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# ACTIVITY REPORT 2004

## CEREA

Research and Teaching Center in Atmospheric Environment

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



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## **CEREA**

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

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

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**Director: Bruno Sportisse**

**Deputy Director: Luc Musson-Genon**

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

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

CEREA organizes its multidisciplinary activities through four research teams: fluid mechanics and dispersion at local scale, dispersion at regional and continental scales, multiphase modelling, and data assimilation. The data assimilation team is also part of an INRIA project, the CLIME project.

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## **RESEARCH TOPICS**

CEREA develops two numerical models: Mercure\_Saturne at local scales (urban environment and vicinity of industrial sites) and Polair3D at regional and continental scales. Some appropriate physical parameterizations and chemical mechanisms are plugged to these models. A specific focus has been devoted to multiphase models.

The resulting 3D models are then validated by model-to-data comparisons. They are used for impact studies and eventually for forecast. In this framework, data assimilation (the methods used for coupling model results and observational data) is a promising approach for improving the model outputs or retrieving input data such as emission fluxes.

### **Local scale and fluid mechanics**

(Group leader: Bertrand Carissimo)

These topics are related to applications of the French Ministry for Transport and Civil Engineering (urban pollution) and of Electricité de France (dispersion at an industrial site). The key tool is the Mercure\_Saturne Computational Fluid Mechanics model.

2003 was a year of transition for Mercure because the numerical kernel has changed from the former kernel ESTET to the new kernel Saturne. The main modification is related to the mesh (unstructured in the new version). This allows to simulate complicated geometries.

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

#### *Reactive dispersion at local scales*

A model for describing the fast chemical reactions has been coupled to Mercure\_Saturne. The application is the formation of NO<sub>2</sub> from NO just after the release of traffic emissions in the atmosphere. A model-to-data comparison has been performed with the data measured in a street of Copenhagen (Jagtveg street). The results indicate that the reactive version of Mercure leads to a better estimation of concentrations.

#### *Dispersion in a urban environment*

These topics are developed through a PhD work (Maya Milliez, from October 2003) that aims at simulating the dispersion in an environment with obstacles.

A first part has been finished with the simulation of an experiment (the Must

experiment in the USA). A series of obstacles was representing an idealized quarter. The results obtained with *Mercure\_Saturne* have been compared to the observational data and good statistics have been obtained.

A new part of this work is the ability of simulating fluctuations of concentrations. Moreover, some tools for dealing with unstructured meshes have been developed with this application.

The next part of this work is devoted to the simulation of thermal and radiative effects.

#### *Microphysical schemes for atmospheric water*

A detailed microphysical parameterization for water has been developed in *Mercure* (PhD work of Emmanuel Bouzereau, defended in December 2004).

This parameterization describes the liquid water content in clouds and in rains. The size distribution of droplets is also modeled. A first application is the model-to-data comparison with the field campaign around the aerorefrigerant tower of Bugey (in the 80s). A second application is the simulation of orographic precipitations with data available in the literature. The results indicate the validity of the developed model.

This work has been performed with the former version of *Mercure* and the transition to the new unstructured version is a work in progress.

#### *Aerosol modelling*

The related works aim at coupling to *Mercure\_Saturne* aerosol models (PhD work of Bastien Albriet). A first phase has been devoted to the improvement of OD aerosol models and the strategy of coupling has been defined. The test case will be a street canyon.

#### *Impact studies*

Impact studies are usually based on yearly averaged concentrations and/or maximal values at a hourly basis. The computational costs are a limitation for the number of configurations. A methodology has been developed in order to select the most representative cases among a data basis of measured pollution episodes. On the basis of this reduced model, the objective is to estimate air pollution impacts with a limited set of situations. This work is under progress with different sets of data (Stéphanie Lacour).

#### **Regional and continental scales**

(Group leader: Luc Musson-Genon)

The main activity is the modelling of air quality at regional (for instance Ile de France

or Southern France) and continental scale (Europe or East Asia). The topics range from forecast to impact studies. The applications are related to the estimation of the impacts of traffic or of energy production (thermal or nuclear).

