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EMULATORS FOR THE RAPID PREDICTION OF CONSEQUENCES IN CASE OF NUCLEAR HAZARDS

Raphaël Périllat[1], Sylvain Girard[1], Irène Korsakissok[2] and Emmanuel Quentric[2]

[1]Phimeca Engineering, Paris, France
[2]IRSN, Fontenay-aux-Roses, France

Abstract: In the event of an accidental release of radionuclides into the atmosphere, the use of emulators (also known as surrogate models) makes it possible to quickly obtain useful results to help decision-making. However, the predictions of high dimension data is complex and the protective actions must be parametrized by a limited number of variable to be predicted by emulators.

***Key words:** Emulator, prediction, gaussian process, accidental release.*

INTRODUCTION

Numerical simulations of the atmospheric dispersion of radioactive particles are used to predict the areas impacted by accidental releases. IRSN use the C3X operational crisis platform to perform these calculations and to propose urgent protective actions (evacuation, sheltering, stable iodine prophylaxis) to decision makers. The protective action guide levels, expressed in terms of dosimetric quantities, are determined by regulation.

For the first response of the emergency center of the IRSN, the maximum distances up to which those protective actions might be proposed, as well as the angular apertures of the territory likely to be concerned, are scalar variables (Figure 1). In emergency response related to a possible or actual atmospheric release, these distances are estimated using the IRSN's operational dispersion models pX (Gaussian puff, used at short distance) and ldX (Eulerian, used at long distance), on the basis of the meteorological situation and source term assessment. In the graded approach applied by the IRSN's emergency center, first response generally relies on pre-calculated scenarios appropriately selected by the responders and for which experts should choose calculation parameters adapted to the situation and to the assessment objective. Precalculated source terms and consequences are made available for the experts for several accidents on several installations. This database has been constructed by calculations made in preparedness phase for a number of accidental scenarios and simple weather situations described by a few parameters (wind direction and speed, atmospheric stability, rain) assumed to be constant and homogeneous over the simulation domain. For each of these typical accidents, pre-calculated data are gathered in an "Accident Type Sheet" (called FAT in french, for "Fiche Accident Type"). Calculations are performed with the Doury Gaussian standard deviations (Doury, 1981), for two stability conditions, normal diffusion (ND) and low diffusion (LD), some wind speed values (3, 7, 13 m/s). A meteorological situation with a rainfall of 2 mm/h is also considered.

However, all possible meteorological situations cannot be covered in a single operational sheet, and the weather condition of the day of the accident rarely matches exactly to one of those described in the FAT. Similarly, other parameters may vary slightly from the calculation assumptions made in the FAT (e.g., the quantity released, the height of release, the standard deviations of Gaussian dispersion, deposition velocities,...). It would be impractical to enrich the FAT to cover all possible situations, that is why providing experts with a tool that instantly provides the response of the simulation for a custom set of parameters would allow operational constraints to be met.

Emulators, also known as metamodels, are surrogate models for the original computational model, used to approximate some of its scalar responses. They are statistical functions built from a large number of simulations, with the aim of predicting new responses with a negligible evaluation time. In this study, Gaussian processes (Roustant et al., 2012) are used for the construction of the emulators based on the pX model.

EMERGENCY PROTECTION ZONES AFTER A NUCLEAR ACCIDENT

We consider here one of the typical accident scenario of a 1300 MWe Pressurized Water Reactor (PWR) of the IRSN FAT catalog, which consists of a break on the primary circuit leading to the total core meltdown within one hour, and to a twenty-four-hours atmospheric release. The pre-calculated projected doses exceeds urgent protective action guide levels over significant distances. Three zones will be considered in this study:

- A sheltering area, where the simulated total effective dose over 24 hours is greater than 10 mSv,
- An evacuation area, where the simulated total effective dose over 24 hours is greater than 50 mSv,
- A stable iodine prophylaxis area, where the simulated equivalent dose to the thyroid due to inhalation over 24 hours is greater than 50 mSv.

