CEREA

Centre d'Enseignement et de Recherche en Environnement Atmosphérique

Research and Teaching Center in Atmospheric Environment

Projet scientifique pour la période 2010-2013

Scientific Project for the 2010-2013 Period

Joint Laboratory Ecole nationale des ponts et chaussées/Electricité de France R&D
Laboratoire commun Ecole national des ponts et chaussées/Electricité de France R&D
http://www.enpc.fr/cerea/

CEREA
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Laboratoire commun ENCP/EDF R&D
Research and Teaching Center in Atmospheric Environment
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Sommaire
Table of Contents

Résumé

Pour la période 2010-2013, le CEREA continuera à concentrer ses activités de recherche en science de l'environnement atmosphérique avec les composantes suivantes :

- Modélisation de la pollution atmosphérique de proximité
- Modélisation de la qualité de l'air aux échelles urbaines, régionales et continentales
- Assimilation de données et modélisation inverse pour des applications environnementales
- Observations de la couche limite de l'atmosphère

L'objectif général du CEREA est d'être reconnu comme l'un des tout premiers groupes de recherche dans le domaine des sciences de l'environnement atmosphérique du point de vue d'une part de la qualité scientifique de la recherche (mesurée par exemple par le nombre de citations des publications du CEREA) et d'autre part de la valorisation de cette recherche (par exemple grâce à des contributions à des outils opérationnels). Dans ce but, chaque composante de la recherche conduite au CEREA devra se concentrer sur des sujets pour lesquels le CEREA peut contribuer de façon significative. Ceci se déclinera par une activité de production scientifique (publications dans des revues internationales avec comité de lecture, thèses de doctorat soutenues) et des activités à caractère plus appliqué concernant des besoins opérationnels et répondant à des attentes sociétales (utilisation de modèles de la qualité de l'air et de dispersion atmosphérique pour évaluer la contribution des secteurs industriels et des transports à la pollution atmosphérique, contributions à des systèmes opérationnels pour la prévision de la qualité de l'air et l'optimisation de réseaux de mesures, dépôt et dissémination de codes en « logiciel libre »).

La réalisation du projet scientifique va inclure diverses activités, parmi lesquelles :

- L'identification de sujets émergents sur lesquels le CEREA a les capacités de se différencier d'autres groupes de recherche comme, par exemple, l'exposition aux particules ultrafines en proximité des routes, le traitement des incertitudes en prévision de la qualité de l'air, l'influence du changement climatique, l'impact des biocarburants, le développement et l'utilisation de méthodes non-linéaires et non-gaussiennes pour l'assimilation de données, l'assimilation de données multi-échelles, la fusion de données pour l'optimisation des réseaux de mesures, la modélisation explicite du climat urbain au moyen de codes de mécanique des fluides, et l'étude de la dispersion près du sol dans des atmosphères stables.
- La réalisation des tâches de recherche et de développement (par les chercheurs permanents, les post-doctorants, les doctorants et les stagiaires).
- La présentation des résultats de la recherche dans des revues scientifiques, ainsi qu'à des congrès, conférences et ateliers.
- Des interactions plus soutenues et d'autres nouvelles avec divers groupes de recherche (y compris la participation à des programmes de recherche français, européens et internationaux) ; la mise en place de partenariats de longue durée

avec des groupes de recherche expérimentale, notamment en chimie atmosphérique, sera particulièrement bénéfique.

- La dissémination de certains produits de la recherche dans la communauté scientifique pour un usage plus important de nos codes numériques et de nos méthodologies.
- Des collaborations actives pour la mise en place de systèmes opérationnels comme le système de prévision de la qualité de l'air Prèv'air ou le futur réseau de surveillance des radionucléides Descartes).
- La valorisation de certaines technologies du CEREA dans l'industrie par le biais d'EDF et dans l'administration à travers des instituts nationaux comme l'IRSN et l'INERIS.
- L'embauche de doctorants et post-doctorants particulièrement prometteurs.
- L'enseignement de cours en sciences de l'environnement et en mathématiques appliquées incluant des travaux pratiques utilisant les outils numériques développés au CEREA.

La réalisation réussie de ces activités de recherche, de développement, d'enseignement et de valorisation devraient permettre au CEREA de devenir un des tout premiers groupes de recherche dans le domaine de la modélisation de la qualité de l'air.

Summary

For the period 2010-2013, CEREA will continue to focus on its major research areas in atmospheric and environmental science, which include the following:

- Short-range atmospheric and dispersion modeling
- Air quality modeling at urban, regional and continental scales
- Data assimilation and inverse modeling for environmental applications
- Atmospheric measurements in the boundary layer

The overall objective for CEREA is to be recognized as one of the premier groups in atmospheric and environmental research both in terms of scientific status (e.g., number of citations of CEREA papers) and application work products (e.g., contributions to successful operational systems). To that end, the goal for each research area is to focus on topics where CEREA can make significant scientific contributions, which will be reflected in terms of scientific output (e.g., publications in the peer-reviewed literature, Ph.D. theses) and practical applications (e.g., application of air quality and atmospheric dispersion models to real-world problems, contributions to operational systems such as air quality forecasting and monitoring network design, registration and distribution of open-source computer codes).

The implementation of the scientific project will include a variety of activities including the following:

- Identification of topics of current or emerging interest for which CEREA has the capabilities to make a difference (e.g., exposure to ultrafine particulate matter near roadways, treatment of uncertainties in air quality forecasting, influence of climate change on air quality, impact of biofuels, non-linear non-Gaussian methods for data assimilation, multi-scale data assimilation, data fusion for optimal design of air quality monitoring networks, explicit modeling of urban climate with computational fluid dynamics, studies of atmospheric dispersion in the stable boundary layer).
- Implementation of the research and development tasks (by permanent staff, post-docs, Ph.D. students and summer interns).
- Presentation of the results of the research in journals, as well as at conferences, seminars and workshops.
- Increased and new interactions with other research groups (including participation in French, European and international research programs); establishing long-term partnerships with experimental research groups (e.g., in atmospheric chemistry) will be particularly beneficial.
- Distribution of selected work products to the scientific community for wider use (e.g., computer codes).
- Active participation in the implementation of operational systems (e.g., the Prev'air air quality forecasting system, the future French radionuclides monitoring network: Descartes).
- Transfer of technology developed at CEREA to industry (e.g., EDF) and government agencies (e.g., IRSN, INERIS).

- Recruitment of talented Ph.D. students and post-doctoral fellows.
- Teaching of courses in environmental science and applied mathematics using simulation tools developed at CEREA.

Successful implementation of these research, development, teaching and technology transfer activities will allow CEREA to become one of the premier groups in the field of air quality modeling.

Scientific Project

This document describes the scientific project of CEREA for 2010-2013. Section 1.1 presents an overview of CEREA. Section 1.2 provides the overall scientific project for the 2010-2013 period. Sections 1.3 through 1.6 describe specific projects planned for each of the four major research areas of CEREA.

1.1 Current Status of CEREA

1.1.1 Organization

The Research and Teaching Center in Atmospheric Environment (CEREA) was established in 2004 as a research center of École nationale des ponts et chaussées (ENPC, a founding member of both Université Paris-Est and the Paris Institute of Technology/ParisTech). CEREA is a joint laboratory between ENPC and the Research & Development Branch of the French electric utility (EDF R&D). It hosts a joint project with the national computer science institute (INRIA) since December 2005, the CLIME project. CEREA has three locations (ENPC at Champs sur Marne, EDF R&D at Chatou, INRIA at Rocquencourt).

CEREA is led by a Director (Christian Seigneur) and two Deputy Directors (Luc Musson-Genon, EDF, and Marc Bocquet, ENPC). The joint project with INRIA (CLIME) is led by Isabelle Herlin, INRIA, Project Director, and Marc Bocquet, ENPC, Deputy Project Director.

The Oversight Committee of CEREA includes 3 representatives each from EDF and ENPC; the Director, the Deputy Directors and the Director of the CLIME project attend the Oversight Committee meetings. The Oversight Committee meets twice a year: in July for the presentation of a Progress Report and in December for the presentation of the results for the past year and a forecast of the activity for the coming year. Four reports are then proposed for approval by the Oversight 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 operation of this joint laboratory is governed by a contract between ENPC and EDF R&D. The current contract covers 2008-2011. At the end of each quadrennial period, an evaluation of CEREA past activities and future plans is conducted by an international scientific committee; the resulting report by this scientific committee is then submitted to the scientific committees of EDF and ENPC.

A contract between ENPC and CEREA to cover the joint CLIME project is being drafted.

Figure 1 depicts the organization of CEREA according to the three host organizations.