This activity is mainly centered around the modelling system *Polyphemus* (freely available at [www.enpc.fr/cerea/polyphemus](http://www.enpc.fr/cerea/polyphemus), V.Mallet and D.Quélo). A key component of this platform is the Chemistry-Transport-Model *Polair3D* for the simulation of the reactive dispersion of gases and aerosols. An access to the archived data of ECMWF allows to have the meteorological fields as inputs to the modelling chain. At smaller scales, the meso-scale models *RAMS* and *MM5* are used for computing the meteorological fields.

In 2004, the main developments have been the improvement of physical parameterizations (vertical turbulence and deposition) and of chemical mechanisms (for instance for mercury). The parameterizations are inserted in the *AtmoData* library.

Numerous applications have been realized with these models.

#### *Air quality forecast*

*Polair3D* has been validated at European scale for the period April-August 2001 through model-to-data comparisons for ozone (242 ground monitoring stations). The forecast skills are satisfactory (typically a Root Mean Square Error of 20 microg/m<sup>3</sup> for ozone peaks). Moreover, the coupling to the *Prév'air* platform operated by INERIS for the operational forecast of photochemistry has been performed. The system runs daily on an experimental basis (PhD work of Vivien Mallet).

At regional scale, a *PREDIT* project devoted to the evaluation of air quality over the region of Lille has been led (D.Quélo, R.Lagache). A first part is the evaluation of the model for year 1998 (ozone and Nox), a second part is devoted to impact studies for 2015 on the basis of different scenarios for traffic emissions.

#### *Impact studies and transfer matrices*

Impact studies require the use of models over long periods and for many emission scenarios. It is therefore crucial to reduce the computational cost. Several reducing methods have been developed in the PhD work of Jaouad Boutahar (defended in September 2004), especially look-up tables and representative chemical situations. A sensitivity analysis with respect to emissions has also been performed with the linear tangent model of *Polair3D* applied to a simplified chemical mechanism (*EMEP* mechanism for acid rains). The follow-up of

this work is the computation of transfer matrices with Polair3D.

#### *Heavy metals and mercury*

The main developments are related to mercury. A new detailed mechanism (including the aqueous phase) has been tested for year 2001 over Europe and compared to the EMEP observational data (PhD work of Yelva Roustan). The results are better than those obtained with the simplified scheme of Petersen (1995) for the dissolved part of mercury in rains. Moreover, a sensitivity analysis with respect to boundary conditions has been performed (Y. Roustan and M. Bocquet). This is a key point due to the large residence time of mercury in the atmosphere.

#### *ESCOMPTE*

CEREA has participated in the modelling exercise led in the framework of the ESCOMPTE campaign (postdoctoral fellowship of M.Taghavi) in southern France (summer 2001). Two Intensive Observation Periods (IOP 2 and 3) have been simulated with RAMS for the meteorological fields and Polair3D for gas-phase species. Moreover, the impact study of the emissions for the Power Plant of Martigues has been performed (study for the thermal branch of EdF).

#### *Multimedia modelling*

The PhD work of Solène Quéguiner aims at coupling to Chemistry-Transport-Models the description of other media (ground, water). One component of this multimedia system is the OURSON model, developed at LNHE/EDF R&D. A first part is devoted to the extension of OURSON to lead and cadmium and then to mercury and POPs.

#### *Dispersion of radionuclides*

An important project is led in a collaborative work with IRSN. The Forecast Center of IRSN now uses for studies Polair3D and the simulation of the Chernobyl's release is a work in progress (D. Quélo, M.Bocquet, J.P.Issartel, B.Sportisse).

#### **Multiphase modelling**

(Group leader: Bruno Sportisse)

The objective is to develop and to validate a multiphase model to be hosted by 3D models such as Mercure\_Saturne or Polair3D.

#### *PAM project*

The work for multiphase modelling (gas, aerosol, aqueous-phase) have been led in the framework of the PAM project (Multiphase Air Pollution) of the French Research Program Primequal-Predit (in collaboration with the research centers LISA and LSCE).

