

# CEREA Summary Report 2003–2007

TEACHING AND RESEARCH CENTER IN ATMOSPHERIC ENVIRONMENT Joint Laboratory École Nationale des Ponts et Chaussées/Électricité de France R&D http://www.enpc.fr/cerea/





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## CEREA Research and Teaching Center in Atmospheric Environment Joint LABORATORY ENPC-EDF R&D

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This reports summarizes the activities of CEREA for 2003-2007. A list of acronyms can be found in Section 14.

## 1 Key features

## 1.1 General presentation

The Research and Teaching Center in Atmospheric Environment (CEREA) was established in 2003 as a research center at École Nationale des Ponts et Chaussées. It was previously nurtured by the Water Research Laboratory of ENPC (CEREVE). In 2004, it became a joint laboratory between ENPC and EDF R&D. It also hosts a joint project with INRIA since September 2003, the CLIME project.

CEREA has three locations (ENPC at Champs sur Marne, EDF R&D at Chatou, INRIA at Rocquencourt).

Its main research activity is devoted to air quality modeling and atmospheric dispersion from short-range to long-range scales. Research works are also dedicated to studying the atmospheric boundary layer (especially for applications related to wind power estimate).

A special focus is given to the assessment of environmental impact of transport and energy production (thermal or nuclear). These activities are connected with the programs of EDF R&D and with research units and technical centers of the French Ministry for Transport through its Research Directorate.

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

As a research laboratory depending both of a company (EDF) and of a graduate school (French "Grande Ecole": ENPC/Paris Institute of Technology), CEREA has a *double* focus on:

- academic works (illustrated by scientific publications and PhD works);
- applied projects with end-users (from impact studies to development of models and methods for environmental forecast).

## 1.2 Organization

CEREA is organized in five groups:

- Atmospheric fluid mechanics and short-range dispersion;
- Multiphase modeling;
- Air quality modeling at regional and continental scales;
- Data assimilation and inverse modeling;
- Observation of the atmospheric boundary layer.

The data assimilation team is also part of the INRIA project hosted by CEREA (CLIME).

#### **1.3** Research topics

CEREA develops modeling activities mainly with two numerical models: an atmospheric CFD (Computational Fluid Dynamics) tool, Mercure\_Saturne, for short-range applications (urban pollution, risk assessment, wind power estimate), and an air quality modeling system, POLYPHE-MUS. POLYPHEMUS includes different models ranging from short-range dispersion (Gaussian and puff models) to long-range dispersion at regional and continental scales (the Chemistry-Transport Models Castor and Polair3D). Some appropriate physical parameterizations and multiphase reactive box models are developed and plugged in these three-dimensional models.

The resulting models are evaluated by comparisons 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 modeling of pollutants.

Apart from modeling, the measurements team is implied in several campaigns in order to improve the knowledge of the atmospheric boundary layer and to support the validation of Mercure\_Saturne.

The research topics and the main results obtained for 2003-2007 are detailed in Section 2.

#### 1.4 Motivations for CEREA

The main objectives for CEREA are:

- 1. to fullfill specific requirements of ENPC and EDF R&D, namely:
  - (a) to propose high-level courses to the students of ENPC (more generally of ParisTech, the Paris Institute of Technology) and to host PhD students;
  - (b) to be inserted in the scientific network of the French Ministry for Transport;
  - (c) to participate in the research programs of EDF R&D;
  - (d) to be able to offer a policy-relevant expertise to the EDF group.
- 2. to produce high-level scientific works, to be assessed by publications in international peerreviewed journals;
- 3. to develop and to maintain an extended network of partnerships through research contracts and/or joint projects with other institutions.

The motivations, strengths and weaknesses of CEREA are also detailed in (unfortunately in French):

Sportisse, B. (2007a). *Management de la recherche publique*, chapter Partenariat recherche publique/entreprise : l'exemple du CEREA, Laboratoire Commun ENPC/EDF R&D. De Boeck

## 1.5 Summary of 2003-2007: key facts

## Academic

- More than 50 articles have been published or accepted for publication in international peer-reviewed journals.
- 10 PhD works and one Research Habilitation (HDR) were defended.
- More than 200 teaching hours are given by CEREA researchers per year (in the framework of ParisTech). More than two thirds of these courses are driven by CEREA researchers and correspond to new courses created during the last 4 years.

One refers to Section 5 for a detailed list of publications, to Section 11 for a detailed list of PhD works and to Section 3 for the description of courses.

## Applications

- CEREA is implied in many projects of EDF R&D (related to the requirements of EDF operational departments, both for nuclear production and thermal production of electricity). This includes for instance the Impact THF and AREA projects (for the impact of thermal power plants), the DIAMAN project (for the impact of nuclear power plants), the LIBECIO project (for wind power production) and the EDF R&D network "Uncertainties".
- CEREA carries out many applied projects with partners such as the Fossil-Fired Generation and Engineering Department of EDF (DPIT, not a part of EDF R&D), ADEME (the French Agency of Environment), CEA (nuclear industry), CETU (Research Center for Tunnels), DGA (Ministry of Defence), ONERA (Institute for Aeronautics), INERIS (the French Institute in charge of chemical and biological risks), IRSN (the French Institute in charge of nuclear safety and radiological protection), SETRA (a technical center of the French Ministry for Transport in charge of road management), etc.

## Key partnerships

- CEREA has two strategic partners:
  - IRSN (nuclear safety).
  - INERIS (chemical and biological risks).

These partners are the technical centers in support of the government departments in charge of a specific risk (nuclear, chemical or biological, respectively). Both include Forecast Emergency Centers (CASU at INERIS and CTC at IRSN) also in charge of impact studies. The joint projects are devoted to model developments to be shared (especially within the POLYPHEMUS system), to developments of new methods (both for forecast and impact studies) and to dedicated applied studies.

Framework Agreements (for a long period: typically 3-5 years) exist with these partners.

• CEREA has a Joint Agreement with the IPSL Institute. This mainly concerns the observational site (SIRTA) in the southern suburb of Paris at Palaiseau. The measurements team of CEREA has deployed its instrumental tools at SIRTA since early 2006 and has taken part in the field campaign ParisFog in 2006/2007.

• CEREA is implied in the network devoted to air quality and impacts of the French Ministry for Transport. The involvement is driven by the Framework Agreement with the Research Directorate of the Ministry (specific to CEREA).

CEREA has a long-term partnership with the Technical Center of the Ministry for northern France (CETE Nord-Picardie). The projects are devoted to air quality modeling at regional scale with a focus on the impact of transport.

- CEREA is an active member of the R2D2 network (Research Network for Sustainable Development, funded by the Ile de France region).
- CEREA has taken part in many projects funded by public national research programs (including PNCA for aerosols and data assimilation, Primequal for the PAM project devoted to aerosol modeling and a project devoted to aircraft soot, ANR for the Atlas project devoted to machine learning with ENS Ulm or LEFE for the ParisFog campaign).
- CEREA is a member of the European Integrated projects NEEDS, HEIMTSA and EX-IOPOL devoted to integrated modeling of air quality impacts (especially with IER Stuttgart).

One refers to Section 4 for the detailed list of international collaborations of CEREA.

## 1.6 Budget

Table 1 gathers the main features of CEREA budget for 2004-2007, as presented to the Managing Committee of CEREA at the end of each year. The total budget also includes the salaries of the permanent staff. "Other" refers to other sources of funds next to EDF and ENPC (contracts, INRIA, etc). At equilibrium, the EDF part ranges in [40-50] %, the ENPC part in [25-30] % and the other part in [25-30] %.

	Total budget (kiloeuros)	ENPC Part	EDF Part	Other
2004	1530	46~%	43~%	10~%
2005	1586	30~%	45~%	25~%
2006	1702	28~%	50~%	22~%
$2007^{\star}$	1960	25~%	44 %	31~%

Table 1: CEREA Budget for 2003-2007. Forecast for 2007<sup>\*</sup>.

Table 2 gives the main features related to the contracts of CEREA, viewed as a research laboratory of ENPC. At equilibrium, CEREA earns contracts in the range [500-600] kiloeuros per year, including [200-350] kiloeuros funded by EDF projects and [200-350] kiloeuros funded by other partners or projects. ENPC funds (for travels, missions, investments) range in [70-125] kiloeuros.

A detailed list of contracts for 2004-2006 can be found in Section 12.

	Total contracts (kiloeuros)	EDF R&D	EDF	Other	ENPC funds
2004	275	101	56	118	70
2005	480	148	42	290	71
2006	513	283	50	180	89
$2007^{\star}$	692	266	50	376	125

Table 2: Left: amount of contracts for CEREA, viewed as ENPC Laboratory. Right: ENPC funds. Period 2004-2007. Forecast for  $2007^*$ .

## 1.7 Management

- CEREA is led by a Director (Bruno Sportisse, ENPC) and a Deputy Director (Luc Musson-Genon, EDF).
- Meetings for the whole staff are organized from 4 to 6 times per year. Each research group organizes, when necessary, its own meetings.
- The Managing Committee of CEREA includes 3 representatives both for EDF and ENPC, the Director and the Deputy Director. It meets two times a year: in July for the presentation of a Progress Report, in December for the presentation of the results for the past year (scientific results, involvements in research programs of EDF and ENPC, teaching at ENPC, contacts, budget) and a forecast of the activitity for the coming year (scientific activity and budget). Four reports are then proposed for approval to the Managing Committee: the Activity Report of CEREA and the Budget Report for the past year, a Program Report and a Budget Report for the coming year.
- The Scientific Committee of CEREA has the following composition:

BERCAMETTI Cillos	CNRS Université Paris XI LISA
DEMGAMET IT GILES	UNITS, Universite I alls AI, LIGA
BRANDT Jorgen	NERI, Denmark
BRUN Eric	Météo France, CNRM
LE DIMET François-Xavier	Université Joseph Fourier and INRIA
ROSSET Robert	CNRS, Université Paul Sabatier, LA
SCHLUENZEN Heinke	University of Hamburg, ZMAW, Germany
GODIN Paul	EDF, Scientific Committee of EDF
POCHAT Rémy	LCPC, Scientific Committee of ENPC

It aims at giving a *scientific* assessment of the works achieved at CEREA for the Scientific Committees of EDF and ENPC.



Figure 1: Water droplet plume from cooling towers at the Bugey power plant. Left: plume photograph taken from the measurement airplane. Right: iso-surface of liquid water concentration from numerical simulations using Mercure\_Saturne (PhD work of E. Bouzereau).

## 2 Research topics

## 2.1 Local scale and fluid mechanics (group leader: Bertrand Carissimo)

The research actions are related to the concerns of the French Ministry for Transport (urban pollution) and those of EDF (dispersion at an industrial site). They mainly rely on the development of a 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 parameterizations suitable for the atmospheric environment (roughness wall law, drag urban canopy parameterizations, transport equation for concentration and fluctuations, microphysical cloud scheme, atmospheric radiative scheme, chemistry model, aerosols model...).

The year 2003 was an important transition for the model Mercure\_Saturne. The solver, which was initially based on the numerical kernel ESTET, a code based on a structured grid approach, moved toward the new kernel Code\_Saturne based on an unstructured grid approach. The resulting modifications are important, especially for the atmospheric parameterizations 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 parameterizations in the unstructured environment and all the existing pre and post processing has to be replaced by new procedures.

In 2004, two key functionalities were added to Mercure\_Saturne. The first one is the ability to take into account chemical reactions; the second one is the microphysical description for water.

In 2005, in addition to further development of the above functionalities, the transport equation for fluctuations of concentration was tested. The modal aerosol model already developed for Polair3D (MAM, Section 2.2) was adapted for small scales and coupled to Mercure\_Saturne. A new activity has also been started in the area of wind energy estimate with the accurate modeling of wind field in complex terrain.

In 2006, in addition to efforts in pre and post processing (creation of mesh for complex terrain and buildings), a new scheme for atmospheric radiative transfert in the presence of buildings was developped.

This modeling activity is strongly connected with the measurements team at CEREA for the observation of the atmospheric boundary layer (Section 2.5).

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

A detailed microphysical parameterization for water was first developed in Mercure\_Saturne (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 was extensively validated by a detailed comparison with data from the field campaign around the aerorefrigerant tower of Bugey (in the 1980s) which include aircraft measurements in the plume (Figure 1). 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\_Saturne and the transition to the new unstructured version has been done as an additional task and the results successfully compared.

The warm cloud microphysical scheme previously developed for the simulation of cooling tower plumes has then been also 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, that can also predict the droplet distribution, is suitable for both applications. Three dimensional simulations and comparisons with the fog measurement campaign ParisFog in the winter of 2006-2007 are ongoing.

#### Key reference:

Bouzereau, E., Musson-Genon, L., and Carissimo, B. (2007). On the definition of the cloud water content fluctuations and its effects on the computation of a second-order liquid water correlation. J. Atmos. Sci., 64:665–669

#### Dispersion in urban environment

These topics were developed through a PhD work (Maya Milliez, defended in December 2006) that aimed at simulating the dispersion in an atmospheric environment with obstacles. A first part was the simulation of the Mock Urban Setting Test (MUST) experiment in the USA (Figure 2). An array of shipping containers (12 rows by 10 columns) was representing an idealized urban quarter. A special unstructured grid was set up to simulate these 120 buildings with a still reasonably sized grid of around one million cells. The results obtained with Mercure\_Saturne were compared to the available observational data for several days and good comparison statistics were obtained. An original part of this work was the ability to simulate fluctuations of concentrations trough 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 were developed.

The last part of this PhD work was 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. The numerical results were compared to simple experiments and existing measurements giving the variation of albedo as a function of solar zenith angle and to temperature measurements taken on several container sides during the MUST experiment.

#### Key references:

Milliez, M. and Carissimo, B. (2007). Numerical simulations of flow and pollutant dispersion in an idealized urban area, for different meteorological conditions. *Boundary-Layer Meteor.*, 122(2):321–342

Milliez, M. and Carissimo, B. (2006). CFD modelling of concentration fluctuations in an idealized urban area. *Boundary-Layer Meteor.* Accepted for publication



Figure 2: Diurnal time evolution of the temperature of various faces of a container during MUST. Top left: observations during the MUST experiment. Top right: numerical simulations using the new atmospheric 3D radiative scheme developped in Mercure\_Saturne for the urban canopy (Maya Milliez PhD Thesis). Bottom: experimental set-up of MUST (Mock Urban Setting Test Experiment, 25 September 2001).

#### Dispersion around an industrial site

In the PhD work of Emmanuel Demael (to be defended at the end of 2007) the first objective was to compare Mercure\_Saturne with models which are classically used for these applications (Gaussian plume models). The differences were quantified and explained, in particular for the behavior very near the source (Figure 3). The work has then followed with the simulation of two actual industrial sites, including buildings and topography, for which the mesh and simulation domain were 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 is therefore characterized by a very complex topography. For these industrial sites detailed wind tunnel measurements are also available and are used for the comparison for both the dynamical fields (wind and turbulence) and the dispersion fields (concentrations 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).

#### Key reference:

Demaël, E. and Carissimo, B. (2006). A comparison between Eulerian CFD and Gaussian Plume models on Prairie Grass Dispersion Experiment. J. Applied Meteor. Accepted for publication

#### Wind potential estimates

In this area, most current studies use very simple linearized models that have shown several limitations in very complex terrain. 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" created in very large wind farms when a large set of wind mills modifies the local flow and can reduce the energy potential (and may modify the local temperature). This work started in 2005 and is performed by introducing this masking effect in Mercure\_Saturne by ways of a drag within the flow (PhD work of Laurent Laporte). Results in two dimensions have already been obtained (Figure 4). The classical case of the Askervein hill has also been carried out to check the modeling results. Finally a real site in southern France will be studied both numerically with Mercure\_Saturne and with a field campaign involving meteorological masts and sodars.

#### Key reference:

Laporte, L. (2006). Simulation d'un sillage d'éolienne avec le code mercure\_saturne. Technical Report H-I88-2006-04532, EDF

#### Small scale reactive dispersion

A chemical mechanism describing the fast atmospheric chemical reactions was coupled to Mercure\_Saturne. The focus is on the  $NO/NO_2$  conversion just after emission. This reactive version of Mercure\_Saturne was compared to data measured in a Copenhagen street, the Jagtveg Street. This data base has already been used for box models. The results were satisfactory and the reactive version of Mercure\_Saturne clearly led to a much better estimation of chemical concentrations in general when the chemical regime is standard (just a few cases were found anomalous).

Additional diagnostics were performed. Computed spatial average concentrations in the street canyon were found to be close to single pointvalues found next to the windward side. The  $NO_2$  roof fluxes were found to be very sensitive to ozone background concentrations. The Mercure\_Saturne reactive version is currently used to study the efficiency of new building materials proposed to reduce  $NO_x$  pollution near busy streets (some comparisons have been performed





Figure 3: Top left: view of the wind tunnel experiment (ECL/IRSN). Top right: simulated concentration field. Bottom: comparison of concentration profiles between wind-tunnel data, Mercure\_Saturne and ADMS 3.0 simulations for the release on the chimney (vertical profile at 400 m in built-up area) (Emmanuel Demael PhD Thesis).



