

# PROPOSAL AND DEMONSTRATION OF A PRACTICAL APPROACH TO IDENTIFY AND PROPAGATE UNCERTAINTIES IN ATMOSPHERIC DISPERSION FOR LONG-TERM IMPACT ASSESSMENT STUDIES



*Sébastien Argence<sup>1</sup>, Patrick Armand<sup>2</sup>, Fabien Brocheton<sup>1</sup>, Thierry Yalamas<sup>3</sup>, François Deheeger<sup>3</sup> and Alexandre Micol<sup>3</sup>*

*<sup>1</sup> NUMTECH, Aubière, France*

*<sup>2</sup> CEA, Arpajon, France*

*<sup>3</sup> PHIMECA, Cournon d'Auvergne, France*

# Previous work & objectives of the study

## ■ Context :

- Request from regulatory administration to quantify uncertainties in environmental impact assessment studies

## ➤ Previous work :

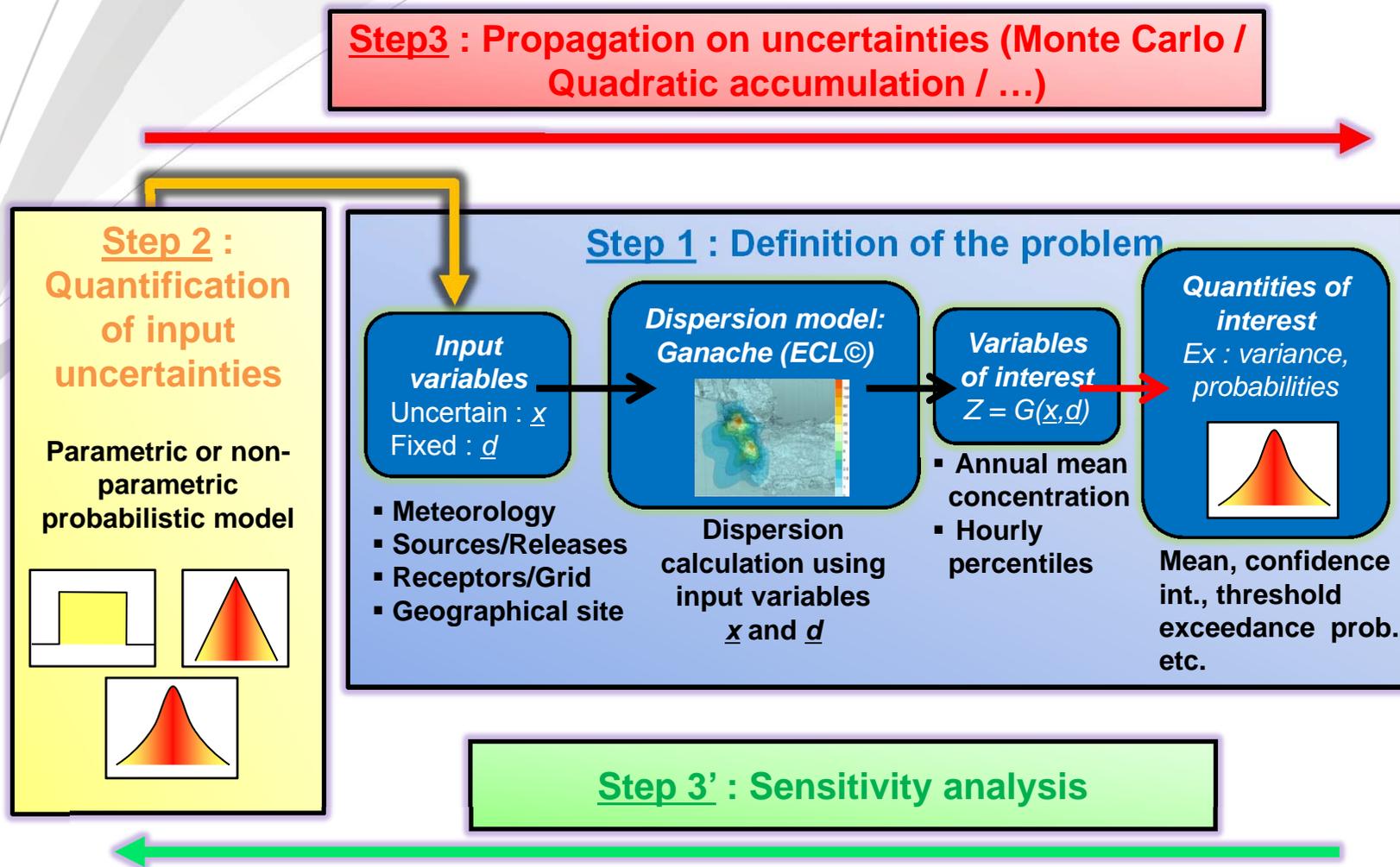
- 1- Global analysis on possible uncertain parameters in atmospheric dispersion models (gaussian plume, puff and lagrangian models)
- 2- Application of a first approach of quantification for chronic impact

## ➤ Objectives :

- Extend the previous work in terms of gaussian model (doury, ...), uncertainty quantification (including sensitivity analysis), ...
- Integrate the chain of treatment in an automatic tool

# Description of the approach

## General overview



Adapted from De Rocquigny et al. (2008)

# Description of the approach

## *Description of each step : definition of the problem*

- Dispersion model : gaussian plume model GANACHE developed at Central School of Lyon (© ECL, France)
  - May use various parameterizations of atmospheric stability (similitude theory, Pasquill-Gifford and Doury classes)
  - Fully integrated to the tool (based on open-turns) that has been developed
  
- Uncertain variables :
  - Meteorology : wind speed/direction, temperature, cloud cover
  - Dispersion site characteristics : surface roughness
  - Release characteristics : emission rate
  - Receptors location and grid height

# Description of the approach

*Description of each step : definition of the problem*

- Variables of interest : annual mean concentration and 95<sup>th</sup> percentiles
- Quantities of interest : mean, confidence intervals, threshold of exceedance probabilities, etc.

