TOXIC RELEASE EVENT RECONSTRUCTION IN A RAIL STATION BY CFD SIMULATIONS AND BAYESIAN INFERENCE

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ABSTRACT

Major public surface rail station has in the past already been concerned and can be again the place of unexpected event like contaminant release during an attack. In such situation, emergency response efforts need to be optimized. The critical questions are: Where is the emission point? How much material was released?

Accurate estimation of the source term is essential to manage the emergency planning and mitigate consequences inside the rail station and in urban vicinity. One solution is to integrate the observed data at sensors with a predictive model to provide probabilistic estimates of the unknown source term parameters. In such semi-confined volumes with many openings and obstacles, flow streamlines and turbulence fields shows complex patterns in and between halls, ticketing rooms, platforms…etc. High-resolution CFD simulations with external meteorological/street scale flow forcing (and possibly internal ventilation forcing) are required for the prediction of the toxic cloud motion. The inverse problem is then solved by a sampling of predictive simulations guided by statistical comparisons with measured data. This approach uses Bayesian Inference with stochastic sampling based on Markov chain (MCMC). The results of the flow analysis may trigger the location of permanent or mobile detection systems. The event reconstruction when performed indicates the probability distribution functions of the source being at a particular location with a release rate.

This paper presents firstly briefly the numerical methodology selected for the source event reconstruction. Then, an application case on the railway station Gare de Lyon in Paris is detailed with a description of the complex flows and some toxic release modeling which have been used for the source term reconstruction testing.

INTRODUCTION

Toxic gas release in confined public area represents one the fearest event for the authorities. When such an accident occurs, the real time following of the concentration fields resulting from the release would be extremely valuable information as support for emergency actions and impact evaluation inside the area itself and its vicinity.

The main objective of this project is to develop an event reconstruction methodology to recover the source parameters. The study aims to determine the location and mass flow rate of the toxic release in a confined area.

The railway station Gare de Lyon in Paris has been selected as a pilot for the performance testing.

The aimed analysis is challenging in such a configuration because of the complex flows patterns inside the station and in the close surrounding. Then, the sensor network which is essential to the source retrieval provides toxic airborne concentration at few places and with specific time samplings. The measurements as the modelling include deviation with natural phenomena. Indded, unsteady meteorological conditions, train movements, opening/closed doors, which are not systematically known, add random events and turbulence to the momentum quantities and the boundary conditions.

The general principle of the methodology is to couple the concentration data recorded at the sensor network with appropriate algorithm for source term determination and 3D dispersion modelling. Regarding the main technical difficulties of the project, the modelling must take into account accurately the complex geometry of the railway station and the source event reconstruction must be performed fastly by using the available concentration recordings.

The proposed technique used to retrieve the source parameters is based the Bayesian inference principle coupled with MCMC stochastic sampling. Such objectives have already been studied in downtown or on opened industrial site but it needs to be adapted to the confined issue.

The project is divided in three phases: a first phase devoted to internal and external flow modeling, the second phase concerns the development of suitable algorithms and the last phase consists in the performance testing of the methodology for different kind of releases. This paper addresses the issue of the development of a source determination algorithm in phase 1 and 2 of the project.

GENERAL DESCRIPTION

In order to identify the location and compute the caracteristics of the source event, a probabilistic approach has been selected. Bayesian inference approach is particularly suited for application where scarce and noisy data are available. The source event reconstruction is firstly based on a windfield database and a concentration database built by unit mass flow rate from all potential sources in the confined area (experience, best place for the attack…). The advection-diffusion equation is supposed to be linear without density effect or chemical reaction.The forward simulation run for unit source strength from the locations of the prior distribution give concentration values at sensor locations which are stored in a database. The precalculated transfer functions between sources and sensors can de used in the inverse process.

A high toxic concentration detected at a sensor in the confined area (threshold detection) triggers the source retrieval which starts by an optimized research of the release parameters (location, mass flow rate and release duration) with a Monte Carlo Markov chain (Chow F.K., B. Kosovic and S.T. Chan, 2006). The release parameters (location, mass flow rate, starting time...) are determined and can be used in a forward dispersion modelling. The real time modelling of this dispersion based on real time weather data would provide valuable information for the emergency planning inside the station and in the nearby surrounding.
The internal/external steady flows are modeled by a CFD code and stored in a database. The 3D CFD (Computational Fluid Dynamic) model Fluidyn-PANEPR (Mazzoldi A., et al., 2008) has been chosen, to simulate the 3D external wind field pattern and the internal flows of the railway station. Taking into account the details of the installations (Hill R;, et al., 2007), this model solves the Navier-Stokes equations including mass, momentum and enthalpy conservation, state law and equations for advection-diffusion. A K-ε model is used for turbulence simulations. This model is used in Eulerian mode to compute wind field pattern and the species dispersion.

The advantage of this probabilistic approach is its robustness since it is based on a comparison between the concentration fields resulting from the most plausible accidental emission release locations and real time observations from a sensor network. In addition, CFD calculation enables a reliable simulation of wind flow and dispersion around complex geometries, taking into account turbulence effects thus giving the proper relationship between concentration fields at short range and source term value (Neuman S., 2006).