In 2004, the developments have focussed on the General Dynamics Equation for aerosols (condensation/evaporation, coagulation and nucleation). Two models are developed: MAM (Modal Aerosol Model, postdoctoral fellowship of Karine Sartelet and PhD work of Bastien Albriet) and SIREAM (Size Resolved Aerosol Model, PhD work of Edouard Debry and postdoctoral fellowship of Kathleen Fahey). The species are inorganic (on the basis of the thermodynamic models ISORROPIA) or organic (on the basis of a parameterized representation of Secondary Organic Aerosols with two-products formulations).

The aqueous phase (fog and clouds) is taken into account through the coupling to the VSRM model developed at Carnegie Mellon University (Kathleen Fahey).

The multiphase models have been coupled to Polair3D and are under evaluation at continental scale (Kathleen Fahey) and at regional scale (Hadjira Foudhil over Lille and Karine Sartelet over Tokyo).

Moreover, the PhD work of Marilyne Tombette has just begun in the framework of a Ile de France project. A first item is devoted to external mixing.

#### *Extension to other applications*

The extension of these models to other applications is a promising approach. For instance, this concerns the short-range dispersion of aerosols in the vicinity of roads (with a gaussian model), radionuclides (in the project with IRSN) and soots related to aircraft emissions (with ONERA). A comprehensive state-of-the-art review has been performed for the radioactive aerosols (Bruno Sportisse). A common project with ONERA has been retained by the Primequal program for studying aircraft soots (Stéphanie Lacour).

#### **Inverse modelling / Data assimilation**

(Group leader: Marc Bocquet)

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

In 2004, the main works have concerned the methods related to data assimilation and inverse modelling of passive tracers.

#### *Inverse modelling of emissions for passive tracers*

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. Thanks to the linear nature of the underlying equations, this can be performed with adjoint solutions called retroplumes.

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

Moreover, some new approaches have been proposed by Marc Bocquet for inverse modelling of passive tracers, on the basis of the maximum entropy principle. The key advantage is the way the a priori knowledge is taken into account. They can be applied to accidental releases (for instance to the ETEX campaign).

This approach also includes variational techniques such as 4D-var PSAS and are equivalent to a projection onto the basis of retroplumes.

Another work is devoted to the assessment of the influence of grid resolution in the framework of inverse problems with entropy regularization. The singular points near sources are then explained. The existence of an optimal resolution has been proved and an indicator of the inverse modelling procedure has been proposed (Marc Bocquet).

#### *Variational assimilation*

The use of 4D-var techniques requires the development of the adjoint model of Polair3D (Denis Quélo). An application is the inverse modelling of Nox emissions at regional scale.

#### *Inverse modelling of Nox emissions*

The emissions fluxes represent one of the main uncertainties in Chemistry-Transport Models. These uncertainties are mainly related to the time distribution. A work has been led over the Lille region (May 1998) on the basis of observational data for ozone and Nox. The control parameters are hourly coefficients applied to emissions of NOx. The forecast of ozone and Nox with the improved emission

fluxes is significantly improved for the learning week and for the two weeks after (Denis Quélo, Vivien Mallet, Bruno Sportisse).

#### *Submission of a MetOp project to ESA*

A project has been submitted to the call of the European Space Agency in order to assimilate data from the MetOp platform (especially vertical profiles of ozone) in the Chemistry-Transport Model Polair3D (Jean-Paul Berroir, Bruno Sportisse, Isabelle Herlin, Marc Bocquet).

#### *Sequential assimilation*

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

#### *Advanced data assimilation techniques*

A preliminary investigation of advanced sequential methods for air quality forecast has been initiated by Marc Bocquet. The methods such as the SIR method are computationally expensive but take into account the non-linearity of models. A Cooperative Research Action of INRIA (ADOQA: Data Assimilation for Air Quality) has been also initiated with other INRIA projects (IDOPT and ASPI) in order to evaluate these approaches.

#### *Sensitivity analysis 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 at continental scale. Adjoint methods have been used in order to quantify the sensitivity of observational data of mercury over Europe with respect to emissions, initial conditions and boundary conditions. The developed tools may also be used in order to perform the inverse modelling of mercury (Yelva Roustan, Marc Bocquet).