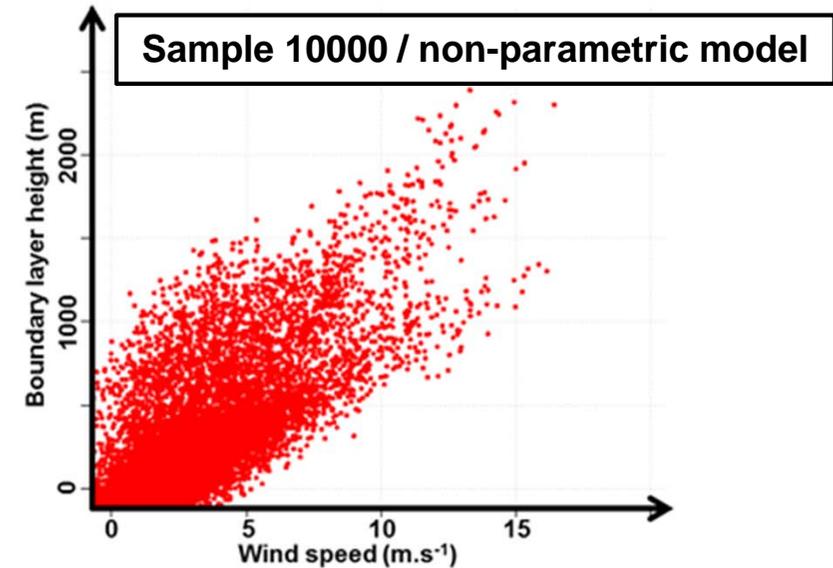
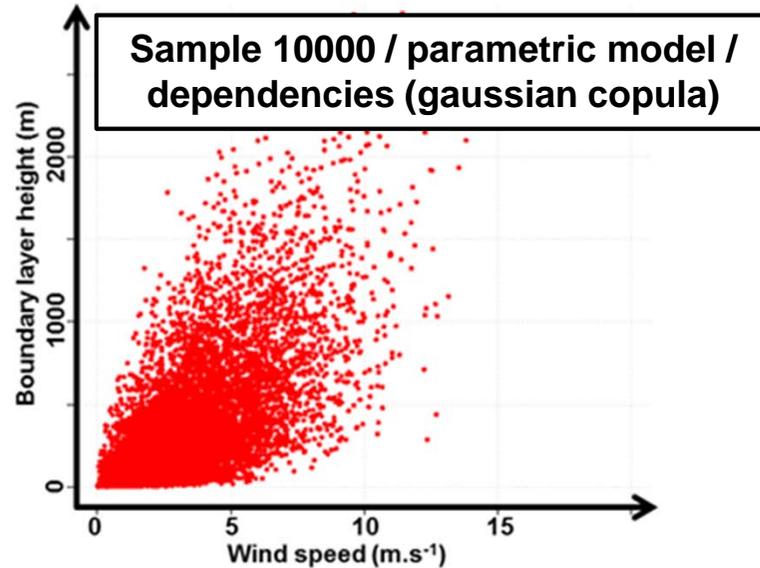
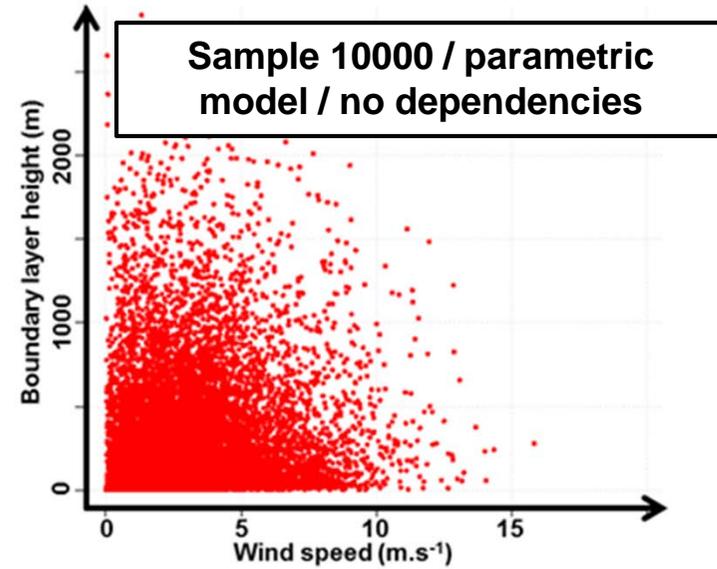
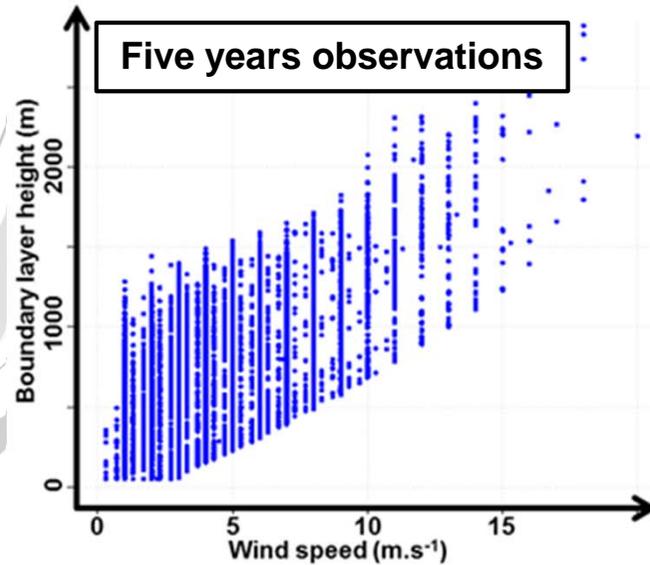
# Description of the approach

*Description of each step : quantification of input uncertainties*

- Characteristics of the release, dispersion site, receptors and grid height : PDFs defined from bibliography/expert judgment
  
  - Choice to construct a probabilistic model for meteorology - Two approaches tested :
    - Parametric : assigning PDF to each uncertain input variable
    - Non-parametric : kernel smoothing distributions
  
