Project Title: " Predictive Numerical Models for Environmental Management ".

Sponsored by: *Subprograma de Proyectos de Investigación Fundamental no orientada, en el marco del VI Plan Nacional de Investigación Científica, Desarrollo e Innovación Tecnológica 2008-2011. Ministerio de Ciencia e Innovación del Gobierno de España.*

Reference: CGL2008-06003-C03-00

Project Coordinator : Prof. Rafael Montenegro Armas.

Web site ULPGC: http://www.dca.iusiani.ulpgc.es/proyecto2008-2011/html_ingles/index.html

1 Aim of the project

Nowadays numerical modelling has become an essential tool for the analysis and prediction of a large number of physical phenomena. The numerical modelling includes the mathematical modelling of the phenomenon and the numerical resolution of the involved mathematical problem. This Project is focused on four environmental phenomena: (1) wind field simulation, (2) air pollution numerical modelling and forecasting, (3) forest fire simulation and (4) solar radiation simulation. Although they are four different problems, there exist many points in common among them. All of them are defined in similar types of domains and thus the same discretization techniques can be used. The wind modelling results critically affect the air pollution and forest fire modelling. Thus the former problem is essential for carrying out the other simulations. In addition, wind modelling has its own applications (wind maps). Air pollution and forest fires are related to unsteady propagation problems which may be mathematically described by a convection-diffusion-reaction equation and thus solved by using similar numerical techniques. The solar radiation modelling is also an environmental problem of which the nature is mostly geometrical. Our experience on adaptive discretization techniques has encouraged us to include this topic in the proposal, as a response to the interest of some companies working on solar radiation maps. Finally, all four phenomena have clear technical applications. Among them, we emphasize: the construction of wind maps, the study and control of pollutant emissions, the planning for anti-fire measures and the construction of solar radiation maps. For this reason, we propose a joint treatment of the four problems in the context of this coordinated project.

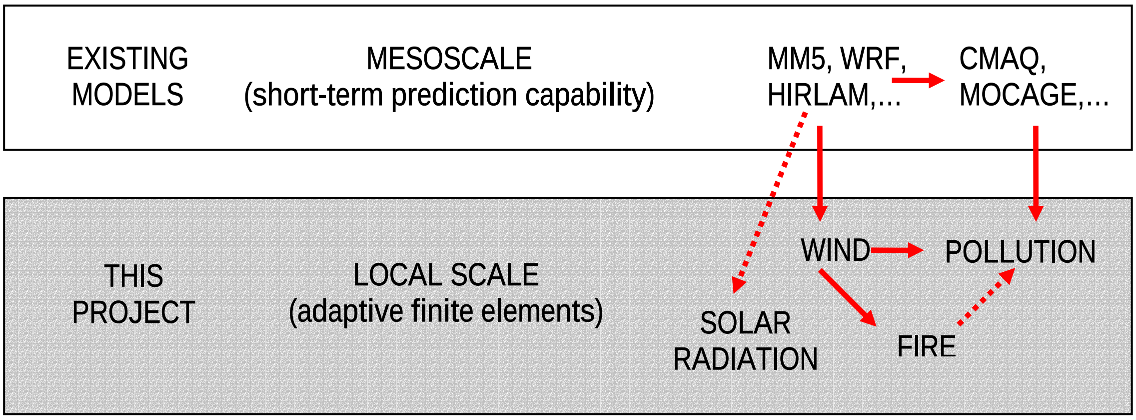

Figure 1: The goal of this project is to develop advanced numerical models at the local scale and to integrate them with existing models at the mesoscale. Solid arrows indicate clear connections while dashed arrows are connections of a more exploratory nature.