The source term, atmospheric dispersion and dose calculation are conducted using conservative assumptions at each step, without taking into account the effect of protective measures, in order to avoid underestimating the impact of the accident.

Each zone is described by three parameters: its maximum distance, its angular aperture and its orientation (see Figure 1), which can be calculated from the dose outputs of the pX model run. The orientation of the plume only depends on the wind direction, assumed to be homogeneous and uniform over the simulation domain, it does not need to be emulated since it is obtained directly from the model input value.

Two emulators (maximum distance and angular aperture) are built for each of the 3 protective action zones. In this paper, we focus on the maximum distances of threshold exceedance of protective action guide levels.

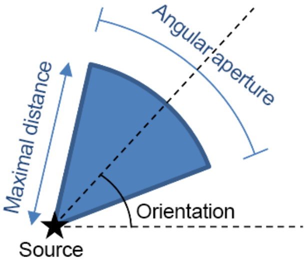


Figure 1. Parameterization of an action zone by three quantities.

Five input parameters of the pX model are considered to be uncertain: the release height of the source term, the source term magnitude, the wind module, the rain intensity and the meandering wind factor, which is a factor increasing the lateral spread of the plume to account for meandering wind direction with a characteristic time between 6 minutes and the meteorological time step (usually one hour). These five variables are selected because they are part of the few parameters that are likely to be modified during the first emergency reponse phase, to take into account either additional clarifications or strong uncertainties on their values. For each of these variables, a range of variation is defined in order to delimit the input space.

EMULATION BY GAUSSIAN PROCESSES

The construction of emulators relies on the simulation of thousands cases to cover a wide range of hypotheses. For each input variable, a draw is made over its range of variation, in order to make the emulators reliable over the entire space of possibilities. In our case, it means to randomly draw points in a space of dimension five. A simulation is then performed with pX for each point of this training sample, with the random values of these parameters. The maximum distances as well as the angular apertures corresponding to the three emergency protection zones can be extracted from the results of these simulations. These quantities are then used in the construction of emulators.

A Gaussian process is defined as a collection of a finite number of random variables having a Gaussian joint distribution. Thus, the response surface described by the output when the inputs vary is modeled as the sum of a constant term and the realization of a centered Gaussian process. If the model output pX is denoted y and the vector of its inputs is denoted x, the emulator f is written as :

$$f(x) = C + \sum_{j=1}^{N} w_j(x)\big(g\big(x^{(j)}\big) - C\big) \tag{1}$$

where *C* is the constant term, *x(j)* is a point in the training sample of size *N*, and *wj (x)* are weights. The determination of *f* by training is performed using the R module DiceKriging (Roustant et al., 2012). In our case, N = 2048 simulations are used to build the metamodels in the normal diffusion mode and 2048 additional simulations are used for the low diffusion mode.

The emulators allow to evaluate very quickly the value of the maximum distance and the aperture of the emergency protection zones, for different dose thresholds and two stability classes. A graphical interface has been developed in order to geometrically represent these parameters, for a better visualization of the results.

Theoretically, with an infinite number of simulations used for their construction, the emulators give results identical to those of the model. But in practice, the number of simulations is limited and the emulators thus constructed can deviate from the model results. To check whether they remain reliable, a common approach is to evaluate the emulator on a test sample and compare the results with the initial model. To do this, we draw M new points in our five-dimensional input space and then run the pX model *M* times with input parameters corresponding to these draws. We then obtain *M* output results (maximum distances and angular apertures) which we can compare with what the emulators predict for the same parameter values. We thus evaluate the quality of our emulators at several points randomly distributed in space, which allows us to quantify the error committed by the emulator on cases it does not know. For this study, we consider a test sample of M = 1000 points.

