2007 in order to bring input and validation data for numerical simulations with Mercure\_Saturne code. The selected site is located in Southern of France and is characterised by strong slopes. The horizontal and vertical heterogeneities of wind and turbulence will be documented by means of 4 instrumented masts and a sodar. These data will allow a comparison between the calculations of wind resource obtained with Mercure\_Saturne and with the linearized model (WASP) generally used up to now (PhD work of Laurent Laporte).

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## Staff

### Scientific Staff

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MICHELANGELI Paul-Antoine (\*\*)  
PLION Pierre  
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TORRES German (\*\*)

## Contracts 2003 - 2005

NAME	2003	2004	2005
<b>ADEME</b>	Uncertainties in traffic and emission models		Aircraft soot
<b>CEA</b>			Resuspension of radionuclides
<b>CETU</b>	<i>Agreement</i>		
<b>CNRS</b>	National Program for Atmospheric Chemistry (PNCA), aerosol project		
	National Program for Atmospheric Chemistry (PNCA), data assimilation project		
<b>CRIEPI (Japon)</b>			<i>Agreement</i>
<b>EDF R&amp;D</b>	<i>Agreement (Joint Laboratory)</i>		
<b>EDR R&amp;D Thermal Branch</b>	Impact study for the power plant of Martigues	Modelling of impacts for the power plant of Martigues	Modelling of impacts for the power plant of Porcheville
<b>INERIS</b>		<i>Agreement</i>	
<b>IRSN</b>	Inverse modelling of emissions in the atmosphere (MIRA project)	Inverse modelling of accidental release (MIRA project)	
	<i>Agreement</i>		
<b>MEDD</b>	<i>PAM Project (Multiphase Air Pollution ), Primequal-Predit</i>		
<b>MELT</b>	<i>Agreement DRAST</i>		
<b>ONERA</b>	Coupling aerosols and turbulence in a jet		

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## **Seminars at CEREa 2003 - 2005**

### **2003**

*January 8, 2003:* Spyros Pandis, Carnegie Mellon University, Etats-Unis.

*February 3, 2003:* Cécile Ferreira-Gago, ONERA.

*February 10, 2003:* Xavier Vancassel, Laboratoire de Physico-Chimie de l'Atmosphère, Université de Strasbourg.

*April 15, 2003:* Laura Gallardo Klenner, Centro de Modelamiento Matematico, Santiago, Chile.

*April 22, 2003:* Patrice Mestayer, Ecole Centrale de Nantes.

*June 10, 2003:* Sylvain Cheinet, LMD.

*July 1, 2003:* Maythili Sharan, Center for Atmospheric Sciences, Indian Institute of Technology, New Delhi.

*July 2, 2003:* Mohammad Thagavi, Laboratoire de Météorologie Physique.

*September 4, 2003:* Christian Seigneur, Atmospheric & Environmental Research, Etats-Unis.

*September 30, 2003:* Kathleen Fahey (CEREa et Carnegie Mellon University).

*October 13, 2003:* German Torres (CEREa et ERCIM).

*October 21, 2003:* Laurent Li, LMD.

*November 4, 2003:* Maya Milliez, CEREa.

*December 17, 2003:* Claire Carouge et Philippe Peylin, LSCE/CEA

### **2004**

*May 25, 2004:* Valery Masson, Météo-France, "Le Micro-climat Urbain : Observations et Modélisation".

*May 27, 2004:* Laura Gallardo Klenner, Centro de Modelamiento Matematico, Santiago, Chile, "Urban Mobile Emission in South American Mega Cities (UMESAM)".

*June 4, 2004:* Jean-Charles Hourcade, CIRED, "Evolution de la Modélisation Intégrée pour le Changement Climatique".

*June 2004:* Workshop CEREa in the framework of the Spring Research days of EDF R&D – Chatou

*November 3, 2004:* Workshop "Air Quality Modelling with Polair3D" – CEREa/EDF Polska

*November 26, 2004:* Philippe Mirabel, Université Louis Pasteur, Strasbourg, Laboratoire de Physico-Chimie de l'Atmosphère. "Modélisation des aérosols dans les traînées de condensation".

*December 6, 2004:* Francesca Muñoz Bravo & Axel Osses, du Centre de Modélisation Mathématique de l'Université du Chili, "Improvement of the Mobile Source Emission Inventory by means of Inverse Modelling in Santiago de Chile".

