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Probabilistic safety analysis for urgent situations following the accidental release of a pollutant in the atmosphere

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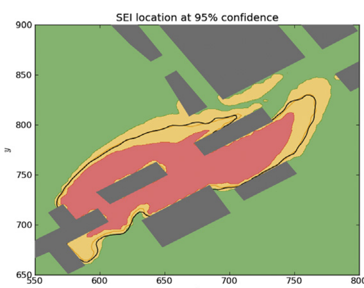
HIGHLIGHTS

- We quantify uncertainty in case of accidental atmospheric dispersion at local scale.
- We account for imprecise knowledge of the meteorological and release conditions.
- We resort to Lagrangian dispersion and to a vector Gaussian process surrogate model.
- We validate the Gaussian process predictors by comparison with Monte Carlo sampling.
- We produce probabilistic risk maps in order to help stakeholders making decisions.

GRAPHICAL ABSTRACT



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ABSTRACT

This paper is an original contribution to uncertainty quantification in *atmospheric transport & dispersion* (AT&D) at the local scale (1–10 km). It is proposed to account for the imprecise knowledge of the meteorological and release conditions in the case of an accidental hazardous atmospheric emission. The aim is to produce probabilistic risk maps instead of a deterministic toxic load map in order to help the stakeholders making their decisions. Due to the urge attached to such situations, the proposed methodology is able to produce such maps in a limited amount of time. It resorts to a *Lagrangian particle dispersion model* (LPDM) using wind fields interpolated from a pre-established database that collects the results from a *computational fluid dynamics* (CFD) model. This enables a decoupling of the CFD simulations from the dispersion analysis, thus a considerable saving of computational time. In order to make the Monte-Carlo-sampling-based estimation of the probability field even faster, it is also proposed to recourse to the use of a vector Gaussian process surrogate model together with *high performance computing* (HPC) resources. The *Gaussian process* (GP) surrogate modelling technique is coupled with a probabilistic *principal component analysis* (PCA) for reducing the number of GP predictors to fit, store

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and predict. The *design of experiments* (DOE) from which the surrogate model is built, is run over a cluster of PCs for making the total production time as short as possible. The use of GP predictors is validated by comparing the results produced by this technique with those obtained by crude Monte Carlo sampling.

1. Introduction

Atmospheric transport and dispersion (AT&D) may originate in releases from facilities under normal operating conditions or submitted to potential or real accidental situations. As the species (gases or aerosols) emitted in these circumstances can constitute a threat for the environment or the human health, AT&D is considered as one of the most important risk sensitive areas. For twenty years, the scientific community and the industrial operators have shown an increasing interest in using methods aiming at determining the uncertainty associated to processes (Saltelli et al., 2008). Various industries (*e.g.* automotive or aeronautics), already take into account uncertainty in the numerical modelling, especially in guarantee and safety studies (car-crash, risk analysis, etc.) (Lemaire and Pendola, 2006). In the same time, public authorities as official entities in charge of national or international regulations tend to request uncertainty to be considered in the industrial activities impact assessment on the population and ecosystems (see *e.g.* National Research Council (NRC) (1983, 1994) or very recently OFCM (2012)).

Nowadays, AT&D simulations are routinely carried out to estimate the consequences of atmospheric releases on the environment and inhabitants in the vicinity of industrial sites. Numerical modelling may be simple or more advanced, but always reflects the influence of the meteorological conditions prevailing during the AT&D event, on the space and time distribution of the pollutants, also possibly affected by physical and chemical transformations and dry or wet deposition on exposed surfaces. Computations are generally performed according to a deterministic approach, *i.e.* by doing a unique realization of the simulation and, of course, not estimating any uncertainty. It is worth noticing that such an evaluation may be already quite challenging when complex modelling is undertaken.

Unfortunately, a deterministic approach may not match the real situation, especially due to the lack of knowledge of the parameters used in the AT&D simulations. As a matter of fact, in numerous accidental situations, there is no meteorological station on the affected industrial site or close to it. Moreover, though necessary for AT&D computations, measurements or estimates of the emissions may not be available at the beginning of the event. These examples point out that the simulations of pollutants transfer through the environmental compartments, especially atmosphere, always go with uncertainty which can lead to extremely different numerical evaluations. And, when it comes to rigorously associating uncertainty with numerical modelling, the stakes are high, particularly in case of an emergency with AT&D and impact assessment being part of stiff human consequences decision making during the crisis management.

Several statistical methods coupled with Lagrangian Particle Dispersion Modelling (LPDM) specially dedicated to risk assessment have been published by Galmarini et al. (2004a,b) with some of them implemented in operational modelling systems. In general, they are adapted to the AT&D of hazardous releases at the mesoscale (from the regional to the continental scale) and have been validated using far-field experimental data, like the ETEX ones (Graziani et al., 1998a,b). Most of the time, these methods are based on an ensemble approach making use of several atmospheric flow and AT&D models, varying the initial and lateral boundary conditions and the numerous physical parametrizations of the models (see *e.g.* Galmarini et al. (2004a,b), Mallet and Sportisse (2008)).

On the other hand, few research papers are dealing with uncertainty in AT&D of accidental releases in the near-field, from 1 to 10 km. At such short distances from the emission source, it is clear that the influence of obstacles, like buildings, on the flow field and on the dispersion should be taken into account. Relevant studies can be found in the thesis by Demaël (2007, Chapter 5) who uses MERCURE, a CFD modelling tool, to assess the distribution of radionuclides released in the course of fictitious accidents affecting the French Nuclear Power Plant of Bugey, in the article by Baumann-Stanzer and Stenzel (2011) who compare the risk distances given by various Gaussian or Lagrangian AT&D models, or in that of Dabberdt and Miller (2000) who take a real accidental situation (oleum release in an industrial suburb of San Francisco) to carry out an uncertainty analysis with the TRIAD Gaussian puff model.

Mallet and Sportisse (2008) have identified different uncertainty origins, all contributing to decreasing the confidence level of the results. They make out the uncertainty of the input data, the uncertainty related to approximations in the modelling, and the uncertainty associated with the numerical schemes. More generally, uncertainty is of two kinds (Der Kiureghian and Ditlevsen, 2009): one is *random*, related to the spread of the results; the other one is *epistemic*, due to a lack of knowledge. For the former, the “actual” value is different from one realization to the other, and the probabilistic approach is universally adopted. For the latter, there is only one value which is not perfectly known. Most researchers including Der Kiureghian and Ditlevsen (2009) consider that the probabilistic approach is still applicable. In this case, the probability is interpreted as the confidence given to the estimate of the value. In this paper, we focus on the epistemic uncertainty.

De Rocquigny et al. (2008) proposed a framework to take uncertainty into account in the numerical modelling of the physical phenomena. Facing a given situation or analysis, they suggest to investigate the large panel of possible scenarios and to consider the variability of the results in order to improve the risk analysis and forecast or to optimize the decision or production processes. Moreover, they propose a general framework divided in four steps:

1. Problem specification.
2. Sources of uncertainty description and quantification.
3. Uncertainty propagation.
4. Sensitivity analysis.

De Rocquigny's method has been much used in numerous academic and industrial applications (see examples given by De Rocquigny et al. (2008)). But, to the best of our knowledge, it has never been applied to the accidental AT&D of hazardous materials, especially at close distances from the emission source, which is the goal of this paper. More precisely, the objective is to set a methodology for estimating the human health risk after an accidental release in order to guide the rescue teams. A particular interest is given to the production of time-varying probabilistic risk maps.