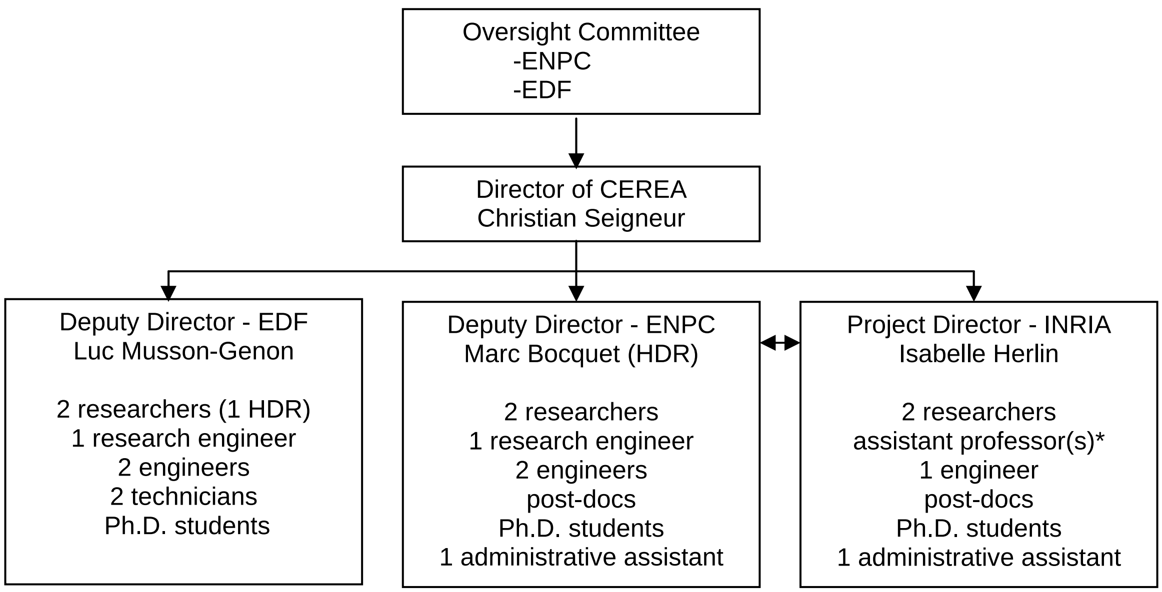

Figure 1. Organization Chart of CEREA for the 2010-1013 period.

* Assistant professors can be assigned to an INRIA project for a two-year period.

The main research activities of CEREA are devoted to air quality and atmospheric dispersion modeling from short-range to long-range scales. Research activities are also dedicated to studying the atmospheric boundary layer (notably for applications related to wind power estimates) and the assimilation of satellite images.

A special focus is given to the assessment of environmental impacts of transportation 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 of Transportation through its Research Directorate.

As a research laboratory co-funded by a private company (EDF) and a graduate school (ENPC), CEREA has a double focus on:

- Academic activities (illustrated by scientific publications and Ph.D. theses);
- Applied projects with end-users (from impact studies to development of models and methods for environmental forecast and monitoring network design).

1.1.2 Overview of Research Activities

Research activities are organized according to four major areas:

- Atmospheric fluid mechanics and short-range dispersion
- Air quality modeling at urban, regional and continental scales
- Data and image assimilation, inverse modeling, network design (CLIME project)
- Observation of the atmospheric boundary layer

CEREA conducts 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, Polyphemus. Polyphemus is a modeling system, which includes different models ranging from short-range dispersion (Gaussian plume 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 incorporated in these three-dimensional models.

The resulting models are evaluated by comparisons to available measurements and used for environmental impact studies or forecasting. The research activities devoted to data assimilation (i.e., integrating observations into the modeling process) aim at improving the ability of models to provide high-quality forecasts and/or perform inverse modeling to improve model inputs.

In addition to modeling activities, a measurement team participates in several campaigns in order to improve the understanding of the atmospheric boundary layer and to support the evaluation of Mercure_Saturne.

1.1.3 Overview of Teaching Activities

CEREA scientists organize and teach courses in air pollution and mathematical modeling at Université Paris-Est, ParisTech (ENPC is a founding member of both), and other universities and engineering schools. Typically, more than 200 teaching hours are given by CEREA staff per year.

1.1.4 Applications and Technology Transfer

CEREA participates in many projects of EDF R&D (related to the requirements of EDF operational departments, both for nuclear production and thermal production of electricity). In addition, CEREA conducts many applied projects with various industrial partners and government agencies. The practical aspect of the applications of CEREA scientific activities can be exemplified by three major operational results:

- The ensemble method for air quality modeling developed at CEREA is currently being tested at INERIS for their national air quality forecasting system.
- The methods developed for monitoring network design at CEREA have influenced the development of monitoring networks implemented by IRSN.
- Environmental impact studies have been conducted with CEREA numerical models for EDF facilities

1.1.5 Key Partnerships

CEREA has three national strategic partners:

- "Institut de radioprotection et de sureté nucléaire" (IRSN; Agency for nuclear safety).
- "Institut national pour l'environnement industriel et les risques" (INERIS; Agency for the industrial environment and risk analysis).
- "Institut Pierre-Simon Laplace" (IPSL) (CEREA focuses mostly on meteorological measurements at the observational site (SIRTA) in the southern suburb of Paris at Palaiseau).

Other current partnerships with French organizations include the following:

- French Ministry of Transportation
- Technical Center of the Ministry of Transportation for northern France (CETE Nord-Picardie).
- R2DS network (Research Network for Sustainable Development, funded by the Ile de France region)
- "Programme national de chimie atmosphérique" (PNCA) for aerosols and data assimilation
- Primequal (research projects sponsored by the Ministry of Ecology)

CEREA has also developed several international partnerships:

- CEREA has a long-term partnership with EDF Polska (the EDF electric utility in Poland)
- CEREA is a member of the European projects HEIMTSA and EXIOPOL devoted to integrated modeling of air quality impacts (especially with IER Stuttgart)
- CEREA participates in MICS Asia (air quality model intercomparison in Asia) and EMS-Beijing (air quality forecasting for Beijing, China).
- CEREA has an active cooperation through the CLIME project with CMM, Chile, the University of Cordoba, Argentina and the environmental monitoring group of CNEA (STIC-AmSud)

1.2 CEREA Project for 2010-2013

As discussed in the Summary Report for 2004-2008, the first four years of CEREA have been quite successful in terms of both academic activities (research and teaching) and applications of work products. The main objectives for the 2010-2013 period are to strengthen the position of CEREA in the academic and applied fields and to increase its recognition at the international level. Specific actions to attain these objectives are articulated below in terms of management, research, teaching, recruitment, financial projections, technology transfer and information.

1.2.1 Management

The main challenges facing CEREA management are twofold:

- Increasing communication among the three sites at Champs sur Marne (ENPC), Chatou (EDF R&D) and Rocquencourt (INRIA)
- Recruiting talented scientists, engineers and technicians (see Section 1.2.4)

Regarding internal communication, regular CEREA meetings where current and future activities will be discussed are planned.

1.2.2 Scientific Plan for Research

The overarching objective of CEREA is to produce policy-relevant, high-level research and modeling tools, that can be used by decision makers in the fields of energy, urban and transportation management. To that end, CEREA aims to be a leader in advanced three-dimensional modeling for environmental impact studies and environmental forecast, with an expertise ranging from state-of-the-science models to advanced numerical methods (data assimilation, ensemble forecast, inverse modeling, monitoring network design). The two work-horses of CEREA for numerical simulations are Mercure_Saturne for computational fluid dynamics (CFD) and Polyphemus for air quality modeling. Note that components of these two modeling system are occasionally coupled when deemed appropriate (e.g., coupling of the aerosol model with CFD model for the simulation of near-roadway air pollution). Furthermore, other models are used at CEREA to address other issues related to air quality, e.g., coupling of Polyphemus with a land/water/foodchain model (Ourson) for assessing multimedia impacts of heavy metals and persistent organic pollutants.

The selection of research topics at CEREA will take into account the existing capabilities of CEREA staff and the importance of the issues for the scientific community and/or policy analysts/decision makers. Thus, one will ensure that the research conducted at CEREA can be successful in terms of both academic results (e.g., publications in the peer-reviewed literature, Ph.D. theses) and practical applications (e.g., operational tools and methods suitable to address real-world problems, registration and distribution of open-source computer codes). CEREA plans to expand its current activities to a level that places it among the top research groups in the modeling of the atmospheric environment by implementing the following actions:

- Identification of topics of current or emerging interest for which CEREA has the capabilities to make a difference (e.g., exposure to ultrafine particulate matter near roadways, treatment of uncertainties in air quality forecasting, development of new data fusion methods for optimal monitoring network design, influence of climate change on air quality, impact of biofuels, development of non-linear non-Gaussian methods for data assimilation, multi-scale data assimilation, explicit modeling of urban climate with atmospheric computational fluid dynamics, studies of atmospheric dispersion in the stable boundary layer)
- Effective implementation of the research and development tasks by permanent staff, post-docs, Ph.D. students and summer interns
- Publication of 15 to 20 articles in international peer-reviewed journals per year

In addition, it will be essential for CEREA to increase its interactions with the measurement community because experimental data are needed for model formulation, inputs and data assimilation, as well as to evaluate the models. The measurement group at CEREA is focused on meteorological measurements; thus, long-term partnerships with research groups active in chemical measurements (both laboratory and field measurements) will help extend the existing relationship between modeling and measurement that currently exists for micrometeorology to include atmospheric chemistry.

The specific research topics that are currently planned to be investigated are presented in detail in Sections 1.3 through 1.6 for each research area. Note that changes are likely to occur between now and 2013 as science evolves rapidly in some areas and we may want to refocus some activities to address problems of highest interest in terms of scientific value. Also, the needs of the user community (e.g., EDF, IRSN and INERIS) are likely to evolve and CEREA will adapt its development activities to meet the demands of those organizations.

1.2.3 Plan for Teaching Activities

Teaching at CEREA includes both training Ph.D. candidates to conduct research on their own and teaching courses at universities and engineering schools. The objectives for the 2010-2013 period are as follows:

- to initiate from 3 to 4 Ph.D. theses per year (each thesis is to be completed in about 3 years); see below for recruitment.
- to teach graduate courses in environmental science, applied mathematics and mathematical modeling at Université Paris-Est, ParisTech and other universities and engineering schools. In particular, CEREA will plan to participate in multidisciplinary Master and “Mastère” programs in environmental science and engineering. The use of CEREA computer simulation codes (numerical models) in courses will be considered.