*December 16, 2004:* Workshop "Numerical simulation for chemistry" - INRIA – B Sportisse (with M. Kern and A. Ern).

### **2005**

*January 14, 2005:* Clémence Pierangelo, LMD/IPSL, "Télédétection infrarouge des aérosols: altitude et épaisseur optique des poussières désertiques depuis l'espace".



*January 28, 2005:* Cathy Clerbaux, Service d'Aéronomie, IPSL, "Monoxyde de carbone : suivi de la pollution par satellite".

*March 18, 2005:* Carole Bedos, INRA UMR Environnement et Grandes Cultures, Equipe Biosphère-Atmosphère Grignon, "Modélisation des sources/puits de polluants atmosphériques dans le continuum sol-végétation-atmosphère et de leur dispersion à courtes distances".

*March 23, 2005:* Workshop of the Scientific Network of the French Ministry for Transport (RST Air).

*May 9, 2005:* Jean-François Vinuesa, University of Minnesota, "Turbulent reacting flows in the atmospheric convective boundary layer".

*June 24, 2005:* Serge Guillas, Georgia Institute of Technology, "Statistical Diagnostic and Correction of a 2-D Model for the Prediction of Total Column Ozone".

*June 27, 2005:* Rachid Abida, Météo Maroc.

*June 2005.* Project meeting of the INRIA Action ADOQA (Data Assimilation for Air Quality).

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## **International collaborations**

CEREA has been honoured to welcome for one week (January 2003) Professor Spyros Pandis from the Carnegie-Mellon University (USA). This has allowed CEREA to strengthen the relations with his team after the mission of Edouard Debry to the States, especially through the post-doctoral position of Kathleen Fahey (2003-2005). The topics are related to aerosol modeling.

A partnership has been initiated with the Center for Atmospheric Sciences of IIT Delhi (Professor Maithilis Sharan). Professor M. Sharan has been welcomed for one month, thanks to the support of the French embassy in Delhi, in 2003 and 2004. Jean-Pierre Issartel has performed two visits at CAS in 2004 and 2005. A new visit of Professor Sharan should allow to build a new project in summer 2006.

CEREA has developed long-term relations (2003-) with the CMM of Santiago de Chile, with topics devoted to inverse modelling of pollutants (mission of Jean-Pierre Issartel to Chile , mission of Laura Gallardo, Francesca Munoz and Ricardo Alcaful at CEREA). This work is supported by CONYCIT/INRIA and ECOSUD. The project is devoted to data assimilation and forecast with the MM5/Polyphemus modelling chain.

A common project has been initiated with GMD First (Berlin, Germany) for air quality forecast and data assimilation, through the post-doc of German Torrès, supported by ERCIM. This work is part of a PROCOPE French German program and is inserted in the CLIME project.

CEREA has a cooperative work inside the CAMP program (Comprehensive Atmospheric Modelling Program) of Georges Mason University (USA). This concerns short-scale dispersion and is led by Bertrand Carissimo.

A joint project with CRIEPI (Center Research Institute for Electric Power Industry, Japan) has been led by Karine Sartelet (with more than 8 months in Japan). This concerns Air Quality modelling over Great Tokyo with Polair3D and the participation in the MICS-Asia exercise. This work has been funded by the Canon Foundation for Research and by CRIEPI. CEREA also takes part in the MICS-ASIA (Phase 2) intercomparison study over East Asia.

In the field of forecast of radionuclides dispersion, CEREA has welcome some foreign researchers to promote collaborative projects, such as Jorgen Brandt (NERI, Denmark ) or Stefano Galmarini (JRC, Italy ), in 2005.

CEREA takes part in the European project NEEDS devoted to Impact studies and Cost-Benefit Analysis of Air Pollution Externalities. This project provides the opportunity for collaborative works with EMEP-West and IER Stuttgart.

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## Members of scientific Committees

### **B. Carissimo:**

Cost Action 732 (Quality Insurance and Improvement of Microscale Meteorological models).

### **L. Musson-Genon:**

Scientific Committee for Primequal/Predit, Journal "Pollution Atmosphérique",  
Conseil Supérieur de la Météorologie/Environmental Committee,  
Cost Action 728 (Atmospheric Dispersion).

### **B. Sportisse:**

Conseil Scientifique "Modélisation" du PREDIT (2003),  
Comité National des Aides de l'ADEME/Qualité de l'Air, Scientific committee of "Pôle de compétitivité  
ville et mobilité durable " (2003-2005).