Figure 4: Mercure\_Saturne 3D simulation of a Rutland wind turbine. Stream lines are colored depending on the turbulent kinetic energy. The mesh and the hub are colored according to the wind speed values (Laurent Laporte PhD Thesis).



Figure 5: Numerical simulation of the reactive dispersion of traffic emissions in a street canyon using Mercure\_Saturne. The wind is at  $45^{\circ}$  angle from the canyon axis. Stream lines indicate the circulation in the street, composed of a classical vortex motion combined with a flow along the canyon. The vertical cross sections indicate respectively : the turbulence with its maximum at roof level, the vertical motion giving a clear signature of the vortex motion and the CO concentration from traffic emissions with a maximum on the leeward side of the street.

with data from the PICADA experiment).

#### Key reference:

Lacour, S. and Schmitt-Foudhil, H. and Carissimo, B. (2007). Detailed modelling of  $NO_x$  and  $NO_2$  dispersion in a street canyon. *Atmos. Env.* Submitted

#### Estimation of pollution induced by tunnels

A project was led with CETU in order to assess the pollution induced by tunnels (Stéphanie Lacour).

The flow velocity inside a tunnel fluctuates due to the unsteady forces related to the vehicular flux. Periodic boundary conditions at the tunnel exit were established in order to take into account heavy duty vehicles passing through the tunnel portal. The reactive version of Mercure\_Saturne was used in order to describe the impact of a tunnel plume. Comparison between passive and reactive dispersion under various pollution situations were performed in order to estimate the impact on the NO<sub>2</sub> concentrations. NO<sub>2</sub> is systematically underestimated in the case of passive dispersion, especially when the ozone concentrations are high. The discrepancy between the reactive and the passive models is less pronounced when the ozone concentrations around tunnel portal. The results were taken into account for the "User's Guide of Air Pollution Study for Tunnels" written by CETU.

An alternative approach, based on a short-range version of Polair3D, was developed for impact studies of roads and tunnels. A classification of pollution was proposed in order to distinguish the "background" component and the "local" component. Some strategies were 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 near the emission point.

#### Key references:

Albriet, B. and Lacour, S. (2003). Etude de la dispersion réactive d'un rejet tunnel dans une rue canyon. Rapport de contrat CETU. Technical Report 2003-6, CEREA

Lacour, S. (2005b). Estimation de la distribution des concentrations horaires annuelles et de leur variabilité à partir d'un nombre limité de simulations. Rapport de contrat CETU. Technical Report 2003-49, CEREA

#### Estimation of pollution near a road in an urban aera

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 near a road work place were extracted from this database. Non-parametric regressions were used to select the data suitable for linking air concentrations to emissions. A dispersion model was used to find out the maximal impact on measured concentrations.

#### *Key reference*:

Lacour, S., Ventura, A., Rangod, N., Carissimo, B., and Jullien, A. (2006b). How to estimate

roadworks emissions factors from traffic and air quality monitoring measurements: a methodological approach. Technical Report 2006-51, CEREA

## Indoor Air Quality

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

## *Key reference*:

Lacour, S. and Sportisse, B. (2007). Estimation of indoor deposition velocity for ozone with a simplified reactive box model. *Atmos. Env.* In revision



Figure 6: The different processes that influence the composition and the size-distribution of aerosols.

## 2.2 Multiphase modeling (group leader: Karine Kata-Sartelet)

The activity of the group is focused on the development and the validation of two multiphase models to be hosted by three dimensional models. 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).

## Development of MAM and SIREAM

The main part of the model development was 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 modeling activities at CEREA, the PAM project took part in the LISAIR Campaign at Paris (led by Partick Chazette, LSCE).

The development of the models MAM (Karine Kata-Sartelet) and SIREAM (Edouard Debry and Bruno Sportisse) 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  $\mu$ m to 10  $\mu$ 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 model ISORROPIA: 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). The different processes that influence the composition and the size-distribution of aerosols are shown in Figure 6.

## Key references:

Sportisse, B., Debry, E., Fahey, K., Roustan, Y., Sartelet, K., and Tombette, M. (2006). PAM project (multiphase air pollution): description of the aerosol models SIREAM and MAM. Technical Report 2006-08, CEREA. Available at http://www.enpc.fr/cerea/polyphemus/

Sartelet, K. N., Hayami, H., Albriet, B., and Sportisse, B. (2005b). Development and preliminary validation of a Modal Aerosol Model for tropospheric chemistry: MAM. *Aerosol Sci. and* 

Technol., 40(2):118–127

Debry, E., Fahey, K., Sartelet, K., Sportisse, B., and Tombette, M. (2007). A new SIze REsolved Aerosol Model: SIREAM. Atmos. Chem. Phys., 7(6):1537–1547

#### Numerical simulation of the GDE

Many appropriate algorithms were 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).

As the GDE for atmospheric aerosol involves several processes, the splitting strategy is important. Coupled methods are well suited methods to solve aerosol dynamics, nevertheless they usually need a large number of size discretization points to be stable. Figure 7 (left panel) shows the error as a function of splitting time step, for splitting and coupled strategies with different splitting sequences between coagulation and condensation.

In SIREAM, because the coagulation between two bins does not exactly fall into one bin, one has to redistribute the coagulation product among bins. Several possibilities to compute the partition coefficients have been proposed in the literature. The error induced by partition coefficients mainly lies in the upper part of the aerosol size spectrum, leading to a numerical diffusion towards large bins. Figure 7 (right panel) shows the error as a function of the number of bins for various kinds of partition coefficients.

In MAM, specific mode merging and splitting were developed to force modes to be of distinct size ranges throughout the simulations (Karine Kata-Sartelet and Bastien Albriet). The importance of mode splitting is stressed in Figure 8, which compares the number distribution during a high-nucleation episode, as computed with MAM (with or without mode splitting) and SIREAM (15 or 50 sections).

New algorithms were also proposed for the redistribution of aerosol Lagrangian bins on a fixed grid (Edouard Debry, Marilyne Tombette and Bruno Sportisse).

#### Key references:

Debry, E., Sportisse, B., and Jourdain, B. (2003). A stochastic approach for the numerical simulation of the General Dynamics Equation for aerosols. J. Comp. Phys., 184:649:689

Debry, E. and Sportisse, B. (2006c). Solving aerosol coagulation with size-binning methods. *Appl. Numer. Math.* doi:10.1016/j.apnum.2006.09.007

Debry, E. and Sportisse, B. (2006a). Numerical simulation of the General Dynamics Equation (GDE) for aerosols with two collocation methods. *Appl. Numer. Math.* In press

Sartelet, K. N., Hayami, H., Albriet, B., and Sportisse, B. (2005b). Development and preliminary validation of a Modal Aerosol Model for tropospheric chemistry: MAM. *Aerosol Sci. and Technol.*, 40(2):118–127

#### 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.



Figure 7: Numerical investigation of the GDE with sectional methods. Left: comparison of splitting and coupled methods for the Collocation/Rosenbrock method (Root Mean Square Error, RMSE, as a function of the splitting timestep). Right: evolution of the RMSE with respect to the number of bins for different partition algorithms.



Figure 8: Comparison of the number distribution during a high-nucleation episode with MAM (with or without mode splitting) and SIREAM (15 or 50 sections).



Figure 9: Percentage of SOA in  $PM_{10}$  over Europe for the year 2001. POLYPHEMUS is runned with two SOA models (AEC and SORGAM).

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 was developed: thermodynamic equilibrium is assumed for small aerosols and dynamic mass transfer is computed for large aerosols (Edouard Debry and Bruno Sportisse).

#### Key reference:

Debry, E. and Sportisse, B. (2006b). Reduction of the condensation/evaporation dynamics for atmospheric aerosols: theoretical and numerical investigation of hybrid methods. J. Aerosol Sci., 37(8):950–966

#### Aqueous-phase chemistry

Further developments concerned the aqueous phase of aerosols by adaptating the cloud model VSRM (Variable Size-Resolved Model, Carneggie Mellon University; Kathleen Fahey, Marilyne Tombette and Bruno Sportisse). This work is a follow-up of works devoted to the numerical modeling of aqueous-phase chemistry (Rafik Djouad and Bruno Sportisse). A simplified aqueous module has also been developed for the description of sulfate production in clouds and is currently under test (Marilyne Tombette).

#### Key reference:

Djouad, R., Audiffren, N., and Sportisse, B. (2003a). Sensitivity analysis using automatic differentiation applied to a multiphase chemical mechanism. *Atmos. Env.*, 37(22):3029:3038

#### Modeling of Secondary Organic Aerosols

The modeling of Secondary Organic Aerosols (SOA) is a challenging issue of aerosol modeling. In previous studies over Europe with Polyphemus and the organic module SORGAM, the concentrations of SOA are under-estimated. The development of a new SOA model has been initiated by Edouard Debry in a joint project with Christian Seigneur (AER and associate researcher at CEREA). The objective is first to update the organic aerosol model for a better description of the hydrophilic/hygrophobic behavior of aerosols, and second to take into account two new SOA precursors (sesquiterpenes and isoprene).

As preliminary results, Figure 9 shows the percentage of SOA in  $PM_{10}$  obtained with the

organic module previously used (SORGAM) and with the new module over Europe. The concentrations of SOA are higher with the new module, which is more realistic.

#### Key reference:

Debry, E. and Seigneur, C. (2007). Tracking organic particulate matter in Europe with the Polyphemus system : development of the SIREAM/AEC module. J. Geophys. Res. In preparation

#### 3D parameterizations for multiphase models

To couple the 3D Chemistry Transport Model Polair3D to the multiphase models SIREAM and MAM, other processes are 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, Karine Kata-Sartelet, Edouard Debry, Yelva Roustan). Sea-salt emissions are parameterized with specific approaches (Karine Kata-Sartelet). The aerosol water content, which is used to compute the aerosol wet diameters, is parameterized using an updated Gerber scheme (Edouard Debry). Specific works were devoted to the parameterization of in-cloud and below-cloud scavenging for gases (Bruno Sportisse).

#### *Key references*:

Sportisse, B. and Du Bois, L. (2003). Numerical and theoretical investigation of a simplified model for the parameterization of below-cloud scavenging by falling raindrops. *Atmos. Env.*, 36:5719–5727

Sportisse, B. and Djouad, R. (2003). Mathematical investigation of mass transfer for atmospheric pollutants into a fixed droplet with aqueous chemistry. J. Geophys. Res., 108(D2):4073

Debry, E. (2007). Optimisation de la formule de Gerber. Technical Report 2007-16, CEREA

Sartelet, K. (2006). Generation of sea-salt aerosols in Polyphemus. Technical Report 2006-12, CEREA

#### Validation at regional/continental scales

The POLYPHEMUS system hosts the coupling of the 3D Chemistry Transport Model Polair3D to SIREAM. This was 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 was validated by comparison to data at regional scale over Tokyo (Karine Kata-Sartelet).

To illustrate the results obtained at the regional scale, Figure 10 compares the  $PM_{10}$  concentrations at a station (Gennevilliers) over Greater Paris.

At the continental scale, for inorganic components of PM over Europe in 2001, Table 4 shows the observed mean, the simulated mean, RMSE, correlation for different databases (EMEP, Airbase and BDQA). The obtained results are satisfactory and correspond to the state-of-thescience. Strong disparities between the observational databases are observed.

Studies to assess the sensitivity of aerosol concentrations to different physical processes (such as coagulation, mass transfer by condensation/evaporation, 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 and Tokyo. For example, Figure 11



Figure 10: Time series of measured versus simulated  $PM_{10}$  concentrations at station Gennevilliers (Paris suburb) for April-October 2001.

	Database	Stations	Obs.	Mod.	RMSE	corr
			mean	mean		
$PM_{10}$	EMEP	26	16.9	15.4	12.5	55.1
	AirBase	537	25.4	15.2	17.0	44.9
	BDQA	23	19.8	15.5	9.6	57.7
$PM_{2.5}$	EMEP	17	12.6	8.3	8.6	54.4
Sulfate	EMEP	57	2.5	2.0	1.7	55.6
	AirBase	11	1.9	2.3	1.7	49.4
Nitrate	EMEP	14	2.6	4.0	3.1	41.3
	AirBase	8	3.5	4.3	2.7	71.7
Amm.	EMEP	9	1.8	2.0	1.3	51.9
	AirBase	8	1.8	2.0	0.9	74.4
Sodium	EMEP	3	1.3	2.4	2.2	62.8
Chloride	AirBase	7	0.9	3.1	3.5	69.8

Table 4: Model-to-data comparison for POLYPHEMUS over Europe in 2001 for aerosols: number of stations (from the networks EMEP, Airbase and BDQA), observed mean ( $\mu g m^{-3}$ ), simulated mean ( $\mu g m^{-3}$ ), RMSE ( $\mu g m^{-3}$ ), correlation (%).



Figure 11:  $PM_{2.5}$  concentration of nitrate at Kudan (Greater Tokyo) for 9 and 10 December 1999. Different configurations of the aerosol model are investigated.



Figure 12: Average simulated AOT at 440nm over year 2005. Aeronet stations are drawn. Marilyne Tombette PhD Thesis.

compares to data the results obtained at Kudan (Greater Tokyo) with Polair3D, CMAQ, Polair3D with heterogeneous reaction  $(N_2O_5)$ , without condensation, with a hybrid scheme for condensation/evaporation instead of assuming thermodynamic equilibrium.

## *Key references*:

Tombette, M. and Sportisse, B. (2007). Aerosol modeling at regional scale: Model-to-data comparison and sensitivity analysis over Greater Paris. *Atmos. Env.* In press

Sartelet, K., Debry, E., Fahey, K., Tombette, M., Roustan, Y., and Sportisse, B. (2007a). Simulation of aerosols and gas phase species over Europe with the POLYPHEMUS system. Part I: model-to-data comparison for year 2001. *Atmos. Env.* doi:10.1016/j.atmosenv.2007.04.024

Sartelet, K., Hayami, H., and Sportisse, B. (2007b). Dominant aerosol processes during high-pollution episodes over Greater Tokyo. J. Geophys. Res. Accepted for publication

Sartelet, K., Taghavi, M., and Musson-Genon, L. (2006). Etude de l'impact du CPT Martigues sur la pollution particulaire dans la région de Marseille-Berre. Technical Report 2006-34, CEREA. Rapport pour la Mission Thermique EDF

Tombette, M., Fahey, K., Sartelet, K., and Sportisse, B. (2005b). Aerosol modelling at regional scale: a sensitivity study with the Polyphemus platform. In *Proceedings of GLOREAM 2005*. Also as Report CEREA 2005-50

## **Aerosol Optical Thickness**

Specific radiative modules have been developed and coupled to the outputs of POLYPHEMUS. The objective is for instance to compute the Aerosol Optical Thickness from outputs of the aerosol model SIREAM (Marilyne Tombette, Patrick Chazette and Bruno Sportisse). Figure 12 shows the average simulated AOT at 440 nm for 2005. High values are observed in North Africa due to Saharan dust. Comparisons have been made to Aeronet data. A sensitivity study shows there are large uncertainties in the computation of AOT.

## Key reference:

Tombette, M., Chazette, P., and Sportisse, B. (2007). Simulation of the Aerosol Optical Thickness over Europe with a 3D size-resolved aerosol model: Comparisons with AERONET data. J.

#### Sulfate concentration in December 2001 (µg m<sup>-3</sup>)



Figure 13: MICS Results: concentration of sulfate over Asia for December 2001 for the set of available models. Polair3D corresponds to Model 8.

Geophys. Res. In submission

## 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 were implied in the 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. Figure 13 shows the concentration of sulfate over Asia for December 2001. A comprehensive sensitivity analysis was also performed. The variability of sulfate and nitrate concentrations induced by using different CTMs is compared to the variability induced by comparing different parameterizations in the aerosol module (Karine Kata-Sartelet).

## Key references:

Sartelet, K., Hayami, H., and Sportisse, B. (2007c). MICS-Asia Phase II: sensitivity to the aerosol module. *Atmos. Env.* doi:10.1016/j.atmosenv.2007.03.005

Carmichael, G., Sakurai, T., Streets, D., Hozumi, H., Ueda, H., Park, S., Fung, C., Han, Z., Kajino, M., Engardt, M., Bennet, C., Hayami, H., Sartelet, K., Holloway, T., Wang, Z., Kannari, A., Fu, J., Matsuda, M., Thongboonchoo, N., and Amann, M. (2007). MICS-Asia II: Model intercomparison and evaluation of ozone and relevant species. *Atmos. Env.* Accepted for publication



Figure 14: Variation of the number distribution of particles as a function of the distance from the road. The condensation of semi-volatile organics is ignored in the left panel while it is taken into account in the right panel. Bastien Albriet PhD Thesis.