Currently, realistic simulations are associated to the availability of meteorological observation data and to the access to the geographic information systems. The meteorological observations are periodically available through different networks and they are the input data for mesoscale models. Among them, perhaps MM5 (Fifth Generation of Mesoscale Model, http://www.mmm.ucar.edu/mm5/, Pennsylvania State University, National Center for Atmospheric Research, USA) is actually the most widespread prognostic model. This is a free communal model supported by NCAR (National Center for Atmospheric Research) to which many research groups have added their own software, both in the model core and in data pre-processing and post-processing. Obviously, other similar models as HIRLAM or WRF are used by the meteorological community. In the field of multiscale air quality models, the CMAQ (Community Multiscale Air Quality Model, NOAA-EPA, USA) has been widely used and it is a reference of this kind of models. The idea is that a mesoscale model (MM5, HIRLAM, WRF, CMAQ, MOCAGE,...) provides the input data for our adaptive high resolution finite element models. So, a main objective of this project is to refine the results of a mesoscale model (with a maximum resolution about 1 Km) in a local scale (about a few meters). This idea is summarized in Figure 1. On the other hand, the communication of our codes with Geographic Information Systems (GIS) is essential in order to be able to carry out realistic simulations. For this purpose, it is necessary to study how to extract data from GIS and how to export our results to GIS.

1.2 Background and current state

The three groups that present this proposal (Universitat Politècnica de Catalunya, UPC, Universidad de Salamanca, USA, and Universidad de Las Palmas de Gran Canaria, ULPGC) have finished together two previous coordinated projects sponsored by Spanish Goverment and FEDER: “Modelización Numérica de Problemas Medioambientales de Convección-Difusión-Reacción” (REN2001-0925-C03; 2002-2004) and “Modelización y Simulación Numérica de Procesos Medioambientales” (CGL2004-06171-C03; 2005-2007). Besides, our groups are currently carring out the bridge project “Modelos Numéricos Predictivos para Gestión Medioambiental” (CGL2007-65680-C03) that will be finalized in 2008. Scientific results of these projects (papers in pdf files, congress communications in ppt files, thesis, congress organization, etc.) can be obtained from http://www.dca.iusiani.ulpgc.es/proyecto0507, http://www-lacan.upc.es, http://web.usal.es/~ferragut, etc. We remark that the present proposal has been developed attending all the suggestions of the reviewers of the project CGL2007-65680-C03.

1.2.1 Wind field simulation

A considerable number of scientific works has been published about wind modelling in 3D along the last thirty years. The ULPGC group has experience in the development and application of this type of models since 1986 (see references [1.1], [1.2], [1.3], [1.4] and [1.5]) in the framework of several projects financed by public institutions. In this new project we will introduce new 3-D mesh generation techniques adapted to GIS for domains defined over complex terrains. The adaptation should be done related to terrain height, rougthness length, coast lines, chimneys, etc. Our objective will always be minimal user intervention and low computational cost. We will design and develop a framework for the mesh generator. This tool will be common for the three subprojects since their simulations are defined on similar domains. On the other hand, we propose a new approach of the initial wind field. For this purpose, our model must construct the initial wind field by using a suitable interpolation of the mesoscale model results. So, an interface between both models should be implemented. Furthermore, GIS will be used for realistic simulations. The final goal is to present several realistic applications of our model for construction wind maps in Canary Islands.

[1.1] G. Montero, R. Montenegro, J.M. Escobar. A 3-D diagnostic model for wind field adjustment, *J. Wind Eng. Industrial Aerodynamics*, 74-76, 249–261 (1998).

[1.2] G. Montero, N. Sanín. 3-D modelling of wind field adjustment using finite differences in a terrain conformal coordinate system. *J. Wind Eng. Industrial Aerodynamics*, 89, 471–488 (2001).

[1.3] G. Montero, E. Rodríguez, R. Montenegro, J.M. Escobar, J.M. González-Yuste. Genetic algorithms for an improved parameter estimation with local refinement of tetrahedral meshes in a wind model, *Advances in Engineering Software*, 6, 3–10 (2005).

[1.4] E. Rodríguez, G. Montero, R. Montenegro, J.M. Escobar, J.M. González-Yuste. Parameter estimation in a three-dimensional wind field model using genetic algorithms, Lecture Notes in Computer Science, 2329, 950–959 (2002).
[1.5] G. Winter, G. Montero, L. Ferragut, R. Montenegro. Adaptive strategies using standard and mixed finite element for wind field adjustment, *Solar Energy*, 54, 46–56 (1995).