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## Publications

### **Articles accepted or published 2003-2005**

#### **Bocquet M.**

Grid resolution dependence in the reconstruction of an atmospheric tracer source, *Nonlinear Processes in Geophysics*, 12, p. 219-234 (2005).

#### **Bocquet M.**

Reconstruction of an atmospheric tracer source using the principle of maximum entropy. I: Theory. *Quarterly Journal of the Royal Meteorological Society*, 131, part B (610), p. 2191 (2005).

#### **Bocquet M.**

Reconstruction of an atmospheric tracer source using the principle of maximum entropy. II: Applications. *Quarterly Journal of the Royal Meteorological Society*, 131, part B (610), p. 2209 (2005).

#### **Boutahar J., Lacour S., Mallet V., Quélo Denis, Roustan Y. and Sportisse B.**

Development and validation of a fully modular platform for numerical modelling of air pollution: POLAIR. *International Journal of Environment and Pollution*. Vol.22, 1-2, p. 17-28, 2004.

#### **Bouzereau E., Musson-Genon L., Carissimo B.**

On the definition of the cloud water content fluctuations and its effects on the computation of a second-order liquid water correlation. Accepted for *Journal of Atmospheric Sciences*.

#### **Debry E., Sportisse B. and Jourdain B.**

A stochastic approach for the numerical simulation of the general dynamics equation for aerosols. *J. Comp. Phys.* 2003. Vol 184, p. 649-689.

#### **Debry E., Sportisse B.**

Reduction of the condensation/evaporation dynamics for atmospheric aerosols: Theoretical and numerical investigation of hybrid methods. Accepted for *Journal of Aerosol Science*

#### **Djouad R., Sportisse B.**

Partitioning techniques and lumping computations for reducing chemical kinetics: APLA, an Automatic Partitioning and Lumping Algorithm. *Applied Numerical Mathematics* 2002. Vol 43, Iss 4, p. 383-398

#### **Djouad R., Sportisse B. and Audiffren N.**

Numerical Simulation of Aqueous-Phase Atmospheric Models: Use of a Nonautonomous Rosenbrock Method. *Atmospheric Environment* (36)5, (2002) p. 873-879

**Djouad R., Audiffren N. and Sportisse B.**

Sensitivity analysis using automatic differentiation applied to a multiphase chemical mechanism. Atmospheric Environment. 2003. Vol 37, nr 22, p. 3029-3038.

**Djouad R., Sportisse B. and Audiffren N.**

Reduction of Multiphase Atmospheric Chemistry. Journal of Atmospheric Chemistry. 2003. Vol 46, p. 131-57.

**Djouad R. and Sportisse B.**

Solving reduced models in Air Pollution Modelling. Applied Numerical Mathematics. 2003. Vol 44, nr 1, p. 49-61.

**Issartel J.P.**

Emergence of a tracer source from air concentration measurements, a new strategy for linear assimilation. Atmos. Chem. Phys. Vol 5-249, 2005, p 249-273.

**Issartel J.-P. and Baverel J.**

Rebuilding sources of linear tracers after atmospheric concentration measurements, Atmos. Chem. Phys., 3, 475-486, 2003

**Mallet V., Sportisse B.**

3-D chemistry-transport model Polair3D: numerical issues, validation and Atmos. Chem. Phys. Disc. 4, 1371:1392. 2004

**Mallet V., Sportisse B.**

A comprehensive study of ozone sensitivity with respect to emissions over Europe with a chemistry-transport model. Journal Geophysical Research, 100, D22 (2005).

**Mallet V., Sportisse B.**

Uncertainty in a chemistry-transport model due to physical parameterizations and numerical approximations: an ensemble approach for ozone modelling. Journal of Geophysical Research 111 (D1). Art. N° D01302

**Mallet V., Sportisse B.**

Ensemble-based air-quality forecasts: a multi-model approach applied to ozone. Accepted for publication in Journal Geophysical Research.

**Milliez M., Carissimo B.**

Numerical simulations of pollutant dispersion in an idealized urban area, for different meteorological conditions. Accepted to Boundary-Layer Meteorology (UAQ 2005 special issue).

**Quélo D., Mallet V., Sportisse B.**

Inverse modelling of NOx emissions at regional scale over Northern France. Preliminary investigations of the second-order sensitivity. Journal Geophysical Research 110 (D24). Art. N° D24310

**Quélo D., Sportisse B., Isnard O.**

Data assimilation for short range atmospheric dispersion of radionuclide: a case study of second-order sensitivity. Journal of Environmental Radioactivity. Vol.84, Issue 3, p. 393-408.