  - How to choose ?
    - Generation of probabilistic models following each method
    - Comparison of the natural relationships between input variables with their artificial relationship when using PDFs
- Example for wind speed / PBLH (see next slide)

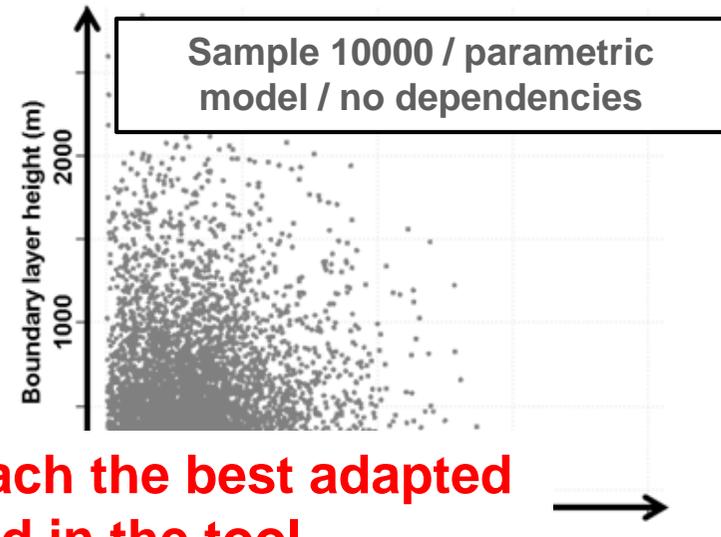
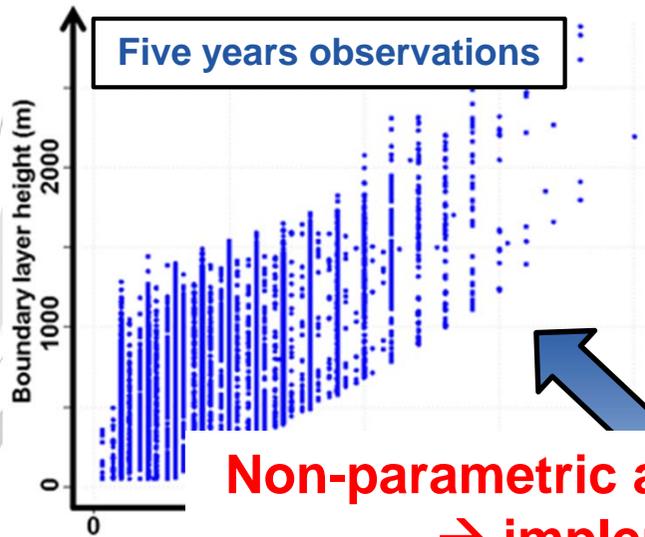
# Description of the approach

*Description of each step : quantification of input uncertainties*

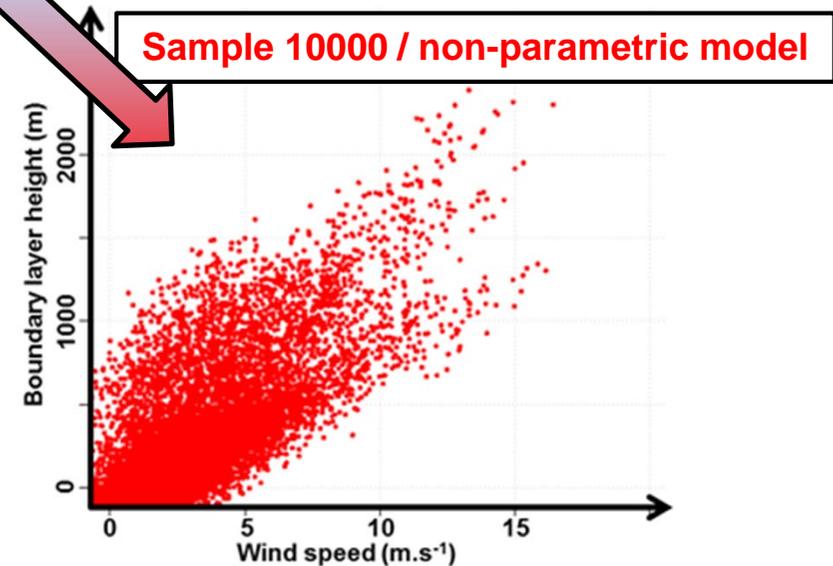
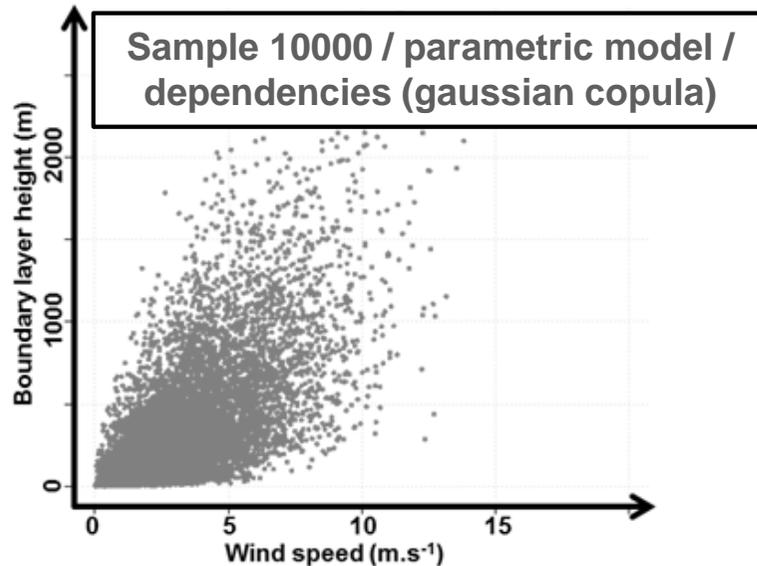


# Description of the approach

Description of each step : quantification of input uncertainties



**Non-parametric approach the best adapted  
→ implemented in the tool**



# Description of the approach

## *Description of each step : propagation method*

- Objective : propagating the joint PDF of each input variable through the dispersion model to generate the PDF of the model results (ground level concentrations)
  