1.2.2 Air pollutant numerical modelling and forecasting

This project focuses in the realistic numerical modelling and forecasting of atmospheric pollutant emissions evolution within the scale of tens of meters to few kilometres. Nowadays, dispersion and photochemical Air Quality Modelling Systems are mainly used to these proposes (see www.epa.gov). Dispersion ones are used to estimate the amount of pollution at ground level near punctual sources (from hundreds of meters to few kilometres), usually considering simplified photochemical models and *lagrangian* approaches of the transport problem. Instead, photochemical ones are used to estimate the impact of all kind of emissions at regional level (from few to hundreds of kilometres), following *eulerian* descriptions of the transport problem, which are discretized with finite differences schemes, and considering the coupling between large amount of chemical components. In photochemical models, areas of special interest are simulated using nested sub-grids [2.1, 2.2], and punctual emissions with dispersion models embedded within the photochemical ones. Both kinds of models have, nowadays, very different focus. Dispersion ones are usually applied to punctual emission impact assessments, and second ones to regional planning and monitoring. However, recent references about the need of coupling punctual emissions with regional planning with hybrid photochemical models can be found [2.1, 2.3]. They are founded in the importance of coupling among key chemical components [2.4], and the increasing awareness about the socioeconomic impacts of punctual emissions and pollution [2.5]. Although hybrid models can couple scales about one kilometre with regional ones, several limitations to this approach has been reported [2.3]. Thus, the search of alternatives is justified.

In this context, the use of the Finite Element Method with unstructured adapted meshes is proposed as an alternative to usual modelling approaches of the local scale. In order to fulfil this goal, the work developed in the previous project with local models [2.6, 2.7] needs to be completed with the coupling with regional models. Stabilized approaches and second order time integration schemes for linear models, as well as second order splitting schemes between transport and reaction for nonlinear ones have been already tested. In this project, adaptive discretizations and high order time integration schemes will be developed and tested in order to reduce the computational effort of local scale computation. Specifically, discontinuous Galerkin schemes for the transport – reaction problem will be applied and analyzed. Moreover, specific domain decomposition schemes will be proposed for coupling both scales, co-ordinately with parallel approaches implemented in standard mesoscale.

Coupling between scales offers the framework to integrate forecasting capabilities at local scale. Different approaches will be compared for coupling wind field from mesoscale models with the local Finite Element model. Work developed in the context of previous projects, where experimental wind measures were used to adjust wind fields in the area of interest, will be extended to this new purpose. Moreover, the coupling of the Finite Element model with Geographic Information Systems is also considered within this project. This will enhance the capabilities of the model of characterizing emissions (as land uses, transport infrastructures, punctual emissaries,…) at the same precision as computations (tens of meters) as well as to facilitate the visualization of engineering outputs (as ground concentration) in the same framework used in territorial planning.

[2.1] M. Taghavi, S. Cautenet, J. Arteta. Impact of a highly detailed emission inventory on modelling accuracy. *Atmospheric Research*, 74, 65–88 (2005).
[2.2] R.S. José, J.L. Pérez, R.M. González. An operational real-time air quality modelling system for industrial plants. *Environmental Modelling and Software*, 22(3), 297–307 (2007).

[2.3] R.E. Morris, G. Yarwood, C.A. Emery, G.M. Wilson. Recent advances in photochemical air quality modelling using the CAMx Model: Current update and ozone modelling of point source impacts . *Proc. AWMA* (2002).
[2.4] T.B. Ryerson, M. Trainer. Observations of ozone formation in power plant plumes and implications for ozone control strategies. *Science*, 292, 719–723 (2001).
[2.5] D.L. Mauzeralla, B. Sultan, N. Kim, D. Bradford. NOx emissions from large point sources: variability in ozone production, resulting health damages and economic costs. *Atmospheric Environment*, 39, 2851–2866 (2005).
[2.6] R. Montenegro, G. Montero, J.M. Escobar, E. Rodríguez, J.M. González-Yuste. 3D adaptive wind field simulation including effects of chimney emissions. *Proc. WCCM VI*, Beijing, China (2004).
[2.7] A. Pérez-Foguet, A. Oliver, J.M. Escobar, E. Rodríguez. Finite element simulation of chimney emissions: a proposal for near field impact assessment in highly complex terrains. *Proc. 5th Int. Conf. on Eng. Comp. Tech.* (2006).