**Roustan Y., Bocquet M.**

Sensitivity analysis for mercury over Europe. Accepted for Journal Geophysical Research.

**Roustan Y., Bocquet M.**

Inverse modelling for mercury over Europe. Accepted for Atmospheric Chemistry and Physics.

**Sartelet K., Hayami H., Albriet B., Sportisse B.**

Development and preliminary validation of a Modal Aerosol for tropospheric chemistry: MAM. Aerosol Science and Technology. 40: 118-127, 2006.

**Sportisse B., Dubois L.**

Numerical and theoretical investigation of a simplified model for the parameterization of below-cloud scavenging by falling raindrops. Atmospheric Environment, 2002. Vol 36, Issues 36-37, Pages 5719-5727

**Sportisse B. and Djouad R.**

Investigation of mass transfer for atmospheric pollutants into a fixed droplet with aqueous chemistry. *Journal of Geophysical Research Atmospheres*. 2003. Vol 108. Nr D2.

**Sportisse B. and Quélo D.**

Data assimilation and inverse modelling of atmospheric chemistry. *Proc. of Indian National Science Academy. Part A Physical Sciences*. Nov. 2003. Vol 69. (Invited Paper)

**Sportisse B., Boutahar J., Debry E., Quélo D. and Sartelet K.**

Some tracks in Air Pollution Modelling. *RACSAM Journal of the Spanish Science Academy, Real Academia de Ciencias de Espana*. 2003. Vol 96. Nr 3. (Invited Paper)

**Wotawa, G., de Geer, L.-E., Denier, P., Kalinowski, M., Toivonen, H., d'Amours, R., Desiato, F., Issartel, J.-P., Langer, M., Seibert, P., Frank, A., Sloan, C., Yamazawa, H.**

Atmospheric transport modelling in support of CTBT verification. Overview and basic concepts, *Atmospheric Environment* 37, 2525-2537, 2003.

***Submitted articles*****Bocquet M.**

High resolution reconstruction of a tracer dispersion event: application to ETEX. Submitted to *QJRMS*.

**Debry E., Sportisse B.**

Numerical simulation of the General Dynamics Equation (GDE) for aerosols with two collocation methods. In revision for *Applied Numerical Mathematics*.

**Debry E., Sportisse B.**

Solving aerosol coagulation with size-binning methods. In revision for *Applied Numerical Mathematics*.

**Demaël E., Carissimo B.**

A comparison between Eulerian CFD and Gaussian Plume models on Prairie Grass Dispersion Experiment. Submitted to *Journal of Applied Meteorology*.

**Krysta M., Bocquet M.**

Source Reconstruction of an Accidental Radionuclide Release at European Scale. Submitted to *Quarterly Journal of the Royal Meteorological Society*.

**Krysta M., Bocquet M., Sportisse B. and Isnard O.**

Data Assimilation for Short-range Dispersion of Radionuclides: An Application to Wind Tunnel Data. In revision for *Atmospheric Environment*.

**Lacour S., Schmitt-Foudhil H., Carissimo B.**

Detailed modelling of NO<sub>x</sub> and NO<sub>2</sub> dispersion in a street canyon. Submitted to *Atmospheric Environment*.

**Sartelet KN., Hayami H, Sportisse B.**

MICS Asia Phase II - Sensitivity to the aerosol module. Submitted to *Atmospheric Environment*

***Articles in French*****Clerbaux C., Hauchecorne A., Bekki S., Granier C., Pirre M., Sportisse B., Issartel J.P et. Attié. J.L.**

Assimilation de données satellitaires et inversion de sources pour l'étude de la composition chimique atmosphérique. *Compte-rendu 2003 du CNFGG*.

**Debry E. et Sportisse B.**

Modélisation de la dynamique des aérosols: le modèle SIREAM. *Pollution Atmosphérique et Journal of Aerosol Sciences*.

**Roustan Y., Bocquet M., Musson-Genon L., Sportisse B..**

Modélisation du mercure, du plomb et du cadmium à l'échelle Européenne. Pollution Atmosphérique.

**Sportisse B.**

Quelques aspects de la modélisation de la pollution atmosphérique. Annales des Ponts et Chaussées, "Modélisation: nouvelles pratiques", 2003.