#### *Short-range inverse modelling*

CEREA is implied in a joint project with IRSN devoted to Inverse Modelling of an Accidental Release in the atmosphere (MIRA). Some experiments have been led in order to invert parameters related to the emission of a point source or physical parameters for turbulent dispersion (PhD work of Monika Krysta). A variational approach has been applied to a puff model with a set of data obtained in the wind tunnel of Ecole Centrale de Lyon (with a

reduced representation of the Bugey power plant). The evaluation of the monitoring network has also been led with cross validation techniques (Monika Krysta, Marc Bocquet, Bruno Sportisse).

#### *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. Some approaches based on reduced look-up tables have been tested by Jaouad Boutahar and Bruno Sportisse.

Moreover, studies devoted to propagations of uncertainties may give the input/output behaviour of models and lead to a focus on key inputs (the most sensitive ones). In order to build an ensemble model for air quality forecast, some efficient Monte Carlo methods have been evaluated (J.Boutahar and B.Sportisse). Some preliminary tests of ensemble forecast have also been performed at continental scale (M.Aissaoui and V.Mallet).

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## **Teaching activities**

CEREA is active in the teaching activities of ENPC and ENSTA and offers a structured set of courses in its research fields: modelling, numerical simulation and data assimilation for atmospheric dispersion.

Inside ENPC, this comprises courses with an applied focus (Air Pollution, Bruno Sportisse, Marc Bocquet and Stéphanie Lacour) but also an involvement in more theoretical courses (Applied Mathematics, Bruno Sportisse). A course of the Mastere TRADD (Transport and Sustainable Development), in the framework of the Renault Foundation, has been created in 2004 by Stéphanie Lacour and Bruno Sportisse (Air Pollution and Transport). Vincent Pircher has also created a course devoted to applications of Meteorology with Météo France.

CEREA is also implied in the management of teaching activities at ENPC (Department VET) through Vincent Pircher.

A master course (DEA M2SAP) is given at ENSTA by Bruno Sportisse and Marc Bocquet (Modelling, simulation and data assimilation for atmospheric chemistry). Moreover, a course devoted to « Computational Physics for Environmental Applications » has also been created in 2004 at ENSTA (Bruno Sportisse with Vivien Mallet and Karine Béranger).

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## **International collaborations**

In 2004, it is noticeable that more than 10 different countries are represented in the staff of CEREA.

CEREA has been honoured to welcome Professor Spyros Pandis from Carnegie-Mellon University (USA). It has strengthened the collaborative work devoted to aerosol modelling (PhD work of Edouard Debry and postdoctoral fellowship of Kathleen Fahey).

The joint project with CAS (Center of Atmospheric Sciences) and Professor Maithili Sharan of IIT Delhi has been strengthened by the visit of Jean-Pierre Issartel in India.

CEREA is also involved in a project with the Center for Mathematical Modelling (CMM) in Santiago de Chile. This project aims at performing inverse modelling of emissions (visit of Jean-Pierre Issartel in Chile and visit of Francesca Munoz at CEREA). This activity is done in the framework of a CONYCIT/INRIA program and is part of the CLIME project.

A joint project with Argentina has also been submitted to the ECOSUD program with the University of Cordoba (after the postdoctoral fellowship of German Torrès). The project is devoted to data assimilation and forecast with the MM5/Polair3D modelling chain.

A project with GMD First (Fraunhofer Institute of Berlin, Germany) is devoted to Air Quality Forecast and Data assimilation (postdoctoral fellowship of German Torrès funded by ERCIM). This is also part of the CLIME project and is funded by the PROCOPE program for german/french relations.

CEREA has a collaborative work with the George Mason University through the CAMP program (Comprehensive Atmospheric Modelling Program) devoted to modelling at local scale (Bertrand Carissimo).

The work of Karine Sartelet for aerosol modelling is led in a joint project with CRIEPI (Japan) and is funded by the Canon Foundation for Research. CEREA also takes part in the MICS-ASIA (Phase 2) intercomparison study over East Asia.