1.2.3 Forest fire simulation

The simulation of forest fire propagation has obvious realistic applications. The main existing models are of different nature (combustion models and propagation models) and are listed below in terms of increasing complexity.

The first type of models is cellular automata [3.1].The main aim of this kind of modelling is to describe forest fire phenomena with universal statistical critical laws assuming that these global characteristics of fire are insensitive to the details of physical interactions. Unfortunately, the transition probabilities are not related, a priori, to any measurable physical parameter, such as humidity, heat capacity, etc. Therefore these types of models fail in the category of black box models, the output of which is mainly the position of the fire front. Up to now they don't fulfil the simulation of interesting magnitudes.

The second group of models is the group of geometrical models. The fire front is seen as a line on a two dimensional surface. The propagation of the fire front is computed by the envelope method [3.2]. These models can be very fast simulating fire spread. However, the geometrical parameters are again difficult to relate a priori to physical parameters.

The third group of models is composed of the empirical models, a balance of energy is considered at the fire front but the rate of spread of the front is given by an empirical law [3.3]. The rate of spread is supposed to be a "scalar" function of the local parameters: load, humidity, slope, wind, etc. Computations are still fast but the empirical laws are usually obtained from laboratory experiments, not from real wildfire measurements.

The two preceding models rely heavily on the concept of normal rate of spread of the front. The fourth group of models is reaction-diffusion models. A 2-D system of partial differential equations, typically reaction-diffusion equations, is considered, corresponding to a leading assumed physical process. The kind of modelling assumes that the vegetation is a continuous medium. Furthermore, the system of equations is usually set on a two dimensional domain although the vegetation lies in a three-dimensional domain, and the fire front is recovered as the curve of points where the temperature is the pyrolysis temperature. The simulation for these type of systems of partial differential equations is relatively slow and the output of the models not only include the position of the fire front but also the state of the physical variables involved in a fire, such as the vegetation temperature or the gas temperature, which can later be compared with experiments. This group of models can be called detailed physical models and can be derived from general conservation laws of mass, energy and momentum [3.4]. The development and numerical resolution of such models was the object of the former projects REN2001-0925-C03-03 and CGL2004-06171-C03-03 of the research group [3.5, 3.6].

The last models developed by the research group are simplified models belonging to the forth group with the aim to simulate fire in small computers and with computing times far below real time but retaining at the same time the main mechanisms of fire propagation. This model has been recently published [3.7] and allows to simulate fires in computing times between five to ten times below real times. The aims of this new project are:

a) The adaptation of the models already developed by the research group and the development of a forest fire simulation system integrated with a GIS and a Mesoscale Meteorological Prediction Systems.
b) The implementation of advanced numerical techniques (domain decomposition and adaptive meshing) allowing on one hand the modelling of wildland fires, with computing times far below real times and on the other hand to improve the quality of the models in order to take into account new physical phenomena to obtain better predictions of fire behaviour, preserving the efficiency of the computation.
c) A complementary aim is the analysis of the qualitative behaviour of the solutions of the models.

[3.1] T. Beer. Percolation theory and fire spread. *Comb. Sci. and Tecnol.*,72, 297-304 (1990).
[3.2] G.D. Richards. An elliptical growth model of forest fire fronts and its numerical solution. *Int. J. Numer. Meth. EnG.,* 30, 1163-1179 (1990).
[3.3] R.C. Rothermel. A mathematical model for predicting fire spread in wildland fuels, *USDA Forest Service Research paper INT-115*, Ogden, Utah, USA, 40 (1972).
[3.4] O. Sero-Guillaume, J. Margerit. Modelling forest fires. Part I: A complete set of equations derived by extended irreversible thermodynamics. *Int. J. Heat Mass Transfer*, 45(8) 1705-1722 (2002).
[3.5] M.I. Asensio, L. Ferragut. On a wildland fire model with radiation. *Int. J. Num. Meth. Eng.,* 54, 137-157 (2002).
[3.6] M.I. Asensio, L. Ferragut, J. Simon. A convection model for forest fire simulation. *Applied Mathematical Letters*, 18, 673-677 (2005).
[3.7] L. Ferragut, M.I. Asensio, S. Monedero. Modelling radiation and moisture content in fire spread. *Commun. Numer. Meth. Eng.,* 23, 819-833 (2007).