**Sportisse B.**

Modélisation et simulation de la pollution atmosphérique. Compte-rendu 2003 du CNFGG.

**Sportisse B.**

Partenariat recherche publique/entreprise: l'exemple du CEREAs, Laboratoire Commun ENPC/EDF R&D In "Management de la recherche publique", Rémi Barré Ed.

## ***Proceedings***

### **2003**

**Lacour S., Megueulle C., Carlotti P., Souhac L. and Sportisse B.**

Unsteady effects on pollutant dispersion around a tunnel portal. In Proceedings of Urban Air Quality Conference (UAQ'4), Prague, march 2003.

**Lacour S. and Joumard R.**

Sampling vehicles for pollutant emission modelling. In Proceedings of the 8<sup>th</sup> Conference on Transport and Air Pollution, Avignon, June 2003.

### **2004**

**Monika Krysta, Marc Bocquet, Olivier Isnard, Jean-Pierre Issartel and Bruno Sportisse.**

Data Assimilation of Radionuclides at Small and Regional Scale. Some preliminary results. July 2004, 10 pages. Proceedings of the NATO ARW, Kluwer

**Henry Quiroz, Laura Gallardo Klenner, Jean-Pierre Issartel.**

Assimilation de données, un révélateur de la qualité des modèles : exemple de l'arsenic minier à Santiago du Chili, Atelier de Modélisation Atmosphérique, Météo-France, Toulouse, November 29-30, 2004.

**K.N. Sartelet, H. Hayami, B. Albriet, B. Sportisse.**

A new modal model of atmospheric aerosols (MAM). ICNAA conference, July 2004.

**K N. Sartelet and Hayami, H.**

Application of the 3D CTM Polair to air quality over Greater Tokyo. Proceedings of the 45th annual meeting of Japan Society for Atmospheric Environment. P.529 - 2004

**Y. Roustan, M. Bocquet, L. Musson-Genon, B. Sportisse.**

Modelling Mercury over Europe with the Chemistry-Transport-Model Polair3D. In Proceedings GLOREAM/EURASAP Workshop. DMI. Denmark.

**K. Fahey, E. Debry, H. Foudhil and B. Sportisse.**

Formulation, development and preliminary validation of the Size Resolved Aerosol Model (SIREAM). In Proceedings GLOREAM/EURASAP Workshop. DMI. Denmark.

### **2005**

**M. Taghavi, K. Fahey, H. Foudhil, B. Sportisse.**

Modelling aerosols with the POLAIR3D/SIREAM model on the mesoscale over an urban area in south-eastern France (ESCOMPTE campaign). European Aerosol Conference, Belgium. September 2005.

**Y. Roustan, M. Bocquet, L. Musson-Genon, B. Sportisse.**

Modelling atmospheric mercury at European scale with the Chemistry Transport Model Polair3D. Proceedings of Gloream 2004.

**E. Demael, B. Carissimo.**

A comparison of Eulerian CFD with Gaussian Plume simulations of Prairie Grass Dispersion Experiments 9th annual George Mason University Conference on Atmospheric Transport and Dispersion Modelling, Fairfax, USA, July 18-20, 2005.

**M. Taghavi, L. Musson-Genon.**

Impact of thermal power plant emissions in Marcheille, Power-Gen Europe Conference, Milan, Italy, June 28-30, 2005.

**M. Taghavi, L. Musson-Genon.**

Intermediate species: does chemistry work in a same way in all models? The Sixth ESCOMPTE Workshop, February 2-4, 2005, Marcheille.

**M. Bocquet and M. Krysta.**

Inverse Modelling of Passive Atmospheric Tracers Using Entropy-based Methods: Methodological Aspects, 2005. Proceedings of the Workshop CEA-EDF-INRIA: Data assimilation and inverse modelling in geosciences. F.-X. Le Dimet and B.Sportisse Eds.

**M. Krysta, M. Bocquet and D. Quélo.**

Source Reconstruction for Accidental Releases of Radio-elements. Proceedings of NATO Advanced Research Workshop, Tabakhmela, Georgia, 2005.

**K. Fahey, E. Debry, H. Foudhil, B. Sportisse.**

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- *SIAM Geosciences, 2005, 6-12 June, Avignon.*

V. Mallet: "Inverse modelling of emissions in a chemistry-transport model".

M. Bocquet: Organization of the mini-workshop "Inverse modelling in air pollution" and oral presentation. "Inverse modelling of passive atmospheric tracers using methods based on the maximum entropy principle".