- Proposed methods :
  - Quadratic accumulation : well adapted for some tests dealing with sensivity analysis for specific hours but not for a study over many years as requested for EIA
  - Polynomial chaos : not adapted as it requires the use of a parametric probabilistic model for input data
  - Monte Carlo simulations was finally chosen

# Description of the approach

## *Description of each step : propagation method*

- Monte Carlo simulations allows to conduct a statistical analysis of the probabilistic distribution of variable of interests
- For percentile/quantiles estimation – 3 additional approaches has been tested:
  - Wilks formula
  - Bootstrap resampling
  - Extreme values analysis (estimation of the law for queue distribution)

# Description of the approach

## *Description of each step : bootstrap resampling*

- Definition : based on the generation of "new samples" obtained by random sampling with replacement from the original dataset → resampling
- Methodology (for each receptor/grid point) :
  - Performing Monte Carlo simulations to obtain a sample of predicted concentration
  - Generation of a new sample obtained by random sampling with replacement from the dataset computed with Monte Carlo
  - A sample of the quantity of interest may then be obtained
  - Computation of its mean, variance and confidence interval following :

$$\left[ \hat{m}_X - t_{\alpha, N-1} \sqrt{\text{Var}[\hat{m}_X]}; \hat{m}_X + t_{\alpha, N-1} \sqrt{\text{Var}[\hat{m}_X]} \right]$$

# Description of the approach

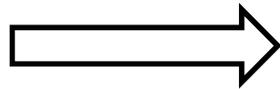
## *Description of each step : extreme values analysis*

- Extreme values analysis relies on the distribution of extreme events. In this study, extreme events are related to very large concentration values
- Methodology (for each receptor/grid point) :
  - Performing Monte Carlo simulations to empirical distribution of predicted concentration
  - Selection of quantiles/data associated with a probability exceeding a given threshold (for example, 0.8 or 0.9). Doing that allows to keep only extreme values of the concentration sample
  - Estimating coefficient of the generalized extreme values law using weighted least squares method
  - Once the optimal law defined, the desired quantile may be obtained

# Application of the approach

## *Case study*

- Five years hourly meteorological data
- Source release : inert gas, 50 m height, 1 m diameter (no plume rise effects)
- Flat terrain and uniform roughness



Negligence of uncertainties associated with topography, obstacles, source geometry, physical and chemical transformations of pollutants

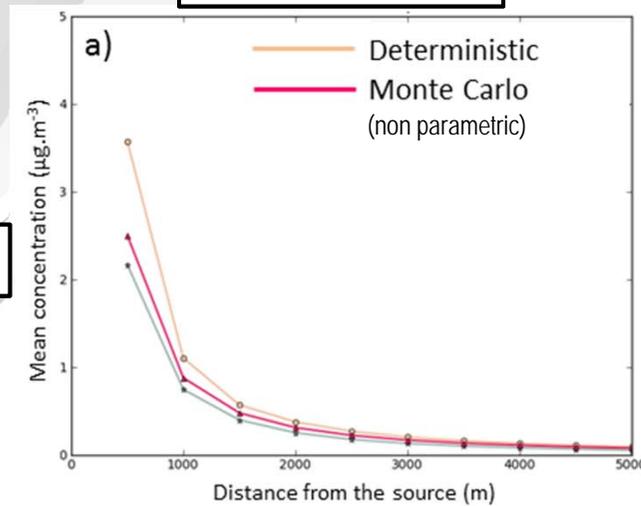
- Numerical calculations conducted for receptors only. Results presented correspond to receptors placed according from two wind directions : D1 (rather infrequent) and D2 (frequent).

# Application of the approach

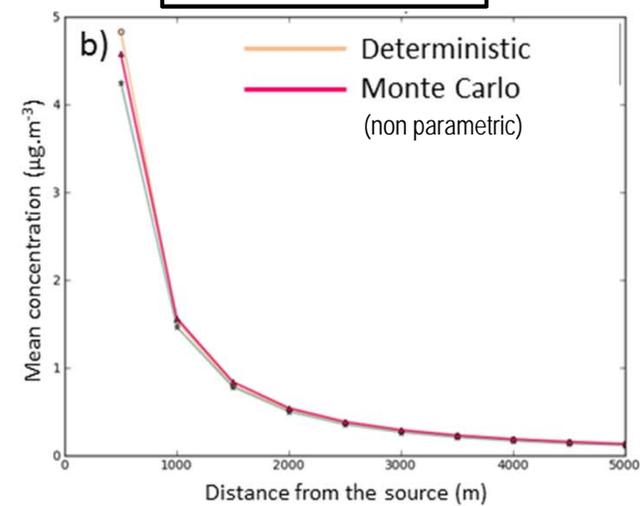
## Annual mean concentration computation

Doury

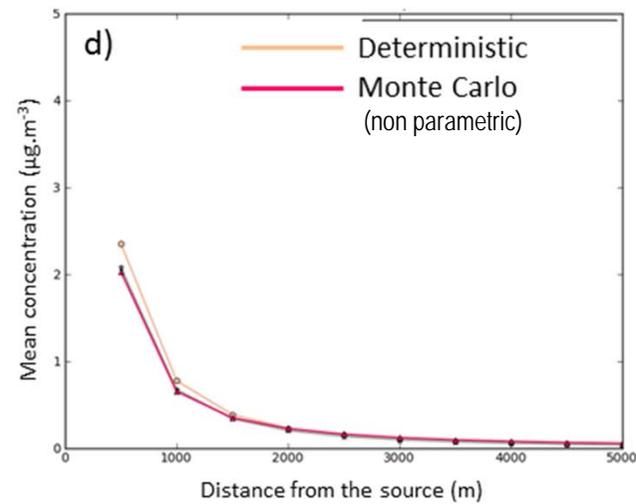
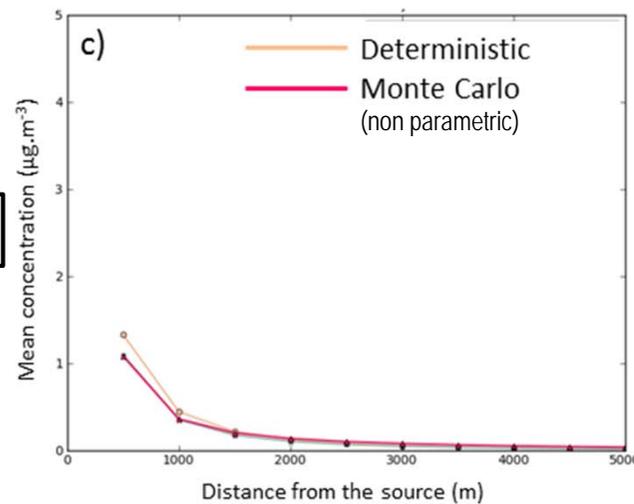
Direction D1



