Inverting time dependent concentration signals to estimate pollutant emissions in case of accidental or deliberate release

Nabil Ben Salem[1], Lionel Soulhac[1], Pietro Salizzoni[1] and Patrick Armand[2]

[1]Laboratoire de Mécanique des Fluides et d'Acoustique, Université de Lyon, CNRS, Ecole Centrale de Lyon, INSA Lyon, Université Claude Bernard Lyon I, Ecully, France

[2]CEA, DAM, DIF, F-91297 Arpajon, France

INTRODUCTION

Accidental releases of toxic substances due to industrial activities or terrorist actions present a major risk for the humans and the environment. The management of the subsequent crisis requires a rapid identification of the position and the strength of the pollutant release source. This can be achieved by using inverse dispersion models. A main limitation of this approach is that the concept of "ensemble average", on which atmospheric dispersion model rely, is no more pertinent as we deal with short accidental or deliberate releases, since these represents a single realisation of the dispersion phenomenon. This study aims in evaluating the statistical properties of the errors obtained in applying an inverse model to real turbulent concentration signals in order to discuss the reliability of this approach for operational purposes.

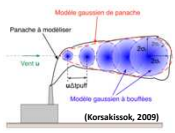
INVERSE MODELLING METHODOLOGY

The inverse modelling can identify the position and the emission rate of a pollutant source by means of :

1. A direct dispersion model of atmospheric pollution - 2. Observations provided by measuring device - 3. Optimization and inverse algorithms.

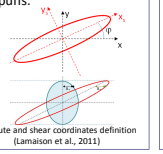
1. Direct Model : SIRANERISK

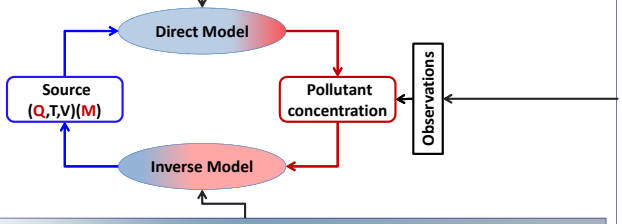
SIRANERISK is an urban dispersion model for operational purposes (Lamaison et al., 2011). It simulates the main effects controlling the dispersion of a substances in a turbulent boundary layer, adopting the same parameterisations implemented in the model **SIRANE** (Soulhac et al., 2011). The dispersion of pollutants is simulated by means of a Gaussian puff model that includes the effect of the mean velocity shear on the dispersion of the puffs.



$$C(x,y,z)=\frac{CTA(\vec{x})\;M}{(2\pi)^{3/2}\,\sigma_y\sigma_z\sigma_{x^*}}\exp\left(-\frac{1}{2}\left(\frac{x^{**2}+y^2}{\sigma_y^{\,2}}+\frac{z^2}{\sigma_z^{\,2}}\right)\right)$$

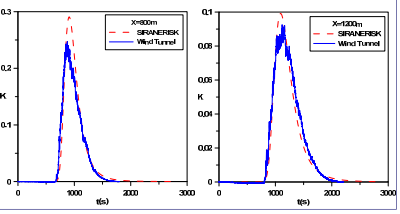
With $\begin{cases}\sigma_{x^*}=\sigma_x\sqrt{1-R_{xz}^{\,2}}\\ x^{**}=x^*\dfrac{\sigma_y}{\sigma_{x^*}}\end{cases}$ Where : $\begin{cases}x^*=x-zR_{xz}\dfrac{\sigma_x}{\sigma_z}\\ R_{xz}=\dfrac{\sigma_{xz}}{\sigma_x\sigma_z}\end{cases}$





Direct Model Validation

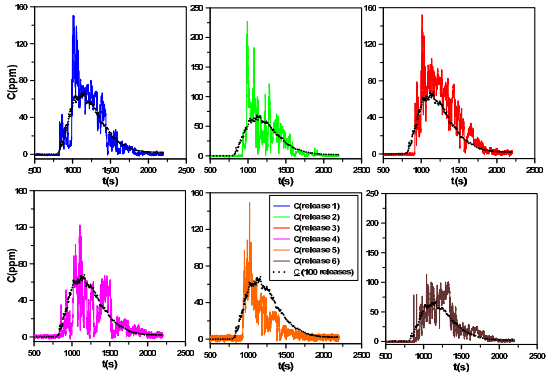
A comparison between model results (dashed line) and wind tunnel measurements (continuous line) shows a good agreement between the two sets of data, considered at two different distances (***X*** = 800m and ***X*** = 1200m) from the source.



2. Wind tunnel experiments

The experimental measurements used in this study are those presented by Cierco et al., (2009b) and carried within the wind tunnel of the Laboratoire de Mécanique des Fluides et d'Acoustique of the Ecole Centrale de Lyon (France).

In the experiments we produced unsteady releases of a passive scalar (ethane) in a turbulent boundary layer over a rough surface. Time dependent signals of passive scalar concentrations were measured downwind the source at fixed positions by means of a Flame Ionisation Detector. In the present study we used only the concentration profiles measured at a single receptor, located at a distance X=2m downwind the source. This corresponds to a real distance of 800m at the 1:400 scale.