B. Sportisse: Plenary speaker "Some issues for Air Pollution Modelling".

- GLOREAM, *Global and Regional Atmospheric Modelling, 2005, 7-9 September 2005, Apeldoorn, the Netherlands.*

M. Krysta: "Inverting sources of an accidental radionuclide release at continental scale".

M. Tombette: "Aerosol modelling at regional scale: a sensitivity study with the Polyphemus platform".

## **SEMINARS**

### **2003**

Issartel J.P., Séminaire du DEA M2SAP X-ENSTA-UVSQ. November 2003. "Modélisation inverse de sources".

Issartel J.P., "Méthode des rétropanaches". 15 May 2003. Université de Calais.

Roustan Y., Journée des doctorants ADEME. 20 May 2003. "Modélisation de l'impact des métaux lourds, du mercure et des particules à l'échelle européenne".

Sportisse B., ERCIM Workshop Environmental Modelling, Sophia Antipolis. February 2003. "Forecasting atmospheric dispersion of radionuclides". Avec V. Mallet, D. Quélo and O. Isnard.

Sportisse B., ESIEE/DEA télédétection. February 2003. "Data assimilation for air pollution modelling".

### **2004**

Issartel J.P., Seminar CMM, Chili, July 2004,

Issartel J.P., Seminar IIT Delhi, Inde, August 2004,

### **2005**

Lacour S. Réseau des économistes des transports. Mécanismes de formation de la pollution atmosphérique, Paris, January 2005.

Sportisse B. EDF R&D Spring Generation Seminar, Chatou. 30-31 May. General presentation of CEREAS.

## **Main missions**

### **2003**

Bocquet M., EGS - AGU - EUG Joint Assembly, Nice (France). April 2003. Session "Assimilation de données".

Bocquet M., école d'été E2Phi 2003 à Bordeaux. August 2003. "*La physique de notre planète, la Terre, et son climat*".

Bocquet M., Annual Seminar 2003 du CEPMMT, Reading (Royaume-Uni). September 2003. "*Recent developments in data assimilation for atmosphere and ocean*"

Issartel J.P., Mission au CMM, Santiago du Chili (Chili). January 2003.

Sportisse B., Journée PNCA/aérosols, Observatoire Midi-Pyrénées, Toulouse. 28 November 2003.

Sportisse B., Journée PNCA/assimilation de données, CERFACS, Toulouse. 2 December 2003.

## 2004

Bocquet M. ERCA2004 (European Research Courses on Atmospheres) (Grenoble, January-February 2004). Oral presentation.

Boutahar J. Casablanca. 24-28 May 2004. EHTP.

Carissimo B. SIG and urban modelling. CERMA, 15 September 2004, Nantes

Carissimo B. Group "Dynamique de l'Atmosphère Habitée", Laboratory of Fluid Mechanics, Ecole Centrale de Nantes, 14 September 2004.

Issartel J.P. Santiago du Chili, 15-31 July 2004, Centro de Modelamiento Matematico, Universidad de Chile & CNRS.

Issartel J.P. Delhi, 19-29 August 2004, Centre for Atmospheric Sciences, Indian Institute of Technology of Delhi.

Mallet V. Summer School for data assimilation in atmospheric sciences. ISSAOS (L'Aquila, Italie).

Milliez M. 5-15 July 2004: Toulouse Meteo France, Capitoul campaign.

Milliez M. 9-10 September 2004 Nottingham (Angleterre) Workshop ERCOFTAC Special Interest Group 5 on Environmental CFD subject: Urban Scale CFD.

Musson-Genon L. Impact study for Martigue's thermal power Plant's emissions on photo-oxydant pollution in Marseille-Berre area, implementation of European environmental Regulation in fossil-fired Power stations of EDF Group, Gdansk, Polska, 27-30 September 2004.

Pircher V. Workshop "Observatoires de Recherche en Environnement (ORE); état des lieux et prospective"; 15-16 November 2004; Paris, Ministry for Research.

Taghavi M. First French-German summer school on "Aerosols, heterogeneous chemistry and climate", Ile d'Oleron, France, September 2004.

## 2005

Carissimo B. DTRO Workshop. Francfurt. June 2005

Carissimo B. Washington. University George Mason. July 2005.

Mallet V. ADOMOCA workshop (INSU/PNCA). Toulouse, December 2005.