Direction D2



Similitude



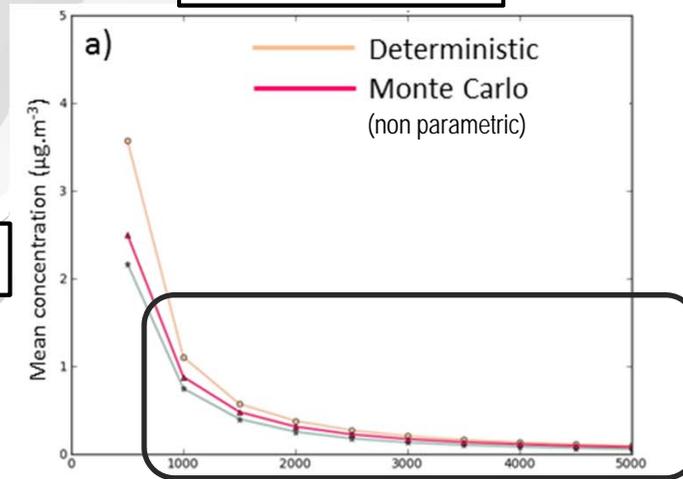
Annual mean concentration as a function of the distance from the release ( $\mu\text{g.m}^{-3}$ )

# Application of the approach

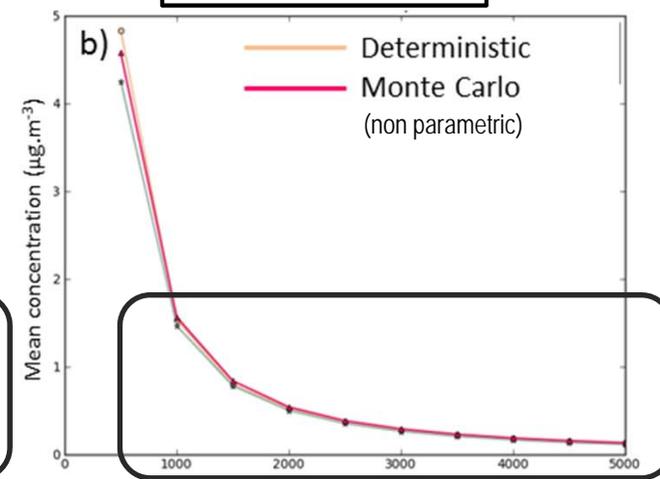
## Annual mean concentration computation

Doury

Direction D1

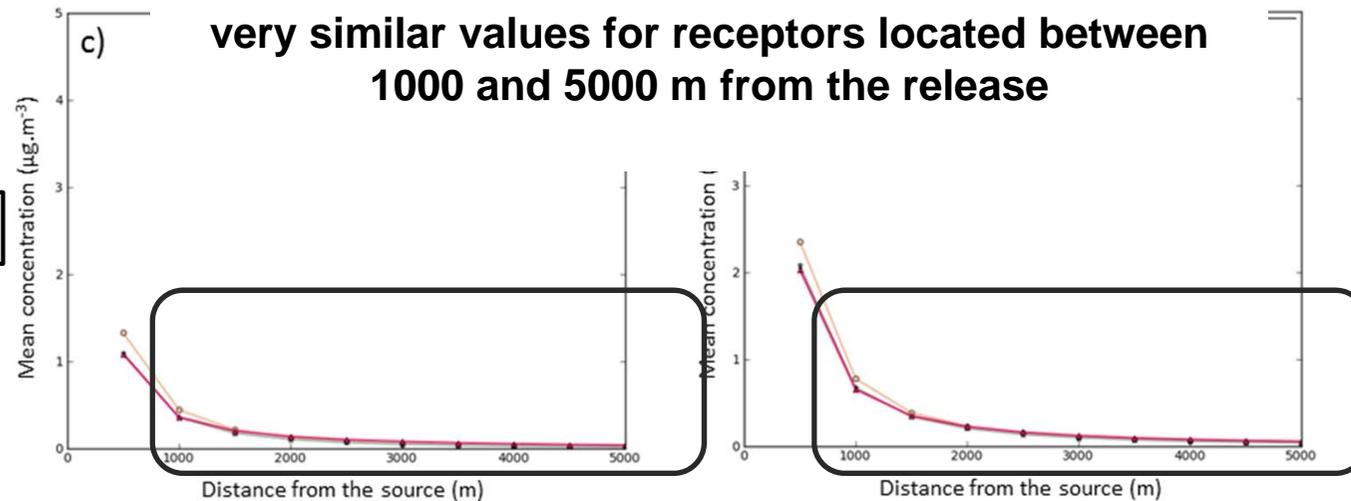


Direction D2



**Deterministic and Monte Carlo simulations exhibit very similar values for receptors located between 1000 and 5000 m from the release**

