



CEREA Prospective Report 2008-2011

TEACHING AND RESEARCH CENTER
IN ATMOSPHERIC ENVIRONMENT

Joint Laboratory École Nationale des Ponts et Chaussées/Électricité de France R&D
<http://www.enpc.fr/cerea/>



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This report describes the prospective of CEREA for 2008-2011. Section 1 is taken from the *CEREA Summary Report 2003-2007*. Section 2 summarizes the key items of the prospective. Section 3 details the research topics.

1 Key Features

1.1 CEREA at a Glance

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

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

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

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

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

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

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

1.2 Organization

CEREA is organized in five groups:

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

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

1.3 Research Topics

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

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

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

The research topics and the main results obtained for 2003-2007 are detailed in Section 3.

1.4 Motivations for CEREA

The main objectives for CEREA are:

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

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

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

1.5 Summary of 2003-2007: Key Facts

Academic

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

Applications

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

Key Partnerships

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

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

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

- CEREA has a Joint Agreement with the IPSL Institute. This mainly concerns the observational site (SIRTA) in the southern suburb of Paris at Palaiseau. The measurements team of CEREA has deployed its instrumental tools at SIRTA since early 2006 and has taken part in the field campaign ParisFog in 2006/2007.
- CEREA is implied in the network devoted to air quality and impacts of the French Ministry for Transport. The involvement is driven by the Framework Agreement with the Research Directorate of the Ministry (specific to CEREA).

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

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

2 CEREA Project for 2008-2011

- 2003-2007 has been a starting and building-up period for CEREA. The main objective for 2008-2011 is to make the activities more perennial by strengthening CEREA both in academic and applied fields.
- CEREA will endeavor to produce policy-relevant, high-level research, to be used by decision makers in the fields of energy, and urban and transport management.
- The first priority is air quality modeling with a focus on atmospheric risk assessment (chemical and biological species, radionuclides).
- The second priority is micro-scale meteorology through modeling and observations for applications ranging from urban canopies to wind power estimate.
- The main focus of CEREA is not the development of new chemical mechanisms or of new physical parameterizations. CEREA aims rather at being a leader in advanced three-dimensional modeling for impact studies and environmental forecast, with an expertise ranging from state-of-the-science models (CFD, multiphase, CTM) to high-level methods (data assimilation, ensemble forecast).

2.1 Background

The background of CEREA, especially for ENPC, will be significantly modified in near future. One can give the following hints:

- ENPC is a founder of “Paris-East University” (jointly with two existing Universities: University of Marne la Vallée and University Paris 12). The research activities of ENPC are about to be imbedded in the coming departments of “Paris-East University”.
- ENPC is also a member of ParisTech (Paris Institute of Technology), an entity which brings together ten of the foremost French institutes of engineering education and research. ParisTech will offer opportunities for fostering research projects with industrial partners.

2.2 Research Topics

The research topics that are planned to be investigated are detailed in Section 3.

2.3 A Few Objectives and Indicators

CEREA will have the following objectives for the period 2008-2011:

1. to initiate from 3 to 4 PhD works per year (to be defended in 3 years).
2. to publish from 15 to 20 articles in international peer-reviewed journals per year.
3. to propose graduate and postgraduate courses in the framework of ParisTech (Paris Institute of Technology) in Air Quality (at ENPC), Fluid Mechanics (at ENPC), Computer Science (at ENPC and ENSTA) and Data Assimilation (at ENPC and ENSTA). The connections to existing Master formations have to be strengthened.
4. to get contracts in the range [500-700] keuros per year (for CEREA as a research laboratory of ENPC) with an increasing part of public funds (through the National Research Agency, ANR).

5. to disseminate, for EDF applications, the open source models *Mercure_Saturne* (led by EDF) and *POLYPHEMUS* (led by ENPC and INRIA) and to extend the user's community of these models.
6. to strengthen the relationship between courses and research led at CEREAs, especially with the use of the developed models in courses.
7. to organize international conferences (for instance as followers of the APMS conferences - Air Pollution Modeling and Simulation- or in the framework of the PNLA conferences -INRIA/CEA/EDF-).
8. to submit a European project as Principal Investigator.
9. to lead a few projects ([2-4]) on the new cluster of EDF R&D (*Blue Gene*) to be chosen among some "logical" candidates (CFD, impact studies, ensemble forecast, network design, etc).

2.4 Partnerships

CEREAs has the following objectives for 2008-2011.

EDF/ENPC

- to increase the applications led for the Fossil-Fired Generation and Engineering Department of EDF (eventually for Eurelectric, the association of the electricity industry 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). CIT and/or CIDEN could enter the development consortium of *POLYPHEMUS*.
- to animate the Air Quality Network of the French Ministry for Transport through joint projects, training sessions and hosting of visiting staff.