#### Local scale

Polair3D-MAM was used to simulate aerosol formation and dispersion in the vicinity of roads (Bastien Albriet, Stéphanie Lacour). Traffic emission leads to high concentrations of sulphuric acid and to high nucleation events (ultra-fine particles of diameter around 1 nanometer). A crucial point is to follow the number distribution, a focus of the future reglementation. Current models only describe the mass distribution. Several measurement campaigns put in evidence the rapid growth of the aerosol diameter close to a traffic source. MAM was coupled to Mercure\_Saturne and process studies were performed in order to evaluate the competition among dilution, nucleation, coagulation and condensation/evaporation. A sensitivity analysis showed that semi-volatile organic compounds can significantly contribute to the growth of nanoparticles by condensation, as illustrated in Figure 14.

#### *Key reference*:

Albriet, B. (2007). Modélisation numérique des aérosols à l'échelle locale. PhD thesis, ENPC

#### Resuspension

In the framework of a project with CEA, models of aerosol resuspension were studied (Stéphanie Lacour). This preliminary work led to a synthesis of available models, parameterizations and measured data to be used by the International Atomic Energy Agency for its Handbooks. A second part of the work is devoted to model developments.

#### *Key reference*:

Lacour, S. (2005c). Resuspension de radionucléides. Rapport de contrat CEA. Technical Report 2005-30, CEREA

#### Aircraft soot

For "aircraft" particles, a project coordinated by ONERA and funded by Primequal/Predit, has just started for the modeling of soot (Stéphanie Lacour, Bastien Albriet, Karine Sartelet).

#### Key reference:

Lacour, S. and Kata-Sartelet, K. (2006). Modélisation du veillissement des suies d'avions, rapport d'avancement du projet CAAT. Technical Report 2006-48, CEREA



Figure 15: POLYPHEMUS is a Cyclops in Odyssey whose name roughly means "multiple speeches". It is consistent with the goals of the system. Left panel: logo. Right panel: flowchart.

#### 2.3 Modeling at regional and continental scales (group leader: Vivien Mallet)

The team focuses on air quality modeling from regional to continental scales. The applications are photochemistry (ozone), heavy metals (such as 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 modeling system, the POLYPHEMUS platform (http://www.enpc.fr/cerea/polyphemus/, Figure 15). Polyphemus is a Cyclops in Odyssey whose name roughly means "multiple speeches". It is consistent with the goals of the system, that is, gathering on the same platform:

- several models: with Gaussian, Eulerian, ... formulations;
- several scales: from small/local scale to continental scale;
- multiple polluants: passive, radionuclides, photochemistry, aerosols, POP, ...
- processing from many inputs (meteorological models, ground data);
- many advanced methods: data assimilation, ensemble forecasting, models coupling, ...

It is written as much as possible with modern computer languages (mainly C++), and only perennial and scalable developments are included. POLYPHEMUS is open. It is open source, distributed under GNU GPL, well documented (for users and developers), and released on a regular basis. Open also means that contributions from other teams are welcome. The developments consortium includes in the core ENPC, EDF and INRIA, and IRSN and INERIS as supporting partners.

Many joint projects with other teams have already been initiated with this modeling 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, Exiopol and Heimtsa) or modeling of the short-range dispersion of pollutants (for INERIS and DGA).

#### Development of the POLYPHEMUS platform

The new approach with POLYPHEMUS is to split the modeling system into 4 distinct levels:

- Physical parameterizations and preprocessing with the object-oriented AtmoData library (potentially shared with any team involved in atmospheric modeling, 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 (for instance Polair3D or Castor, a C++ clone of Chimere, 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-modeling approach through the available parameterizations. This system has been used for numerous applications (itemized below), implying a growing number of teams in joint projects.

Moreover, a training session for the users of POLYPHEMUS was organized in March 2007 (with 13 participants from INERIS, IRSN, CEA, ARIA Technology, University of Lille, Ministry for Transport and EDF/CIDEN). A training session devoted to inverse modeling and data assimilation will be organized in June 2007 in Santiago de Chile for South America (with more than 10 expected participants coming from Chile, Argentina and Brazil).

POLYPHEMUS is also used in courses at ParisTech (ENPC and ENSTA: "Air Pollution", "Computational physics for Environment", "Data assimilation and inverse modeling for geophysical flows"). The improvement of POLYPHEMUS for the ParisTech OpenCourse Ware will be funded by ParisTech for summer 2007.

#### *Key references*:

Mallet, V., Quélo, D., Sportisse, B., Ahmed de Biasi, M., Debry, É., Korsakissok, I., Wu, L., Roustan, Y., Sartelet, K., Tombette, M., and Foudhil, H. (2007b). Technical Note: The air quality modeling system Polyphemus. *Atmos. Chem. Phys. Discuss.*, 7(3):6,459–6,486

Ahmed de Biasi, M., Mallet, V., Korsakissok, I., Debry, E., and Wu, L. (2007). Polyphemus 1.1. User's Guide. Technical Report 2007-17, CEREA

Polyphemus website: http://www.enpc.fr/cerea/polyphemus/

#### Numerical analysis for Chemistry-Transport Models

Solving the Partial Differential Equations that describe the atmospheric dispersion of atmospheric reactive species is still a challenging issue due to the wide range of timescales and the large dimension of the resulting systems.

A comprehensive study of the numerical issues was investigated for a few real cases (air quality modeling over Europe for summer 2001 and simulation of the Chernobyl accident).

Another specific point is related to the so-called mass consistency problem related to the off-line coupling between atmospheric dispersion models and meso-scale numerical models that provide meteorological fields such as wind velocity.

#### Key references:

Mallet, V., Pourchet, A., Quélo, D., and Sportisse, B. (2007a). Investigation of some numerical issues in a Chemistry-Transport Model: gas-phase simulations. *J. Geophys. Res.* Accepted for publication

Sportisse, B., Quélo, D., and Mallet, V. (2007). Impact of mass consistency errors for atmospheric dispersion. *Atmos. Env.* Accepted for publication



Figure 16: Ensemble forecast with the POLYPHEMUS system (ozone, summer 2001). Left panel: an *ensemble* for hourly profiles of ozone (averaged over Europe and over four months). The points indicate the ensemble forecast. Right panel: ensemble relative variance (in %).

#### Air quality ensemble forecast

Due to the wide range of uncertainties, a promising approach for air quality forecast is related to ensemble techniques (Figure 16). The PhD work of Vivien Mallet (defended in December 2005) focused on the assessment of the *a priori* uncertainties in the outputs of a Chemistry-Transport Model through Monte Carlo methods and a multi-modeling 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 Prév'air platform of INERIS was achieved (Hervé Njomgang, Christelle Bordas, Yelva Roustan and Vivien Mallet) and the computation of an extensive set of model-to data statistics was initiated (Christelle Bordas and Vivien Mallet). The POLYPHEMUS platform has been performing an operational test since July 2006, on the Prév'air platform for ensemble photochemical forecast.

#### Key references:

Mallet, V. and Sportisse, B. (2006b). Ensemble-based air quality forecasts: a multi-model approach applied to ozone. J. Geophys. Res., 111(D18):18302

Mallet, V. and Sportisse, B. (2006d). Uncertainty in a chemistry-transport model due to physical parameterizations and numerical approximations: an ensemble approach applied to ozone modeling. J. Geophys. Res., 111(D01302)

#### Mercury and heavy metals

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

The development of the mercury model was completed with two available models (a simple one based on the so-called Petersen formulation and a model based on a multiphase chemical mechanism, Figure 17). Model-to-data comparisons were performed for year 2001 over Europe (Figure 18). Moreover, an innovative sensitivity analysis was developed and inverse modeling with respect to boundary conditions was performed (see Section 2.4). Another model version was developed with the coupling to the gas-phase mechanism RACM, which showed that only



Figure 17: Chemical mechanism for mercury developed by Yelva Roustan in his PhD work on the basis of state-of-the-science models.



Figure 18: Comparison of model outputs from POLAIR3D and observational data for wet mercury (dissolved in rain droplets). Monthly averaged values in g km<sup>-2</sup> yr<sup>-1</sup>. The modified values are computed with the "right" precipitation fields.

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 were 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 model SIREAM. An intercomparison and model-to-data comparisons were performed.

#### Key reference:

Roustan, Y. and Bocquet, M. (2006b). Sensitivity analysis for mercury over Europe. J. Geophys. Res., 111(D14304)

#### Air Quality Modeling over Lille

CEREA took 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 modeling chain was 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 was validated over year 1998 by model-to-observation comparisons with good results.

A joint project with the University of Lille (Valérie Nollet) has been submitted to the Nord-Pas-de-Calais region to build an operational air quality forecast system at regional scale.

#### Key references:

Quélo, D., Mallet, V., and Sportisse, B. (2005a). Inverse modeling of  $NO_x$  emissions at regional scale over Northern France. Preliminary investigation of the second-order sensitivity. *J. Geophys. Res.*, 110(D24310)

Quélo, D., Lagache, R., and Sportisse, B. (2004). Etude de l'impact qualité de l'air des scénarios PDUs sur Lille à l'aide du modèle de Chimie-Transport Polair3D. Technical Report 2004-28, CEREA. Rapport PREDIT

Lagache, R., Declercq, C., Quélo, D., Sportisse, B., Palmier, P., Quetelard, B., and Haziak, F. (2006a). Evaluation du PDU de Lille-Métropole sur le trafic, les concentrations de polluants atmosphériques et la mortalité. In *Actes de la 15ième conférence sur les transports et la pollution de l'air* 

#### Impact studies at continental scale

A work assessed the sensitivity of ozone concentrations with respect to emissions (Vivien Mallet and Bruno Sportisse). The sensitivity study dealt with the temporal, spatial and chemical features of  $NO_x$  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 (Yelva Roustan). The project should allow joint works with EMEP/West and IER Stuttgart. Two followers of NEEDS (HEIMTSA and EXIOPOL) have been retained in FP6 and have begun in 2007.

Moreover, POLYPHEMUS is used by EDF Polska and by the consortium of associated Polish Universities (especially AGH University of Science and Technology, Krakow). The objective is to assess air quality in Polska and the related transboundary fluxes with a focus on Krakow.

In the framework of the CAFE process (Clean Air For Europe/National Emission Ceiling), the impact for the year 2005 of the emissions from the French thermal power plants was computed for the Fossil-Fired Generation and Engineering Department of EDF (Figure 19).



Figure 19: Impact for the year 2005 of the emissions from the French thermal power plants (EDF and SNET). The target is  $PM_{2.5}$ . The indicator is a relative impact computed in % by comparing a reference simulation and a simulation without the emissions.

#### Key references:

Mallet, V. and Sportisse, B. (2005). A comprehensive study of ozone sensitivity with respect to emissions over Europe with a chemistry-transport model. J. Geophys. Res., 110(D22)

Roustan, Y., Lasry, F., and Sportisse, B. (2007). Modélisation de l'impact des émissions des centrales EDF et SNET en France sur le transport atmosphérique des  $PM_{10}$  et  $PM_{2.5}$ . Technical Report 2007-9, CEREA

#### **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. POLYPHEMUS is the support of the new operational forecast system at IRSN for the regional scale.

An extensive work (Denis Quélo and Bruno Sportisse) was devoted in 2005 and 2006 to the simulation of the Chernobyl accident. A sensitivity analysis was 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). Another sensitivity study based on adjoint modeling led to a quantitative description of any measurement sensitivity to dry deposition and wet scavenging parameterization schemes for the Chernobyl accident (Marc Bocquet and Yelva Roustan).

Other applications dealt with the simulations of the ETEX exercise and of the Algeeiras accident (Monika Krysta and Marc Bocquet).

Key references:



Figure 20: Model-to-data comparison (scatter plot) for cesium 137 for the first two weeks after the Chernobyl release.

Sportisse, B. (2007c). A review of parameterizations for modeling dry deposition and scavenging of radionuclides. *Atmos. Env.*, (41):2683–2698

Quélo, D., Krysta, M., Bocquet, M., Isnard, O., Minier, Y., and Sportisse, B. (2007). Validation of the POLYPHEMUS system: the ETEX, Chernobyl and Algeciras cases. *Atmos. Env.* doi:10.1016/j.atmosenv.2007.02.035

#### Escompte

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

For the Fossil-Fired Generation and Engineering Department of EDF, a dedicated study was 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.

#### *Key references*:

Taghavi, M., Musson-Genon, L., and Sportisse, B. (2004). Impact des rejets de la centrale thermique de Martigues sur la qualité de l'air. Modélisation avec Polair3D. Technical Report 2004-27, CEREA. Rapport pour la Mission Thermique EDF

Sartelet, K., Taghavi, M., and Musson-Genon, L. (2006). Etude de l'impact du CPT Martigues sur la pollution particulaire dans la région de Marseille-Berre. Technical Report 2006-34, CEREA. Rapport pour la Mission Thermique EDF

## Multi-media modeling

Impact of air quality pollutants on human health is a new field of application of our modeling system, with a focus on thermal power plant impact. In the PhD thesis of Solen Quéguiner, the outputs of POLYPHEMUS for lead and cadmium (air concentration and ground deposition) were coupled to the ground transfer model OURSON developed at LNHE (Department of EDF R&D). OURSON allows to describe pollution in the ecosystems, the cultures and hydrological networks in order to estimate doses for human beings.

A model devoted to Persistent Organic Pollutants (POP) is under development and validation within POLYPHEMUS.

#### *Key references*:

Quéguiner, S. (2006b). Note de principe "OURSON-atmosphère" pour les métaux lourds. Equations de transfert dans l'environnement terrestre. Technical Report H-I88-2007-00501-FR, EDF R&D

Quéguiner, S. (2006a). Description et modélisation des Polluants Organiques Persistants dans le modèle atmosphérique Polair3D. Technical Report H-I88-2007-00912-FR, EDF R&D

## Hemispheric modeling

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 the base CTM of POLYPHEMUS was initiated with simple modifications of the limited area model (Denis Wendum).

#### Key reference:

Wendum, D. (2006). Passage du code Polair3D en mode global ou hémisphérique: Note de principe. Technical Report 2006-33, CEREA

Model	FB	NMSE	MG	VG	Corr	FAC2
Observations	0.00	0.00	1.00	1.00	1.00	1.00
ADMS	0.56	3.62	—	_	0.64	0.46
AERMOD	0.00	1.87	—	—	0.75	0.76
ISCST3	0.06	1.76	_	—	0.72	0.62
Polyphemus - Briggs	0.0	1.83	1.23	1.47	0.78	0.74
Polyphemus - Doury	0.46	4.47	1.05	7.16	0.42	0.27
Polyphemus - Similarity theory	-0.08	1.25	0.72	1.57	0.82	0.61

#### **Plume-In-Grid models**

Table 5: BOOT statistics for several Gaussian models: comparison of maximum arc concentration for simulation and observation - 43 trials in Prairie Grass Experiment.

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). Some statistics for the Prairie Grass Experiment are given in Table 5 (see also Figure 21).

A Plume-In-Grid ability has also been developed in POLYPHEMUS (to date for passive dispersion). These works are applied to risk modeling in joint projects with DGA and INERIS for biological tracers and aerosols.



Figure 21: Scatter plot of maximum arc concentrations for observations and simulations with similarity theory parameterization. Prairie Grass experiment, 43 trials. Run with one model configuration of POLYPHEMUS.

## Key reference:

Korsakissok, I. (2007). Performance evaluation of Polyphemus Gaussian models with Prairie Grass experiment. Technical Report 2007-15, CEREA



Figure 22: Left: A two-dimensional representation of the reconstructed source of ETEX-I, integrated in time. The inversion is based on the MEM principle. The reconstruction is based on all available positive measurements, the triangles mark the stations whose data were used in this inversion. Right: temporal profile of the solution in the true release grid-cell. 342 kg are recovered (222 kg in the correct grid-cell) against 340 kg known to have been released.

## 2.4 Inverse modeling and data assimilation (group leader: Marc Bocquet)

This group is also part of the INRIA/ENPC project hosted by CEREA, CLIME, devoted to data assimilation and modeling systems for environmental applications. A subsequent action of CLIME, the ADOQUA (Data Assimilation for Air Quality) cooperative action from INRIA, promotes scientific exchange between the three INRIA projects CLIME, ASPI and MOISE.

#### Inverse modeling of tracer source

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 of 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 (Jean-Piere Issartel and Jérôme Baverel). The problem is more intricate for diffuse emissions. A geometric interpretation of the retroplumes was proposed by Jean-Pierre Issartel and applied to the retrieval of arsenic emissions in Chile (joint project with Laura Gallardo Klenner, CMM Chile).