1.2.4 Recruitment

Recruitment of talented Ph.D. students and Post-docs has been a challenge as science and engineering students can typically obtain suitable employment in the private sector and government. We plan to increase our aggressive recruiting through various means including:

- Establishing lasting relationships with foreign universities to offer desirable post-doc position to our graduating Ph.D. students and to recruit Ph.D. students and post-docs from those universities
- Recruiting Ph.D. students among student trainees (including the civil servants of the “Corps des Ponts”)

1.2.5 Financial Plan

Our base funding from ENPC and EDF R&D is established for the 2008-2011 period. In addition, the INRIA CLIME project team is assigned to CEREA until 2009. The CEREA base funding is augmented via outside funding from several strategic partners (IRSN, INERIS) for long-term research and development projects as well as from other industrial companies and government agencies for specific research projects and applied studies. We intend to increase outside funding as follows:

- Obtaining research funding from French government agencies such as ANR, INSU, and the Ministry of Ecology (Primequal)
- Obtaining research funding from European agencies and programs as a Principal Investigator
- Approaching industrial organizations for sole-source or competitive projects
- Strengthening relationships with some key scientific organizations such as “Institut Pierre-Simon Laplace” (IPSL) and international research programs (e.g., MICS-Asia, STIC-AmSud)
- Exploring possibilities of new international funding (e.g., China, South America, North America)

The distribution of the base funding among the various research areas is decided by the CEREA management team and proposed to the Oversight Committee for approval.

1.2.6 Technology Transfer

CEREA is an R&D laboratory and it is essential that its major work products be transferred to third-party organizations for operational applications. To that end, CEREA will continue to emphasize the transfer of technology to government agencies, industrial organizations and the scientific community. Ongoing and planned activities include the following:

- Incorporation of ensemble modeling methods into the air quality forecasting platform Prév'air at INERIS as well as the future European air quality systems (PROMOTE and GMES)
- Application of methods developed at CEREA for the optimization of monitoring networks for radioactive material by IRSN
- Application of optimal network design techniques for urban air pollution by AIRPARIF (the Paris air quality agency) and INERIS
- Application of air quality models to EDF sites to assess potential air quality impacts of emissions from fossil-fuel fired and nuclear power plants
- Use of the CEREA air quality modeling system for ensemble modeling of air pollution by the Institute of Atmospheric Physics of the Chinese Academy of Sciences

Other opportunities to transfer key work products of CEREA research and development activities will be identified and implemented on an ongoing basis. For example, specific efforts will be made to increase the applications led for the Fossil-Fuel-Fired Generation and Engineering Department of EDF (eventually for Eurelectric, the association of the electric utilities in Europe) and to develop joint projects with CIT and CIDEN (the technical centers of EDF in charge of thermal production and nuclear production engineering, respectively), as well as to play a major role in the Air Quality Network of the French Ministry of Transportation through joint projects, training sessions and hosting of visiting staff. Developing joint projects with Météo France (the French weather service) will be considered. Another possibility is to promote projects inside the Advancity ("ville et mobilité durables") research cluster ("Pôle de Compétitivité"), which is devoted to the urban sustainable development.

In addition, CEREA and INRIA plan to register the Polyphemus computer code with the "Agence pour la Protection des Programmes" (APP). The code will be open source.

1.2.7 Information

CEREA will disseminate information related to its research and development activities in various ways including:

- Publications in the peer-reviewed scientific literature (15-20 per year)
- Presentations at conferences (20-30 per year)
- Invited seminars at universities, engineering schools and workshops
- Distribution via Internet to existing and potential users of the Polyphemus air quality modeling system, which is an open source code
- Polyphemus annual workshops (organized to facilitate communication among users of the Polyphemus air quality modeling system)
- Distribution of Mercure_Saturne, which is a computational fluid dynamics open source code (http://retd.edf.fr/code_saturne)
- Organization of an international conference

1.3 Scientific Plan for Short-Range Modeling

The interest for micro-scale modeling of the atmosphere is growing for environmental applications related, for example, to energy production, transport and urban development. The key issues are first to describe the complicated geometry due to buildings in industrial or urban sites sometimes in complex orography and second to describe the complex local meteorological conditions that can arise, such as the local thermal circulations found in sea breeze or the inhomogeneous formation of fog patches.

Even if simplified approximate parameterizations of these effects are actually often used for these studies, this is not always justified and three-dimensional detailed modeling with appropriate Atmospheric CFD (ACFD) models is required to better quantify these effects.

The main fields of application can be grouped according to the following two criteria : effect of the atmospheric environment on the human activities and the reverse effect.
The first group comprises for example the effect of strong wind on the resistance of industrial infrastructure (buildings, roof, cooling tower, electric lines, ..), the effect of the urban climate on energy consumption (with indirect effects such as the cooling of cities in a changed climate) and the estimation of wind power potential (turbulence and fluctuations of production).

The second group includes human activities that release effluents in the atmosphere: local impact of industrial activities and energy production, local impact of traffic in proximity of road infrastructure, including acoustic propagation. One may also add the effects of accidental releases such as the rupture of a storage tank of flammable or toxic material, and intentional releases of NBC materials (terrorist attack).
For these different domains of application the main scientific challenges for micro-scale meteorological modeling are:

- The description of the atmospheric thermal stratification in the ACFD modeling, especially turbulence in the stable layers where pollutant dispersion is low and can lead to strong pollution events. This could be further complicated by the presence of clouds or fog and is specifically difficult in urban or industrial area due to the presence of buildings.
- The numerical simulation of NBC dispersion which requires a detailed description of interactions between gas chemistry, aerosols and cloud or fog droplets including explicit or parametric description of size distribution.
- Data assimilation in ACFD modeling in order to better describe initial state or external forcing but, more particularly, to merge model and measurement data to obtain the best possible knowledge of the flow and dispersion structure for impact or accidental studies.
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To these scientific topics, technical computing challenges can be added regarding the software development and the optimal use of computer resources (massively parallel architectures).

According to these objectives, the main actions for the group and around the Mercure_Saturne code for 2010-2013 period can be structured in the following way. The detailed actions related to wind power estimate and to the SIRTA observatory are described in Section 1.6.

1.3.1 Software Development

Mercure_Saturne is the atmospheric version of the general purpose CFD Code_Saturne. This code has now been released as Open Source (GPL License) since 2007. The first objective is to follow this path with an Open Source version of Mercure that could be activated as an option in the Code_Saturne modeling system. An added benefit of this policy would be a better integration in the computing environment (code coupling), geometry handling and massively parallel computing (Code_Saturne runs on the Blue Gene machine EDF has recently acquired). The validation database will be extended to cover more application cases, according to the new developments. This validation database is rerun for each new version as part of the software quality procedure. This procedure will also be improved in the framework of the European program COST 732 (Quality Assurance and Improvement of Micro-Scale Meteorological Models). In addition, a special effort will be made to improve the pre processing procedures to generate the mesh in the difficult cases where buildings are mixed with complex topography (a valley, a cliff). We will also improve the interface with the various databases containing geometrical descriptions of cities.

1.3.2 Data Assimilation

Data assimilation is an important topic for meteorological models to improve the quality of simulated fields. For Mercure_Saturne, our goal is to implement a nudging procedure, conceptually similar to that found in MM5 or WRF but adapted to unstructured grids. This is a challenging issue as this type of procedure has never been implemented in complex geometries (such as for example in the urban canopy). Because the full adjoint model is not available (and there are no plans to develop one) we will restrict ourselves to using the adjoint of the transport-diffusion equation, which can be easily implemented. With this approach, we will carry out inverse modeling of dispersion in complex geometries with fixed meteorological conditions, in order to locate source terms based on concentration measurements. This will be tested on the Bugey power plant for which we have wind tunnel measurements, extensive experience of direct modeling and of inverse modeling with simpler tools. This will be achieved in collaboration with the assimilation team at CEREA (Section 1.5).

1.3.3 Urban Canopy Modeling

So far, the vast majority of urban canopy modeling has been performed in neutral conditions. As said above, the simulation of the thermal effects in the urban canopy is a difficult task. To that end, we will further develop the 3D atmospheric radiative scheme available in Mercure_Saturne to be able to simulate the urban canopy in stable and unstable conditions. A number of applications are envisioned such as the dispersion of pollutants in extreme meteorological cases, energy consumption in cities (thermal budget) and acoustic propagation.

In the context of climate change, the modeling of the atmosphere in Megacities, where 80% of population could be living in the future, is an important objective in terms of energy consumption, and public health (heat waves, air quality). The growing of computer power and ACFD possibilities leads us to consider the explicit computational modeling of the urban atmosphere possible. Following the Ph.D. thesis of Maya Millez (2006), we propose, in cooperation with the CSTB and Météo France, to adapt Mercure_Saturne to the modeling of the energetic exchanges in a town district by coupling thermal building codes with real meteorological large scale conditions given by Météo-France (MUSCADE project submitted to the ANR). This work can be achieved and validated with the data concerning the city of Toulouse collected during the CAPITOUL experiment.

An extension of this work to air quality modeling could be considered with the different chemical schemes developed by the other teams in CEREA. This could then be applied to the study of the future evolution of cities under an important climate change (for example detailed simulations of green / white roofs, local influence of heating/cooling, etc). This work should be included in the projects following the Agora 2020 discussion of the French Ministry for Transport.