1.2.4 Solar radiation simulation

In this project we propose an adaptive solar radiation model as a new tool for generating solar radiation maps [4.1]. We introduce an improvement to existing models [4.3, 4.4] with mesh adaptation to terrain height, albedo distribution and coast lines [4.2]. This adaptive approach will allow us to develop more efficient codes with a reduction in the computational cost for a given accuracy. It should also be interesting the treatment of shadow boundaries by using adaptive procedures. On the other hand, there are some parameters involved in the solar radiation model, of which values are not easily available or their optimal values are unknown. We propose a strategy to optimize those parameters from experimental or predicted data by using genetic algorithms. Once the clear-sky radiation is computed, the results will be corrected by using the data in order to obtain the real-sky radiation. The solar radiation values will be integrated for a month or for a year for constructing solar radiation maps.

[4.1] F. Cerezo, J.M. Escobar, G. Montero, R. Montenegro, E. Rodríguez. Modelo numérico para la generación de mapas de radiación solar, Proc. of the CMNE/CILAMCE (2007).
[4.2] J.M. Escobar, G. Montero, R. Montenegro, E. Rodríguez. An algebraic method for smoothing surface triangulations on a local parametric space, Int. J. Num. Meth. Eng. 66, 740–760 (2006).
[4.3] K. Scharmer, J. Greif. The European Solar Radiation Atlas. Vol. 1 Fundamentals and Maps, *Les Presses de l'Ecole des Mines*, Paris (2000).
[4.4] M. Šúri, J. Hofierka. A new GIS-based solar radiation model and its application to photovoltaic assessments, *Transactions in GIS*, 8(2), 175–190 (2004).

1.3 Related national and international groups

In Spain there are several research groups in meteorology (Fundamental Physics, Modelling of mesoscale and synoptic scale meteorological phenomena, global change, Statistic Análisis, etc.). Many of them provide important contributions in the field of numerical simulation in meteorology. The ULPGC group belongs to the international network "Red Ibérica MM5/WRF" (http://redibericamm5.uib.es) which involves 47 scientific groups on applications of MM5 and WRF leaded by "Grupo de Meteorología" of the Universidad de las Islas Baleares. The main contribution of our groups is on numerical methods in Applied Science and Engineering. We are connected to the main Spanish groups in this area, in the context of the “Sociedad Española de Métodos Numéricos en Ingeniería” (SEMNI) and of the “Sociedad Española de Matemática Aplicada” (SEMA).

We are collaborating with very prestigious international groups on Numerical Methods and Computational Mechanics (Ticam, Berkeley, Bonn, Delft, Nantes, Lieja, Université Blaise Pascal, Santiago de Chile, Concepción, Bath, Edimburgh). The most important collaborations are the following: Department of Aeronautics & Astronautics del Massachusetts Institute of Technology (USA), Department of Civil Engineering de la University of Wales Swansea (UK), École Normale Supérieure de Cachan (Francia), Department of Mathematics and Institute for Physical Science and Technology, University of Maryland, Maryland (United States of America), Istituto di Analisi Numérica, Consiglio Nazionale delle Richerche, Pavia (Italia), Ecole National Supérieure d´Electricité et de Mécanique, Nancy (France), Université Blaise Pascal, Clermond-Ferrand (France), Universidad de Chile and Universidad de Concepción (Chile), University of Bath (U.K.) and Heriot-Watt University (U.K.).

During previous projects we have worked on building a bridge between the community of Numerical Methods for Environmental Applications and of Meteorological Phenomena Prediction. With this purpose, we have organized Special Sessions on Environmental Modelling in several national and international numerical methods conferences keeping the connection between both communities.

Several figures, obtained with our codes, are included in this section to illustrate the main objectives of the project: wind, solar radiation, air pollution and fire propagation; see figures 2, 3, 4 and 5.