French Partnerships

- to maintain the key partnership with IRSN and INERIS, especially with the works devoted to the *POLYPHEMUS* system.
- to maintain the involvement in the SIRTAs observational site and to take part in the dedicated field campaigns.
- to strengthen the relationship with Patrick Chazette's team (aerosol measurements), now at IPSL/LMD.
- to develop joint projects with Météo France (AROME team, urban modeling, stratospheric modeling).
- to strengthen the position of CEREAs inside scientific committees of the French academic community, especially through the LEFE program.

The "Paris-East University" project can also be an opportunity for strengthening CEREAs, which motivates the search for possible connections to existing teams (especially LISA at the University Paris 12).

Foreign Partnerships

- to maintain the partnership with IER Stuttgart (Germany) devoted to integrated modeling.
- to maintain the partnership with CRIEPI, especially through the involvement in the phase 3 of the MICS campaign.
- to maintain the partnership with EDF Polska and the AGH University of Science and Technology (Krakow, Poland).
- to develop joint projects with the CMAQ/WRF community (USA), especially through Christian Seigneur.
- to develop a joint project with a Chinese partner (eventually through the LIAMA Laboratory of INRIA).

Industrial Partnerships

- to develop a strong relationship to a research and development facility (either an existing one or a start-up to be created from CEREAs).
- to promote projects inside the VMD research cluster (“Pôle de Compétitivité”) devoted to the urban sustainable development.

2.5 Human Resources

CEREAs suffers from a lack of permanent staff. The target for the period 2008-2011 is to reinforce:

- the team at the regional scale through ENPC,
- the Mercure_Saturne team through EDF,
- the data assimilation team through INRIA.

Another key point (to be improved) is the ability for CEREAs to host PhD works of young “Ingénieur des Ponts et Chaussées” (civil servants from the Ministry for Transport).

2.6 Organization and Management

CEREAs will be structured in 5 teams:

- short-range modeling;
- aerosol modeling;
- regional modeling;
- INRIA/ENPC CLIME project devoted to data assimilation and inverse modeling;
- observation of the atmospheric boundary layer.

The Director of CEREAs will be helped by two Deputy Directors, one from EDF (Luc Musson-Genon) and one from ENPC (Marc Bocquet).

The Executive Committee of CEREAs, to meet every three months, will be composed of the Director, of the Deputy Directors, of the group leaders and of the INRIA head of the CLIME project (Isabelle Herlin).

3 Research Axes for 2008-2011

3.1 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.

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 2008-2011 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 3.5.

3.1.1 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.

3.1.2 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 CERE (Section 3.4).

3.1.3 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 PhD work 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 CERE. 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.

3.1.4 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 PhD work 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 `Saturne_Code`. 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 (especially for the French Ministry for Transport).

3.1.5 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.

3.1.6 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).

3.1.7 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 $k - \varepsilon$ 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.

3.1.8 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 3.2) 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 works. 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.

3.2 Aerosol Modeling

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:

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

2. MAM, a modal aerosol model:

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

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).

Many articles have described the development, comparisons to observational data and applications of these models. One can cite for instance for the main applications (over Europe, over Asia and at regional scale, respectively):

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

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

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

Both models are embedded in the POLYPHEMUS system. MAM is also coupled to the CFD model Mercure_Saturne.

There are of course still many challenging issues in aerosol modeling. The main objectives for the period 2008-2011 are to improve the quality of the parameterizations and to extend the range of applications. Moreover, these models have begun to be used by other teams (for instance, MAM is currently used by a NOAA team which develops CMAQ, the American Community Multiscale Air Quality modeling system).

The following topics will be investigated.

3.2.1 Update of the Current Available Aerosol Models

This first item is related to an improvement of the existing models, for instance:

1. SIREAM and MAM are currently coupled to a version of ISORROPIA that takes into account sodium, sulphate, nitrate, ammonium and chloride. They will be coupled to other existing thermodynamic models, especially for having a better description of the mineral (crustal) components;
2. 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.

3. 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.

3.2.2 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 is currently being updated to include:

- the description of hydrophilic/hydrophobic effects (on the basis of existing works);
- 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.

This is based on a collaborative work with Christian Seigneur. After validation of the new SOA module, further work will concern:

- 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.

3.2.3 Modeling of Traffic-Induced Ultrafine Particles

Ultrafine particles (with a diameter of a few hundreds of nanometers) are a key concern at local scales 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 works already initiated will be continued through a partnership with observational teams. Contacts with car manufacturers should be initiated.

3.2.4 Soot Aerosols

Soot has not a spherical form and can be 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.

3.2.5 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 fixed 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 will be

determined experimentally. Another key application is the study of the radiative effects of the aerosol composition.

A collaborative work could be initiated with Laboratoire d'Aérodologie (Toulouse, University Paul Sabatier and CNRS; Marc Mallet). A joint project was submitted to the ANR in 2006 but was unfortunately rejected.

