**18th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
9-12 October 2017, Bologna, Italy**

A NEW METHOD FOR ASSESSING THE UNCERTAINTY ASSOCIATED WITH 3D DISPERSION SIMULATIONS IN ANY VARIABLE METEOROLOGICAL CONDITIONS

Christophe Duchenne [1], *Patrick Armand* [1], *Marine Marcilhac* [2], *Sylvain Girard* [2] *and Thierry Yalamas* [2]

[1]CEA, DAM, DIF, F-91297 Arpajon, France
[2]Phimeca Engineering, Paris, France

Abstract: Whether for danger studies or emergency preparedness and response, relevant methods and models are needed to simulate the atmospheric transport and dispersion of hazardous materials in the atmosphere. This is especially the case when computations of the hazmat spatio-temporal distribution are run to help deciding an appropriate course of actions in a context characterised by a high level of uncertainty. Among the various sources of uncertainties, this study focuses on the wind field conjecture used as input to local scale atmospheric flow and dispersion simulations. A probabilistic model of this uncertainty adapted to operational contexts is proposed. It comprises two perturbation schemes, an additive perturbation and a time warp, that were compared on a realistic case study in a complex environment with an uneven terrain and highly fluctuating meteorological conditions.

Key words: *local scale, wind field, dispersion, perturbation, time warp, uncertainty propagation.*

CONTEXT AND PROBLEM FORMALISATION

Dispersion simulations of hazardous materials released within complex industrial or urbanised sites most often require 3D models capable to take account of the combined influence of the topography and buildings. There is an increasing demand for such 3D simulations from civilian security institutions for assessing precisely and realistically the impact of noxious releases on human health, both for regulatory purpose and emergency preparedness. These simulations are usually carried out using a deterministic set of parameters for the release and the meteorological conditions. Yet these quantities are partially unknown and a major source of uncertainties on the flow and dispersion patterns. Hence, methods for propagating these uncertainties through the 3D models are needed for enlightened decision making.

This study is a continuation of previous efforts to design an efficient computational chain for flow and atmospheric dispersion simulations at local scale (from 1×1 up to 50×50 km²) aimed at both risk studies achievement and decision making in an emergency (Aguirre Martinez *et al*., 2016; Armand *et al*., 2014).

Dispersion simulation following a real or hypothetical atmospheric release starts from a meteorological “conjecture” based on numerical simulations or available observations. The word “conjecture” is used in a deliberately loose sense: it is chosen to avoid semantic clash with cognates from related scientific domains such as data assimilation or machine learning. Informally, it is “something we believe in about what will happen”. In this paper, we investigate how the uncertainty of the wind field conjecture impacts the atmospheric dispersion prediction.

Basically, it was decided to use a unique wind field as the conjecture. Indeed, local scale meteorological ensembles are difficult to obtain. The wind field exhibits limited temporal statistical stationarity which precludes fitting stochastic processes such as ARMA (autoregressive moving average) or conditioning simulations with a kriging model. Fully inferring the uncertainty structure as well as its amplitude solely from available data is not possible here, and the amount of arbitrariness in the model augments accordingly. Yet, a careful inquiry of expert knowledge and operational requirements allows subduing this arbitrariness to a restricted set of intelligible parameters. Four specifications of a wind uncertainty simulator applicable to our specific context were thus elicited:

1. Confidence in the conjecture – Uncertain wind simulations should be close to the conjecture. Different metrics of proximity can be thought of, but more importantly the level of confidence should be explicitly controllable by the user.
2. Physical origin of spatio-temporal structures – Spatio-temporal structures in the conjecture are assumed to originate from physical phenomena. They should therefore be preserved as much as possible when applying the modelled uncertainty. Correlation is one possible characterisation of such structures.

3. Link between uncertainty and conjecture variability – Experts in atmospheric dispersion expect the wind conjecture to be more uncertain when it is intrinsically highly variable than when it is stable. Hence, there should be a link between the variability of the conjecture and the amplitude uncertainty.
4. Operational constraint – The uncertain simulator should be automatic and not require parameter tuning or unconstrained data analysis. Decision from the user is not ruled out but it should be organised into a preset plan.