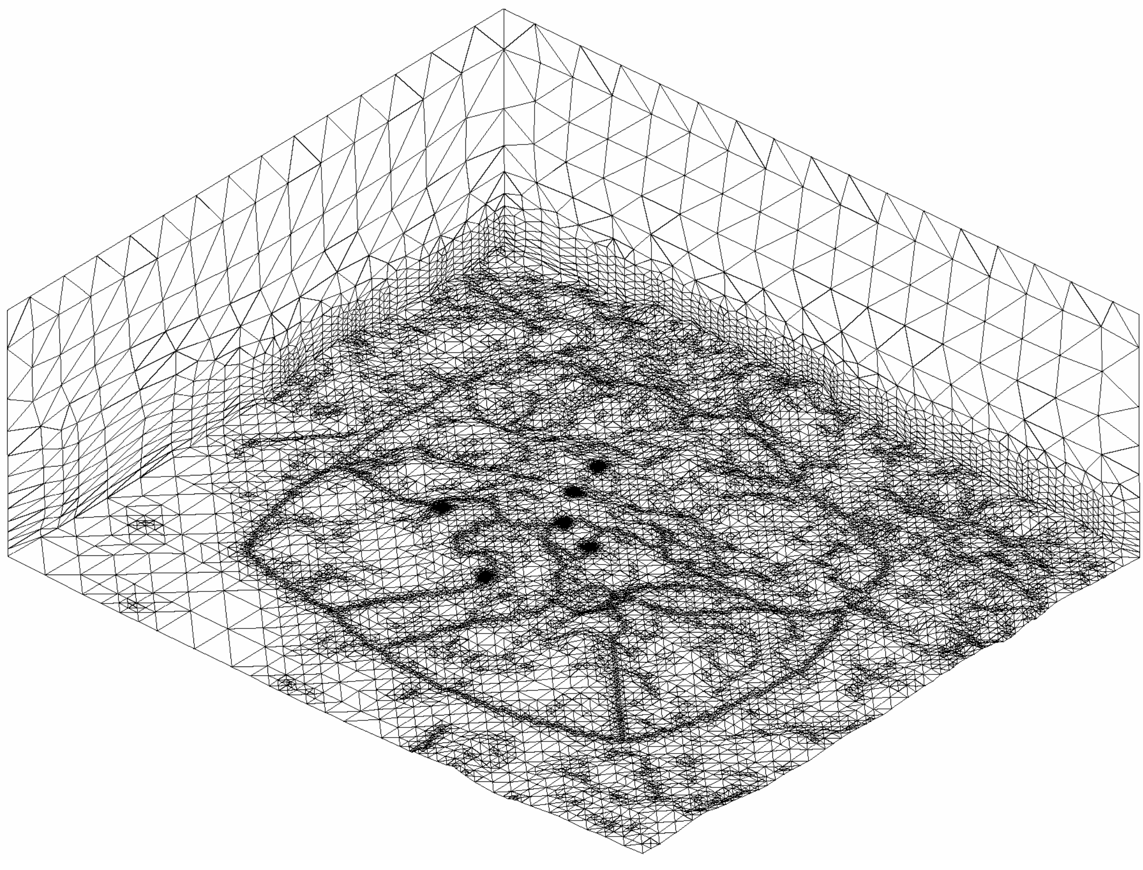

Figure 2: Three-dimensional mesh of a wind farm constructed by Desarrollos Eólicos, S.A., in the province of Lugo (Spain). The mesh has been generated by our code and it is adapted to the terrain height, to the terrain roughness length and on a circular region around six measurement stations.