Comparison between the concentration measurements for six different realizations and the average concentration (dashed line) over 100 realizations in receptor located at coordinates (***X*= 1200m**, ***Y*=0**, ***Z*= 24m**, ***X*** being the wind direction).

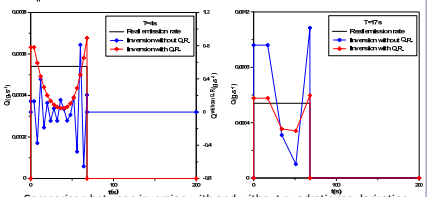
3. Inverse algorithm

The inverse model can lead to the identification of the position and the strength of a pollutant source Q, inverting a linear equation system : $C(m,n)=ATC(m,n)*Q(n,1)$. The inversion algorithm varies depending on the number of pollutant sources n and on the number of receptors m. We are here particularly concerned with the case ***m>n***. In case that ***Rank(ATC)=n*** and that the problem is over-determined, solution that can be determined by minimizing the quadratic cost function :

$$J=\frac{1}{2}\|\varepsilon\|^2+2\lambda\|DQ\|^2$$

Where : $\begin{cases}\varepsilon=C-ATC*Q\\ \lambda=\arg\min_{\lambda\in IR}\left\|\int_{t_0}^{t_f}q^{true}*\Delta t-\int_{t_0}^{t_f}q^{est.}*\Delta t\right\|\end{cases}$ with λ is a regularization parameter that is used to minimize the uncertainty due to the noise in the time dependent signal.

Role of quadratic regularisation:
An example of the results obtained inverting the ensemble averaged signal of concentration at a fixed receptor, with and without regularisation parameter and for two different time steps of the source emission rate.



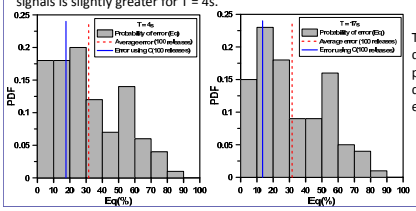
Comparison between inversion with and without quadratic regularization (Q.R.) algorithm for cases T=4s and T=17s

RESULTS

We evaluate the performance of the inverse model to estimate the mass of pollutant rejected by an impulsive emission using respectively the max relative error ***Er*** and the relative error of mass quantities ***Eq***.

$$E_q(\%)=\left(\left(\int_{t_0}^{t_f}q^{true}*\Delta t-\int_{t_0}^{t_f}q^{est.}*\Delta t\right)*100\right)/\int_{t_0}^{t_f}q^{true}*\Delta t$$

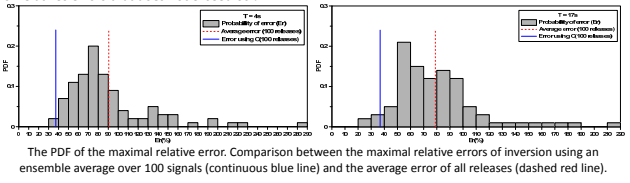
The relative error of mass quantities provides global information for the quality of inversion because it represents only the difference between the inverted and true mass quantities. ***Eq*** does not exceed 90% for any of the inverted signal. The average relative error of mass quantities is almost the same in two cases (T = 4s and T = 17s) but the average maximum relative errors found using the ensemble average over 100 signals is slightly greater for T = 4s.



The PDF of the relative error of mass quantities. The continuous blue line presents the relative error of mass quantities estimated using an ensemble average over 100 signals.

$$E_r(\%)=\max\left(\left(q_{true}^{t_i}-q_{est.}^{t_i}\right)*100\right)/q_{true}^{t_i}$$

The relative error ***Er*** represents the local and instantaneous gap between signals i.e. it resumes the difference between the forms of the inverted and true signals. ***Er*** can reach 286% in the case T = 4s and 213% in the case T = 17s. This shows that the choice of the time step is important if we want to determinate the time dependence of the emission rate. With T = 4s, the error ***Er*** usually is greater than 30% and we have more than 25% of errors that exceed 100%. In the cases T = 17s, we have more than 25% of relatives errors that does not exceed 60 %.



The PDF of the maximal relative error. Comparison between the maximal relative errors of inversion using an ensemble average over 100 signals (continuous blue line) and the average error of all releases (dashed red line).

Conclusions and perspectives

In this study we examined the reliability of an inverse model in reproducing the unsteady pollutant emissions from concentration signals recorded at fixed receptors. We have discussed the role of a quadratic regularization to reduce the effects of the noise in the signals and we tested our inverse code using synthetic concentrations provided by the direct model SIRANERISK. The inverse model is shown to reliably estimate the total amount of mass emitted at the source. However the model has to face major difficulties when we aim in identifying the time variability of the emission. In the future, a sensitivity analysis will be completed in order to identify for different receptors the optimal time step, providing the lowest error in the estimate of the pollutant emission rate at the source.

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