1.3.4 Modeling Cooling Towers

Cooling towers have important industrial applications and generate atmospheric plumes which impact the atmospheric environment (interactions with low clouds, fog, reduction of visibility, solar radiation). The accurate simulation of the cooling tower plumes is therefore required to improve the situation. This can be performed by coupling the modeling of the atmospheric dispersion with Mercure_Saturne to the modeling of the internal flow and thermodynamics using Code_Saturne with its specific modules adapted to cooling towers (exchange packs, fans). After the Ph.D. thesis of Emmanuel Bouzereau (2005) concerning the modeling of the atmospheric part, it is now possible to use the specificities of non-structured meshes as for Code_Saturne. This could be coupled with the ASTER code (mechanics of structure, EDF R&D). In addition the effect of strong winds on the structure and performance is an important modeling aspect that will be addressed with these tools. Other applications are also possible in collaboration with INERIS concerning industrial cooling tower. A cooperation should be considered to benchmark several models using liquid water plume description on an experimental data set providing from a experiment campaign schedulded in 2009 involving CSTB, INERIS.

1.3.5 Impact Studies for Nuclear Plants in Complex Terrain

Up to now, long term impact studies for nuclear power plants have been performed with simple tools that are not suited for buildings and complex terrain. Previously, a few cases have been simulated (typically 10 different wind directions). The aim is to carry out real impact studies by modeling the dispersion over a long period (typically a year). This will require a massive amount of computations but also a long term validation with a measurement database such as that performed on the SIRTA experimental site (Section 3.5). The case studies could be the plants of Flamenville, Penly and Chooz.

1.3.6 Sensitivity Analysis and Uncertainties

ACFD simulations can produce very accurate values for given specified inputs. However, in practice, there are many uncertainties in these inputs such as the large scale meteorological conditions. The goal is then to characterize these uncertainties in the simulated values by means of sensitivity analyses. This involves a large number of simulations, together with optimization techniques to try to reduce the required number for a given accuracy. Different approaches will be theoretically investigated on small cases (with a low computational burden).

1.3.6 Large Eddy Simulation (LES)

In some identified cases (such as dispersion close to the source, flow zones with very large gradients, very unstable boundary layers or dissipation of fog patches) the Reynolds Average Navier Stokes (RANS) equations, that we usually solve with a k-ε approach, have shown limitations. These cases will be further investigated using a LES approach, with a particular emphasis on inhomogeneous conditions and complex geometries, which have been rarely investigated previously. This requires large computing resources and will be performed after the massively parallel version is operational.

1.3.7 Modeling Local Traffic Pollution and Exposure

Traffic is a major source of local pollution both for gases and aerosols. Detailed simulations with ACFD tools is a decisive aid in better design of road infrastructures and various protections. New possibilities will be implemented in Mercure_Saturne to cover these needs. For example the effect on local pollution of acoustic protection will be studied in details. For the study of particle formation in the near field, the modal aerosol model of CEREA (MAM, Section 1.4) will be further adapted to be able to handle all cases from rural roads to urban traffic.

Coupling outdoor air quality (simulated with Mercure_Saturne) with indoor air quality (simulated by Code_Saturne) is also a possible extension of current work. This should be done in close collaboration with CSTB. A good case study could be the site of ENPC or of CSTB at Champs sur Marne.

1.4 Scientific Plan for Air Quality Modeling

CEREA has developed during the period 2004-2007 a new modeling system, Polyphemus. The Polyphemus is characterized by the following features:

- it covers the local, regional and continental scales
- it hosts different models (Gaussian models, Puff models, aerosol models, two Chemistry-Transport Models)
- it allows different uses of models viewed as black boxes to be driven (forward simulation, data assimilation with sequential and variational algorithms, ensemble forecast)
- it includes different "kinetics" (photochemistry, radioactive species, heavy metals, mercury, Persistent Organic Pollutants).
-

The objectives for the period 2010-2013 is twofold: (1) to improve the physical and chemical components of the air quality models that constitute Polyphemus and (2) to extend and improve the capabilities of the modeling platform Polyphemus and its applications.

1.4.1 Update of the Current Available Aerosol Models

Particulate matter is a key component of air quality, both through health impact (fine particles) and radiative effects.
CEREA has developed two aerosol models during the period 2003-2007:

1. SIREAM, a size resolved aerosol model:
2. MAM, a modal aerosol model:

Both describe the inorganic and organic components. Both models are based on the same physical parameterizations and only differ by the size discretization (modal versus sectional).

- SIREAM and MAM are currently coupled to a version of ISORROPIA that takes into account sodium, sulphate, nitrate, ammonium, chloride and water. They will be coupled to other existing thermodynamic models, especially for having a better description of the mineral (crustal) components;
- The parameterizations used for the heterogeneous reaction probability for N_2O_5 will be updated in order to take into account the aerosol chemical composition, temperature and humidity. This update is expected to decrease the high nitrate concentrations simulated over Europe in winter.
- In SIREAM, the number distribution needs to continue to be better described. Currently, the number distribution is simply deduced from the mass distribution, assuming that the density is constant and that the volume of particles is a function of the cube of the mean diameter. The use of a moving-diameter approach will offer the possibility to treat both number and mass concentrations jointly. This feature will be particularly useful when addressing both ultrafine particulate

matter (UFPM) and $PM_{2.5}$ (or PM_{10}) because the number concentration is relevant for UFPM whereas the mass concentration is relevant for $PM_{2.5}$ and PM_{10}.

1.4.2 Secondary Organic Aerosols

The current organic aerosol model does not have a precise description of the organic components, although the partition of anthropogenic and biogenic secondary organic aerosols is taken into account. As simulations over Europe with Polyphemus under-estimate the formation of SOA, the organic aerosol model was recently updated to include:

- the description of hydrophylic/hydrophobic effects (on the basis of existing work);
- the inclusion of sesquiterpenes and isoprene as new SOA precursors;
- the description of polymerization effects;
- the description of the production of semi-volatile organic compounds.

Further work will address:

- the description of the formation of SOA from aqueous-phase reactions of organic species;
- the description of the formation of SOA from nucleation events;
- the description of the formation of organo-sulphates and organo-nitrates.
- the treatment of high-NO_x and low-NO_x regimes for SOA formation
- improvement of current parametrizations as new experimental data become available

Regarding the last item, we will actively pursue partnerships with experimental groups in Europe and the United States in order to participate in the design of experiments being conducted on SOA formation so that they can be focused on the issues that we perceive to be the most important for improving air quality models.

1.4.3 Modeling of Traffic-Induced Ultrafine Particles

Ultrafine particles (with a diameter of a few hundreds of nanometers) are a key concern at local scales near roadways for the health impact. The application is related to the management of the exhaust emissions through the assessment of the efficiency of filters.
This topic is related to a finer description of the competition between nucleation and condensation. As nucleation is associated to a large number of ultrafine particles of small mass, the impact of aerosol processes on the number distribution, rather than the mass distribution, is crucial. The work already initiated will be continued through a partnership with experimental measurement teams. Contacts with car manufacturers will be initiated to identify co-funding for large experimental programs that can be used to evaluate the models developed at CEREA.

1.4.4 Soot Aerosols

Soot is not spherical and is best represented by particles with a fractal dimension. The objective is then to extend the available models.
Applications will be the air pollution induced by aircrafts (with the partner ONERA) and air pollution induced by traffic.

1.4.5 External Mixing

The current aerosol models are based on the assumption of *internal mixing*. This means that there is a unique chemical composition for a given size. This does not take into account the "history" of the aerosol. Close to sources, emitted aerosols may not instantaneously mix with background aerosols to form an internally mixed population.
The objective is to develop a version of SIREAM based on *external mixing* (a set of aerosol families for a given size). Validation will be done using data from the Escompte campaign, for which the types of mixture of aerosols on a rural site and on an industrial site were determined experimentally. Another key application is the study of the radiative effects of the aerosol composition. A collaboration could be initiated with Laboratoire d'Aérologie (Toulouse, University Paul Sabatier and CNRS; Marc Mallet).

1.4.6 Radiative Effects and Photolysis

Radiative effects are strongly controlled by the vertical distribution of aerosol composition and optical properties. Comparisons of simulated profiles to lidar data will be done by teaming with Patrick Chazette (IPSL, LMD). The radiative effect of clouds on photolysis rates will be taken into account by coupling the radiative transfer scheme FAST-J or TUV to the CTMs of Polyphemus. Currently, clear-sky photolysis rates are preprocessed data, which are tabulated using climatological values of temperature, pressure and ozone. In the coupling with a radiative transfer scheme, the modeled values of temperature, pressure and ozone will be used, together with the modeled aerosol profiles for extinction and scattering.

1.4.7 Multiphase Processes for Radionuclides

Part of the radioactive species associated with an accidental release in the atmosphere are bound to existing aerosols. This is for instance the case for cesium. They can also participate in multiphase processes (for instance iodine either in elemental or in organic forms, eventually dissolved). The objective is to develop a multiphase model for radioactive chemicals. A first item is the coupling of the aerosol model SIREAM to a radioactive model describing daughter products. A second item is the development of a model with multiphase processes.

1.4.8 Numerics for the General Dynamic Equation

The General Dynamic Equation (GDE) describes the time evolution of the aerosol size distributions, governed by nucleation, coagulation and condensation.
The numerical simulation of the GDE is also still a challenging issue, especially with the increase in complexity to arise in near future (see the points above). A key point is also the coarse discretization (for the size distribution) used for 3D modeling. The objective is to develop robust algorithms for the GDE. Adaptive gridding of the aerosol size distribution should also be investigated. Such a modeling approach will be particularly useful to address both UFPM and $PM_{2.5}/PM_{10}$ problems jointly as a finer size resolution will be needed for the ultrafine particles (i.e., >0.1 μm) than for the other fine and coarse particles.

1.4.9 On-the-fly Developments and Software Developments

A parallel version of the base CTM of Polyphemus, Polair3D, will be developed in 2008-2009, especially for aerosol models and thermodynamics. Quality software-developments will also be performed: unit tests, procedure of automatic validation for the new releases, usability, etc. The target for the dissemination (Polyphemus is open source and distributed under GNU GPL) is to release a new version every six months and to organize a training session every year.