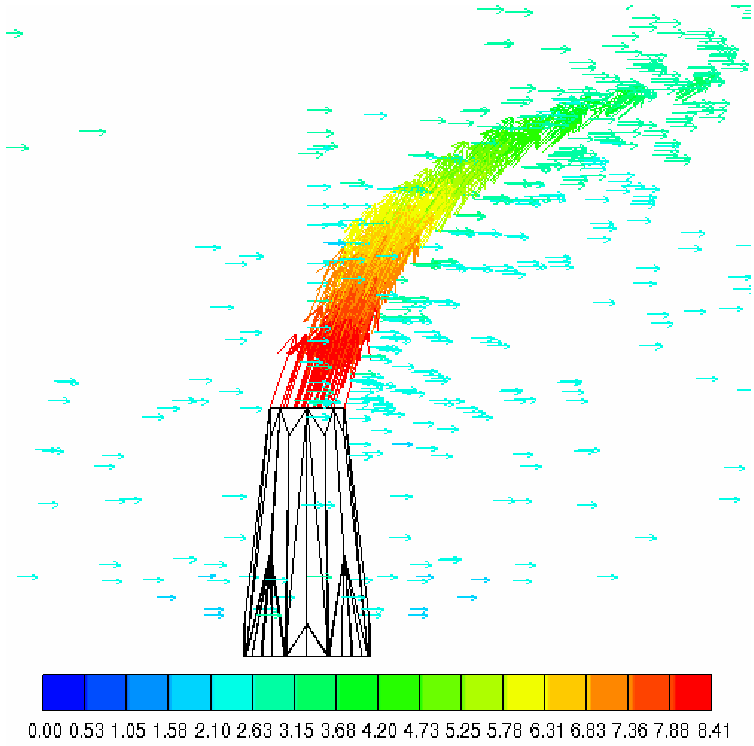

Figure 3: Example of a modified wind field including the effects of chimney emissions. The colormap represents the wind velocity in m/s.

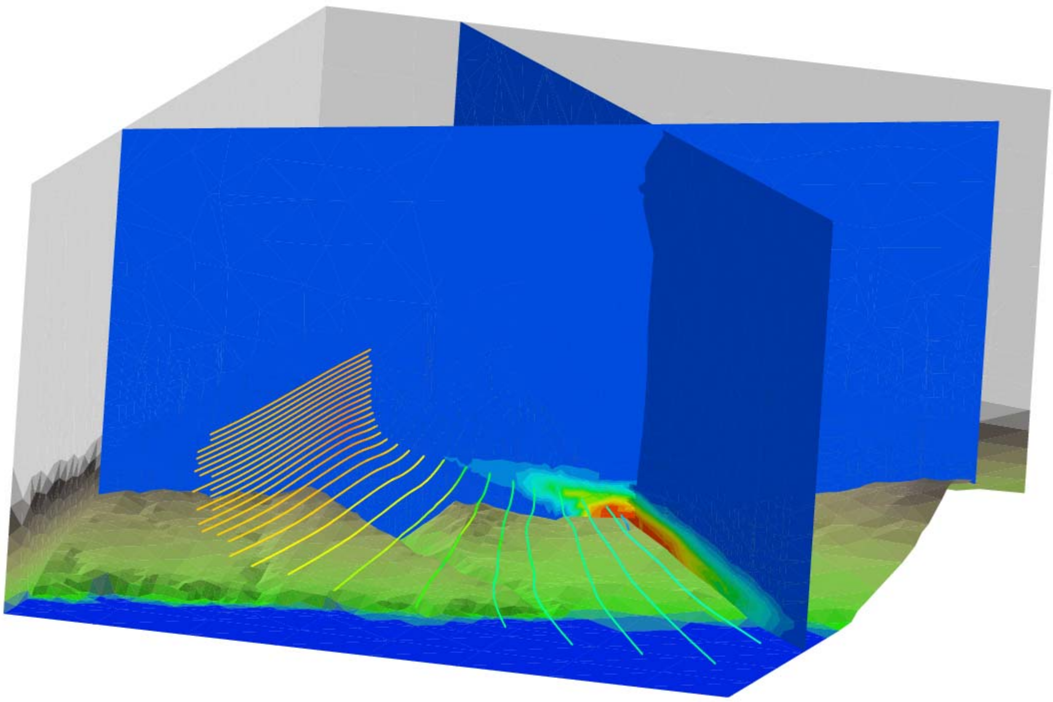

Figure 4: Example of chimney plume in La Palma Island (Spain). Colormap represents the pollutant concentration in gr/m^3. Wind streamlines starting over the chimney are also indicated.