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## Personnel

### Scientific Staff

ALBRIET Bastien (\*)  
BOCQUET Marc  
BOUTAHAR Jaouad (@)  
BOUZEREAU Emmanuel (#)  
CARISSIMO Bertrand  
DEBRY Edouard (#)  
DEMAEL Emmanuel (\*)  
DUPONT Eric  
FAHEY Kathleen (\*\*)  
FOUDHIL Hadjira  
GARNIER François (@)  
ISSARTEL Jean-Pierre  
KRYSTA Monika (\*)  
LACOUR Stéphanie  
LAGACHE Rémy (\*)  
MALLET Vivien (\*)  
MILLIEZ Maya (\*)  
MOUFOUMA-OKIA Wilfran (#)  
MUDGAL Shailendra (#)  
MUSSON-GENON Luc  
QUEGUINER Solen (\*)  
PIRCHER Vincent  
PLION Pierre  
QUELO Denis  
RADICCHI Alessandro (\*, @)  
ROUSTAN Yelva (\*)  
SARTELET Karine  
SPORTISSE Bruno  
TAGHAVI Mohammad (\*\*)  
TOMBETTE Maryline (\*)  
TORRES German (@)  
WENDUM Denis

(\*) PhD

(#) No longer member of CEREAs from January 2005

(\*\*) Postdoctoral fellow

(@) Associated member

### Master thesis 2004

AISSAOUI Mohamed (DEA)  
GARAU Damien (ENPC)  
GRAIEDSKI Leonardo (DEA)  
HUYN Laurent (ENPC)  
JOLY Marc (ENPC)  
JUHEL Bénédicte (Ecole Centrale Nantes)  
LEBRUN Frédéric (DEA)  
MILTON Jonathan (Alban program)  
NJOMGANG Hervé (ENSTA)  
SALAMEH Tamara (DEA)  
SOH Chi Sian (ENPC)  
ZEKIOUK Tarik (DEA)

### Administrative Staff

BARRES Karine

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## Teaching activities

Applied Mathematics, ENPC.  
Bruno SPORTISSE, Vivien MALLET.

Air Pollution, ENPC.  
Bruno SPORTISSE.  
Marc BOCQUET, Stéphanie LACOUR, Rémy LAGACHE, Luc MUSSON-GENON.

Modelling, simulation and data assimilation for atmospheric chemistry, ENSTA and DEA M2SAP (X-UVSQ).  
Bruno SPORTISSE.  
Marc BOCQUET.

Computational Physics for Environmental Applications, ENSTA.  
Bruno SPORTISSE.  
Vivien MALLET.

Air Pollution and Transport, master TRADD (ENPC/Renault Foundation).  
Stéphanie LACOUR.  
Bruno SPORTISSE.

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## Articles and reports

### Accepted or published (with peer review)

**D. Quélo, B. Sportisse et O. Isnard.**  
Data assimilation for short range atmospheric dispersion of radionuclides: a case study. J. of Env. Radioact., 2004, accepted.

**J.P. Issartel.**  
Emergence of a tracer source from air concentration measurements, a new strategy for linear assimilation, Atmos. Chem. Phys. Disc, 5, 249-273, 2 February 2005.

**J. Boutahar, S. Lacour, V. Mallet, D. Quélo, Y. Roustan & B. Sportisse.**  
Development and validation of a fully modular platform for numerical modelling of air pollution: Polair3D. International Journal of Environmental Pollution 2004, volume 22, numéro 1-2.

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

### Marc Bocquet

Reconstruction of an atmospheric tracer source using the principle of maximum entropy. I: Theory, accepted for publication QJRMS.

**Marc Bocquet.**

Reconstruction of an atmospheric tracer source using the principle of maximum entropy. II: Applications, accepted for publication QJRMS.

**Marc Bocquet.**

Grid resolution dependence in the reconstruction of an atmospheric tracer source, accepted for publication in Nonlinear Process in Geophysics.

**Submitted publications**

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

Development and preliminary validation of a new Modal Aerosol Model for tropospheric chemistry. MAM, Submitted to Aerosol Science and Technology.

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

Use of Proper Orthogonal Decompositions for the reduction of atmospheric chemistry. Linear Algebra and its Applications. Special issue devoted to Model Reduction 2004.