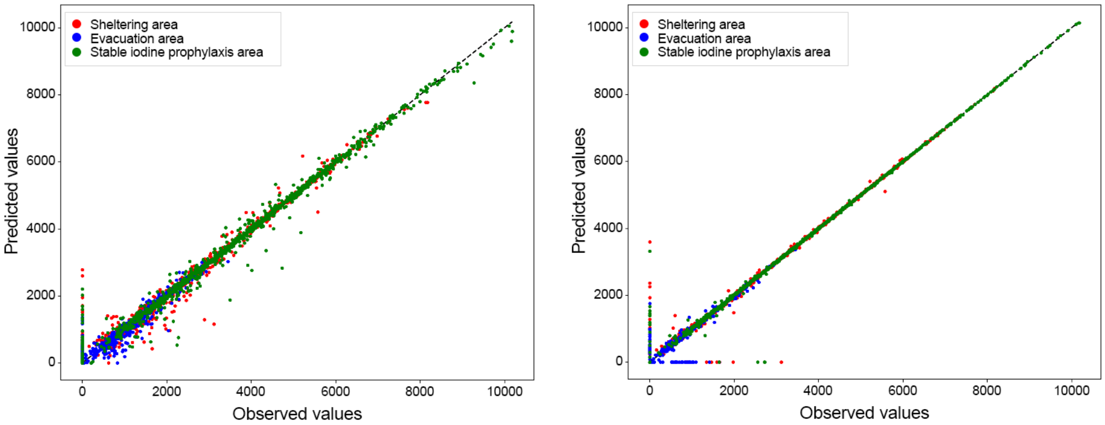
CLASSIFICATION METHODS FOR THE IMPROVEMENT OF PREDICTIONS

The distances of threshold exceedance of protective action guide levels may be all zero for some values of the input variables and that creates a discontinuity that is difficult for emulators to reconstruct. To avoid this problem, we use a classification method to determine, prior to emulation, whether or not the distances are going to be zero, using a nearest k-neighbor method (Altman, 1991). For a given dose threshold, the input space of the model can be divided into two subspaces: a first one in which the distance is zero and a second one in which it is strictly positive. The purpose of the classification is to estimate whether a point P in the space is located in one or the other of these subspaces.

To carry out this classification, we have used the same N points that were used to build the emulator. By then constructing two classes, $\{d = 0\}$ and $\{d > 0\}$, it is possible to assign to all the points in space one of these classes, depending on the state of its k-nearest neighbors. In our study, we have chosen $k = 5$ and we have weighted the influence of each of its 5 points by the inverse of the distance separating it from the point to be evaluated. This distance is defined as the Euclidean distance between the points in a 5-dimensional space normalized so that the range of variation of each variable is between 0 and 1.

Once this classification has been done, the evaluation of whether a point in the space will give a distance of zero is almost instantaneous with this method. It can therefore be used upstream of the emulator to predict whether a result will be zero or whether it needs to be evaluated by an emulator.

The main advantage of this method is to be able to build an emulator only on the restricted space of the inputs where the distances are non-zero. Emulators constructed in this way are more accurate, because the points where the distances behave differently are removed for its construction. Then when we want to evaluate a point in space, we first determine whether the classification predicts that it will have a non-zero distance. If this is the case, the algorithm stops, otherwise the emulator allows us to evaluate the distance.



(a) Emulator without any classification

(b) Emulator associated with a classification by k-nearest neighbors

Figure 2. Comparison between the maximum distances observed (pX simulations) and the values predicted by the emulator without any classification and associated with a classification by k-nearest neighbors, for the three dose thresholds considered, for a sample of 1000 test points, in the case of normal diffusion stability.

However, the classification setup is not perfect and depends on the points that were used for its construction. It is possible that the classification gives erroneous results, especially in the area close to the interface between the two subspaces we are trying to define, as it can be seen in Figure 2 where several points are located on the lines y = 0 and x = 0. To evaluate the results of this classification, we use an uniform test sample of 1000 points to estimate the number of false positives and false negatives predicted by classification. With the combination of classification followed by emulation, there are still some false positive or negative cases (between 1.8 and 8.0%), but these numbers are much lower than when no classification was made (between 3.7 and 46.0%). Moreover, the evaluation of the emulator on areas where distances are non-zero is in most cases much better, as shown by the estimation errors in Table 1.