3.2.6 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.

3.2.7 Multiphase Processes for Radionuclides

Part of the radionuclides associated to an accidental release in the atmosphere are bound to existing aerosols. This is for instance the case for cesium. They can also be implied in multiphase processes (for instance iodine either in elemental or in organic forms, eventually dissolved).

The objective is to develop a multiphase model for radionuclides. A first item is the coupling of the aerosol model SIREAM to a radioactive model describing fission. A second item is the development of a model with multiphase processes.

3.2.8 Numerics for the General Dynamics Equation

The General Dynamics Equation (GDE) describe 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.

3.3 Air Quality Modeling at the Regional Scale

CEREA has developed during the period 2003-2007 a new modeling system, POLYPHEMUS. The key reference is (with many references therein):

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

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, radionuclides, heavy metals, mercury, Persistent Organic Pollutants).

The objectives for the period 2008-2011 is first to extend and to improve the abilities of POLYPHEMUS (especially with a better resolution – parameterizations and discretization), second to promote it by hosting new models.

3.3.1 On-the-fly Developments and Software Developments

A parallel version of the base CTM of POLYPHEMUS, Polair3D, will be developed in 2007-2008, 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.

3.3.2 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 knowledge 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.

The “Paris-East University” is a good framework for developing a strong relationship with LISA, a laboratory with a recognized expertise in chemistry.

3.3.3 Update and Extension of the Chemical Mechanisms

Other photochemical mechanisms have to be plugged to POLYPHEMUS (for instance SAPRC). 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 “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 studies (for the hemispheric scale);
- etc.

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

3.3.4 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 K_z), 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.

3.3.5 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).

3.3.6 Short-Range Dispersion

There is a strong need for short-range dispersion models, specifically for applied studies. The current Gaussian models hosted by POLYPHEMUS should be extended to cover ADMS features and be further validated to constitute an open-source alternative to ADMS and other such models. This includes the addition of parameterizations to take into account complex geometries.

POLYPHEMUS currently lacks a Lagrangian model to complete its range of model classes. Coupling POLYPHEMUS with well-known Lagrangian models should then be investigated.

3.3.7 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 works led at CEREAs have 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 work with Météo France (AROME project, François Bouttier).

3.3.8 On Line 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 CEREAs 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, CEREAs 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).

3.3.9 Next Generation CTM

The grid resolution may have a strong impact on the results. The future generation of 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 can 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).

3.3.10 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 is implied, jointly with the IER - University of Stuttgart (where the EcoSense model is currently developed), in two European projects starting 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 Hourcade), 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 R2D2 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.

3.3.11 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).

3.3.12 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 radionuclides);
- 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 automatization. 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 Transport either at regional scale (similar to the traffic study performed for Lille) or at national scale (to study the impact of new gasolines 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. CEREAs lacks a Chinese partner, typically for an application to Beijing.
- CEREAs 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 (CEREAs had the opportunity of joining the Eurodelta exercise but POLYPHEMUS was still in development).

3.4 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 help 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.

3.4.1 Satellite Data

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_x 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_2 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 CEREAs should maintain some activity in this domain. 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.

3.4.2 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 than satellite data.

The Adelira project, lead by Patrick Chazette (IPSL/LMD), should help define and implement campaigns with the use of such devices. If the project is accepted by ANR, CEREAs will be PI or co-PI of two work-packages: data assimilation of such lidar data into POLYPHEMUS (with ARIA) and network design to define optimal locations of mobile lidar.

3.4.3 Data Assimilation for Air Quality

The benchmark of data assimilation methods for air quality is still a challenging point (sequential versus variational algorithms). It is the subject of a Research Action at INRIA that joints 3 projects: ADOQA for Data Assimilation for Air Quality.

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.

3.4.4 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 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 error model as much as possible (for instance with EOF/POD methods).

3.4.5 Ensemble Forecast

Previous works 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 (Section 3.3). 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.

3.4.6 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. CERE and IRSN/CTC are part of the European DETECT project, in the FP7 Euratom framework, which has just been submitted (May 2007). An exchange and intercomparison exercise on assimilation of radionuclides 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.

3.4.7 Network Design

The natural field of applications are radionuclides/accidental pollutant monitoring, and photo-chemistry air monitoring.

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.

3.4.8 Image and Air Quality

One of the main themes of CLIME is the exploration of the use of images as raw data to be assimilated into a 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.

3.4.9 Inverse Modeling, Uncertainties and Non-Linearities

The works on second-order modeling carried out at CEREAs (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.

3.4.10 Challenging Statistical and Representation Issues in Air Quality Models

Past works testify of the statistical and mathematical skills developed at CEREAs 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. Works related to downscaling should also be initiated.