**E. Debry and B. Sportisse.**

Reduction of the General Dynamics Equation for atmospheric aerosols: theoretical and numerical investigation, submitted to Journal of Aerosol Science,

**Proceedings**

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

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

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

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

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

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

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

Modelling Mercury over Europe with the Chemistry-Transport-Model Polair3D.

In Proceedings GLOREAM/EURASAP Workshop. DMI. Denmark.

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

Formulation, development and preliminary validation of the Size Resolved Aerosol Model (SIREAM).

In Proceedings GLOREAM/EURASAP Workshop. DMI. Denmark.

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**Reports**

**Report 2004-1:** Rapport de synthèse des travaux réalisés dans le cadre de la convention EDF/ENPC pour l'année 2003. Bruno Sportisse. 7 janvier 2004. 9 pages.

**Report 2004-2:** Modélisation de la qualité de l'air en région PACA et effets de scénario de transport sur des épisodes photochimiques, Moufouma-Okia Wilfran, Lacour Stéphanie, janvier 2004, 31 pages.

**Report 2004-3:** Modélisation de la pollution atmosphérique et des impacts l'échelle locale en interaction avec le RST, Lacour Stéphanie, janvier 2004, 15 pages.

**Report 2004-4:** Etude de l'impact des missions de la centrale de Martigues sur la pollution photo-oxydante en région PACA, Moufouma-Okia Wilfran, Musson-Genon Luc, Sportisse Bruno, janvier 2004, 40 pages.

**Report 2004-5:** Modélisation de la dispersion réactive des oxydes d'azote à l'échelle locale avec Mercure, Lacour S., Carissimo B., janvier 2004, 44 pages.

**Report 2004-6:** Modélisation de l'impact des métaux lourds, du mercure, et des particules (PM2.5, PM10) à l'échelle du continent Européen., Roustan Y., Rapport d'avancement ADEME/EDF 3, février 2004, 30 pages.

**Report 2004-7:** Impact des missions des avions sur la qualité de l'air autour des plates formes aéroportuaires, Huynh Laurent, juillet 2004.

**Report 2004-8:** Rapport de synthèse des travaux réalisés dans le cadre du Projet Assimilation de Données pour le PNCA, Bruno Sportisse, Mai 2004, 23 pages.

**Report 2004-9:** Projet MIRA. Rapport numéro 2, Monika Krysta, Juin 2004, 20 pages.



**Report 2004-10:** Data Assimilation of Radionuclides at Small and Regional Scale. Some preliminary results, Monika Krysta, Marc Bocquet, Olivier Isnard, Jean-Pierre Issartel, and Bruno Sportisse, Juillet 2004, 10 pages.

**Report 2004-11:** Code, tools and methods at CEREA, V. Picavet, avril 2004, 26 pages.

**Report 2004-12:** Documentation of MM5toPOLAIR, G.A.Torrès.

**Report 2004-13:** Rapport de stage Damien Garreau et Marc Joly.

**Report 2004-14:** Rapport de stage Terik Zebouk : Panache sous-maille dans Polair3D.

**Report 2004-15:** Reduction of the General Dynamics Equation for atmospheric aerosols: theoretical and numerical investigation, article soumis à Journal of Aerosol Science, E. Debry et B. Sportisse, Juillet 2004, 32 pages.

**Report 2004-17:** Etat d'avancement des travaux engagés dans le contexte de la convention cadre IRSN/CEREA, Bruno Sportisse, 4 pages.

**Report 2004-18:** Etude de la propagation d'incertitudes dans un modèle de Chimie-Transport, Polair3D. Rapport de stage DEA M2SAP. Mohamed Aissaoui.

**Report 2004-19:** Estimations de ratios moyens de NO<sub>2</sub>/NO<sub>x</sub> au voisinage du débouché d'un tunnel en tranche en milieu urbain, Stéphanie Lacour, 16 pages.