Table 1. The mean error, quantile 95% of the error, the number of cases where the emulators, associated with a k-nearest neighbors classification method or not, give a non-zero response when it should be at zero (false positive) and where it gives a zero response when it should be positive (false negative), on a test sample of 1000 simulations, for the threshold exceedance of Total Effective Dose (TED) and Inhalation thyroid dose (ITD). The error rate correspond to the sum of false positive and false negative divided by the number of simulations in the sample.

Emulator	**Stability**	**Threshold**	**Mean error**	**Q95% of the error**	**False positive**	**False negative**	**Error rate**
Emulator without any classification	Normal diffusion	TED ≥ 10 mSv	109 m	189 m	38	1	3.9 %
		TED ≥ 50 mSv	97 m	66 m	233	3	23.6 %
		ITD ≥ 50 mSv	116 m	293 m	36	1	3.7 %
	Low diffusion	TED ≥ 10 mSv	419 m	874 m	368	0	36.8 %
		TED ≥ 50 mSv	390 m	361 m	460	0	46.0 %
		ITD ≥ 50 mSv	462 m	1391 m	399	1	40.0 %
Emulator associated with a k-nearest neighbors classification	Normal diffusion	TED ≥ 10 mSv	53 m	142 m	11	9	2.0 %
		TED ≥ 50 mSv	60 m	78 m	45	35	8.0 %
		ITD ≥ 50 mSv	42 m	230 m	50	4	1.8 %
	Low diffusion	TED ≥ 10 mSv	101 m	646 m	18	26	4.4 %
		TED ≥ 50 mSv	414 m	222 m	20	27	4.7 %
		ITD ≥ 50 mSv	67 m	492 m	18	25	4.3 %

It is important to identify which errors are acceptable and which are not in this context. An error of a few hundred meters over a maximum distance of 1 km may seem less acceptable than an identical error over a maximum distance of 15 km, but in terms of surface, the area of the zone where the emulator gives a bad prediction will be much smaller in the first. In practice, these values are not used as exact values, but it is rather their order of magnitude that determines the actual areas over which actions will be carried out (often over administrative entities). Therefore, the error committed on the estimation of distances must be smaller than the margins that are taken by decision-makers for safety reasons.

To further reduce the number of false positives and false negatives in the classification, it is possible to use a classification by Gaussian process. Then the number of false points is still lower (between 0.3 and 4.3%), but the call to the classification is much slower, which makes the use of the emulator much less reactive: of the order of 2 seconds for an evaluation, compared to only 0.2 seconds with a classification by nearest neighbor. The first classification is thus more interesting in cases where a very large number of evaluations is to be expected.

CONCLUSION

Emulators allow to obtain a quasi-instantaneous estimate of the areas where protective action guide levels might be exceeded for a given accidental scenario and meteorology. As soon as a catalog of emulators is built on the basis of the "typical" accident scenarios, the production of expertise, and therefore the provision of technical advice for decision-makers, can be accelerated, particularly in the early phases of the crisis when uncertainties reign so much. Prior to this operational use, these emulators must be evaluated against test samples to verify their reliability and sometimes complemented by classification methods to increase their performance.

The first emulation phase has highlighted the main sources of inaccuracy. Upstream classification tools to predict a null output result or a 360° zone have greatly improved the output results of the emulators, but also sometimes slow down the emulator thus created.

One perspective to improve the results is to study a different parameterization of the output data, using dimension reduction methods, in order to reduce the dose maps to a few scalar parameters which can then be emulated. This would allow to avoid the use of thresholds and thus to avoid discontinuities related to threshold effects, but also to be able to go beyond the prediction of distance and aperture of a sector-shaped zone and predict 2D dose maps.

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