3.4.11 Intensive Computing Issues

Many of the works 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 runned on the Blue Gene computer of EDF R&D (a cluster of about 10 000 processors).

3.5 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 CEREAs 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 ...
- 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.

3.5.1 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 CEREAs at the end of 2007, with the associated systems of acquisition, transmission and storage of the data. By combining IPSL and CEREAs 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.

- Area 3: sodar measurements (Remtech PA1).
- 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 traffic ...), and for wind energy resource assessment. In this comparison, *Mercure_Saturne* will be used in RANS mode with $k - \varepsilon$ 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 operationnaly 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*. CEREIA 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 16 IOPs (Intensive Observation Period) including additional measurements (radiosoundings, tethered balloon, aerosols and droplets measurements). A 1D version of *Mercure_Saturne* will be 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 be performed (PhD 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 $k - \varepsilon$ 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 2008-2011, 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.

3.5.2 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, and especially for sites characterized by complex orography and/or forest.

The sodars campaign performed during winter 2005-2006 by CEREAs 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 and the reduction of uncertainty.

The first step of the work planned for the next years is a 6-month campaign of wind and turbulent measurements on a future wind energy production site. This campaign is planned for June-December 2007 and aims at studying which improvement can bring a combination sodar / CFD code on the resource assessment for a complex site. The selected site is located in southern France and is characterized both by strong slopes and forests. The horizontal and vertical heterogeneities of wind and turbulence will be documented by means of 4 instrumented masts and 2 sodars. These data will be analyzed and used into 2 directions. First, the behavior of the sodar on a difficult site with strong ground clutters and strong winds will be studied. 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. Secondly, a comparison between the measurements, and the calculations of wind resource obtained with *Mercure_Saturne* and with the linearized model *WAsP* will be performed (PhD thesis of Laurent Laporte). Different options will be tested in the application of *Mercure_Saturne*, which includes the required number of simulations for a long-term representativity, the boundary conditions, the forest modeling, data assimilation methods ...

A further step 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, RISO (Denemark), CENER (Spania), Armines, and EDF-R&D, has been submitted in the framework of the Seventh Framework Programme 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 turbines wake is still an important source of uncertainty in the wind power estimation. Some numerical simulations have already been performed with *Mercure_Saturne* (PhD work of Laurent Laporte) by introducing a drag term to represent the far wake effect (after 2 to 3 times the turbines' diameter). A collaboration with the Laboratoire de Mécanique et d'Énergétique (Polytech'Orléans) has started in 2007 for 3 years, which will allow to compare the numerical results with wind tunnel measurements, on several configurations, the last one including both orography and wake effects on a real case. A data set of on-site measurements will be also searched for. As this kind of data set seems to be very difficult to find, the opportunity to organize or participate to a campaign devoted to this subject will be studied.

3.5.3 Advances in Observational Methods

This part of the measuring activity will probably 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 CEREAs 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. CEREAs is in contact with several manufacturers (especially *LEOSPHERE*) and the first campaigns of comparison with reference measurements are very promising. The Doppler lidar offers

some advantages in comparison to sodar: it does not generate any noise and is not disturbed by ambient noise, and it has less limitations for the measurements of strong winds. Moreover, after some developments, 2D and even 3D scanning will probably be possible. CEREAs will be involved with EDF-Energies Nouvelles in the course of 2007 in a campaign of comparison (on wind and turbulence) between the LEOSPHERE lidar and anemometers measurements, and CEREAs will then continue to follow the further developments on this instrument. Moreover, the Doppler lidar could be involved (through some collaboration) in campaigns related to wind energy applications (determination of an "equivalent wind speed", measurements in a turbine wake). 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 far 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 distortions 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 CEREAs.

3.5.4 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, in collaboration with CRA. 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.

4 Acronyms

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

LISA	Laboratoire Interuniversitaire des Systèmes Atmosphériques (CNRS/Universities Paris 7 and 12).
LMD	Laboratoire de Météorologie Dynamique (X/ENS/CNRS).
LSCE	Laboratoire Surveillance du Climat et de l'Environnement (CEA/CNRS).
MEDD	Ministère de l'Ecologie et du Développement Durable.
MTETM	Ministère des Transports, de l'Équipement, du Tourisme et de la Mer.
ONERA	Office National d'Études et de Recherches Aérospatiales.
PREDIT	Programme pour la Recherche, le Développement et l'Innovation dans les transports terrestres.
PRIMEQUAL	Programme Interministériel d'Étude de la Qualité de l'Air.
R2D2	Réseau de Recherche sur le Développement Durable (Research Network of region Ile de France).
SFEN	Société Française de l'Énergie Nucléaire.
SIRTA	Site Instrumental de Recherche par Télédétection Atmosphérique.
VMD	Research cluster devoted to the urban sustainable development (Pôle de Compétitivité Ville et Mobilité Durable).