Similitude



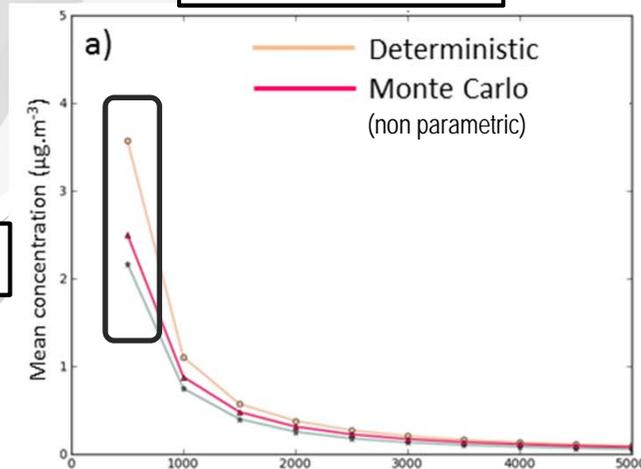
Annual mean concentration as a function of the distance from the release ( $\mu\text{g}\cdot\text{m}^{-3}$ )

# Application of the approach

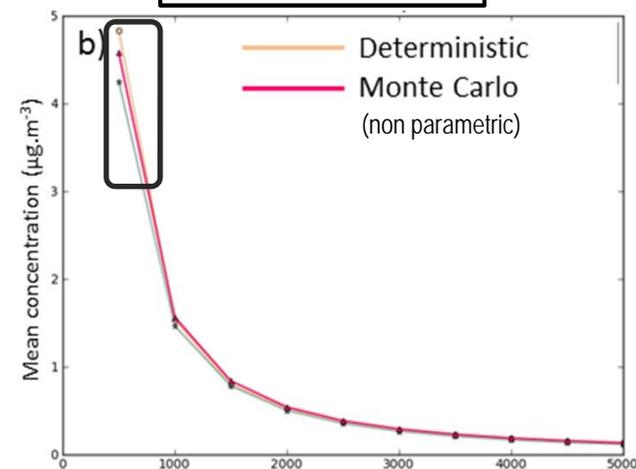
## Annual mean concentration computation

Doury

Direction D1

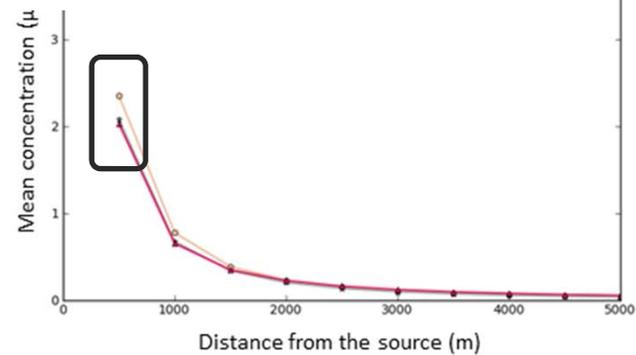
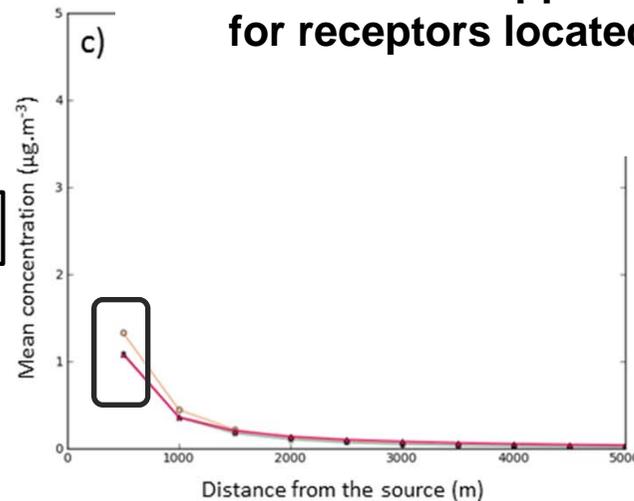


Direction D2



Main differences appear in the vicinity of the source, for receptors located at 500 m of the release

Similitude



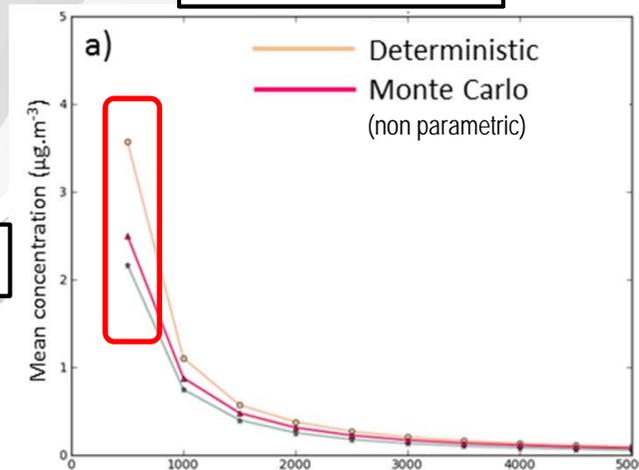
Annual mean concentration as a function of the distance from the release ( $\mu\text{g}\cdot\text{m}^{-3}$ )

# Application of the approach

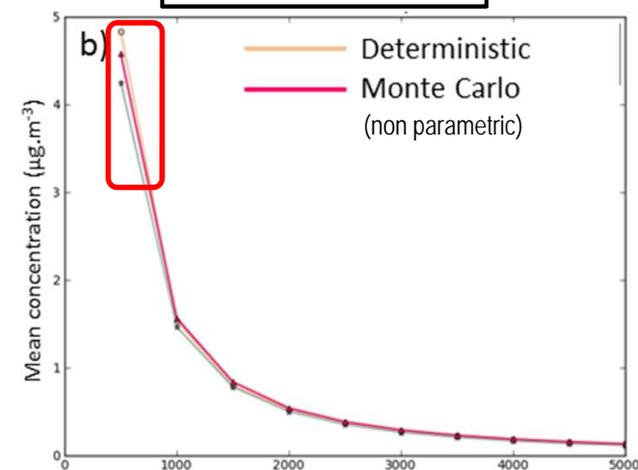
## Annual mean concentration computation