1.4.10 Physical Models Development and Evaluation

As a new laboratory, with its own new models, CEREA has mostly filled the initial gap between its modeling tools and state-of-the-art systems. There is a need to further develop the physical models, to improve their performances for dedicated targets and to acquire accurate knowledge about their behaviour.
As a first step, dispersion itself should be improved: better control of the models discretization, improved turbulent parameterization, parameterized convection, ...Even if there are upcoming changes with respect to meteorology (fine discretizations, coupling with aerosol models), this work is necessary to compete with the best models in the following years.

A second step is the need for detailed analysis of the chemical mechanisms. CEREA should increase its own expertise in chemistry in order to perform sensitivity analyses (to emissions, to photolysis rates), to compare different mechanisms, to improve the mechanisms for given targets, ... Among the concrete objectives, there are:

- forecasts for Prév'air platform on which Polyphemus models should bring the best forecasts, especially through ensemble forecasts;
- the ability to simulate columns of ozone and aerosols (link with satellite observations);
- taking accurately into account very-long-range or global-range transport (e.g. ozone transport over Atlantic or over Asia);

- evaluation of the models with strong topography or unusual meteorological conditions.
-

Université Paris-Est offers the opportunity for developing a strong relationship with LISA, a laboratory with a recognized expertise in chemistry.

1.4.11 Update and Extension of the Chemical Mechanisms

Other photochemical mechanisms have to be plugged to Polyphemus (for instance SAPRC and CB05). The main objective is to improve the ability to perform ensemble forecasts and to estimate the reliability of impact studies (for instance for COV/NO_x reductions with ozone as a target).

The currently available models devoted to mercury and heavy metals will be updated and coupled to aerosol models. This may have a strong impact through deposition processes. The POP model has to be updated on the basis of state-of-the-science parameterizations. New species and kinetic mechanisms have to be inserted in the model for new applications:

- biological tracers (in the framework of a joint project with INERIS);
- pollens;
- CO;
- tracer for the hemispheric scale

For each application, a comparison to the available sets of observational data will be performed.

1.4.12 Subgrid Parameterization

Subgrid parameterization is a key component of geophysical models. Many *unresolved* processes have indeed characteristic scales much finer than the resolved numerical scale (typically the size of a cell in a Finite Differences framework). The applications for air pollution modeling are related to the vertical turbulent fluxes (parameterization of), the microphysical mass transfer, the coupling between chemistry and turbulence and plume-in-grid modeling. These examples illustrate the need for rigorous approaches in order to derive the appropriate parameterizations. An alternative approach is based on numerical sampling used in order to define the parameterization. A Probability Density Function is then computed on the basis of repeated calls to a microphysical function.

This method is an illustration of "micro/macro" methods that are used in other fields. The principle is to couple a deterministic "macro" model to a stochastic "micro" model. The application of such methods to air quality modeling should be investigated. The typical application is the coupling between chemistry and turbulence (segregation effects), to be investigated by different techniques in near future. Another example is mass transfer (with reactive surface reactions, currently not taken into account). A specific point is devoted to the coupling to an existing parameterization of the convective processes for the CTMs of Polyphemus. This cannot be considered as a research action (no new results are expected): the objective is only to fill one of the last identified weaknesses in comparison to state-of-the-science models.

1.4.13 Plume-In-Grid Modeling

Emissions of point sources in a large grid cell induce a numerical artefact by creating artificial diffusion. One way to reduce this diffusion is to parameterize short-term dispersion of freshly emitted pollutants as an alternative to the use of refined meshes (see above). The parameterizations are usually based on Gaussian models (stationary solutions of the dispersion equation). An issue is the rigorous coupling between long-range Eulerian models and short-range Gaussian models for reactive flows. This will be investigated for multiphase models, evaluated by model-to-data comparisons and applied to the continental scale (for instance for the evaluation of the impact of the thermal power plants - a similar work has already been led in the northeastern USA).

1.4.14 Improvement of Atmospheric Dispersion Models for Short-Range Dispersion

It appears desirable to identify the best features of existing atmospheric dispersion models and to incorporate them into a single modeling framework (i.e., Polyphemus) in order to offer potential users with the ability to conduct both regulatory-type atmospheric impact studies and research-grade investigations. The objectives will be to first assess the current state-of-the-science in atmospheric dispersion modeling and second implement the best algorithms within Polyphemus. This includes the addition of parameterizations to take into account complex geometries. Evaluation of the new model against available observations and comparison with standard models such as AERMOD, ADMS, CALPUFF and SCIPUFF will be conducted. The Lagrangian “particle” model developed at EDF could be part of this package.

1.4.15 Ensemble Forecast and Probabilistic Outputs

A promising approach is not to rely on one single model but to use a set (an *ensemble*) of models or of model configurations to deliver the forecast. To date, the work performed at CEREA has focused on ozone. The extension to the multiphase models (more generally to any model outputs of Polyphemus) should be investigated. One objective is to routinely deliver probability density functions of the model outputs (a key point for forecast and impact studies). Another approach to be investigated is the use of ensemble meteorological forecasts. The impact of the spread in the meteorological fields for the CTMs has to be investigated. This could be the opportunity of a joint effort with Météo France (AROME project, François Bouttier).

1.14.16 Coupling

The American projects WRF and WRF-Chem are ambitious projects with a growing community of developers and users. The relationship to these projects has to be carefully evaluated. A key point is to evaluate the opportunity of having available at CEREA a CTM with on-line coupling (such as WRF-Chem or/and BRAMS-CPTEC, see below).
Due to its expertise and to the human resources, CEREA is not able to develop its own on-line coupled model and Polyphemus will continue to be based on off-line coupling in near future. However, it may be relevant to initiate projects that evaluate the impact of on-line coupling (especially for forecast and regional scale).

1.14.17 Next Generation Chemical Transport Models

The grid resolution may have a strong impact on the results. The future generation of chemical transport models (CTM) will have a fine resolution (let say 0.1 for the horizontal dimension, less than 5 kilometers) in coherence with the high-resolution meteorological models, currently under development. One may also wonder if the next generation of CTM will not be based on unstructured methods, similar to those used in CFD (Computational Fluid Dynamics). Adaptive gridding and unstructured methods have to be investigated for CTM (especially for zooming, as an alternative to parameterizations of subgrid processes). The boundary conditions for continental- and regional-scale models are typically obtained from a global model. We will explore whether CEREA should develop its own global model or develop a long-term relationship with a group that supports an exiting global model (e.g., GEOS-Chem of the Harvard group)

1.4.18 Integrated Modeling

Following Jan Rotmans (Rotmans J. and van Asselt M.B.A., *Uncertainty in integrated assessment modelling: A labyrinthic path*, Integrated Assessment, Vol. 2, pp 43-55, 2001), “integrated assessment models are frameworks to organise and structure various strands of recent scientific knowledge”. Generally these models aim at answering specific issues of interest for the public policies and are expected to serve the decision-making process. This kind of approach is strongly supported by the European Union. The current inputs of CTM are emission data (based on the so-called SNAP classification). The current outputs are time evolutions of 2D (fluxes) or 3D fields (concentrations) related to the modelled species.

Extending the current models to integrated modeling chains starting from economic activities to exposure of population is of great interest. However, until now only rather simple parameterizations (possibly derived from complex models) are used mainly due to the computational time requirements. It should be interesting to couple more comprehensive dispersion models (as those provided by Polyphemus) to already existing frameworks or include them in the development of new ones. CEREA participates, jointly with the IER - University of Stuttgart (where the EcoSense model is currently developed), in two European projects started in 2007:

- EXIOPOL (a new Environmental accounting framework using eXternality data and Input-Output tools for POLicy analysis), mainly devoted to the valuation of externalities.
- HEIMTSA (Health and Environment Integrated Methodology and Toolbox for Scenario Assessment), focusing on exposure and health impact assessment.

Moreover, a joint project should be initiated with another research laboratory depending from ENPC, CIRED (Jean-Charles Hourcarde), in order to build an integrated model devoted to air quality. A first work could be the assessment of the uncertainties related to existing models such as GAINS/RAINS. A joint project should be submitted to the R2DS network. The objective is to have an integrated framework around Polyphemus in 2011 to perform Cost Benefits Analysis and Health Impact Assessments based on economic scenarios at regional and continental scales.

1.4.19 Hosting New Models

To date, Polyphemus hosts two of the three French Chemistry-Transport Models, namely Chimere (through a C++ clone, Castor) and Polair3D. The opportunity of hosting Mocage, the global CTM developed by Meteo France, is relevant in order to share parameterizations, algorithms (especially for data assimilation or ensemble forecast) and to save time for the three concerned teams. This will also allow Polyphemus to run global simulations. Hosting global CTM with a stronger scientific basis (for instance Mozart or GEOS-CHEM) has also to be investigated in close connection to the development teams.
Hosting BRAMS-CPTEC, that already use components of Polyphemus (multiphase chemistry) is a project under way in the framework of the STIC/AMSUD project led by the Clime project (with Brazil, Chile and Argentina). The main application is biomass burning (with an hemispheric scale). It will also allow Polyphemus to support on-line coupling with the meteorological model RAMS. Contacts with other teams (including the teams in charge of the development of LOTOS, DREAM, etc) will be taken. Hosting new models also means hosting models for other media (for instance for multi-media impact: a first attempt has been made for the modeling of POP with a soil model). Joint projects with the Water Research Laboratory of ENPC (CEREVE) should be investigated. These are only examples and it does not exclude other models (for instance FARM/STEM developed by G. Carmichael and ARIA-Italy).