Milliez M. European Research Course on Atmospheres Grenoble. January 2005.

Musson-Genon L. EDF, Polska,

Quélo D. EDF, Polska. December 2005.

Sportisse B. Needs Project (Integrated Project, EU), Stuttgart. February 2005.

Taghavi M. Scientific collaboration with Meteo Iran. June & October 2005.

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## Teaching activities

CEREA is involved in the teaching activities at Ecole Nationale des Ponts et Chaussées. This includes courses devoted not only to applications (Air Pollution) but also to academic fields (Applied Mathematics). CEREA is also active in teaching activities at ENSTA with two courses: one devoted to Computational Physics for geophysics, one devoted to data assimilation.

CEREA is implied in the animation of the Teaching Department ENPC/VET through Vincent Pircher.



CEREA is also involved in the teaching program of Master TRADD with a course devoted to Air Pollution and Transport. Some courses (Atmospheric Modelling) have been given in Research Master SGE.

**Air Pollution, ENPC.**

Bruno SPORTISSE, Stéphanie LACOUR.

**TRADD Mastère (Air Pollution and Transport), ENPC.**

Stéphanie LACOUR, Bruno SPORTISSE.

**Applied Mathematics, ENPC (1st year).**

Bruno SPORTISSE.

**Atmospheric Environment, ENPC (3rd year).**

Vincent PIRCHER.

**Data assimilation and inverse modelling, ENSTA.**

Bruno SPORTISSE, Marc BOCQUET, Vivien MALLET.

**Computational Physics for Environment, ENSTA.**

Bruno SPORTISSE, Vivien MALLET.

**Atmospheric Environment, Centrale Marseilles.**

Bertrand CARISSIMO.

**Atmospheric Modelling, Master Recherche SGE, Option AQA.**

Bertrand CARISSIMO, Edouard DEBRY, Vivien MALLET.

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## **Textbooks for teaching activities**

(Available at [www.enpc.fr/cerea](http://www.enpc.fr/cerea) as ParisTech courseware)

Air Pollution Modelling (ENPC)

B. Sportisse

Air Pollution and Transport: emission inventories (ENPC)

S. Lacour

Data Assimilation and inverse modelling (ENSTA)

B. Sportisse and D. Quélo (part 1)

M. Bocquet (part 2)

Computational Physics for Environmental Problems (ENSTA)

B. Sportisse and V. Mallet

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## **PhD Works**

*Theses in progress*

R. ABIDA

Construction optimale de réseaux de mesure pour la pollution atmosphérique. ENPC.

B. ALBRIET

Modélisation des aérosols à l'échelle locale et régionale. ENPC.

E. DEMAEL

Modélisation de la dispersion sur un site nucléaire. ENPC.

M KRYSTA

Modélisation inverse de la dispersion des radionucléides dans l'atmosphère. Paris 12.

R. LAGACHE

Couplage de modèles pour l'estimation des impacts de la pollution atmosphérique liée aux transports à l'échelle locale. ENPC.

D. LAPORTE

Amélioration de l'estimation du productible éolien en terrain complexe. ENPC.

H. MALAKOOTI

Modélisation de la qualité de l'air dans une "Megacity". Application à Téhéran. ENPC.

M MILLIEZ

Modélisation thermique au sein du modèle Mercure\_Saturne. Application à la modélisation de l'environnement urbain. ENPC.

S. QUEGUINER

Modélisation multi milieux de la pollution atmosphérique. ENPC.

M. TOMBETTE

Modélisation des aérosols à l'échelle régionale. ENPC.

#### *Theses defended*

J. BOUTAHAR 30/09/2004

Réduction de modèles de qualité de l'air pour les études d'impact à l'échelle européenne. ENPC.

E. BOUZEREAU 14/12/2004

Modélisation de l'eau liquide dans le modèle Mercure\_Saturne. Paris 6.

E. DEBRY 13/12/2004

Modélisation numérique de la dynamique des aérosols. ENPC.

D. QUELO 8/12/2004

Assimilation de données variationnelle pour la chimie atmosphérique. ENPC.

V MALLET 6/12/05

Estimation de l'incertitude et prévision d'ensemble avec un modèle de chimie-transport – Application à la simulation numérique de la qualité de l'air. ENPC.

Y. ROUSTAN 12/12/05

Modélisation de la dispersion atmosphérique du mercure, du plomb et du cadmium à l'échelle Européenne. ENPC.