Doury

Direction D1

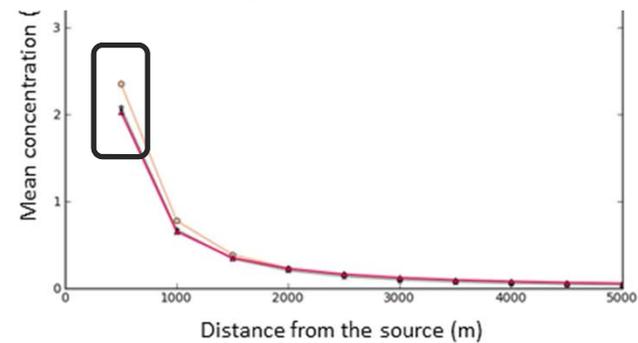
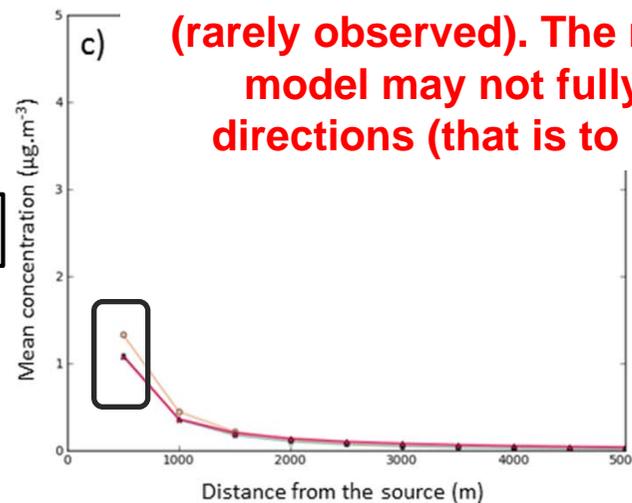


Direction D2



Differences are more important for wind direction D1 (rarely observed). The non-parametric meteorological model may not fully represent infrequent wind directions (that is to say with the right frequency)

Similitude



Annual mean concentration as a function of the distance from the release ( $\mu\text{g}\cdot\text{m}^{-3}$ )

# Application of the approach

## *Annual mean concentration computation*

Approach	Direction D1	Direction D2
<b>Doury – Deterministic (5 years)</b>	3.57	4.83
<b>Doury – Monte Carlo simulations (sampling size 10000)</b>	2.50 [2.31 ; 2.68]	4.57 [4.32 ; 4.83]
<b>Similitude – Deterministic (5 years)</b>	1.32	2.35
<b>Similitude – Monte Carlo simulations (sampling size 10000)</b>	1.08 [0.99; 1.17]	2,03 [1.92 ; 2.13]

*Annual mean concentration for receptors located at 500 m from the release ( $\mu\text{g}\cdot\text{m}^{-3}$ ) and 95% confidence intervals (in square brackets)*

# Application of the approach

*Estimation of 95<sup>th</sup> percentiles of the predicted concentration*

Approach	Direction D1	Direction D2
<b>Doury – Deterministic (5 years)</b>	0.25	16.89
<b>Doury – Monte Carlo simulations (sampling size 10000)</b>	13.84	38.98
<b>Similitude – Deterministic (5 years)</b>	8.90	13.92
<b>Similitude – Monte Carlo simulations (sampling size 10000)</b>	2.75	14.84

*95<sup>th</sup> percentiles of the predicted concentration for receptors at 500 m from the release ( $\mu\text{g.m}^{-3}$ )*

# Application of the approach

*Estimation of 95<sup>th</sup> percentiles of the predicted concentration*

Approach	Direction D1	Direction D2
<b>Doury – Deterministic (5 years)</b>	0.25	16.89
<b>Doury – Monte Carlo simulations (sampling size 10000)</b>	13.84	38.98
<b>Similitude – Deterministic (5 years)</b>	8.90	13.92
<b>Similitude – Monte Carlo simulations (sampling size 10000)</b>	2.75	14.84

*95<sup>th</sup> percentiles of the predicted concentration for receptors at 500 m from the release ( $\mu\text{g}\cdot\text{m}^{-3}$ )*

**Monte Carlo simulations using similitude theory are able to reproduce the order of magnitude of deterministic 95<sup>th</sup> percentiles**

# Application of the approach

*Estimation of 95<sup>th</sup> percentiles of the predicted concentration*

Approach	Direction D1	Direction D2
<b>Doury – Deterministic (5 years)</b>	0.25	16.89
<b>Doury – Monte Carlo simulations (sampling size 10000)</b>	13.84	38.98
<b>Similitude – Deterministic (5 years)</b>	8.90	13.92
<b>Similitude – Monte Carlo simulations (sampling size 10000)</b>	2.75	14.84

*95<sup>th</sup> percentiles of the predicted concentration for receptors at 500 m from the release ( $\mu\text{g}\cdot\text{m}^{-3}$ )*

**Doury approach led Monte Carlo simulations to strongly overestimate 95<sup>th</sup> percentiles values, particularly for receptors located in the wind direction D1**

# Application of the approach

*Estimation of 95<sup>th</sup> percentiles of the predicted concentration*

Approach	Direction D1	Direction D2
<b>Doury – Deterministic (5 years)</b>	0.25	16.89
<b>Doury – Monte Carlo simulations (sampling size 10000)</b>	13.84	38.98
<b>Similitude – Deterministic (5 years)</b>	8.90	13.92
<b>Similitude – Monte Carlo simulations (sampling size 10000)</b>	2.75	14.84