Moreover, new approaches have been proposed for inverse modeling of passive tracers, using the maximum entropy on the mean principle (MEM, Marc Bocquet). The main advantage of this set of methods is the way the a priori knowledge is taken into account. In particular the positivity of the source can be numerically enforced, rigorously and efficiently. New cost functions, one for each prior, are generated by the MEM principle and can be especially devised for several types of application. They can be generated both in the state space or in the dual space of observations. The generated cost function is 4D-Var (4D-Var PSAS in the dual space), when the hypotheses on the source and the errors are Gaussian. In this latter case, it was shown to be equivalent to a projection onto the basis of retroplumes. These methods can be applied to accidental releases (for instance to the ETEX campaign), where they have been demonstrated to be very efficient. Besides, the optimization of the cost function can be performed both in the state space and in the space of observations (dual approach). When the number of observations is low compared to the number of unknown variables, the dual approach proves numerically fast. The method were tested on ETEX-I and ETEX-II. As for ETEX-I, the total mass is recovered and the correct grid-cell of the release is found, with about 65~% of the total mass in this grid cell (Figure 22).

Another work is devoted to the assessment of the influence of grid resolution in the frame-


Figure 23: Total PMCH (340 kg were released in ETEX-I in Monterfil) reconstructed mass (full line) and reconstructed mass around Monterfil (dashed line) against time (a). Relative entropy for the source (full line) and relative entropy for the errors (dashed line) against time (b). The time origin corresponds to 23 October 1994 15:00 UTC, one hour before the start of the release.

work of inverse problems with or without entropy regularization. The singular points in the retrieved sources around the monitoring stations are then explained. The existence of an optimal resolution has been proved and an indicator of the inverse modeling procedure has been proposed (Marc Bocquet).

### Key references:

Bocquet, M. (2005c). Reconstruction of an atmospheric tracer source using the principle of maximum entropy I : Theories. *Quart. J. Roy. Meteor. Soc.*, 131(Part B(610)):2191–2208

Bocquet, M. (2005d). Reconstruction of an atmospheric tracer source using the principle of maximum entropy II : Applications. *Quart. J. Roy. Meteor. Soc.*, 131(Part B(610)):2209–2223

Bocquet, M. (2005a). Grid resolution dependence in the reconstruction of an atmospheric tracer source. *Nonlinear Process in Geophysics*, 12:219–234

#### Advanced data assimilation for pollutants of linear physics

A natural follow-up of previous works was to use the best estimation of an accidental source of pollutant to forecast the pollutant plume. This was explained and demonstrated on ETEX-I (Marc Bocquet). Besides, one can adapt this technique to emergency situations where data come as the crisis unfolds, and where the best forecast is needed throughout the crisis. It was shown that in the context of ETEX-I, 15 hours were necessary to identify the source term, for a satisfying forecast of the plume to be given (Figure 23).

#### Key reference:

Bocquet, M. (2007b). High resolution reconstruction of a tracer dispersion event: application to ETEX. *Quart. J. Roy. Meteor. Soc.* In press

#### Short-range inverse modeling

Since 2003, CEREA has been implied in a joint project with IRSN devoted to Inverse Modeling of an Accidental Release in the atmosphere (MIRA). A preliminary work was accomplished in 2004-2005 with twin experiments (Denis Quélo and Bruno Sportisse). Some experiments were



Figure 24: Reconstructed profiles of an accidental release of Cs-137 in Algeciras, Spain, using especially devised cost-function. Some  $[2.96 \times 10^{11}; 2.96 \times 10^{12}]$  Bq released between 01:00 and 03:00 UTC on 30 May 1998. Time of the release corresponds to 215-217 on the horizontal axis. Reconstructed activity:  $2.96 \times 10^{12}$  Bq.

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 was 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 was also completed with cross validation techniques (Monika Krysta, Marc Bocquet and Bruno Sportisse).

#### Key references:

Quélo, D., Sportisse, B., and Isnard, O. (2005b). Data assimilation for short-range dispersion of radionuclides: a case study for second-order sensitivity. *J. Environ. Radioactivity*, 84:393–408

Krysta, M., Bocquet, M., Sportisse, B., and Isnard, O. (2006). Data assimilation for short-range dispersion of radionuclides: an application to wind tunnel data. *Atmos. Env.*, 40(38):7267–7279

#### Inverse modeling of radionuclides accidental release at European scale

First experiments in inverse modeling 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 localization of sources were analytically derived and tested numerically on two hypothetical accidents in Europe. The sensitivity of the inversion with respect to the monitoring network spatial distribution, the meteorological conditions, the number of observations, was studied. The methods were then applied to the Algeciras radioactivity release incident (Monika Krysta and Marc Bocquet). The temporal inversion leads to satisfactory results while a reasonable 3D reconstruction is proven to be impossible with the available data (Figure 24).

The MEM method was also applied to the Chernobyl accident (Xavier Davoine and Marc Bocquet). The location was supposed to be known, and a two-dimensional (temporal and vertical) profile is sought for. The isotopes available for long-range transport were investigated: <sup>131</sup>I, <sup>137</sup>Cs, and <sup>134</sup>Cs. It appeared that the inversions were very sensitive to the mass scale that entered the definition of the prior which enforces the positivity of the source, in addition to the usual ratio of covariances between background and errors. The L-curve semi-empirical approach



Figure 25: A typical solution of the Chernobyl source inversion problem based on a Bernoulli source prior, and a uniform Gaussian error prior. The left-hand-side figure (a) is a density graph representing the activity released per unit of time and unit of altitude (in Bq m<sup>-1</sup> s<sup>-1</sup>). The right-hand-side figure (b) are reconstructed hourly and day-to-day (dashed line) profiles of the iodine-131 release rate.

has been used to estimate the value of these parameters. The total activity reconstructed for the three species has been shown to be only within 10% to 30% of the previous official estimations (Figure 25).

#### Key references:

Krysta, M. and Bocquet, M. (2007). Source reconstruction of an accidental radionuclide release at European scale. *Quart. J. Roy. Meteor. Soc.*, 133:529–544

Davoine, X. and Bocquet, M. (2007). Inverse modelling-based reconstruction of the Tchernobyl source term available for long-range transport. *Atmos. Chem. Phys.*, 7:1549–1564

#### Inverse modeling of ozone precursors using variational assimilation

The use of 4D-Var techniques requires the development of the adjoint model of Polair3D (Denis Quélo). An application was the inverse modeling of  $NO_x$  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 was completed over the Lille region (May 1998) on the basis of observational data for ozone and  $NO_x$ . The control parameters are hourly coefficients applied to emissions of  $NO_x$  (Figure 26). The forecast of ozone and  $NO_x$  with the improved emission fluxes is significantly improved for the learning week and for the next two weeks after the learning period (Denis Quélo, Vivien Mallet and Bruno Sportisse).

#### Key reference:

Quélo, D., Mallet, V., and Sportisse, B. (2005a). Inverse modeling of  $NO_x$  emissions at regional scale over Northern France. Preliminary investigation of the second-order sensitivity. *J. Geophys. Res.*, 110(D24310)

#### Sensitivity analysis and inverse modeling of mercury over Europe

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



Figure 26: Optimized time distributions of  $NO_x$  emissions over different periods (Lille run).



Figure 27: Sensitivity to emissions of the mercury annual average modeled air concentration measurement. Application to transboundaries pollution issues for Germany (a), France (b) and the Czech Republic (c). In the case of the Czech Republic examples of monthly averaged sensitivities are also given to demonstrate the intra-year variability of the sensitivity ((d), (e) and (f)).



Figure 28: Monthly averaged ground measurement of gaseous mercury (in ng m<sup>-3</sup>) at four EMEP sites for the year 2001. The observations data of the first two stations are used for the assimilation process.

at continental scale. Adjoint methods were used in order to quantify the sensitivity of observational data of mercury over Europe with respect to emissions, initial conditions and boundary conditions (Yelva Roustan and Marc Bocquet). 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 (Figure 27, see also Section 2.3).

These tools were also 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 (Figure 28).

#### Key references:

Roustan, Y. and Bocquet, M. (2006b). Sensitivity analysis for mercury over Europe. J. Geophys. Res., 111(D14304)

Roustan, Y. and Bocquet, M. (2006a). Inverse modeling for mercury over Europe. Atmos. Chem. Phys., 6:3085–3098

#### Comparison of sequential and variational methods in Air Quality

German Torrès 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 were developed and some preliminary applications to an academic case were performed.



Figure 29: Left: time evolution of ozone concentrations against available observations at EMEP station Montandon, for the reference simulation (without assimilation), the simulation with assimilation (OI, EnKF, RRSQRT and 4D-Var). The assimilation is performed for a coarse model configuration with one day of assimilation (2001-07-01) followed by one day of prediction. The vertical line delimits the assimilation period. Right: time evolution of root mean square error of ozone concentrations compared with all available observations. The total RMSE over two days is 27.5 for reference, 18.9 for OI, 21.7 for EnKF, 22.1 for 4D-Var, and 24.4 for RRSQRT.

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 (Lin Wu and Vivien Mallet). A secondary aim is to study the impact of non-linearities in air quality data assimilation (main topic of ADOQA, a Research Action of INRIA). The drivers for 4D-Var and several variants of the Kalman filter are now implemented in POLYPHEMUS, and they are being extensively tested (Figure 29).

#### Key reference:

Mallet, V., Quélo, D., Sportisse, B., Ahmed de Biasi, M., Debry, É., Korsakissok, I., Wu, L., Roustan, Y., Sartelet, K., Tombette, M., and Foudhil, H. (2007b). Technical Note: The air quality modeling system Polyphemus. *Atmos. Chem. Phys. Discuss.*, 7(3):6,459–6,486

#### Ensemble methods for air quality forecast

Ensemble methods for air quality forecast (Vivien Mallet and Bruno 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.

#### Key reference:

Mallet, V. and Sportisse, B. (2006b). Ensemble-based air quality forecasts: a multi-model approach applied to ozone. J. Geophys. Res., 111(D18):18302



Figure 30: Monitoring networks (100 stations) optimized for the best extrapolation of radionuclides concentration fields over the French territory, on a yearly database of 7000 fictitious accidents. The red rhombuses represent the sources (civil nuclear sites), and the blue crosses represent the network stations. Each of the networks is optimized on the basis of a different cost function which is parametrised by  $\alpha$ . The last network results from a geometric optimization: no simulation is used.

#### Network design for atmospheric dispersion

A research project in network design for air quality started in January 2006 with the PhD work of Rachid Abida (ENPC/IRSN support). IRSN asked CEREA to help define its future aerosol station network for the evaluation of an accidental radionuclides release in France (Descartes project). The results of the preliminary work were given in a first report (Nikki Vercauteren and Marc Bocquet). A basis of 15000 radiological accident simulations were computed using POLAIR3D, for two types of accident, and one species (among three possible). An objective function was then defined to evaluate any monitoring network. The capability of a network to extrapolate activity measurements on the ungauged grid cells of the domain is the primary objective. The cost function is therefore a measure of the discrepancies between the extrapolation and the true values as read in the simulation database, for all accidents of the database. Several methods of extrapolation were considered: closest-point approximation, ordinary kriging, splines. A simulated annealing optimization was then performed, for a fixed number of stations, to reach a close to optimal network. The first phase of the work consisted in implementing this program using one month of simulations from the database, and developing the parallel algorithm (Lam MPI and POSIX threads) on the CEREA PCs. In the second phase (Rachid Abida and Marc Bocquet), the study was extended to one year of simulation. The sensitivity of the network performance to the number of stations was tested. One of the key result is the very high sensitivity of the design to the definition of the cost function, and in particular to the norm that pounders the discrepancies. It was shown that, because of the sharp gradients in an accidental dispersion, the usual least-square criterion arranges all stations around the source, neglecting the evaluation of the subsequent plume far way from the source (Figure 30). A milder norm was therefore advocated  $(l_1 \text{ or } l_{1/2} \text{ norm})$ .

A similar project is also carried out in a joint project with DGA (Irène Korsakissok, Vivien Mallet and Bruno Sportisse). The aim is to design and evaluate networks for defence applications at regional and local scale (on the battlefield). A tool was designed to evaluate networks performance in terms of detection probability and saturation time. It was tested on networks designed by taking the sensors that have the best detection probability or the best saturation time. A sensitivity study was also achieved for parameters such as wind speed and angle variation, the species type (biological, radioactive or chemical) and diameter to be detected, and the number of sensors in the network (Figure 31).

#### Key references:

Sportisse, B. and Quélo, D. (2002). Observational network design, adaptive observations and targeting strategies in atmospheric data assimilation: sketch of a methodological review. In *INRIA-CEA-EDF Summer School on Data Assimilation for Geophysical flows* 

Vercauteren, N. and Bocquet, M. (2006). Projet de développement d'un réseau automatisé de télésurveillance des particules radioactives dans l'air - Etude pour l'optimisation du réseau. Technical Report 2006-41, CEREA. Rapport de contrat IRSN

Korsakissok, I. and Sportisse, B. (2006). Simulations et évaluation de réseaux pour la détection de traceurs à l'échelle locale. Technical Report 2006-46, CEREA. Rapport de contrat DGA

Abida, R. and Bocquet, M. (2007). Projet de développement d'un réseau automatisé de télésurveillance des particules radioactives dans l'air. Etude pour l'optimisation du réseau. Rapport final. Technical Report 2007-7, CEREA. Rapport de contrat IRSN

Bocquet, M. (2007a). Construction optimale de réseaux de mesures : application à la surveillance des polluants aériens. Technical Report 2007-6, CEREA. Notes de cours ENSTA





Figure 31: Network design on a battlefield (regional scale). Map of detection probability at regional scale for all possible sensors, as well as the sensors positions for the ten sensors having the best detection probability.

#### Reduced models and propagation of uncertainties

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 (Rafik Djouad, Jaouad Boutahar and Bruno Sportisse).

#### Key references:

Djouad, R. and Sportisse, B. (2003). Solving reduced models in air pollution modelling. *Appl. Numer. Math.*, 44(1):49:61

Djouad, R., Sportisse, B., and Audiffren, N. (2003d). Reduction of multiphase atmospheric chemistry. *Journal of Atmospheric Chemistry*, 46:131–157

Sportisse, B. and Djouad, R. (2007). Use of Proper Orthogonal Decompositions for the reduction of atmospheric chemistry. J. Geophys. Res., 112(D06303)



Figure 32: Influence of the wind speed at 80 meters (measured by sonic anemometer) on bias (dotted lines) and standard deviation (solid lines) between sodar and sonic measurements, for 2 of the 3 tested sodars, during the campaign of winter 2005-2006.

# 2.5 Meteorological Measurements (group leader: Eric Dupont)

This activity has been existing at EDF-R&D for many years and was integrated in CEREA at the beginning of 2005. The projects are related to the needs of EDF for atmospheric dispersion at an industrial or urban site, and for wind energy resource assessment, in close link with the Mercure\_Saturne team. The field campaigns are primarily devoted to the constitution of data bases for numerical simulations, and to the tests of instruments, especially wind profilers (sodar, UHF radar). This activity involves 2,5 people.

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



Figure 33: Comparison between computation and measurement of wind speed at 80 m, for a one-year data set (December 2004 to December 2005), with two methods: one using normalized vertical profiles measured by sodar (left panel), one using a simple power law (right panel).

## Sodars intercomparison

2005 was dominated by a campaign of intercomparison for sodars, in collaboration with CSTB. The goal was to evaluate the quality of measurements and the acoustic disturbance of several commercialized mini-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 very flat and without obstacles, therefore well adapted for intercomparisons. During two months, four sodars were compared with a 80-meter mast instrumented with cup and sonic anemometers, and to a reference sodar which has been extensively evaluated in the past. The data were analyzed in terms of availability rate of validated data, and statistical differences on wind and standard deviation of the vertical velocity. The results show significant differences of behaviour between the 4 tested sodars, especially for very windy or rainy situations, which generally correspond to unfavourable conditions for sodars. Two sodars exhibit very good statistical comparisons with sonic anemometers, without any calibration or data filtering. But only one was able to measure the strongest winds encountered during the campaign (18 m s<sup>-1</sup> at 80 meters), and to keep a very good data quality for these winds (Figure 32). Thus, this sodar fulfills the specific needs of wind energy applications. A simple method using the sodar data was tested to calculate the annual mean wind speed at hub height (here 80 m), whose accuracy determines the quality of the electric power assessment. This method consists in the computation of sodar vertical profiles of wind speed, normalized at 40 m and averaged by direction sectors. With this method, the sodar data provided by the two-month campaign combined with one-year measurements of a cup anemometer (at 40 m level) allow a decrease by a factor of 3 of the relative error for the mean annual wind speed at hub height, when compared to a vertical extrapolation by a power law (Figure 33).