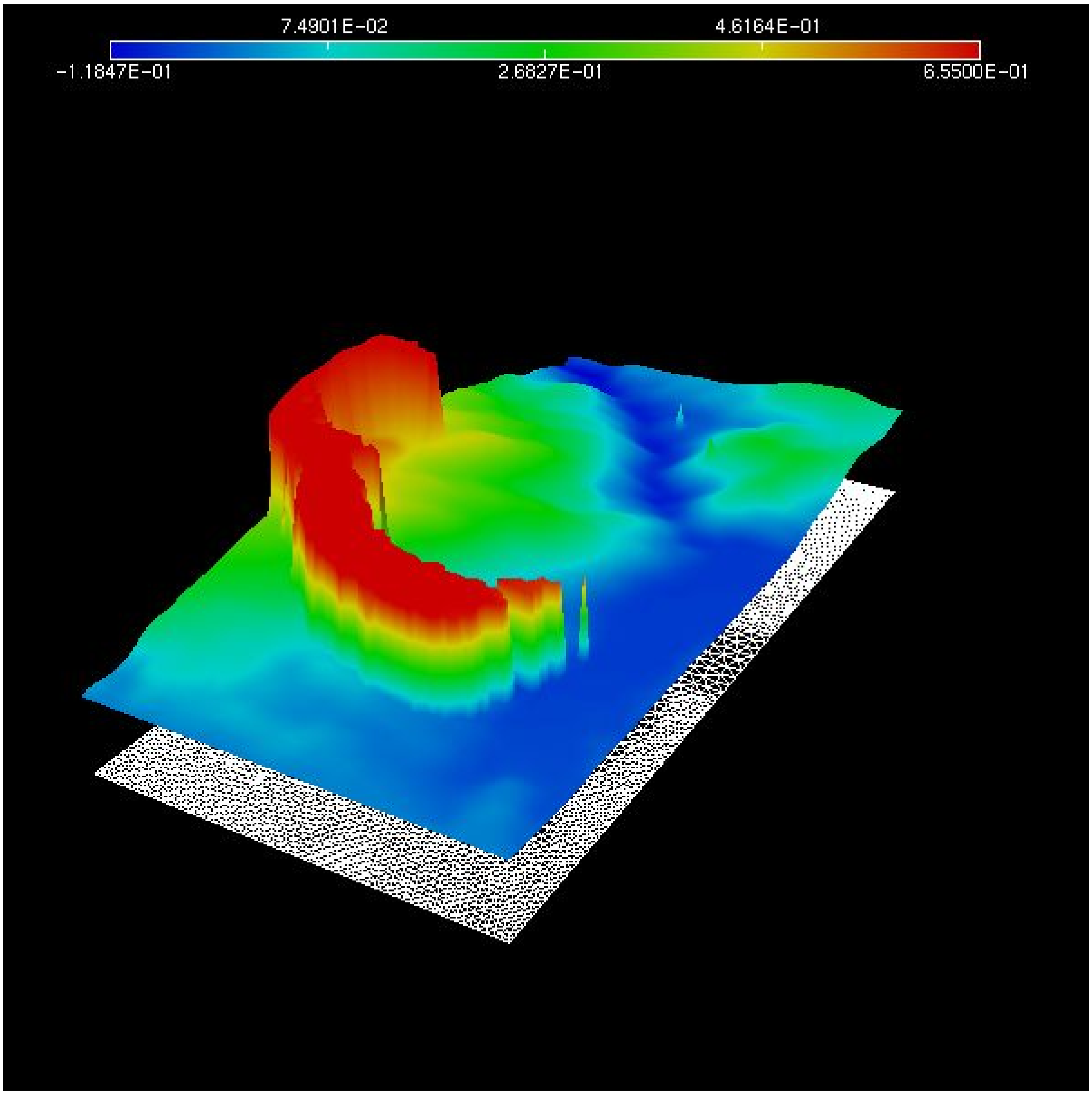

Figure 5: Application of our 2.5-D fire propagation model in a river basin (6 km long x 3 km width) after 5 hours. Computation time 35 minutes.