1.4.20 Applications

The main applications of Polyphemus will be related to the needs of:

- EDF for impact studies at regional and continental scales, and possibly air quality forecast at regional scales (a project under way with CIT/EDF);
- IRSN (forecast of radioactive chemicals);
- INERIS (short-range dispersion of chemical and biological tracers, impact studies at continental scale, air quality forecast).

The following points should be investigated in the framework of applied projects:

- The abilities of Polyphemus for performing impact studies have to be improved, especially through automation. A concrete objective could be to reduce to one day the time required for preparing the runs of an impact study of a power plant. The relationship to the Fossil-Fired Generation and Engineering Department of EDF should be strengthened with a possible extension to Eurelectric. This could be also the opportunity of having projects with EPRI (USA).

- The same kind of projects could be done for the French Ministry for Transportation either at regional scales (similar to the traffic study performed for Lille) or at national scale (to study the impact of new fuels or of new road infrastructures). The availability of a new detailed National Emission Inventory (all the more managed by Christian Seigneur) is a key point.
- For forecast (IRSN/CTC and INERIS/CASU and Prév'air), Polyphemus will systematically extend its outputs to probabilistic outputs.
  The joint projects with foreign teams have to be strengthened in order to increase the number of applications to Megacities. To date, this includes Santiago de Chile, Tokyo, Delhi and Sao Paulo on the basis of current projects under way. CEREA lacks a Chinese partner, typically for an application to Beijing.
- CEREA should take part in a benchmarking exercise in Asia (phase 3 of the MICS project). A corresponding exercise should be planned for South America. It is a key point to take part in a possible corresponding exercise for Europe (CEREA had the opportunity of joining the Eurodelta exercise but Polyphemus was still in development).
- Applications to develop matrices of source-receptor transfer coefficients and the development of new methodologies to optimize the development of such transfer matrices.

1.4.21 Effect of Climate Change on Air Quality

Climate change will affect air quality in several ways: changes in emissions that are affected by wind, temperature and precipitation, changes in local and regional meteorology that will affect the transport, dispersion and removal of air pollutants, and changes in chemical transformations due to changes in temperature and solar radiation. CEREA can take the output of global climate change models applied by other research groups to perform downscaling of the meteorology; then, this new meteorology will be applied to calculate new emissions and air quality. The implications of climate change for future air quality policies can be investigated and various emission scenarios can be tested to provide decision makers with quantitative information on the potential effect of climate change on the air quality and various options to mitigate those effects.

1.4.22 Effects of Biofuels on Air Quality

The use of biofuels on air quality has been limited mostly to detailed investigation of the changes in mobile source emissions on air quality or relatively simple cradle-to-grave studies of the effect of all emission sources. There is presently a dire need to develop more comprehensive analyses of all emissions associated with biofuel production and usage (including but not limited to changes in land use, biogenic emissions related to biofuels, transportation of raw material to biofuel production plants, emissions from those plants, transportation of biofuels from the plants to distribution centers and usage of biofuels by mobile sources). Such an effort will require teaming with other research groups with expertise in economics, agriculture and engineering to perform a defensible inventory of all emissions associated with biofuels.

1.5 Scientific Plan for Data Assimilation and Inverse Modeling

The specificity of data assimilation and inverse modeling in geophysical applications is that it applies to very large systems. As a consequence, the applied mathematics methods should be as efficient, if not simple, as possible. It has been successfully used in meteorology (where data assimilation is operational and helps produce forecasts every six hours), and oceanography. Inverse modeling is more specifically used in Earth sciences.
In atmospheric chemistry and especially air quality (in the boundary layer), applications are much more recent (beginning of the decade). The number of control variables is even larger because of the number of species to account for. Besides inverse modeling and data assimilation are closely related. Indeed a good forecast in air quality that makes use of data (data assimilation), is a forecast capable of indirectly estimating the emissions (inverse modeling). Finally, the dynamics differs from meteorology and oceanography since it is essentially non-chaotic, though possibly highly nonlinear with chemistry.
The data assimilation and inverse modeling group is also focussed on other applications where applied mathematics play a significant role such as: ensemble forecast, multi-model approaches, model reduction, network design, or new applications that require new couplings between models and data such as satellite data assimilation into chemistry transport models.

1.5.1 Satellite Data Assimilation into CTMs

Satellite data have been assimilated for years into meteorological models (most of the assimilated data are actually from satellite origin). Observables such as temperature and water vapour (after "deconvolution" from the radiance signal) are assimilated. More recently trace gas observations from satellite have also been assimilated (ozone, methane, etc.). This is especially useful in the monitoring of the stratospheric ozone layer over the poles. However, reaching as deep as the boundary layer and extracting ozone or NO_2 concentrations for air quality purposes is a much more challenging problem. Yet recent non-operational space platforms possess IR spectrometers offering products such as column of NO of direct interest to air quality modeling, and a column between 0 and 6 kilometres of ozone. So that first papers on the assimilation of such products (NO_2 columns) into CTM have appeared three years ago. No dramatic improvements are expected in the precision of these products from new instruments in the coming years. Yet, the possibility of assimilating such data into CTM is so promising, that CEREA should maintain some activity in this domain. Thanks to a contract with the European Space Agency, we have been granted access to the data of MetOp , launched October 2006, and the ozone data of IASI will be exploited. We are also participating in the definition of the modeling applications of the TRAQ platform, in the short-list of the ESA Earth missions.

1.5.2 Data Assimilation for Aerosols

Besides ground observations and spaceborne observations, exists the active sounding of the gas constituents from the ground (or even space). From the ground, the lidar allows the height-resolved probing of optical thickness of the boundary layer (and above). Up to

very recently, deploying a lidar was a difficult task. But new mobile, low budget and safe lidar have appeared (LEOSPHERE). So that it is possible to use a dozen of such lidar to monitor the air quality over an urbanized region. For boundary-layer air quality, this offers very promising perspectives, maybe even more that satellite data.
CEREA is collaborating on a regular basis with a team of IPSL/LMD.

1.5.3 Data Assimilation for Air Quality

The benchmark of data assimilation methods for air quality is still a challenging point (sequential versus variational algorithms). Our air quality data assimilation system implemented in Polyphemus has been tested and validated. It is the baseline to any further developments, in particular towards improving forecast through data assimilation.
Another interesting point could be to optimize with respect to other “appropriate” control parameters (for instance eddy coefficient, emissions, dry deposition velocities, kinetic rates, etc). The case study is logically the Prév'air platform operated by INERIS for air quality forecast.

1.5.4 Model Error

Model error is and is likely to remain at the heart of the improvement of data assimilation methods. A typical source of errors for pollutants is their lack of mixing nearby the emission area (turbulence, up and downdraft). This affects the kinetic rates of reactions, which are different from the kinetic rates of perfectly mixed pollutants in a numerical model grid cell. Improvement of these sources of error will involve subgrid parameterization. At a statistical level, it may involve stochastic parameterization, closely related to the weak formulation of variational data assimilation. Error model can be the by-product of the intentional reduction of models. In this case, the process can be optimized so as to minimize model error as much as possible (for instance with EOF/POD methods).

1.5.5 Ensemble Forecast

Previous work focused on ozone with gas-phase models. Monte Carlo simulations and ensemble simulations were carried out with changes in input data, numerical schemes and physical formulation. This work should be extended to other species and to multiphase models, which requires a rather comprehensive set of alternative physical parameterizations. A key objective of ensemble forecasts is the estimation of uncertainties. From the data assimilation point of view, there are important steps:

- building an ensemble that properly estimates the uncertainties: based on comparisons between observations and ensemble forecasts, the ensemble quality (that is, its ability to approximate the concentrations probability density function) may be assessed;
- extending the *a priori* uncertainty estimations to *a posteriori* uncertainty estimations, where the target is the conditional probability density function of the concentrations, given past observations.

Current ensemble method (to linearly combine different models) compute weights at observation locations. Further work should address models aggregation of 2D fields. Hence the weights associated to the models should be applied in the whole simulation domain. Among other open questions with need for theoretical developments, one may point out the coupling between data assimilation methods and ensemble approaches. For instance, parameter estimation is severely limited by the strong uncertainties arising everywhere in the models. The natural outcome of inverse modeling should be probabilistic estimations of the optimized parameters.

1.5.6 Inverse Modeling and Advanced Data Assimilation for Accidental Releases

The implementation of the methods that have been developed and validated will be carried on at pre-operational level, in partnership with IRSN. ENPC/CEREA and IRSN/SESUC are part of the European DETECT-2 project, in the FP7 Euratom framework, which has just been submitted (May 2008). An exchange and intercomparison exercise on assimilation of radioactive chemicals is also scheduled with M.Sofiev and his team (Finnish Meteorological Institute), and has just been partly funded by INSU (LEFE-Assimilation program). New applications should be considered, such as biological tracers, or dirty bombs in a urban environment setting. With very similar methods that have been used at continental scale, but with Puff models and/or a CFD tool like Mercure_Saturne, one could extend previous studies to urban inverse modeling scenarios.

1.5.7 Network Design

The natural field of applications are radionuclides/accidental pollutant monitoring, and photo-chemistry air monitoring. IRSN is continuing to finance part of these efforts in this field (2008-2010), especially with the optimisation of the IRSN observation network Descartes, to be built in the next five years. A similar effort will be directed towards air quality (photochemistry) monitoring, through a Région Ile-de-France project R2DS, over 2008-2010, with possible collaborations with AirParif and INERIS. New sources of observational data could be used: new “light” networks for air quality (and also meteorology): Harvard University/BBN Technologies (ARPANET)/Cambridge, Massachusetts, Wiki sensors (CitySense), but also mobile lidar network (see above). It considerably extends the coverage of monitoring so that stations selection is not anymore a luxury. Adaptive design should also be investigated in two contexts: near-field to mesoscale in case of a radiological accidental release, and mesoscale to regional for urban pollution with mobile stations.