The first two specifications provide a general bearing towards the kind of *structure* that should be investigated for the uncertainty model. Meanwhile, specification 1 and 3 constrain the amplitude of its variability, and outline the *decision plan* mentioned in specification 4.

Now, the question of the uncertainty structure can be further narrowed by considering that different inputs of a high dimensional physical model (here a black box including all data post-processing) may result in very similar outputs. Consider for instance a physical model that averages a lot of independent uncertain inputs. The central limit theorem states that the distribution of the outputs of this model approaches a Gaussian distribution as the inputs dimension. It is then fully characterised by two parameters, mean and variance, and is uninfluenced by the distribution of the inputs apart from their own mean and variance.

Another commonplace example, now from a signal processing standpoint, is the case of frequency filters. Thermal inertia as modelled by Fourier's law, and phenomena that admit similar mathematical formulation, are examples of low-pass filters. Two inputs time series to such a model, identical up to some high frequency fluctuation, will result in identical outputs.

This particular instance of equifinality (Beven, 2006) implies that while the diversity of possible uncertainty structures should be explored as exhaustively as our imagination allows, the resulting probabilistic models can probably be sieved to achieve a simple and concise formulation. Indeed, what we are ultimately interested in modelling is the uncertainty of the hazardous materials spread and their potential impact. Modelling wind field uncertainty is but a means towards this end.

PROBABILISTIC MODEL OF WIND FIELD UNCERTAINTY

So as to fill specifications 1 (confidence in conjecture) and 2 (physical origin of structures) straight-forwardly, we framed the probabilistic model of wind field uncertainty as perturbations of the conjecture. We have devised two probabilistic models whose expectation is the conjecture: an additive perturbation scheme and a time warp. Both perturbations apply to either wind velocity or direction. At this stage, notice that only wind direction and wind velocity were considered amongst the meteorological conditions for the sake of simplicity.

Additive perturbation

With the additive perturbation scheme, the perturbed field is simply the sum of the conjecture and a perturbation with null expectation:

$$Z(x,h,t) = z_0(x,h,t) + \varepsilon(x,h,t) \qquad (1)$$

where Z denotes the chosen variable, x the spatial (horizontal) coordinates, h the altitude and t the time. Specifications 1 and 2 are verified as long as the perturbation ε is *small enough* compared to the conjecture z_0. One way to simultaneously verify specifications 3 (variability link) and 4 (automation) is to algorithmically link the variance of the perturbation ε to the variance of the conjecture z_0. One of the simplest structures that an additive perturbation can assume is the *constant perturbation* that depends on the position, altitude and time only through its variance:

$$Z_{constant}(x,h,t) = z_0(x,h,t) + \varepsilon_c \, \alpha \, \sigma_c(h,t) \qquad (2)$$

where ε_c follows a standard Gaussian distribution, α is an arbitrary *confidence factor* and σ_c (h,t) a temporally local estimate of the conjecture variance. We choose here to use for the latter the rolling standard deviation of the conjecture, averaged over every location x.

Time warp

The additive perturbation scheme is able to represent conjecture errors such as global discrepancies or unforeseen fluctuations. Another source of error, with possibly important consequence on the final predictions, is to get the *dynamics* of the phenomena wrong. We propose to account for this eventuality with random functions distorting the considered time frame of total duration T. At any given instant *t*, an *interval warp* function φ expands or contract a time interval Δt by a factor β(t) that varies in time:

$$\varphi : t, \Delta t \quad \varphi(t, \Delta t) = \beta(t)\Delta t \tag{3}$$

From there, the associated *time warp* function ϕ mapping any instant t_i from $\{t_0 = 0, t_1 \dots t_K = T\}$ to the warped instant is defined as:

$$\phi(t_i) = \frac{T}{\sum_{k=0}^{K-1} \varphi(t_k, t_{k+1} - t_k)} \sum_{k=0}^{i} \varphi(t_k, t_{k+1} - t_k) \tag{4}$$

and preserving the time origin:

$$\phi(t_0 = 0) = t_0 = 0 \tag{5}$$

Equation (4) can be condensed by assuming a constant time step Δt and denoting by β' the function β including the scaling factor of the right hand side:

$$\phi(t_i) = \Delta t \sum_{k=0}^{i} \beta'(t_i) \tag{6}$$

It follows from this definition that the time warp functions also preserve the total duration:

$$\phi(t_K = T) = t_K = T \tag{7}$$

This property is convenient as it avoids truncation or extrapolation of the sequence of instants. Finally, denoting by Φ the distribution of time warp functions, the time warp perturbation scheme is:

$$Z_{warp}(x, h, t) = z_0(x, h, \Phi(t)) \tag{8}$$

In practice, the warped time series $Z_{warp}(x,h,t)$ are obtained by interpolating the conjecture at the sequence of warped instants $\{t_0, t_1 \dots t_K\}$. As for the distribution of Φ, it seems reasonable to assume that the interval warp function varies slowly and smoothly in time, namely that $\beta'(t) \approx \beta'(t + \Delta t)$. This is achieved by using oscillating functions for β obtained by summing low frequency sine waves with random phases.

APPLICATION: SHORT TIMED EMISSION FROM A COMPLEX TERRAIN

We have compared the variability induced by an additive perturbation of the direction versus a time warp of both direction and velocity on a realistic case study. We supposed one unit of mass (1 u) of hazardous material, either radionuclide or a chemical, to be emitted during 10 min within a 3 hours time frame, and dispersed in the atmosphere over an 8×5 km^2 domain. The terrain is complex: the source is hypothetically located on the talweg of a river running between two plateaus, through a valley 90 m deep and 1 km wide. The flow and dispersion have been computed with PMSS (Parallel-Micro-SWIFT-SPRAY), a modelling system developed by ARIA Technologies, ARIANET, MOKILI, and CEA (Tinarelli *et al*., 2013).

PMSS is dedicated to the high resolution simulation (from 1 meter to a few tens of meters) of the flow field and dispersion in variable meteorological conditions taking account of the topography and buildings.

PMSS comprises PSWIFT, a mass-consistent flow diagnostic model and PSPRAY, a Lagrangian particle dispersion model. Both models have been efficiently parallelized (Oldrini *et al*., 2017).
Here, the wind conjecture is a set of vertical profiles of the horizontal wind components issued from WRF reconstruction and forecast meso-scale system. As we are mostly interested in highly fluctuating meteorological conditions, we contracted a 24 h original WRF sequence to 3 h. PMSS computational chain is fed with the resulting 2 min time-step sequence, starting with PSWIFT. The spatial resolution in the domain centred on the river valley is 1 km, and there are 31 vertical layers. As stated above, the applied perturbations are independent of the location, and solely depend on the vertical layer and time.
Two samples of 100 uncertain wind fields were simulated: one with constant additive perturbation of the direction, and the other with time warped direction and velocity. Additionally, a constant additive perturbation was applied to both samples as a nuisance factor. The computation lasted about 300 h, using 28 cores of a CEA cluster at the CCRT (*Centre de Calcul Recherche et Technologie*).

Figure 1 shows 4 of those simulations, each column corresponding to one of the two samples.

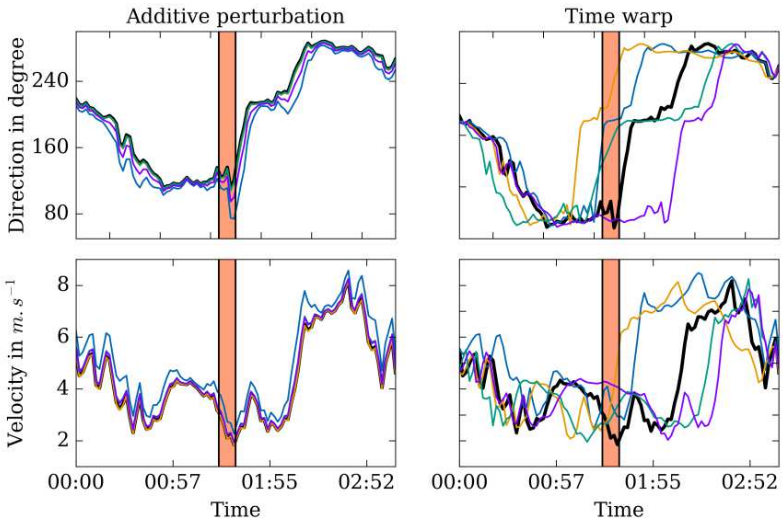

Figure 1. Four uncertain wind field realizations at 10 m above the ground. The conjecture is plotted as a thick black line. The orange vertical bar spans the emission time frame. Notice the sharp direction swing starting at about 1:40.