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## **Softwares**

### ***AtmoData***

Library for data processing and parameterizations in atmospheric chemistry and physics.

V. Mallet, D. Quélo, H. Njomgang.

ENPC

### ***AtmoPy***

AtmoPy, statistical and graphical python library for analyzing Chemistry Transport model output concentrations: comparison to observations, comparison between simulations.

V. Mallet, V. Picavet.

### ***MAM***

Modal Aerosol Model for particulate matter dynamics.

K. Sartelet, B. Albriet, B. Sportisse.

ENPC

### ***Mercure\_Code Saturne***

CFD model for the Atmospheric Boundary Layer.

E. Bouzereau, B. Carissimo, E. Dupont, H. Foudhil, S. Lacour, M. Milliez, L. Musson-Genon.  
EDF R&D

***Polair3D***

Chemistry transport model.

J. Boutahar, D. Quélo, K. Fahey, K. Sartelet, B. Sportisse, M. Tombette.  
ENPC

***Polyphemus***

Modelling system for atmospheric modelling ([www.enpc.fr/cerea/polyphemus](http://www.enpc.fr/cerea/polyphemus)) V. Mallet, D. Quélo,  
B. Sportisse.

***SIREAM***

Size Resolved Aerosol Model.

E. Debry, K. Fahey, K. Kata-Sartelet, B. Sportisse, M. Tombette.  
ENPC

***Spack***

Simplified Preprocessor for Atmospheric Chemical Kinetics.

B. Sportisse, P. Plion, R. Djouad (at University of York, Canada)  
ENPC

## **List of acronyms**

ADEME	Agence pour le Défense de l'Environnement et la Maîtrise de l'Energie
CEA	Commissariat à l'Energie Atomique
CEFIPRA	Centre Franco-Indien pour la Promotion de la Recherche Avancée
CEPMMT	Centre Européen de Prévision Météorologique à Moyen Terme
CEREA	Centre d'Enseignement et de Recherche sur l'Environnement Atmosphérique
CETE	Centre d'Etudes Techniques de l'Equipement
CETU	Centre d'Etude des Tunnels
CNFGG	Comité National Français de Géodésie et de Géophysique
CNRS	Centre National de Recherche Scientifique
CONICYT	Comision National de Investigacion Cientifica y Tecnologica de Chile
CRIEPI	Central Research Institute for Electric Power Industry (Japon)
CSTB	Centre Scientifique et Technique du Bâtiment
DGA	Délégation Générale à l'Armement
DRAST	Direction de la Recherche et des Affaires Scientifiques et Techniques du METMLT
ECL	Ecole Centrale de Lyon
EDF R&D	Electricité de France Recherche et Développement
ENPC	Ecole Nationale des Ponts et Chaussées
ENSTA	Ecole Nationale Supérieure des Techniques Avancées
ERCIM	European Research Consortium for Informatics and Mathematics
ESA	European Spatial Agency
GMD FIRST	German National Research Institute for Information Technology
IAEA	International Atomic Energy Agency
INRIA	Institut National de Recherche en Informatique et Automatique
INERIS	Institut National sur l'Environnement et les Risques Industriels et Sanitaires
INRETS	Institut National de Recherche et d'Etude sur les Transports et la Sécurité
IPSL	Institut Pierre-Simon Laplace
IRSN	Institut de Radioprotection et de Sûreté Nucléaire
LISA	Laboratoire Interuniversitaire des Systèmes Atmosphériques (Paris 7, Paris 12, CNRS)
LMD	Laboratoire de Météorologie Dynamique (X-ENS-CNRS)
LSCE	Laboratoire Surveillance du Climat et de l'Environnement (CEA/CNRS)
M2SAP	DEA Modélisation, Simulation, Applications à la Physique (X-ENSTA-UVSQ)
MEDD	Ministère de l'Ecologie et du Développement Durable
ONERA	Office National d'Etudes et de Recherches Aérospatiales
PNCA	Programme National de Chimie Atmosphérique
PPF	Plan Pluriannuel de Formation
PREDIT	Programme pour la Recherche, le Développement et l'Innovation dans les transports terrestres
PRIMEQUAL	Programme Interministériel d'Etude de la Qualité de l'Air
PROCOPE	Programme d'action intégrée franco-allemand
UMLV	Université de Marne La Vallée
UVSQ	Université de Versailles-Saint Quentin
VET	Département Ville-Environnement-Territoire de l'ENPC

# Synopsis

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