**Report 2004-20:** Modélisation de la dispersion atmosphérique réactive dans une rue, rapport de stage Tamarra Salameh.

**Report 2004-21:** Paramétrisation de la vitesse de dépôt sec pour un modèle de chimie-transport de polluants, rapport de stage de première année l'ENPC, Chi-Sian Soh, 58 pages.

**Report 2004-22:** Modal aerosol model (MAM) - Technical description, Karine Sartelet, 24 pages.

**Report 2004-23:** Development and preliminary validation of a new Modal Aerosol Model for tropospheric chemistry: MAM. Article soumis à Atmospheric Research, K.N. Sartelet, H. Hayami, B. Albriet, B. Sportisse, 17 pages.

**Report 2004-24:** Assimilation de données. 1ère Partie : Eléments théoriques. Bruno Sportisse et Denis Quélo. Octobre 2004.

**Report 2004-25:** Assimilation de données. 2ème Partie : Implémentation dans Polair3D. Denis Quélo et Bruno Sportisse. Octobre 2004.

**Report 2004-26:** Coupling the SIREAM model to Polair3D, preliminary results. Kathleen Fahey, Hadjira Foudhil et Bruno Sportisse. 2004

**Report 2004-27:** Impact des rejets de la centrale thermique de Martigues sur la qualité de l'air. Modélisation avec Polair3D. M. Taghavi, L. Musson-Genon et B. Sportisse.

**Report 2004-28:** Etude de l'impact qualité de l'air des scénarios PDUs sur Lille l'aide du modèle de Chimie-Transport POLAIR3D. D. Quélo, R. Lagache et B. Sportisse. Novembre 2004.

**Report 2004-29:** AtmoData Library: data processing and parameterizations in atmospheric sciences. V. Mallet.

**Report 2004-30:** Reconstruction of an atmospheric tracer source using the principle of maximum entropy. I: Theory, Marc Bocquet, article soumis QJRMS.

**Report 2004-31:** Reconstruction of an atmospheric tracer source using the principle of maximum entropy. II: Applications, Marc Bocquet, article soumis QJRMS.

**Report 2004-32:** Grid resolution dependence in the reconstruction of an atmospheric tracer source, Marc Bocquet, article soumis Nonlinear Process in Geophysics, Septembre 2004.

**Report 2004-33:** Assimilation de données, un révélateur de la qualité des modèles: exemple de l'arsenic minier Santiago du Chili, Henry Quiroz, Laura Gallardo Klenner, Jean-Pierre Issartel, article publié dans les actes des Ateliers de Modélisation Atmosphérique organisés par Météo-France, Toulouse les 29 et 30 novembre 2004.

**Report 2004-34:** Etude des lois de la couche limite de l'atmosphère. Frédéric Lebrun. Stage DEA/Ecole Centrale de Nantes.

**Report 2004-35:** Modélisation de la pollution atmosphérique et des impacts à l'échelle locale en interaction avec le RST. Rapport de convention DRAST. S. Lacour.

**Report 2004-36:** Projet MIRA. Modélisation inverse sur la base des données de la soufflerie ECL. Monika Krysta, Marc Bocquet et Bruno Sportisse. 74 pages.

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## Theses in progress

B. ALBRIET

Modélisation d'une distribution d'aérosols aux échelles locales et régionales. ENPC.

E. DEMAEL

Dispersion de radionucléides à petite échelle. ENPC.

M KRYSTA

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

R. LAGACHE

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

V MALLET

Prévision de la qualité de l'air et méthodes non linéaires d'assimilation de données. ENPC.

M. MILLIEZ

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

S. QUEGUINER

Modélisation multi-milieux de la pollution atmosphérique. ENPC.

Y. ROUSTAN

Modélisation de la dispersion du mercure et des métaux lourds à l'échelle européenne. ENPC.

M. TOMBETTE

Modélisation des aérosols à l'échelle régionale. ENPC.

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## Theses defended

J. BOUTAHAR 30/09/2004

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

E. BOUZEREAU 14/12/2004

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

E. DEBRY 13/12/2004

Modélisation numérique de la dynamique des aérosols. ENPC.

D. QUELO 8/12/2004

Assimilation de données variationnelle pour la chimie atmosphérique. ENPC.