Figure 2 compares the effects of the two perturbations on the probability of the integrated concentration (or *dosage*) to exceed a critical threshold (here 10^{-7} u.s.m^{-3}) which could correspond to a danger zone for the human health or the taking of countermeasures. The probability surface resulting from the additive perturbation assumes the same overall shape as the exceedance region of the conjecture. On the contrary, time warp spreads the simulations all over the northern part of the domain. Of particular interest for emergency management are the low probability contour lines, displayed over the conjecture in the lower left corner. With time warp, the delimited zone spans most of the northern plateau, while it is notably smaller with additive perturbation.

Principal component analysis of the samples provides additional insights about their respective effects:

- The additive perturbation has two prominent effects: rotating the plume within a limited domain of about 45° (40% of the variance), concentrate or spread the plume symmetrically on either side of its main axis (20% of the variance).
- The effect of the time warp can be split as a switch effect (30% of the variance) selecting one of the two angles prominent in the lower right map of **Figure 2** and a rotation of the plume between those extreme positions. The latter clearly ensues from the emission occurring just before a significant swing in wind orientation.

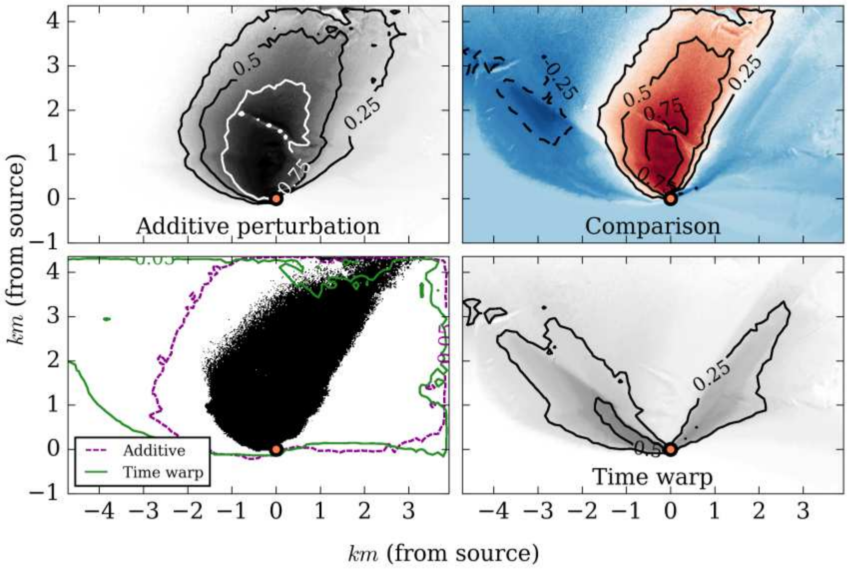

Figure 2. Empirical probabilities of the dosage exceeding 10^{-7} u.s.m^{-3} under additive perturbation (upper left) and time warp (lower right). Differences of those probabilities are mapped in the upper right corner. The exceedance zone for the conjecture is drawn in black in the lower left corner, where level lines indicate the 5% probability of exceedance for both perturbations. The source location is marked by an orange dot.

CONCLUSION AND PERSPECTIVES

Despite its relative simplicity, our model is able to capture some of the diversity of wind field uncertainty. It is highly flexible and should accommodate the diversity of topographic and meteorological conditions. The two compared perturbation schemes are equally acceptable and should probably be combined in practice. It is worth noticing that our approach could be adapted to other sources of uncertainties, whether meteorological, such as the Monin-Obukhov length (characterizing the atmospheric stratification), mixing layer height or rate of precipitation, or source term related, location, height and rate of emission. Then, sensitivity analysis could help to select the most relevant sources of uncertainty, so as to keep the model concise. Further work will be focused on calibrating the confidence levels and testing the uncertainty propagation in operational contexts: impact assessment, risk studies and simulated emergency.

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