# Key references:

Musson-Genon, L., Dupont, E., and Wendum, D. (2007). Reconstruction of the surface boundary layer vertical structure of wind temperature and humidity at two levels. *Boundary-Layer Meteor.* Accepted for publication

Dupont, E., Flori, J., Lefranc, Y., Demengel, D., Wendum, D., and Heute, A. (2006b). Evaluation des performances de sodars pour la mesure du vent dans le domaine de l'éolien. Technical Report H-I88-2006-01230-FR, EDF R&D

Dupont, E., Flori, J., Lefranc, Y., Demengel, D., and Heute, A. (2006a). Evaluation des performances de sodars pour une utilisation sur site nucléaire. Technical Report H-I88-2006-03959-FR, EDF R&D

Dupont, E. and Flori, J. (2007). Comparison of sodars with ultrasonic and cup anemometers for wind energy applications. In *Proceedings EWEC conference* 

# Tests of a UHF radar and derivation of turbulent parameters

A Degréane UHF radar was extensively tested during several years in collaboration with the Centre de Recherches Atmosphériques (Laboratoire d'Aérologie) 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 was 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 availability rate of validated data at the first level of the radar (85 m) is now larger than 90%, and that the measurements of wind speed and direction at this level are in very good agreement with the measurements of the reference sodar



Figure 34: Comparison between spectral width measured on UHF vertical beam and standard deviation of vertical velocity measured by sonic anemometer (left panel). Also between standard deviation of vertical velocity measured by sodar and sonic anemometer (right panel).

Remtech PA2 and the ultrasonic anemometer (bias less than  $0.5 \text{ m s}^{-1}$  and  $5^{\circ}$  speed and direction, standard deviation about 1 m s<sup>-1</sup> and 30°). Moreover, the use of the spectral width of the UHF meteorological peak allows to determine some turbulent parameters such as the dissipation rate of kinetic energy. The comparison of the spectral width on the UHF vertical beam with the standard deviation of vertical velocity measured by a sonic anemometer shows a reasonable agreement during daytime, but large differences during nighttime. Figure 34 shows that, on the whole, the correlation is lower than the one between sodar and sonic measurements of standard deviation of vertical velocity. It is therefore necessary to improve the methodology to extract a reliable turbulence information from UHF radar data, especially in stable situations.

#### Key reference:

Dupont, E., Lohou, F., Campistron, B., Demengel, D., and Lefranc, Y. (2006c). Evaluation des performances du radar UHF Degréane : Résultats de la campagne de l'été 2005 et ses conclusions. Technical Report 2006-36, CEREA. Also as EDF Report H-I88-2006-00975-FR

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

In the framework of a collaboration with the IPSL Institute, an important set of meteorological instruments was installed during 2006 on the experimental site of IPSL (SIRTA, located about 25 km south-west of Paris, Ecole Polytechnique). SIRTA gathers a large set of teledetection instruments (lidars and radars) and is implied in international networks of experimental sites devoted to research on aerosols and clouds. CEREA has primarily brought instruments for wind and turbulence measurements (UHF radar, sodar, sonic anemometers), but also radiative, temperature and humidity sensors (Figure 35). 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 with SIRTA a regional observatory for research on meteorology and air quality.

Measurements are performed on a routine mode in order to constitute a long term (several years) data set. This data set will allow an extended validation of the Mercure\_Saturne code including a wide range of meteorological situations. This comparison between measurements and simulations will focus especially on the ability of this code to simulate correctly the micro-scale meteorological heterogeneities induced by the complex land use of SIRTA (buildings, trees, water) and by the near valleys. Four areas, with distances ranging from several hundreds of meters to one kilometer, have been or are about to be instrumented on the site in order to



Figure 35: Views of the radar UHF (left) and the 30-meter mast (right) installed on the SIRTA site.

document these heterogeneities. This includes one area near a building.

CEREA instruments are also used in the framework of campaigns in collaboration with other laboratories on specific scientific objectives. CEREA is currently involved with IPSL and Météo-France in the ParisFog project, which is supported by the French research atmospheric program LEFE. This project is dedicated to the observation and numerical simulation of turbulent, radiative, dynamical, and microphysical processes involved in the life cycle of fog. The field campaign took place at SIRTA between November 2006 and March 2007. Most of the instruments have worked continuously, but 14 IOPs (Intensive Observation Period), including additional measurements (radiosoundings, thetered balloon, aerosols and dropplets measurements), have been documented. These IOPs correspond to different kinds of fog, in terms of physical processes, spatial heterogeneity, and time evolution. 1D simulations are currently performed with Mercure\_Saturne in order to validate the physical parameterizations, and 3D simulations will then follow, primarily on radiative fog events of the campaign.

# Key references:

Lefranc, Y. and Dupont, E. (2006). Dispositif instrumental installé par le CEREA au SIRTA. Technical Report H-I88-2006-04593-FR 1.0, EDF R&D

Challet, J., Carissimo, B., Dupont, E., Musson-Genon, L., and Samba, C. (2007). First applications of Mercure\_Saturne microphysics scheme to fog simulation. Poster Journée Scientifique du SIRTA

Elias, T., Haeffelin, M., Bergot, T., Musson-Genon, L., Rangognio, J., Gomes, L., and co authors (2007). The Paris-Fog experiment. In *Proceedings Int. Conf. on Fog, Fog collection and Dew* 

### Campaign for wind resource assessment in complex terrain

Still now, wind resource assessment is generally performed with linearized models like WAsP. However, the limitations of this kind of models in complex terrain are well known, and CFD codes are more and more considered as valuable tools for sites characterized by complex orography and/or forest. Moreover, the sodars campaign performed during winter 2005-2006 has shown that sodars measurements can contribute to improve the methodology to calculate the mean annual wind speed at hub height. A six-month campaign of wind and turbulent measurements on a future wind energy production site is planned for June-December 2007 in order to study what improvement can bring a combination sodar / CFD code on the resource assessment for a complex site. The selected site is located in southern France and is characterized both by strong slopes and forest. The horizontal and vertical heterogeneities of wind and turbulence will be documented by means of 4 instrumented masts and 2 sodars. These data will allow a comparison between the measurements, and the calculations of wind resource obtained with Mercure\_Saturne and with the linearized model WAsP (PhD work of Laurent Laporte). Sodar measurements will be compared to those of a 80-meter mast in order to evaluate the behaviour of this sodar on a difficult site with strong ground clutters and strong winds.

#### Key reference:

Laporte, L. Progress report of the PhD Thesis "Wind Resource Assessment in complex terrain". EDF CR-I88/06/069

# 3 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, Fluid Mechanics). CEREA is also active in teaching activities at EN-STA with two courses (Computational Physics for Environment, Data Assimilation and Inverse Modeling).

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. A few courses (Atmospheric Modeling) are given in the Research Master SGE.

In 2006, a new course devoted to Air Pollution was offered at ENTPE (Ecole Nationale des Travaux Publics de l'Etat). This gives to CEREA a central position for teaching these topics inside the Scientific Network of the French Ministry for transport.

Moreover, the POLYPHEMUS system is used in courses at ENPC and ENSTA (Air Pollution, Computational Physics for Environment, Data Assimilation and Inverse Modeling). POLYPHE-MUS is also supported by ParisTech in the framework of the OpenCourse Ware program ("Libres savoirs").

# 3.1 Courses

# Air Pollution, ENPC.

Bruno SPORTISSE. 42 hours.

# TRADD Master (Air Pollution and Transport), ENPC.

Stéphanie LACOUR, Bruno SPORTISSE. 30 hours.

# Air Pollution, ENTPE.

Stéphanie LACOUR. 20 hours.

# Applied Mathematics, ENPC.

Bruno SPORTISSE. 30 hours.

# Fluid Mechanics, ENPC.

Bertrand CARISSIMO. 30 hours.

# Data assimilation and Inverse Modeling, ENSTA/ENPC.

Marc BOCQUET, Vivien MALLET and Bruno SPORTISSE. 36 hours.

# Computational Physics for Environment, ENSTA/ENPC. Bruno SPORTISSE, Vivien MALLET. 25 hours.

# Atmospheric Modeling, SGE Master, AQA Option.

Bertrand CARISSIMO, Edouard DEBRY, Vivien MALLET. 6 hours.

# Atmospheric Environment, Ecole Supérieure de Mécanique de Marseille [2001-2006].

Bertrand CARISSIMO, Luc MUSSON-GENON. 24 hours.

# 3.2 Textbooks for teaching activities

The following textbooks are available at www.enpc.fr/cerea as ParisTech OpenCourse Ware.

Bocquet, M. (2007a). Construction optimale de réseaux de mesures : application à la surveillance des polluants aériens. Technical Report 2007-6, CEREA. Notes de cours ENSTA

Bocquet, M. (2005b). Introduction aux principes et méthodes de l'assimilation de données en géophysique. Technical Report 2005-60, CEREA. Notes de cours ENSTA. 118 pages

Lacour, S. (2005a). Cours de pollution atmosphérique ENPC: dispersion locale de polluants. Technical Report 2005-31, CEREA

Lacour, S. (2006a). Cours TPE "qualité de l'air et santé". Volet 1: introduction à la pollution atmosphérique. Technical Report 2006-59, CEREA

Lacour, S. (2006b). Cours TPE "qualité de l'air et santé". Volet 2: émissions de polluants atmosphériques. Technical Report 2006-60, CEREA

Mallet, V. (2007b). Prévision d'ensemble. Notes de cours ENSTA, B10-2. Technical Report 2007-4, CEREA

Mallet, V. (2007a). Introduction aux modèles de chimie transport pour la qualité de l'air. Notes de cours Master SGE-AQA. Technical Report 2007-5, CEREA

Sportisse, B. (2007d). Une introduction à la pollution atmosphérique: processus et modélisation. En cours de publication. Notes de cours ENPC. 230 pages

Sportisse, B. and Mallet, V. (2005). Calcul Scientifique pour l'Environnement. Cours ENSTA. 86 pages

Sportisse, B. (2004). Assimilation de données. I Eléments théoriques. Technical Report 2004-24, CEREA. Notes de cours ENSTA et DEA M2SAP

Sportisse, B. and Quélo, D. (2004). Assimilation de données. II Implémentation des approches variationnelles: le cas d'un modèle de Chimie-Transport. Technical Report 2004-25, CEREA. Notes de cours ENSTA et DEA M2SAP

# 4 International collaborations and visiting scientists

CEREA fosters visits of foreign colleagues to receive training and collaborate on developing and applying its models.

- CEREA was honoured to welcome for one week (January 2003) Professor Spyros Pandis from the Carnegie-Mellon University (USA). This 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 and aqueous-phase chemistry.
- A partnership was initiated with the Center for Atmospheric Sciences (CAS) of IIT Delhi (Professor Maithilis Sharan, Director of CAS). Professor Sharan visited CEREA for one month, thanks to the support of the French embassy in Delhi, in 2003 and 2004. Jean-Pierre Issartel performed two visits to IIT Delhi in 2004 and 2005.

CEREA is also involved in a project led by INRIA (Principal Investigator: Jérome Jaffré), funded by CEFIPRA/IFCPAR (Indo-French Centre for the Promotion of Advanced Research). This project with IIT Bangalore focuses on Partial Differential Equations for environmental applications.

• CEREA has developed a long-term relationship (2003-) with the CMM of Santiago de Chile, with topics devoted to air pollution modeling and inverse modeling of emissions (visit of Jean-Pierre Issartel in Chile, visits of Laura Gallardo, Francesca Munoz and Ricardo Alcafuz at CEREA). This work is supported by CONYCIT/INRIA and ECOSUD.

A new project for Southern America (AirPol) is also funded by STIC/AMSUD (Air Pollution Forecast and Data Assimilation with POLYPHEMUS, 2006-). A training session for POLYPHEMUS will be organized in Santiago in June 2007 with more than 10 participants coming from Brazil, Argentina and Chile and the visit of Irène Korsakissok and Meryem Ahmed de Biasi in Chile.

Following the one-week visit of Karla Longo (CPTEC/INPE, Brazil) in April 2007, three south-american researchers (one from the University of Cordoba, Argentina, Ricardo Alcafuz and Pablo Saide from Chile) will visit CEREA in July 2007 for two weeks.

- In 2003-2004, a joint project was initiated with GMD First (Fraunhofer Institute, Berlin, Germany) for air quality forecast and data assimilation, through the post-doc of German Torrès, supported by ERCIM. This work was also funded by the PROCOPE French-German program and was included in the CLIME project.
- CEREA has a cooperative work with the CAMP program (Comprehensive Atmospheric Modeling Program) of Georges Mason University (USA). This concerns short-scale dispersion and is led by Bertrand Carissimo (several visits in the USA).
- A joint project with CRIEPI (Center Research Institute for Electric Power Industry, Japan) is led by Karine Sartelet (with a 8-month visit in Japan in 2005). This concerns Air Quality modeling over Greater Tokyo with Polair3D. This work was funded by the Canon Foundation for Research and by CRIEPI. CEREA also took part in the MICS-ASIA (Phase 2) intercomparison study over East Asia.
- CEREA participates in the European Integrated Projects NEEDS (2005-), HEIMTSA and EXIOPOL (2007-) dedicated to Impact studies and Cost-Benefit Analysis of Air Pollution Externalities. These projects provide the opportunity for collaborative works with IER Stuttgart around POLYPHEMUS.

- CEREA has a joint project with the AGH University of Science and Technology (Krakow, Poland), funded by EDF Polska. The objective is to simulate with POLYPHEMUS the air quality in Poland and in Krakow, and to assess the impact of the emissions of EDF Polska. Artur Wyrwa visited CEREA in 2005, 2006 and 2007. Janusz Zisk came to CEREA for a 4-month visit in 2006 in the framework of the European program Leonardo de Vinci.
- In 2006, Vivien Mallet achieved a three-month visit at CWI (Amsterdam, The Netherlands) in the team of Professor Jan Verwer. The topics were related to the numerical simulation of aerosol dynamics.

# 5 Publications 2003-2007 (at the date of May 1st, 2007)

# 5.1 Articles in international peer-reviewed journals

# 2003

- 1. Debry, E., Sportisse, B., and Jourdain, B. (2003). A stochastic approach for the numerical simulation of the General Dynamics Equation for aerosols. J. Comp. Phys., 184:649:689
- 2. Djouad, R., Sportisse, B., and Audiffren, N. (2003c). Numerical simulation of aqueousphase atmospheric models : use of a non-autonomous Rosenbrock method. *Atmos. Env.*, 36:873–879
- 3. Djouad, R., Audiffren, N., and Sportisse, B. (2003b). Sensitivity analysis using automatic differentiation applied to a multiphase chemical mechanism. *Atmos. Env.*, 37(22):3029:3038
- 4. Djouad, R., Sportisse, B., and Audiffren, N. (2003d). Reduction of multiphase atmospheric chemistry. *Journal of Atmospheric Chemistry*, 46:131–157
- 5. Djouad, R. and Sportisse, B. (2003). Solving reduced models in air pollution modelling. Appl. Numer. Math., 44(1):49:61
- 6. Issartel, J.-P. (2003). Rebuilding sources of linear tracers after atmospheric concentration measurements. Atmos. Chem. Phys., (3):2111–2125
- 7. Issartel, J.-P. and Baverel, J. (2003). Inverse transport for the verification of the Comprehensive Test Ban Treaty. Atmos. Chem. Phys., 3:475–486
- Sportisse, B. and Du Bois, L. (2003). Numerical and theoretical investigation of a simplified model for the parameterization of below-cloud scavenging by falling raindrops. *Atmos. Env.*, 36:5719–5727
- Sportisse, B. and Djouad, R. (2003). Mathematical investigation of mass transfer for atmospheric pollutants into a fixed droplet with aqueous chemistry. J. Geophys. Res., 108(D2):4073
- 10. Sportisse, B. and Quélo, D. (2003). Data assimilation and inverse modeling of atmospheric chemistry. *Proc. of Indian National Science Academy. Part A Physical Sciences*, 69
- Wotawa, G., De Geer, L., Denier, P., Kalinowski, M., Toivonen, H., D'Amours, R., Desiato, F., Issartel, J.-P., Langer, M., Seibert, P., Frank, A., Sloan, C., and Yamazawa, H. (2003). Atmospheric transport modelling in support of CTBT verification - overview and basic concepts. *Atmos. Env.*, 37(18):2529–2537

# 2004

- Boutahar, J., Lacour, S., Mallet, V., Quélo, D., Roustan, Y., and Sportisse, B. (2004). Development and validation of a fully modular platform for numerical modelling of air pollution: Polair3D. Int. J. Env. and Pollution, 22(1-2)
- Mallet, V. and Sportisse, B. (2004). 3D Chemistry-Transport Model Polair3D: numerical issues, validation and automatic-differentiation strategy. Atmos. Chem. Phys. Discuss., (1):1371:1392