1.5.8 Image and Air Quality

One of the important themes of CLIME is the exploration of the use of images as structured data to be assimilated into an environmental model (ADDISA project, accepted by ANR). The first applications of image assimilation are meteorology and oceanography (clouds, gyres, vortices, hurricanes, etc.). The idea is to assimilate qualitative, but extremely useful, features (such as the shape of a vortex) into a numerical model of evolution. However the translation of such features into information on the control variables of the numerical model is not immediate and may involve an intermediary complex physical model. The central question is to know whether to perform the assimilation in the space of the control variables of the numerical model or in the space of the features. Applications to air quality can be contemplated: for example the plume of biomass burning observed from space can be used to identify the fires, and / or feed a model of fire evolution through data assimilation.

1.5.9 Assimilation of Satellite Data and Images in a Multiscale/Multiresolution Context

The assimilation of satellite data and images within environmental forecast models (meteorology, oceanography, etc.) should be formulated in a multiscale framework. Models are actually organized in networks, from the global to the local scale, and on another hand satellite image data are available at different resolutions. Structures can be mathematically represented at different scales. The researches will tend to identify, given a model, the relevant observation resolutions allowing the assimilation of adequate data and structures (appropriate for constraining the model and obtaining better forecasts), to define multiscale observation operators linking the state variables and the image data, to define control methods for assimilating structured data according to their resolution. Last, the impact of the multiple assimilation of an image within nested models is still to be understood.

1.5.10 Toward Physical Image Models

Obtaining pseudo-observations from satellite data requires the definition of Image Models describing the image dynamics and properties. Two distinct usages of these Image Models are, indeed, identified:

- Assimilation of images and image structures within a geophysical simulation model. The Image Model serves as an intermediate layer: in a first step images and structures are assimilated within the Image Model to provide pseudo-observations of the state variables. In a second step these pseudo-observations are assimilated within the simulation model. The Image Model satisfies the following requirements: it is designed to be consistent with the physics of the simulation model; it must describe the dynamics of visible image structures that have a potential to constrain the simulation.
- Ill-posed image processing problems solved within the framework of data assimilation. Two cases are considered:
  - Physical information is available to explain the dynamics of the observed phenomena. The Image Model is then built from this physical information, if necessary completed with heuristics on images.
  - If such information is not available, the Image Model is either derived from a generic model adapted to a class of images, or built by inference from the sole data analysis.

1.5.11 Inverse Modeling, Uncertainties and Non-Linearities

The work on second-order modeling carried out at CEREA (sensitivity of the solution of an inverse problem to parameters) should be continued. This is especially important when the physics is nonlinear and/or the retrieval scheme is nonlinear. Then Gaussian approximation of statistics is inefficient and a generalized probabilistic approach is needed. This is more generally related to the estimation of uncertainties that affect the solution of an inverse modeling problem. This activity is also related to the OpenTurns project of EDF R&D in the framework of the network "Uncertainties". The involvement in this network should increase in near future with a focus on probabilistic inverse modeling.

1.5.12 Challenging Statistical and Representation/Multiscale Issues in Air Quality Models

Past publications testify of the statistical and mathematical skills developed at CEREA towards air quality. This effort should be carried on. Several issues have been and will continue to be considered: impact of the space resolution in data assimilation and especially inverse modeling, definition and extraction of a typical meteorological configuration over a period of time, representativity of observations (a question related to subgrid parameterization), representation issues of control variables (such as the positivity of concentrations, sources), etc. On this very subject, an ANR project submitted to the SYSCOMM call, named MSDAG for "Multiscale Data Assimilation for Geophysics" has been accepted in July 2008. Four partners are involved (PI: M.Bocquet): CEREA/CLIME (M.Bocquet), LJK/MOISE (L.Debreu), INRIA Rennes (E.Mémin), IPSL/LSCE (P.Rayner). The project is three-year long (2009-2011), and 480k€ are granted (about 140k€ for CEREA). It should concentrate many of our efforts.

1.5.13 Intensive Computing Issues and Codes

Many of the tasks ahead will involve large computing capabilities. Among them: ensemble forecast (or any Monte Carlo based method), network design, inverse modeling, uncertainty and second-order studies. For some of these applications, parallel computing is not trivial and requires specific developments, on different hardware architecture. A few projects should be proposed to be run on the Blue Gene computer of EDF R&D (a cluster of about 10 000 processors).

It is planned to forge a universal library of data assimilation methods. The language would be high-level (C++) , so as to foster re-usability, and an easy integration in other codes. Given the expertise of CEREA and CLIME on the matter, the methods to be implemented could range from basics techniques (BLUE-based) to advanced ones (Bayesian inference, non-Gaussian approaches, machine learning), a few of them developed by CEREA members.

1.6 Scientific Plan for Observations of the Atmospheric Boundary Layer

A common tendency to use more and more complex tools is observed in atmospheric dispersion and wind energy domains. In both cases, micro-scale numerical modeling is increasingly used and is about to replace in the future the current operational tools, at least for cases in which the expected improvement in accuracy is important due to the complex orography or the complex land use (buildings, vegetation, water ...). This results in an increasing need for detailed measurements in order to provide input and validation data adapted to the simulated physical processes and spatial scales, and to the final goals of the simulations.

The main role of the observations team at CEREA is to provide the data necessary for the development and the validation of the numerical models of the Laboratory. More specifically, the "meteorological measurements" activity is primarily linked to the micro-scale numerical modeling with Mercure_Saturne, and to the development of new methodologies involving this model and/or the instruments.

In this context, the main objectives for the next years are:

- the acquisition of long term data sets, in order to validate Mercure_Saturne on a large range of situations in view of a future use in impact studies, and to develop a new methodology for wind resource estimation.
- the acquisition of data sets on more specific subjects such as turbulence in a stable layer, interactions between microphysical and radiative processes, wake effect of wind turbines, use of remote sensing for wind energy applications ...
- the use of the data set of the ParisFog campaign especially for the study of fog microphysics and influence of complex terrain on fog evolution.
- to keep informed of the evolutions of meteorological instruments and their performances, and to participate to campaigns of tests in collaboration with the manufacturers or/and other laboratories, for the future instrumentation needs of both EDF R&D and operational services of EDF.
- to develop methodologies to derive from the measurements "secondary" parameters, which are not directly measured.

In order to achieve these objectives, the "measurements" activity of the next years will consist in the following actions.

1.6.1 Measurements and Numerical Modeling on SIRTA Site

The collaboration with the IPSL Institute gives the possibility to acquire on the SIRTA site a very well documented data set including dynamics, turbulence, radiative, aerosols, clouds measurements, over periods of several years. Four areas will have been instrumented by the CEREA at the end of 2008, with the associated systems of acquisition, transmission and storage of the data. Two of these areas are operational since

2006. By combining IPSL and CEREA instruments, the SIRTA provides in particular the following measurements :

- Area 1: wind and turbulence measurements with ultrasonic anemometers at 10 m and 30 m on a 30-meter mast, and at 10 m on another mast, vertical profile of wind with one UHF radar and one X-band radar, clouds parameters with a 95 GHz doppler radar, radiative, rain, surface temperature and humidity measurements.
- Area 2 (near buildings and on roof): aerosols extinction and backscattering with one lidar, detailed radiative measurements at ground and roof (15 m) levels, temperature and humidity at 8 m near buildings, sonic anemometer measurements at 10 m (partly to be installed).
- Area 3: sodar measurements (to be installed)
- Area 4: sonic anemometers, temperature and humidity, at 10 m and 30 m, sodar (Scintec SFAS) (when not used for other campaigns).

All these instruments (except lidar) are operational on a routine mode, and are available for the specific campaigns which will be decided in agreement with IPSL and possibly with other laboratories or institutes. After quality control, the data are stored on IPSL servers where they are freely accessible.

The SIRTA data set will be primarily used for the validation and the development of Mercure_Saturne. The two instrumental modes are associated to different objectives.
The routine mode is devoted to a long term comparison with Mercure_Saturne simulations which will allow an extended validation of this code on a large range of meteorological situations. The analysis of the comparison will focus on the ability of Mercure_Saturne to reproduce the micro-scale (some hundreds of meters) heterogeneities associated to the complex land use of the site (buildings, trees, water) and the local scale circulations induced by the orography. The final goal is to improve the operational abilities of Mercure_Saturne, and thus to prepare a future use of this code for impact studies (for EDF power plants, roads trafic ...), and for wind energy resource assessment.
In this comparison, Mercure_Saturne will be used in RANS mode with k-ε turbulent closure. Due to its unstructured grid resolution, Mercure_Saturne will be able to take into account explicitly the buildings. The effect of the trees will be taken into account with a porosity-drag approach, consisting in adding terms in the equations of motion and turbulence variables. The lateral boundary conditions will be provided by the MM5 model which is operationally runned by IPSL, or by Meteo-France models analysis (ALADIN, AROME). A part of the observations will also be assimilated in the model with the nudging method (see Section 3.1).