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## Contracts

Agreement 2004 EDF R&D

EDF R&D

Agreement 2004 DRAST

S. Lacour, R. Lagache, B. Sportisse

METLMT

Modelling of impacts for the Power Plant of Martigues

M. Taghavi, L. Musson-Genon, B. Sportisse  
Thermal Branch EDF R&D.

Reduced models for air quality modelling at continental scale

J. Boutahar, L. Musson-Genon, B. Sportisse  
EDF R&D

Inverse modelling of accidental release (MIRA project)

M Bocquet, M. Krysta, D. Quélo, B. Sportisse  
IRSN

Agreement IRSN

M. Bocquet, D. Quélo, B. Sportisse, D. Wendum  
IRSN

Agreement INERIS

B. Albriet, V.Mallet, Y. Roustan, B. Sportisse, K. Fahey  
INERIS

National Program for Atmospheric Chemistry (PNCA), aerosol project

Debry E., Fahey K., Sportisse B.  
CNRS

National Program for Atmospheric Chemistry (PNCA), data assimilation project

Bocquet M., Quélo D., Sportisse B.  
CNRS

Dispersion of pollutants at a tunnel portal

S. Lacour, B. Albriet  
CETU

PAM project (Multiphase Air Pollution), program Primequal-Predit

E. Debry, K. Fahey, H. Foudhil, K. Sartelet, M. Taghavi, B. Sportisse  
MEDD

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## **Conferences, seminars, missions**

### **Conferences**

Jaouad Boutahar, 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, Bulgarie

Mohammad Taghavi, 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, HO<sub>2</sub>, H<sub>2</sub>O<sub>2</sub>, HNO<sub>3</sub>, RO<sub>2</sub>s, The Second ESCOMPTE Modelling Workshop, 18-19 November 2004, Meteo France, Toulouse, France.

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

Bertrand Carissimo, 8th Annual George Mason University Transport and Dispersion Modelling Conference July 2004, Fairfax, Virginia, U.S.A.

Workshop 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

Jean-Pierre Issartel, Nice, 27, 28, 29 April 2004, EGU, session Atmospheric Environment, Modelling, Monitoring and Assessment: 'Filtering the redundancy from continuous space or time data'.

Jean-Pierre Issartel, 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'.

Jean-Pierre Issartel, 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'.

Maya Milliez, 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).

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

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

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

Karine Sartelet, 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.

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

Stéphanie Lacour. Workshop Environment and Lifecycle. LCPC Nantes. October 2004.

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

### **Séminars**

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

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

### **Main missions**

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

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

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

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

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

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

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

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

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

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

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

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

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### **Seminars at CEREA**

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

27 May 2004: Laura Gallardo Klenner, Centro de Modelamiento Matematico, Université du Chili, Santiago, « Urban Mobile Emission in South American Mega Cities (UMESAM) ».

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

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

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

### **Organisation of conferences**

Workshop CEREA in the framework of the Spring Research days of EDF R&D – Chatou – June 2004.

Workshop « Numerical simulation for chemistry » - INRIA – 16 December 2004 – B Sportisse (with M. Kern and A. Ern).

Workshop « Air Quality Modelling with Polair3D » – CEREA/EDF Polska – 3 November 2004.

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### **Softwares**

#### *AtmoData*

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

V Mallet  
ENPC

#### *Mam 1.0*

Modal Aerosol Model for particulate matter dynamics

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

#### *Mercurie\_Code Saturne*

CFD model for the Atmospheric Boundary Layer.

E. Bouzereau, B. Carissimo, E. Dupont, S. Lacour, M. Milliez  
EDF R&D

#### *Polair 1.3*

Chemistry-Transport Model, version 2.1.

J. Boutahar, H. Foudhil, V. Mallet, D. Quélo, Y. Roustan, B. Sportisse

ENPC

*Siream 1.0*

Size Resolved Aerosol Model.

E. Debry, K. Fahey, P. Plion, B. Sportisse

ENPC

*Spack*

Simplified Preprocessor for Atmospheric  
Chemical Kinetics.

B. Sportisse, P. Plion

ENPC

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**List of initials used**

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