- 14. Bocquet, M. (2005a). Grid resolution dependence in the reconstruction of an atmospheric tracer source. *Nonlinear Process in Geophysics*, 12:219–234
- Bocquet, M. (2005c). Reconstruction of an atmospheric tracer source using the principle of maximum entropy I: Theories. Quart. J. Roy. Meteor. Soc., 131(Part B(610)):2191–2208
- Bocquet, M. (2005d). Reconstruction of an atmospheric tracer source using the principle of maximum entropy II : Applications. Quart. J. Roy. Meteor. Soc., 131(Part B(610)):2209– 2223
- 17. Issartel, J.-P. (2005). Emergence of a tracer source from air concentration measurements: a new strategy for linear assimilation. *Atmos. Chem. Phys.*, 5:249–273
- Mallet, V. and Sportisse, B. (2005). A comprehensive study of ozone sensitivity with respect to emissions over Europe with a chemistry-transport model. J. Geophys. Res., 110(D22)
- Quélo, D., Mallet, V., and Sportisse, B. (2005a). Inverse modeling of NO<sub>x</sub> emissions at regional scale over Northern France. Preliminary investigation of the second-order sensitivity. J. Geophys. Res., 110(D24310)
- Quélo, D., Sportisse, B., and Isnard, O. (2005c). Data assimilation for short-range dispersion of radionuclides: a case study for second-order sensitivity. J. Environ. Radioactivity, 84:393–408
- Sartelet, K. N., Hayami, H., Albriet, B., and Sportisse, B. (2005b). Development and preliminary validation of a Modal Aerosol Model for tropospheric chemistry: MAM. *Aerosol Sci. and Technol.*, 40(2):118–127

#### $\mathbf{2006}$

- Debry, E. and Sportisse, B. (2006b). Reduction of the condensation/evaporation dynamics for atmospheric aerosols: theoretical and numerical investigation of hybrid methods. J. Aerosol Sci., 37(8):950–966
- 23. Demaël, E. and Carissimo, B. (2006). A comparison between Eulerian CFD and Gaussian Plume models on Prairie Grass Dispersion Experiment. J. Applied Meteor. Accepted for publication
- Krysta, M., Bocquet, M., Sportisse, B., and Isnard, O. (2006). Data assimilation for short-range dispersion of radionuclides: an application to wind tunnel data. *Atmos. Env.*, 40(38):7267–7279
- 25. Mallet, V. and Sportisse, B. (2006b). Ensemble-based air quality forecasts: a multi-model approach applied to ozone. J. Geophys. Res., 111(D18):18302
- 26. Mallet, V. and Sportisse, B. (2006d). Uncertainty in a chemistry-transport model due to physical parameterizations and numerical approximations: an ensemble approach applied to ozone modeling. J. Geophys. Res., 111(D01302)
- 27. Mallet, V. and Sportisse, B. (2006a). Air quality modeling: from deterministic to stochastic modeling. *Computers and Mathematics with Application*. In press
- Roustan, Y. and Bocquet, M. (2006b). Sensitivity analysis for mercury over Europe. J. Geophys. Res., 111(D14304)

29. Roustan, Y. and Bocquet, M. (2006a). Inverse modeling for mercury over Europe. Atmos. Chem. Phys., 6:3085–3098

#### 2007

- 30. Bocquet, M. (2007b). High resolution reconstruction of a tracer dispersion event: application to ETEX. Quart. J. Roy. Meteor. Soc. In press
- Bouzereau, E., Musson-Genon, L., and Carissimo, B. (2007). On the definition of the cloud water content fluctuations and its effects on the computation of a second-order liquid water correlation. J. Atmos. Sci., 64:665–669
- 32. Carmichael, G., Sakurai, T., Streets, D., Hozumi, H., Ueda, H., Park, S., Fung, C., Han, Z., Kajino, M., Engardt, M., Bennet, C., Hayami, H., Sartelet, K., Holloway, T., Wang, Z., Kannari, A., Fu, J., Matsuda, M., Thongboonchoo, N., and Amann, M. (2007). MICS-Asia II: Model intercomparison and evaluation of ozone and relevant species. *Atmos. Env.* Accepted for publication
- 33. Davoine, X. and Bocquet, M. (2007). Inverse modelling-based reconstruction of the Tchernobyl source term available for long-range transport. Atmos. Chem. Phys., 7:1549–1564
- Debry, E., Fahey, K., Sartelet, K., Sportisse, B., and Tombette, M. (2007). A new SIze REsolved Aerosol Model: SIREAM. Atmos. Chem. Phys., 7(6):1537–1547
- 35. Debry, E. and Sportisse, B. (2006c). Solving aerosol coagulation with size-binning methods. *Appl. Numer. Math.* doi:10.1016/j.apnum.2006.09.007
- 36. Debry, E. and Sportisse, B. (2006a). Numerical simulation of the General Dynamics Equation (GDE) for aerosols with two collocation methods. *Appl. Numer. Math.* In press
- 37. Krysta, M. and Bocquet, M. (2007). Source reconstruction of an accidental radionuclide release at European scale. *Quart. J. Roy. Meteor. Soc.*, 133:529–544
- Mallet, V., Pourchet, A., Quélo, D., and Sportisse, B. (2007a). Investigation of some numerical issues in a Chemistry-Transport Model: gas-phase simulations. J. Geophys. Res. Accepted for publication
- Mallet, V., Quélo, D., Sportisse, B., Ahmed de Biasi, M., Debry, É., Korsakissok, I., Wu, L., Roustan, Y., Sartelet, K., Tombette, M., and Foudhil, H. (2007b). Technical Note: The air quality modeling system Polyphemus. *Atmos. Chem. Phys. Discuss.*, 7(3):6,459–6,486
- Milliez, M. and Carissimo, B. (2007). Numerical simulations of flow and pollutant dispersion in an idealized urban area, for different meteorological conditions. *Boundary-Layer Meteor.*, 122(2):321–342
- 41. Milliez, M. and Carissimo, B. (2006). CFD modelling of concentration fluctuations in an idealized urban area. *Boundary-Layer Meteor*. Accepted for publication
- 42. Musson-Genon, L., Dupont, E., and Wendum, D. (2007). Reconstruction of the surface boundary layer vertical structure of wind temperature and humidity at two levels. *Boundary-Layer Meteor.* Accepted for publication
- 43. Quélo, D., Krysta, M., Bocquet, M., Isnard, O., Minier, Y., and Sportisse, B. (2007). Validation of the POLYPHEMUS system: the ETEX, Chernobyl and Algeciras cases. Atmos. Env. doi:10.1016/j.atmosenv.2007.02.035

- 44. Sartelet, K., Debry, E., Fahey, K., Tombette, M., Roustan, Y., and Sportisse, B. (2007a). Simulation of aerosols and gas phase species over Europe with the POLYPHEMUS system. Part I: model-to-data comparison for year 2001. Atmos. Env. doi:10.1016/j.atmosenv.2007.04.024
- 45. Sartelet, K., Hayami, H., and Sportisse, B. (2007b). Dominant aerosol processes during high-pollution episodes over Greater Tokyo. J. Geophys. Res. Accepted for publication
- 46. Sartelet, K., Hayami, H., and Sportisse, B. (2007c). MICS-Asia Phase II: sensitivity to the aerosol module. *Atmos. Env.* doi:10.1016/j.atmosenv.2007.03.005
- 47. Sportisse, B. (2007b). A review of current issues in air pollution modeling and simulation. Journal of Computational Geosciences. doi:10.1007/s10596-006-9036-4
- 48. Sportisse, B. (2007c). A review of parameterizations for modeling dry deposition and scavenging of radionuclides. *Atmos. Env.*, (41):2683–2698
- 49. Sportisse, B. and Djouad, R. (2007). Use of Proper Orthogonal Decompositions for the reduction of atmospheric chemistry. J. Geophys. Res., 112(D06303)
- 50. Sportisse, B., Quélo, D., and Mallet, V. (2007). Impact of mass consistency errors for atmospheric dispersion. *Atmos. Env.* Accepted for publication
- 51. Tombette, M. and Sportisse, B. (2007). Aerosol modeling at regional scale: Model-to-data comparison and sensitivity analysis over Greater Paris. *Atmos. Env.* In press

# 5.2 Articles in french

- 1. Bocquet, M. and Sportisse, B. (2007). Modélisation inverse pour la qualité de l'air : éléments de méthodologie et exemples. *Pollution Atmosphérique*. Accepted for publication
- Clerbaux, C., Hauchecorne, A., Bekki, S., Granier, C., Pirre, M., Sportisse, B., Issartel, J.-P., and Attié, J. (2003). Assimilation des données satellitaires et inversion de sources pour l'étude de la composition chimique atmosphérique. Compte Rendu du Comité National Français de Géophysique, CNFGG
- Roustan, Y., Bocquet, M., Musson-Genon, L., and Sportisse, B. (2006). Modélisation du mercure, du plomb et du cadmium à l'échelle du continent européen. *Pollution Atmo*sphérique, (191):317–327
- 4. Sportisse, B. (2003b). Ozone des villes, ozone des champs: qualité de l'air et pollution photochimique. *PCM Le Pont*
- 5. Sportisse, B. (2003a). Modélisation et simulation de la pollution atmosphérique. Compte Rendu du Comité National Français de Géophysique, CNFGG
- 6. Sportisse, B. (2003c). Quelques aspects de la modélisation de la pollution atmosphérique. Annales des Ponts et Chaussées, 107-108:44–55
- 7. Sportisse, B. (2007a). *Management de la recherche publique*, chapter Partenariat recherche publique/entreprise : l'exemple du CEREA, Laboratoire Commun ENPC/EDF R&D. De Boeck

# 5.3 Proceedings

# 2003

- 1. Lacour, S., Megueulle, C., Carlotti, P., Soulhac, L., and Sportisse, B. (2003). Unsteady effects on pollutant dispersion around a tunnel portal. In *Proceedings of the 4th Urban Air Quality Conference*. Prague
- 2. Lacour, S. and Joumard, R. (2003). Sampling vehicles for pollutant emission modelling. In *Proceedings of the 8th Conference on Transport and Air Pollution*. Avignon

# $\boldsymbol{2004}$

- 3. Krysta, M., Bocquet, M., Isnard, O., Issartel, J., and Sportisse, B. (2004). Data Assimilation of Radionuclides at Small and Regional Scale. Some preliminary results. In *Proceedings of the NATO ARW*. Kluwer
- 4. Quiroz, H., Gallardo-Klenner, L., and Issartel, J.-P. (2004). Assimilation de données, un révélateur de la qualité des modèles : exemple de l'arsenic minier à Santiago du Chili. In *Atelier de Modélisation Atmosphérique*. Météo-France
- 5. Sartelet, K., Hayami, H., Albriet, B., and Sportisse, B. (2004). A new modal model of atmospheric aerosols (MAM). In *Proceedings of the ICNAA Conference*
- 6. Sartelet, K. N. and Hayami, H. (2004). Application of the 3D CTM Polair to air quality over Greater Tokyo. In *Proceedings of the 45th annual meeting of Japan Society for Atmospheric Environmnent*
- 7. Roustan, Y., Bocquet, M., Musson-Genon, L., and Sportisse, B. (2004). Modelling Mercury over Europe with the Chemistry-Transport-Model Polair3D. In *Proceedings of the GLOREAM/EURASAP Workshop*. DMI. Denmark
- 8. Fahey, K., Debry, E., Foudhil, H., and Sportisse, B. (2004). Formulation, development and preliminary validation of the Size Resolved Aerosol Model (SIREAM). In *Proceedings of the GLOREAM/EURASAP Workshop*. DMI. Denmark

# 2005

- 9. Taghavi, M., Fahey, K., Foudhil, H., and Sportisse, B. (2005). Modelling aerosols with the POLAIR3D/SIREAM model on the mesoscale over an urban area in south-eastern France (ESCOMPTE campaign). In *Proceedings of the European Aerosol Conference*. Belgium
- 10. Demael, E. and Carissimo, B. A comparison of Eulerian CFD with Gaussian Plume simulations of Prairie Grass Dispersion Experiments
- 11. Taghavi, M. and Musson-Genon, L. (2005). Impact of thermal power plant emissions in marseille. In *Power-Gen Europe Conference*. Milan
- 12. Taghavi, M. (2005). Intermediate species: does chemistry work in a same way in all models? In *Sixth ESCOMPTE Workshop*. Marseille
- 13. Bocquet, M. and Krysta, M. (2005). Inverse Modelling of Passive Atmospheric Tracers Using Entropy-based Methods: Methodological Aspects. In Dimet, F.-X. L. and B.Sportisse, editors, *Proceedings of the Workshop CEA-EDF-INRIA: Data assimilation and inverse* modelling in geosciences

- 14. Krysta, M., Bocquet, M., and Quélo., D. (2005). Source reconstruction for accidental releases of radio-elements. In *Proceedings of NATO Advanced Research Workshop*. Tabakhmela, Georgia
- 15. Fahey, K., Debry, E., Foudhil, H., and Sportisse, B. (2005). The incorporation of Aerosol processes in Polair3D. In *Proceedings of Gloream 2004*
- Boutahar, J. and Sportisse, B. (2005). Reduction methods and uncertainty propagation: Application to a Chemistry-Transport Model. In *Proceedings of the TAM/TAM Confer*ence. Tunis
- 17. Tombette, M., Fahey, K., Debry, E., and Sportisse, B. (2005a). Aerosol modelling at regional scale: a sensitivity study with the Polyphemus platform. In Builtjes, P., editor, *Proceedings of Gloream 2005.* TNO. Apeldoorn, The Netherlands
- Krysta, M. and Bocquet, M. (2005). Inverting sources of an accidental radionuclide release at continental scale. In Builtjes, P., editor, *Proceedings of Gloream 2005*. TNO. Apeldoorn, The Netherlands
- Sartelet, K. and Hayami, H. (2005). MICS. Asia Phase II: sensitivity to the aerosol module. In Proceedings of the workshop of the Japanese atmospheric environmental society,. Nagoya, Japan
- 20. Sartelet, K., Hayami, H., and Sportisse, B. (2005a). Application of Polair3D to the model inter-comparison study MICS-Asia Phase II for March 2001. In *Proceedings of MICS Asia 7th workshop, IIASA*. Laxenburg, Austria
- 21. Isnard, O., Krysta, M., Bocquet, M., Dubiau, P., and Sportisse, B. (2005). Data assimilation of radionuclides atmospheric dispersion at small scale: a tool to assess the consequences of radiological emergencies. In *Proceedings of the IAEA Conference*. Rio, Brazil

#### $\mathbf{2006}$

- 22. Joumard, R., Laurikko, J., Geivanidis, S., Samaras, Z., Oláh, Z., Weilenmann, M., André, J., Cornelis, E., Gribe, M., Lacour, S., Prati, M., Vermeulen, R., and Zallinger, M. (2006). Accuracy of exhaust emissions measurements on vehicle bench. In *FISITA 2006, World Automotive Congress*. Yokohama, Japan
- 23. Lacour, S., Ventura, A., Rangod, N., Carissimo, B., and Jullien, A. (2006a). How to estimate roadworks emissions factors from traffic and air quality monitoring measurements A methodological approach. In *Proceedings of the 15th Workshop Transport and Air Pollution*. Reims, France
- 24. Lagache, R., Declercq, C., Sportisse, B., Quélo, D., Palmier, P., Quetelard, B., and Haziak, F. (2006b). Évaluation de l'impact du plan de déplacements urbains de Lille-Métropole sur le trafic, les concentrations de polluants atmosphériques et la mortalité. In *Proceedings of the 15th Workshop Transport and Air Pollution*. Reims, France
- 25. Mallet, V. and Sportisse, B. (2006c). Peut-on modéliser la qualité de l'air de manière déterministe ? In *Proceedings of "38e Journées de Statistique"*. SMS. Paris
- 26. Milliez, M., Musson-Genon, L., and Carissimo, B. (2006b). Validation of a radiative scheme for CFD modeling of heat transfers between buildings and flowin urban canopies. In *Preprints of the 6th International Conference on Urban Climate*. Goteborg, Sweden

27. Milliez, M., Musson-Genon, L., and Carissimo, B. (2006a). Radiative transfers in CFD modeling of the urban canopy. In *Proceedings of the 28th NATO International Technical Meeting on Air Pollution Modeling and its Applications*. Leipzig, Germany

# 5.4 Technical reports

2003

Report 2003-1: J. Boutahar and B.Sportisse. Propagation d'incertitude dans un modèle de chimie-transport. Premières applications à un modèle 0D. Rapport de contrat EDF. 19 pages.

Report 2003-2: B. Sportisse. Proposition de programme de travail pour la convention IRSN/ENPC "Dispersion atmosphérique de radionucléides". 7 pages.

Report 2003-3: B. Sportisse. Compte-rendu scientifique du projet "Modélisation de la chimie multiphasique". Rapport pour le Programme National de Chimie Atmosphérique (INSU/PNCA). 13 pages.

Report 2003-4: Y. Roustan. Modélisation de l'impact des métaux lourds, du mercure, et des particules (PM2.5 et PM10) à l'échelle du continent Européen. Rapport d'avancement ADEME/EDF. 15 pages.