The second instrumental mode, consisting in short and intensive campaigns in the framework of national or international projects, will be associated with the development and the validation of specific parameterizations of Mercure_Saturne. CEREA currently participates in collaboration with IPSL and Météo-France, to such a project, the ParisFog project, which is devoted to the study of radiative, microphysical and dynamical processes involved in the life cycle of the fog. The field campaign has allowed to document about 20 situations of fog or favourable to fog formation between November

2006 and March 2007, among which 15 IOPs (Intensive Observation Period) including additional measurements (radiosoundings, tethered balloon, aerosols and dropplets measurements). A 1D version of Mercure_Saturne has been used in order to develop and validate schemes for: microphysical interactions between aerosols and fog droplets through nucleation process using a parametric description of the size distribution (log-normal), deposition velocity, interactions with solar and infra-red radiations. 3D simulations will now follow (Ph.D. thesis of Xiaojing Zhang), primarily on radiative fog events of the campaign, in order to study the impact of SIRTA spatial heterogeneities of land use on the fog evolution, from formation to dissipation. The code will be first applied in RANS mode with k-ε turbulent closure. LES simulations should be achieved (first on an homogeneous domain) to better study the turbulent structures. This work could be extended to polluted fog simulations. During the period 2010-2013, other campaigns will be possibly decided in collaboration with IPSL, on scientific subjects related to the physical processes in the boundary layer and their representation in numerical models. In that field a passive gas tracer experiment should be scheduled in 2009 on SIRTA site in order to investigate dispersion in stable stratification both in a small homogeneous area for fundamental studies and in a building area for comparison with Mercure-Saturne.

1.6.2 Measurements and Numerical Modeling for Wind Energy Applications

Still now, wind resource assessment is generally performed using simple cup anemometers and linearized models like WAsP. However, the limitations of these tools are more and more pointed out. Cup anemometers need high masts to measure up to hub height, and their measurements can be affected by mast distorsion, turbulence, and flow inclination. The application of linearized models in complex terrain can lead to very high errors in the estimation of the wind resource. For these reasons, remote sensing instruments and CFD codes are more and more considered as valuable tools for wind energy applications, especially for sites characterized by complex orography and/or forest.

The sodars campaign performed during winter 2005-2006 by CEREA in collaboration with CSTB has shown that some sodars commercially available fulfill the specific needs of wind energy. However, both for remote sensing instruments and CFD codes, there is still a need of development of methodologies in order to find the best compromise between the cost of their use and the reduction of uncertainty.

The first step of the work planned for the next years is the analysis of the data set obtained during a 1-year campaign performed between June 2007 and June 2008 on a future wind energy production site. This site is located in southern France and is characterized both by strong slopes and forest. This campaign has provided a well documented data set for the definition and the validation of a new methodology of wind resource estimate with the Mercure_Saturne code. The other goal of the campaign is to evaluate the behaviour of a mini-sodar in very difficult conditions (complex terrain, strong ground clutters and strong winds). Moreover, the work on the methodologies to calculate the mean annual wind speed at hub height, initiated in 2006 on a flat site, will be carried on for this complex site.

The Ph.D. thesis of Laurent Laporte is currently in its last stage and is concluded by a first wind resource estimate with Mercure_Saturne. This work is going to be carried on in the framework of a partnership with the Spanish National Centre of Renewable Energies (CENER), which will focus on methodologies of coupling between mesoscale and microscale, using assimilation of local measurements and well adapted to the simulation of long time periods.

Another part of the work will consist in performing a campaign on a site with turbines, in order to study, especially in complex terrain, the relationship between the turbine production and the vertical profiles of wind and turbulence. Remote sensing instruments (sodars, lidars) are well adapted to this objective. A European project (SAFEWIND) involving, among other partners, RISOE (Denmark), CENER (Spain), Armines, and EDF-R&D, has been accepted in the framework of the Seventh Framework Program of the European Union (FP7). This project includes two measurements campaigns, with some objectives related to comparisons between the instruments, and to the determination of an "equivalent wind speed" more adapted to the electric power estimation or forecast than the single wind at hub height.

Lastly, the collaboration initiated with the Laboratoire de Mécanique et d'Energétique (Polytech'Orléans) will continue until 2009. This collaboration aims to compare Mercure_Saturne simulation of wind turbines wake with wind tunnel measurements. After comparisons on a simple configuration including one wind turbine, more complex arrangements are going to be studied. A data set of on-site measurements will be also searched for..

1.6.3 Advances in Observational Methods

This part of the measuring activity will decrease in the coming years as compared to the previous period. However, it is necessary to keep informed of the instrumental evolutions both for the needs of CEREA related to the previous points, and for those of the operational services of EDF.

A key point is the recent arrival of the Doppler lidar on the market of wind instruments. The Doppler lidar offers some advantages in comparison to sodars: it does not generate any noise and is not disturbed by ambient noise, and it has fewer limitations for the measurements of strong winds. Moreover, 2D and even 3D scanning are possible with this technology.. CEREA is currently involved in the VMT (Virtual Meteorological Tower) project supported by ADEME which consists in performing and analyzing 2 campaigns of Doppler lidar measurements. As for sodars, these campaigns aim both to evaluate the quality of the measurements of wind and turbulence, and to study the possible improvement brought by the instrument in the wind resource assessment methodology. Several instrumented masts with cup and sonic anemometers give the reference measurements. The data are going to be analyzed during the next months. The possibility of using a Doppler lidar for wind turbine power curve measurement will be evaluated. The possible applications of other types of lidar (backscattering lidar, Raman lidar, DIAL lidar ...) will be also investigated, for aerosols or droplets characterization, determination of the boundary layer height, determination of species concentrations ... Another subject to explore is the turbulence sensing with a scintillometer. This instrument measures the structure constant of refractive index fluctuations spatially averaged over the line of sight. The spatial scale of averaging varies from some tens or hundreds meters for the surface layer scintillometer, to several kilometers for the boundary layer scintillometer. In both cases, the heat flux can be derived, and the first one can also determine the dissipation rate of turbulent kinetic energy, and the momentum flux. These instruments allow a better temporal resolution than the conventional point sensors (like ultrasonic anemometers) as they do not need temporal averaging, and they do not suffer from flow distorsions caused by the sensor and its mounting on mast. The possibilities and applications of this instrument will be investigated with a surface layer scintillometer which will be installed at the SIRTA site by CEREA.

1.6.4 Methodologies to Derive Turbulent Parameters

Remote sensing instruments like sodars and UHF radars provide the vertical profile of wind speed and direction, but give also some information on turbulence. Concerning UHF radars, a method to retrieve the turbulent dissipation rate and turbulent fluxes has been defined by the CRA (Centre de Recherches Atmosphériques, Lannemezan) in collaboration with EDF R&D during previous years. However, this method is still limited to convective cases and has been validated on a limited number of data sets. The possibility to keep on this work in order to extend the applicability of the method will be studied. The same kind of work could be performed with sodar data. The retrieval of vertical profiles of turbulent variables should permit an extension of the validation of Mercure_Saturne to the SIRTA site, as the current possibilities of turbulence comparison are limited to surface values measured by sonic anemometers.

2. Hygiène et sécurité

L’hygiène et la sécurité sont gérées au CEREA selon les organisations hôtes des trois sites du laboratoire (ENPC, EDF R&D et INRIA).

En terme d’accident de travail sur la période précédente, on a signalé seulement un accident de trajet en deux roues (bicyclette) ayant entraîné un arrêt de travail de 5 mois d’un membre du CEREA du site EDF R&D (voir Bilan – CEREA, chapitre 5). Devant la recrudescence de ce type d’accident de trajet, un stage de sensibilité à la sécurité routière, spécifique « deux roues » sera organisé au niveau de la R&D d’EDF.

D’autres mesures ne semblent pas nécessaires à ce moment, mais nous nous réservons la possibilité de mettre en place des mesures ou formations si des problèmes d’hygiène ou de sécurité devaient se présenter.

ACRONYMS - ABBREVIATIONS

ACFD	Atmospheric Computational Fluid Dynamics
ADEME	Agence de l'Environnement et de la Maîtrise de l'Energie
ANR	Agence Nationale de la Recherche
CASU	Cellule d'Appui aux Situations d'urgence (Emergency Center at INERIS)
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)
CMM	Centre de Modelamiento Mathematico (Center for Mathematical Modeling)
CIT	Centre d'Ingénierie Thermique (EDF)
CNEA	Comisiòn Nacional de Energia Atòmica (Argentina)
CNRS	Centre National de la Recherche Scientifique
COV	Composés organiques volatils
CSTB	Centre Scientifique et Technique du Bâtiment
CTC	Centre Technique de Crise (Emergency Center at IRSN)
CTM	Chemistry Transport Models
EDF R&D	Electricité de France Recherche et Développement
ENPC	Ecole Nationale des Ponts et Chaussées
EPRI	Electric Power Research Institute (USA)
FP	Research Framework Programme (European Union)
GMES	Global Monitoring for Environment and Security
INERIS	Institut National de l' Environnement Industriel et des Risques
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
ISORROPIA	Equilibrium in Greek ; équilibre en grec
LEFE	Les Enveloppes Fluides et l'Environnement (CNRS/INSU Program.)
LMD	Laboratoire de Météorologie Dynamique (X / ENS / CNRS)
MAM	Modal aerosol model
NBC	Nuclear, biological and chemical
NO_x	Nitrogen oxides
ONERA	Office National d'Etudes et de Recherches Aérospatiales
PRIMEQUAL	Programme Interministériel d'Etude de la Qualité de l'Air
PROMOTE	Protocol Monitoring for the GMES Service Element
SIREAM	Size-resolved Aerosol Model
SIRTA	Site Instrumental de Recherche par Télédétection Atmosphérique
STIC-AmSud	Sciences et Technologies de l'Information et de la Communication – Amérique du Sud
UFPM	Ultra Fine Particulate Matter
WRF	Weather & Forecast Model (meteorological model)
WRF-Chem	WRF with Chemistry (meteorological and air quality model)