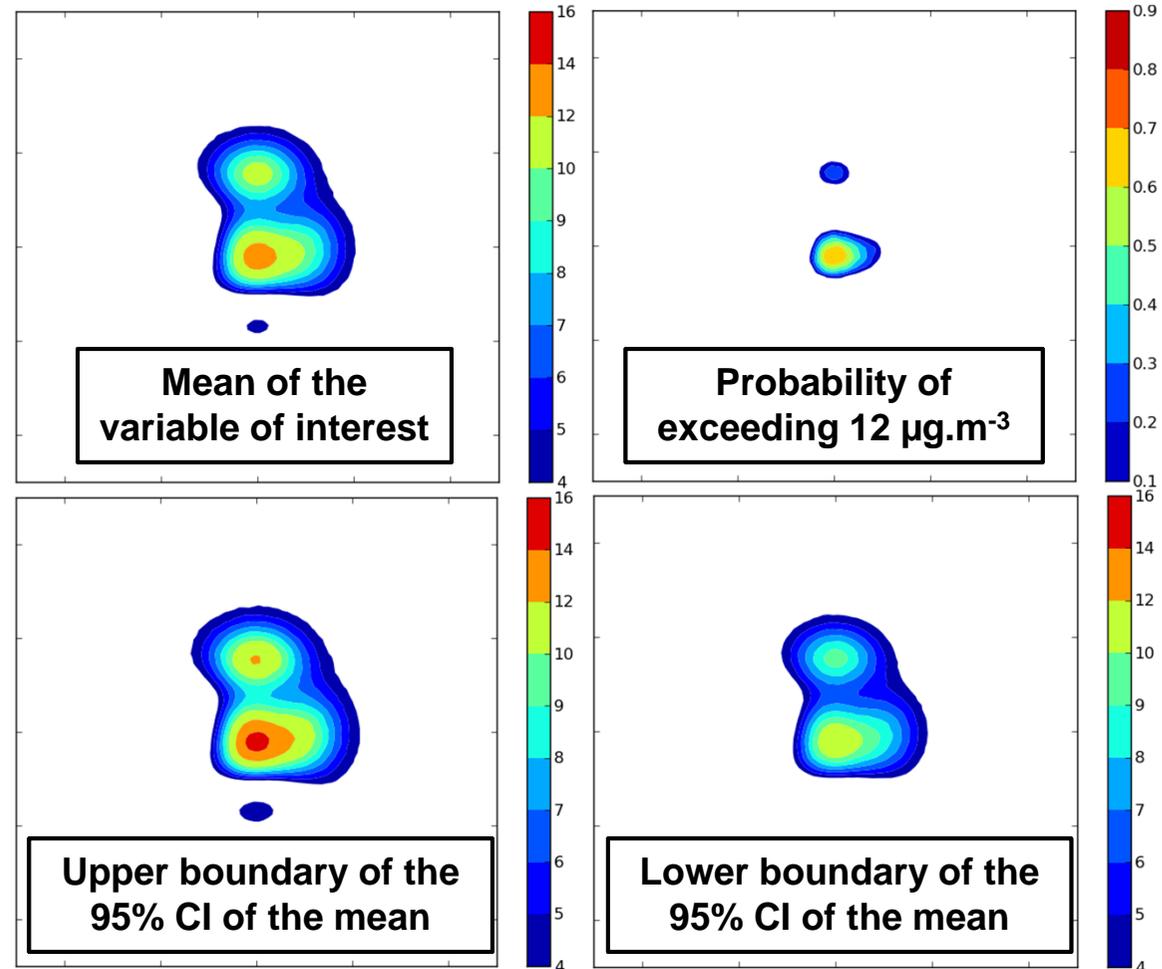
*95<sup>th</sup> percentiles of the predicted concentration for receptors at 500 m from the release ( $\mu\text{g}\cdot\text{m}^{-3}$ )*

**Possible explanation : a detailed analysis of the results revealed the strong sensitivity of high order percentiles estimation to both the large proportion of simulated zero values and to the shape of the tail of simulated concentrations distribution**

# Presentation of results associated with an uncertainty analysis

## Examples

- Probabilistic mean estimation
- Boundaries of a given confidence interval (giving the possible minimum and maximum values accounting for input uncertainties)
- Probability of threshold exceedance
- ....



*Graphical representation of the results of an uncertainty study conducted over a full grid with idealized data*

# Conclusions and future work

## *Conclusions*

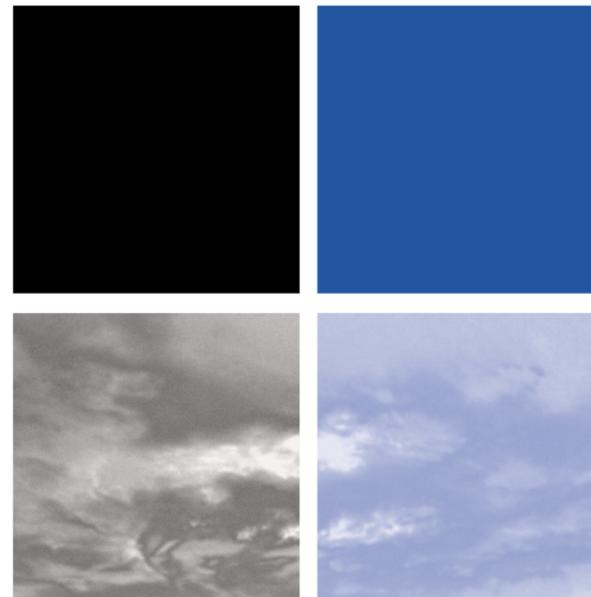
- A complete chain for the treatment of uncertainties associated with a gaussian model has been developed
- This chain contains all aspects of an uncertainty analysis from the quantification of uncertainties associated with input variables to the statistical postprocessing of predicted ground level concentrations (mean, percentiles, confidence intervals, threshold exceedance probabilities, etc.) and sensitivity analysis
- The whole chain is based on Python scripts and is computationally efficient (parallelization of computation).
- The chain has been validated using a practical case study and now constitutes an operational and fully automatized tool that may be easily coupled to other Gaussian dispersion models (the only modifications of the chain consist in modifying subroutines that deal with input and output files of the model used)

# Conclusions and future work

## *Perspectives*

- Extending our approach to other variables of interest (daily percentiles for example)
- Using this tool for more complex case studies (with topography and multiple sources, for example)
- Coupling this chain with more complex dispersion models like puff or lagrangian models. Doing this, we will assess the feasibility of using this chain to conduct impact studies for both accidental and chronic releases

NUMTECH



**NUMTECH**  
L'ATMOMODÉLISATION

[www.numtech.fr](http://www.numtech.fr)

6, Allée Alan Turing  
Parc Technologique de la  
Pardieu

63170 Aubière France

Tel. : (33) 4 73 28 75 95

Fax : (33) 4 73 28 75 99