Report 2003-5: I. Mabrouki and S. Lacour. Modélisation de la qualité de l'air à l'intérieur d'un bâtiment. 53 pages.

Report 2003-6: B. Albriet and S. Lacour. Etude de la dispersion réactive d'un rejet tunnel dans une rue canyon. Rapport de contrat CETU. 45 pages.

Report 2003-7: J. Boutahar et B. Sportisse. Application de la méthode HDMR à un Modèle de Chimie-Transport 3D: POLAIR 3D. Rapport de contrat EDF. 24 pages.

Report 2003-8: S. Panzarella. Modélisation numérique de la dispersion de polluant en milieu urbain idéalisé (expérience MUST). Rapport de stage DEA. 158 pages.

Report 2003-9: J. Boutahar, S. Lacour, V. Mallet, D. Quélo, Y. Roustan and B. Sportisse. Development and validation of a fully modular platform for the numerical modelling of Air Pollution: Polair. Preprint article submitted to International Journal of Environmental Pollution. 21 pages.

Report 2003-10: Y. Roustan. Modélisation de l'impact des métaux lourds, du mercure et des particules à l'échelle du continent Européen. Rapport d'avancement ADEME/EDF numéro 2. 41 pages.

Report 2003-11: P. Pommier. Localisation de source de polluant atmosphérique et application à l'accident de Tchernobyl. Rapport de stage scientifique ENPC. 43 pages.

Report 2003-12: C. Ferreira-Gago. Guide d'utilisation de FLUDILES. Rapport de contrat ON-ERA. 32 pages.

Report 2003-13: M. Krysta, M. Bocquet and B. Sportisse. Identification des paramètres d'assimilation de données. Eléments bibliographiques et premières applications au modèle de

dispersion de l'IRSN. Rapport de contrat IRSN. 50 pages.

Report 2003-14: E. Debry and B. Sportisse. Modélisation numérique de la dynamique des aérosols: le module SIREAM (SIze REsolved Aerosol Model). Actes Congrès de l'ASFERA. 6 pages.

Report 2003-15: D. Quélo and B. Sportisse. Data assimilation for short range atmospheric dispersion of radionuclides: a case study. Preprint article submitted to J. of Env. Rad. 27 pages.

Report 2003-16: V. Mallet and B. Sportisse. 3D chemistry-transport model Polair: numerical issues, validation and inverse-modelling strategy. Preprint article submitted to Atmos. Chem. Phys. Discuss. 8 pages.

Report 2003-17: B. Albriet. Modèles gaussiens pour la dispersion des particules. Calculs préliminaires. 20 pages.

Report 2003-18: B. Albriet. Merging dans les modèles modaux d'aérosols. 10 pages.

Report 2003-19: S. Lacour. Dispersion de particules liées aux transports routiers - Eléments bibliographiques. Rapport de contrat DRAST. 12 pages.

Report 2003-20: R. Lagache. Effets sur la santé liés à la pollution atmosphérique. 5 pages.

### $\boldsymbol{2004}$

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Report 2007-5: V. Mallet. Introduction aux modèles de chimie transport pour la qualité de l'air. Notes de cours master SGE-AQA. 24 pages.

Report 2007-6: M. Bocquet. Construction optimale de réseaux de mesures : application à la surveillance des polluants aériens. Notes de cours de l'ENSTA. Révision 1.10. 39 pages.

Report 2007-7: R. Abida and M. Bocquet. Projet de développement d'un réseau automatisé de télésurveillance des particules radioactives dans l'air. Etude pour l'optimisation du réseau. Rapport de contrat IRSN.

Report 2007-8: V. Mallet, D. Quélo, B. Sportisse, E. Debry, I. Korsakissok, L. Wu, Y. Roustan, K. Sartelet, M. Tombette, M. Ahmed de Biasi and H. Foudhil. Technical note : the air quality modeling system POLYPHEMUS. Preprint article submitted to Atmos. Chem. Phys. and Discuss. 9 pages.

Report 2007-9: Y. Roustan, F. Lasry and B. Sportisse. Modélisation de l'impact des émissions des centrales EDF et SNET en France sur le transport atmosphérique des PM10 et PM2.5.
Rapport de contrat Mission Thermique EDF. 23 pages.

Report 2007-10: M. Ahmed de Biasi, V. Mallet, I. Korsakissok, E. Debry and L. Wu. Polyphemus  $1.1\alpha$  User's Guide. 140 pages.

Report 2007-11: I. Korsakissok. Simulations et évaluations des réseaux à l'échelle régionale. Rapport de contrat DGA. 70 pages.

Report 2007-12: I. Korsakissok and B. Sportisse. Simulation et évaluation des réseaux à l'échelle locale et régionale. Rapport de synthèse. Rapport de contrat DGA. 11 pages.

Report 2007-13: B. Sportisse. Air pollution Modeling and Simulation. Manuscript for Research Habilitation. 75 pages.

Report 2007-14: B. Sportisse. Modélisation et Simulation de la pollution atmosphérique. Manuscrit d'Habilitation à Diriger les Recherches. 79 pages.

Report 2007-15: I. Korsakissok. Performance evaluation of POLYPHEMUS Gaussian plume models with Prairie Grass experiment. 23 pages.

# 6 Staff

# 6.1 Staff at May 1, 2007

### Scientific Staff

BOCQUET Marc	ENPC	
CARISSIMO Bertrand	$\mathrm{EDF}$	
DUPONT Eric	$\mathrm{EDF}$	
KATA-SARTELET Karine	ENPC	
LACOUR Stéphanie	ENPC	
MALLET Vivien	ENPC	
MUSSON-GENON Luc	$\mathrm{EDF}$	
SEIGNEUR Christian	ENPC and AER	
SPORTISSE Bruno	ENPC	
WENDUM Denis	$\mathrm{EDF}$	
Administrative staff		
DEHLINGER Véronique	ENPC	Secretary
PIRCHER Vincent	Météo France	Teaching Department VET
Technical staff		
DEMENGEL Dominique	EDF	
LEFRANC Yannick	EDF	
Research engineers		
AHMED DE BIASI Meryem	INRIA	
SCHMITT-FOUDHIL Hadjira	ENPC	

### Postdoctoral fellows

ALBRIET Bastien	ENPC
DEBRY Edouard	ENPC
LE CREUER Benjamin	ENPC
ROUSTAN Yelva	ENPC
WU Lin	INRIA

### PhD

ABIDA Rachid	ENPC
DEMAEL Emmanuel	EDF
KORSAKISSOK Irène	ENPC
LAGACHE Rémy	ENPC
LAPORTE-DAUBE Damien	EDF
MALAKOOTI Hossein	ENPC
QUEGUINER Solen	EDF
TOMBETTE Marilyne	ENPC
ZHANG Xaojing	ENPC

#### 6.2 Former staff

#### Scientific Staff

ISSARTEL Jean-Pierre (now at DGA)

#### Administrative staff

BARRES Karine (now at Ministry of Transport)

#### **Research engineers**

QUELO Denis (now at IRSN) VERCAUTEREN Nikki (now at EPFL, Switzerland)

#### Postdoctoral fellows

FAHEY Kathleen (now at EPA, USA)
FERREIRA-GAGO Cécile (now at CEA)
KEIKO Alex (now at Melentiev Energy Systems Institute, Russian Academy of Sciences, Russia)
LASRY Fanny (now at ARIA)
MICHELANGELI Paul-Antoine (now in a private company)
RADICCHI Alexandre (now at University of Triest, Italy)
TAGHAVI Mohammad (now at University of Columbia, Canada)
TORRES Germán (now at University of Cordorba, Argentina)

### PhD

BOUTAHAR Jaouad (now at EHTP, Morocco) BOUZEREAU Emmanuel (now in a private company) DJOUAD Rafik (now at Qatar Petroleum) KRYSTA Monika (now at INRIA, postdoctoral fellowship) MILLIEZ Maya (maternity leave)

#### Former master thesis

AISSAOUI Mohamed (Univ. Versailles) BAVEREL Jérôme (ENSTA) BORDAS Christelle (ENSTA) DUBOIS Laurent (ENPC) DAVOINE Xavier (ENSTA) EL ATTAR Abdel (Univ. Pierre & Marie Curie) GARAU Damien (ENPC) GIRAULT Laëticia (Univ. Pierre & Marie Curie) GRAIEDSKI Leonardo (Univ. Versailles) HUYN Laurent (ENPC) JOLY Marc (ENPC) JUHEL Bénédicte (Centrale Nantes) LEBRUN Frédéric (Centrale Nantes) MABBROUKI Intissar (ENPC) MILTON Jonathan (Alban program, Argentina) NJOMGANG Hervé (ENSTA) PANZARELLA Sébastien (UMLV) POMMIER Pierre (ENPC) POURCHET Adélaïde (ENSTA) PUERTA Julien (Centrale Marseille) RAUWEL Fanny (ENPC) RISZK Pierre (ENPC) SALAMEH Tamara (Univ. Versailles) SAMBA Céline (Centrale Lyon) SOH Chi Sian (ENPC) ZEKIOUK Tarik (Univ. Claude Bernard, Lyon)

## 7 Members of Scientific Committees and Editorial Boards

M. Bocquet:

- Associate member of the Scientific Committee LEFE/Data assimilation.
- B. Carissimo
  - French Representative for the Cost Action 732 (Quality Insurance and Improvement of Microscale Meteorological models).
  - Associate member of the Scientific Committee LEFE/IDAO.

#### L. Musson-Genon:

- Scientific Committee for Primequal/Predit.
- Editorial Board of "Pollution Atmosphérique".
- Conseil Supérieur de la Météorologie/Environmental Committee.
- French Representative for the Cost Action 728 (Atmospheric Dispersion) [2004-2006].
- Scientific Committee SIRTA/IPSL.

#### B. Sportisse:

- Scientific Committee "Modeling" of PREDIT [2003-2004].
- Comité National des Aides de l'ADEME/Qualité de l'Air [2003-2006].
- Scientific committee of "Pôle de compétivité ville et mobilité durable" (Research cluster "Sustainable Urban Development").
- Editorial Board of Journal of Computational Geosciences (Springer Verlag).

### 8 Awards

- The Young Researchers EURASAP award for the third price was given to Maya MILLIEZ at ITM 2006 (International Technical Meeting for Air Pollution Modeling and its Applications, NATA/CCMS) for her work devoted to "Radiative transfers in CFD modeling of the urban canopy".
- In 2006, an award of the SFEN (French Nuclear Energy Society) was given to Emmanuel BOUZEREAU for his PhD work devoted to the modeling of cooling tower plumes.

### 9 CEREA Seminar Series 2003 - 2006

#### 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 and Carnegie Mellon University.

October 13, 2003: German Torres, CEREA and ERCIM.

October 21, 2003: Laurent Li, LMD.

November 4, 2003: Maya Milliez, CEREA.

December 17, 2003: Claire Carouge and Philippe Peylin, LSCE/CEA.

#### $\mathbf{2004}$

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 Muno Bravo and Axel Osses, 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).

#### 2006

February 9, 2006: Jean-Paul Chilès, Serge Séguret et Hans Wackernagel. Centre de Géosciences - Ecole des Mines de Paris. "Les problèmes géostatistiques de l'assimilation de données. Analyse géostatistique de données de validation d'un modèle de prévision de la pollution atmosphérique".

March 8, 2006: Jean-Michel Rosant. DAH/LMF - Ecole Centrale de Nantes. "Mesures micro-météorologiques dans une rue canyon : l'expérience JAPEX".

March 10. 2006: Faouad Badran, Charles Sorror, Sylvia Thiria. LOCEAN - Université de Paris VI. "YAO : une méthodologie logicielle pour l'implémentation de modèles numériques (schéma direct, adjoint et assimilation variationnelle)".

March 17, 2006: Thierry Bergot. Centre National de Recherches Météorologies. "Recherche sur le brouillard au CNRM".

April 28, 2006: Alberto Carrassi. ISAC-CNR, Bologna - Italy. "Adaptive observations and assimilation in the unstable subspace (AUS)".

May 5, 2006: Remus Hanea. Department of Applied Mathematics Analysis, Delft University of Technology. "Kalman filter algorithms for large scale atmospheric chemistry applications".

May 23, 2006: Benoît Noetinger. Institut Français du Pétrole. "Les techniques de changement d'échelle des écoulements, une approche physique : applications aux problèmes de l'industrie pétrolière et à la gestion des incertitudes".

June 15, 2006: Gérald Nicolas, Electricité de France R&D - Département SINETICS. "Adaptation de maillages avec le logiciel HOMARD".

June 27, 2006: Sylvain Dupont. INRIA-EPHYSE. "Modélisation des écoulements atmosphériques en zones urbaines et rurales à fine résolution spatiale".

July 12, 2006: Patrick Chazette. Laboratoire des Sciences du Climat et de l'Environnement - CEA & CNRS. "Un lidar compact pour l'étude de la troposphère".

October 19, 2006: Alain Clappier. Laboratoire de Pollution de l'Air et des Sols - Ecole Polytechnique Fédérale de Lausanne. "Modélisation méso-échelle de la qualité de l'air en milieu urbain".

## 10 Conferences, seminars, missions

#### 10.1 Conferences

#### $\boldsymbol{2003}$

Debry E., Congrès annuel de l'ASFERA (Association Française d'Etudes et de Recherche sur les Aérosols), Paris (France). December 2003. "Le modèle SIREAM pour la dynamique des aerosols". With B. Sportisse.

Issartel J.-P., Pan-American Advanced Studies Institute, Centro de Modelamiento Matematico, Santiago (Chili). 6-18 January 2003. "Inverse modelling of atmospheric tracers".

Issartel J.-P., Simposio de Cambio global: hacia una vision sistematica, Punta Arenas (Chili). January 2003.

Issartel J.-P., EGS - AGU - EUG Joint Assembly, Nice (France). April 2003.

Issartel J.-P., Atelier de Modélisation Atmosphérique de Météo-France, Toulouse (France). 5 December 2003.

Lacour S., Urban Air Quality Conference (UAQ'4), Prague. March 2003. "Unsteady effects on pollutant dispersion around a tunnel portal". With C. Megueulle, P. Carlotti and L. Soulhac.

Lacour S., Conference on Transport and Air Pollution, Avignon (France). June 2003. "Sampling vehicles for pollutant emission modelling". With R. Joumard.

Lacour S., Colloque de l'ADEME "Modélisation des émissions du transport routier", Paris (France). April 2003. "Intercomparaison d'outils et de méthodes d'inventaires d'émission d'origine routière".

Mallet V., EGS - AGU - EUG Joint Assembly, Nice (France). April 2003. "Validation of the 3D chemistry-transport model POLAIR and preliminary results on inverse modelling of emissions". With J. Boutahar, D. Quélo, K. Sartelet and B. Sportisse.

Mallet V., GLOREAM-Eurasap Workshop, Cologne (Allemagne). 29/09-01/10 2003. "Sensitivity analysis with the 3D chemistry-transport model POLAIR". With D. Quélo and B. Sportisse.

#### **2004**

Boutahar J., Workshop "Numerical Chemistry". 16 December 2004. INRIA "Méthodes de réductions pour les systèmes d'advection-diffusion-réactions; applications à la pollution atmosphérique".

Krysta M, Presentation: "Inverse Modelling of radionuclides: some preliminary tests from local to regional scales" NATO Advanced Research Workshop Advances in Air Pollution Modelling for Environmental Security 8-12 May 2004, Borovetz, Bulgary.

Taghavi M., Musson-Genon L., Sportisse, B.: Modelling of an intensive observation period using the POLAIR chemistry/transport model (Preliminary results), The First ESCOMPTE Modelling Workshop, 5-6 May 2004, Meteo France, Toulouse, France.

Taghavi M., Musson-Genon L., Sportisse B.: Modelling study of photochemical air pollution over an urban area in south eastern-France (ESCOMPTE campaign), 8th Scientific Conference of IGAC, 4-9 September 2004, Christchurch, New Zealand.

Taghavi M., Musson-Genon L., Sportisse B.: Evaluation and model/model comparisons for OH, HO2, H2O2, HNO3, RO2s, The Second ESCOMPTE Modelling Workshop, 18-19 November 2004, Meteo France, Toulouse, France.

Bocquet M., EGU meeting 2004, Nice. Oral presentation.

Carissimo B., 8th Annual George Mason University Transport and Dispersion Modelling Conference July 2004, Fairfax, Virginia, U.S.A. Worshop ERCOFTAC on Urban Flows, 9 and 10 September, Nottingham, UK. Workshop on the Uncertainty in the Prediction of Atmospheric Transport of CBRN Hazards, 8 - 10 November 2004, Cranfield University, Shrivenham, UK.

Issartel J.P., Nice, 27, 28, 29 April 2004, EGU, session Atmospheric Environment, Modelling, Monitoring and Assessment: "Filtering the redundancy from continuous space or time data".

Issartel J.P., Nice, 27, 28, 29 September 2004, 4th Annual Meeting European Society of Meteorology, session Urban Meteorology, Atmospheric Pollution and Climate: "Identification of pollution sources, assimilation versus quantum theory".

Issartel J.-P., Toulouse, 30 November 2004, Ateliers de Modélisation Atmosphérique de Météo-France, Henry Quiroz et Laura Gallardo Klenner: "Assimilation de données, un révélateur de la qualité des modèles : exemple de l'arsenic minier à Santiago du Chili".

Milliez M., 4-15 May 2004: Kiev (Ukraine) NATO ASI (Advanced Study Institute) Flow and Transport Processes in Complex Obstructed Geometries: from cities and vegetative canopies to industrial problems (presentation: detailed numerical modelling of local atmospheric dispersion in an idealized urban area).

Roustan Y., 2nd GLOREAM / EURASAP workshop "Modelling Mercury over Europe" 6-8 September 2004. Copenhague.

Albriet B., 2nd GLOREAM/EURASAP Workshop "Aerosol modelling with MAM/SIREAM models", September 2004 Copenhague.

Sartelet K., A new modal model of atmospheric aerosols (MAM), July 2004. ICNAA conference K.N. Sartelet. H. Hayami. B. Albriet. B. Sportisse.

Sartelet K., Application of the 3D chemistry transport model POLAIR3D to air quality over Greater Tokyo, KN Sartelet, H Hayami, October 2004. Conference of Japanese atmospheric environmental society.

Sartelet K., A new modal model of atmospheric aerosols (MAM). ICNAA conference, July 2004. K.N. Sartelet, H. Hayami, B. Albriet, B. Sportisse.

Lacour S., Workshop Environment and Lifecycle. LCPC Nantes. October 2004.

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

#### 2005

M. Milliez. Conference on Urban Air Quality (UAQ 5), Valencia, Spain, 29-31 March 2005. Numerical simulations of plume transport in an idealized urban area for different meteorological conditions.

K. Sartelet, H. Hayami, B. Sportisse. 7th MICS Asia workshop, IISA, Laxenburg, Austria, 14-15 February 2005. Application of Polair3D to the model inter-comparison study MICS-Asia Phase II for March 2001.

K. Sartelet. H. Hayami. Workshop of the Japanese atmospheric environmental society, Nagoya, Japan, 6-9 September 2005. MICS Asia Phase II: sensitivity to the aerosol module.

Y. Roustan. EMEP/TFMM Workshop on MSC-E model review, Moscow, Russia, 13-14 October 2005-11-17. Oral presentation.

V. Mallet. B. Sportisse. Workshop ERCIM. Combining observations and ensemble air-quality forecasts.

M. Bocquet. IPAM/SAMSE Workshop, "Mathematical Issues and Challenges in Data Assimilation for Geophysical Systems:Interdisciplinary Perspectives", UCLA, Los Angeles (2005). Poster presentation.

M. Bocquet. 4th WMO Symposium on data assimilation, Prague, Czech Republic (2005). Poster presentation.

M. Krysta. Air, Water and Soil Quality Modelling for Risk and Impact Assessment. NATO Advanced Research Workshop, 16-20 September 2005, Tabakhmela. Georgia.

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

EGU, European Geophysical Conference. 2005, 24-29 April, Vienna.

K. Fahey, E. Debry, H. Foudhil, B. Sportisse: "Size-resolved aerosol treatment in Polair3D: Model development and preliminary validation".

Y. Roustan: Poster.

M. Bocquet, Y. Roustan: "Inverse modelling for mercury over Europe".

EAC, European Aerosol Conference, 2005, 28 August - 1st September, Ghent - Belgium.

K. Fahey, E. Debry, H. Foudhil, B. Sportisse: "Incorporation and Validation of Size Resolved Aerosol Processes in Polair3D".

M. Taghavi: "Modelling aerosols with the POLAIR3D/SIREAM model on the mesoscale over an urban area in south-eastern France (ESCOMPTE campaign)".

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 Lecture, "Some issues for Air Pollution Modelling and Simulation".

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".

#### $\mathbf{2006}$

EGU, European Geophysical Conference. 2006, 2-6 April, Vienna, Austria. M. Krysta and M. Bocquet.

ITM06, May 2006, Leipzig, Germany. M. Milliez.

GLOREAM (Global and Regional Atmospheric Modeling)/ACCENT Meeting, 11-13 October 2006, Paris. M. Bocquet, E. Debry, B. Sportisse.

The 6th Conference on Urban Air Quality, Gothenburg, Sweden, 11-16 June 2006. M. Milliez, B. Carrissimo, R. Lagache.

2nd Conference Environment & Transport / including 15th Conference Transport and Air Pollution Reims, France, 12-14 June 2006. S. Lacour, B. Albriet, R. Lagache.

Conference "Journées statistiques de la SMS", May 2006, Paris. V. Mallet.

Workshop Primequal, February 2006, Strasbourg, France. B.Sportisse.

#### 10.2 Seminars

#### $\boldsymbol{2003}$

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". With V. Mallet, D. Quélo and O. Isnard.

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

#### $\boldsymbol{2004}$

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 CEREA.

#### $\mathbf{2006}$

Sportisse B. "Uncertainties in Chemistry-Transport Models". Presentation for the Scientific Committee of Institut Français du Pétrole (18 January 2006). Paris, France.

Sportisse B. "Air pollution modeling". 8th Workshop Transport/Energy/Environment. 22 May 2006. Paris.

Sportisse B. "Atmospheric dispersion of radionuclides: some modeling approaches". EMRAS Tritium Meeting, IAEA/EDF, June 2006. Chatou, France.

Mallet V. "Uncertainties in Air Quality Modeling". CWI Seminar. October 2006.

Bocquet M. "Advanced Inverse Modeling of radionuclides". LMD, Paris. December 2006.

Bocquet M. "Modélisation inverse en chimie atmosphérique". Summer school "Data Assimilation" CEA/INRIA/EDF. July 2006.

#### 10.3 Main missions

#### 2003

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

Bocquet M. Summer school E2Phi 2003, Bordeaux (France). August 2003. "La physique de notre planète, la Terre, et son climat ".

Bocquet M., ECMWF Annual Seminar 2003, Reading (UK). September 2003. "Recent developments in data assimilation for atmosphere and ocean".

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

Sportisse B., Workshop PNCA/aerosols, Observatoire Midi-Pyrénées, Toulouse (France). 28 November 2003.

Sportisse B., Workshop PNCA/data assimilation, CERFACS, Toulouse (France). 2 December 2003.

#### $\boldsymbol{2004}$

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 photooxydant 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. and 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.

#### $\mathbf{2006}$

Mallet V. CWI, Amsterdam. August - November 2006.

Debry E. Workshop Needs RS1b- Stuttgart, Germany. November 2006.

Lacour S. Workshop "Particles" Primequal, Avignon, France. March 2006.

Wu L., Y. Roustan, M. Bocquet, M. Krysta. Workshop "Assimilation de données" (LEFE/CNRS), Toulouse, France. May 2006.

Bocquet M. Workshop Accent/WMO, Genève, Switzerland. April 2006.

Malakooti H. Field campaign for aerosols over Tehran (Iran). July and November 2006.

Abida R. Summer school: STATGIS06. Klagenfurt, Austria. September 2006.

Bocquet M., L. Wu. Meeting ARCs (INRIA), Grenoble, France. October 2006.

Tombette M. Summer school (Turbulence in the Atmospheric Boundary Layer). Barcelona, Spain. November 2006.

## 11 PhD Thesis and Research Habilitation

### PhD Thesis in progress

Rachid ABIDA	Construction optimale de réseaux de mesure pour la pollution atmosphérique. ENPC.
Emmanuel DEMAEL	Modélisation de la dispersion sur un site nucléaire. ENPC.
Irène KORSAKISSOK	Changements d'échelles en modélisation de la qualité de l'air et estimation des incertitudes associées. ENPC.
Rémy LAGACHE	Couplage de modèles pour l'estimation des impacts de la pol- lution atmosphérique liée aux transports à l'échelle locale. ENPC.
Laurent LAPORTE-DAUBE	Amélioration de l'estimation du productible éolien en terrain complexe. ENPC.
Hossein MALAKOOTI	Modélisation de la qualité de l'air dans une "Megacity". Application à Téhéran. ENPC.
Solène QUEGUINER	Modélisation multi milieux de la pollution atmosphérique. ENPC.
Marilyne TOMBETTE	Modélisation des aérosols à l'échelle régionale. ENPC.
Xaohling ZHANG	Modélisation du brouillard à l'aide du code Mercure_Saturne. ENPC.

### PhD Thesis Defended

Bastien ALBRIET (defended 26 January 2007)	Modélisation des aérosols à l'échelle locale et régionale. ENPC.
Jaouad BOUTAHAR (defended 30 September	Réduction de modèles de qualité de l'air pour
2004)	les études d'impact à l'échelle européenne.
,	ENPC.
Emmanuel BOUZEREAU (defended 14 Decem-	Modélisation de l'eau liquide dans le modèle
ber 2004)	Mercure_Saturne. Paris 6.
Edouard DEBRY (defended 13 December 2004)	Modélisation numérique de la dynamique des
	aérosols. ENPC.
Rafik DJOUAD (defended 28 June 2002)	Contribution à la modélisation et à la simula-
	tion de la chimie atmosphérique multiphasique.
	Université de Rouen.
Monika KRYSTA (defended 14 September 2006)	Modélisation inverse de la dispersion des ra-
	dionucléides dans l'atmosphère. Paris 12.
Maya MILLIEZ (defended 14 December 2006)	Modélisation thermique au sein du modèle
	Mercure_Saturne. Application à la
	modélisation de l'environnement urbain.
	ENPC.
Denis QUELO (defended 8 December 2004)	Assimilation de données variationnelle pour la
	chimie atmosphérique. ENPC.
Vivien MALLET (defended 6 December 2005)	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.
Yelva ROUSTAN (defended 12 December 2005)	Modélisation de la dispersion atmosphérique du
	mercure, du plomb et du cadmium à l'échelle
	Européenne. ENPC.

### **Research Habilitation**

Bruno SPORTISSE. University Pierre et Marie Curie (Paris 6). Air Quality Modeling and Simulation. 4 June 2007.

# 12 List of contracts and grants for 2004-2007

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Partner	Amount (kiloeuro)	Topics
IRSN	88	Data assimilation & POLYPHEMUS
DRAST	18	Short-range dispersion
INERIS	12	Uncertainties
EDF/DPIT	56	Impact Study

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Partner	Amount (kiloeuro)	Topics
ADEME	6	Aircraft soot
CEA	30	Resuspension of radionuclides
CETU	10	CFD
DRAST	30	Short-range dispersion
INERIS	65	Aerosol modeling and POLYPHEMUS
IRSN	60	Data assimilation and POLYPHEMUS
MEDD	57	Aerosol modeling
CRIEPI	34	Aerosol modeling and POLYPHEMUS
EDF/DPIT	42	Impact Study

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Partner	Amount (kiloeuro)	Topics
ONERA	20	Aircraft soot
IRSN	40	Data assimilation and POLYPHEMUS
DRAST	25	Short-range
DGA	64	Network design and POLYPHEMUS
MEDD	25	Aerosol modeling
R2D2	5	Integrated modeling
EDF/DPIT	42	Impact Study

## 2007 (Forecast)

Partner	Amount (kiloeuro)	Topics
CEA	50	Deposition and scavenging of radionuclides
DGA	16	Network design and POLYPHEMUS
DRAST	35	Short-range dispersion
INERIS	25	POLYPHEMUS (uncertainties, mercury, etc)
IRSN	100	Framework agreement (atmospheric dispersion
		of radionuclides) and network design project
LEFE/INSU	10	Grant for measurements
R2D2	60	Grant for air quality modeling
SETRA	30	Short-range dispersion of particles
EDF/DPIT	50	Automatization of POLYPHEMUS for impact
		studies

### 13 Software

#### AtmoPy

Statistical and graphical Python library for analysing Chemistry Transport model output concentrations: model-to-data and model-to-model comparisons.

V. Mallet, V. Picavet (INRIA). ENPC.

#### AtmoData

Library for data processing and parameterizations in atmospheric chemistry and physics. V. Mallet, D. Quélo, I. Korsakissok. ENPC.

#### Castor

V. Mallet, based on code from Chimere team (developers: L. Menut, J.-L. Monge, R. Vautard). ENPC.

#### Gaussian models

I. Korsakissok, V. Mallet, H. Foudhil.

#### MAM

Modal Aerosol Model. K. Sartelet, B. Albriet, B. Sportisse. ENPC.

#### Mercure\_Saturne

CFD model for the Atmospheric Boundary Layer.

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

#### SIREAM

Size Resolved Aerosol Model. E. Debry, K. Fahey, K. Sartelet, B. Sportisse, M. Tombette. ENPC.

#### Polyphemus

Modeling system for atmospheric modeling (www.enpc.fr/cerea/polyphemus).

V. Mallet, D. Quélo, B. Sportisse, M. Ahmed de Biasi, E. Debry, I. Korsakissok, L. Wu, Y. Roustan, K. Sartelet, M. Tombette and H. Foudhil. ENPC and INRIA.

#### Polair3D

Chemistry transport model.

V. Mallet, L. Wu, D. Quélo, Y. Roustan, B. Sportisse. ENPC.

# 14 Acronyms

ADEME	Agence de l'Environnement et de la Maîtrise de l'Energie.
ANR	Agence Nationale de la Recherche.
ARC	Action de Recherche Concertée (INRIA).
CASU	Cellule d'Appui aux Situations d'Urgence (Emergency Center at INERIS).
CEA	Commissariat à l'Energie Atomique.
CEREA	Centre d'Enseignement et de Recherche en Environnement Atmosphérique.
CEREVE	Centre d'Enseignement et de Recherche Eau, Ville, Environnement.
CETE	Centre d'Etudes Techniques de l'Equipement.
CFD	Computational Fluid Dynamics.
CIDEN	Centre d'Ingénierie, Déconstruction et Environnement (EDF).
CIT	Centre d'Ingénierie Thermique (EDF).
CMAQ	Community Multiscale Air Quality modeling system.
CNRS	Centre National de Recherche Scientifique.
CONICYT	Comision National de Investigacion Científica y Tecnologica de Chile.
CRIEPI	Central Research Institute for Electric Power Industry (Japon).
CSTB	Centre Scientifique et Technique du Bâtiment.
CTC	Centre Technique de Crise (Emergency Center at IRSN).
CTM	Chemistry Transport Models.
CWI	Centrum voor Wiskunde en Informatica (Center for Mathematics and Com-
	puter Science, The Netherlands).
DRAST	Direction de la Recherche et des Affaires Scientifiques et Techniques du
DDIT	MTETM.
DPIT	Division Production Ingenierie Thermique (EDF, Fossil-Fired Generation
DOI	and Engineering Department).
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.
ENTPE	École Nationale des Travaux Publics de l'Etat.
EPRI	Electric Power Research Institute (USA).
ESA	European Spatial Agency.
EURASAP	European Association for the Science of Air Pollution.
FP	Research Framework Programme (European Union).
IAEA	International Atomic Energy Agency.
IDAO	Interactions et Dynamique de l'Atmosphère et l'Océan (CNRS/INSU Pro- gram).
IER	Institut für Energiewirtschaft und Rationelle Energieanwendung (University
	of Stuttgart, ermany)
INERIS	Institut National de l'Environnement Industriel et des Risques.
INRETS	Institut National de Recherche et d'Etude sur les Transports et la Sécurité.
INRIA	Institut National de Recherche en Informatique et en Automatique.
INSU	Institut National des Sciences de l'Univers (CNRS)
IPSL	Institut Pierre-Simon Laplace.
IRSN	Institut de Radioprotection et de Sûreté Nucléaire.
LCPC	Laboratoire Central des Ponts et Chaussées.
LEFE	Les Enveloppes Fluides et l'Environnement (CNRS/INSU Program).
LISA	Laboratoire Interuniversitaire des Systèmes Atmosphériques (CNRS/Universities Paris 7 and 12)
LMD	Laboratoire de Météorologie Dynamique (X/ENS/CNRS).

LSCE	Laboratoire Surveillance du Climat et de l'Environnement (CEA/CNRS).
MEDD	Ministère de l'Ecologie et du Développement Durable.
MTETM	Ministère des Transports, de l'Equipement, du Tourisme et de la Mer.
ONERA	Office National d'Etudes et de Recherches Aérospatiales.
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.
R2D2	Réseau de Recherche sur le Développement Durable (Research Network of
	region Ile de France).
SFEN	Société Française de l'Energie Nucléaire.
SIRTA	Site Instrumental de Recherche par Télédétection Atmosphérique.
VMD	Research cluster devoted to the urban sustainable development (Pôle de
	Compétitivité Ville et Mobilité Durable).