RECONSTRUCTION PROBLEM FORMULATION

Bayesian inference

A probablistic theory like Bayesian inference in the source event reconstruction enables to compute the likeliest parameters on the sensors data basis (Keats A., F.-S. Lien and E. Yee, 2006).The posterior probability is a conditional probability which is the link between the hypothesis and the concentration at sensors and the prior information.
The general formulation for conditionnal probability is

$$P(X|Y,Z) \tag{1}$$

- X : proposal
- Y : conditionnal information
- Z : context

By considering the vector m of parameters which includes the release caracteristics:

$$m = (loc, q_s, t_{on}, d)$$

Where loc is the release location, q is the mass flow rate, t_{on} is the turn on time and d is the release duration. The source reconstruction algorithm computes probability density function which after a statistical analysis provides the most probable values.
If the Bayesian theory is applied to the source event determination, the posterior probability for the m vector with the concentration C at sensors and the prior data E

$$P(m|C,E) = \frac{P(m|E)P(C|m,E)}{P(C|E)} \tag{2}$$

- $P(C|E)$ is a normalization constant. The posterior probability function is proportional to the product of the prior probability and $P(C|m,E)$:

$$P(m|C,E) \propto P(m|E)P(C|m,E) \tag{3}$$

- $P(C|m,E)$ is the probablity to get the C concentration measured at sensors for a selected m vector. This probability estimates the deviation between the C concentration recoreded at sensors and the C_{mod} modeled concentration provides by the atmospheric dispersion model for the m set of parameters. This deviation includes the measurements and numeric models errors. By hypothesis, the deviation between the measured concentration at i detector and the real concentration follows a normal law distribution. The same statement is done for the theorical concentration at I detector and the real concentration. The two noise components are supposed to get null average and σ_C and σ_{Cmod} variances.
  The probability that the measured concentration be foreseen by the dispersion model for the m vector can be computed by the following relation:

$$P(C|m,E) \propto Exp\left[-\frac{1}{2}\sum_i \frac{\left(C_i - C_{mod,i}(m)\right)^2}{\sigma_C{}^2 + \sigma_{Cmod}{}^2}\right] \tag{4}$$

- $P(m|E)$ is the prior probability for the m set of parameters. In this project, this probablity is set as a constant that means there is no most probable release in one source than in another.

$$P(m|E) = constant \tag{5}$$

Nevertheless, it is obvious that the m parameters are defined in a range between 0 and the maximal realistic value (for instance the maximal flow rate based on the process caracteristics in the hazard study). Then, it is supposed that the release can't occur in a building and the probability is set at 0 inside buildings.

- $P(m|C,E)$ is the posterior probability for the m vector based on the measured concentrations at sensors and the parameter space E. The relation for the probability density function (PDF) is:

$$P(m|C,E) \propto Exp\left[-\frac{1}{2}\sum_i \frac{\left(C_i - C_{mod,i}(m)\right)^2}{\sigma_C{}^2 + \sigma_{Cmod}{}^2}\right] \tag{6}$$

Sampling procedure by Markov Chain

The combinaison of the Bayesian inference technique and a sampling method as the MCMC (Monte Carlo Markov Chain) enables a reliable release parameters determination.

Indeed, the PDF is a huge space which must be sampled. A classical Monte Carlo sampling is not an appropriated methodology for a multidimensional function. If this sampling is done with a Markov chain which includes the PDF value, the method is highly efficient. There is no waste in time in exploring non useful parts of the parameters space which have low contribution in the PDF.

Various algorithms exist for MCMC samplings. In the present study for a set of m parameters (loc, q, t_{on}, d) the posterior probability is computed by the Metropolis algorithm. The Markov chains are initialized by taking samples from the prior distribution (building excluded, mass flow rate range...). The stored concentrations can be rescaled depending on the proposed source release rate for a particular source location. In this algorithm, the candidate state is sampled from a proposal distribution at each iteration and it is accepted if it improves the PDF value of the previous set. If the comparison is worse, the proposal is not automatically rejected. The sample is compared with a randomly chosen value to know whether it is accepted or not. If rejected, the next point is selected based on the last accepted value. Each new part of the Markov chain m_k depends on the previous part m_{k-1}. The MCMC process is repeated for a large number of iteration (20000 to 40000 iterations) and generates a point series as a chain. It is expected that the distribution of these proposals follows the target $P(m|C,E)$ distribution. Based on the MCMC results, a statistical analysis (histogram, mean value, standard deviation…) can be done for each parameter.

RAILWAY STATION CASE STUDY

In case of an attack in a complex railway station like Gare de Lyon in Paris with buildings in the vicinity and concentration measurements at few locations, retrieve the contaminant source location and strength is a challenging problem. The domain size is 4km*4km and was subdivided into 782 201cells with an unstructured mesh. The cells inside the station have been refined with a structured mesh.

For the present case, eleven sensors have been used to perform the source reconstruction. Only half of the platforms are taken by a train.

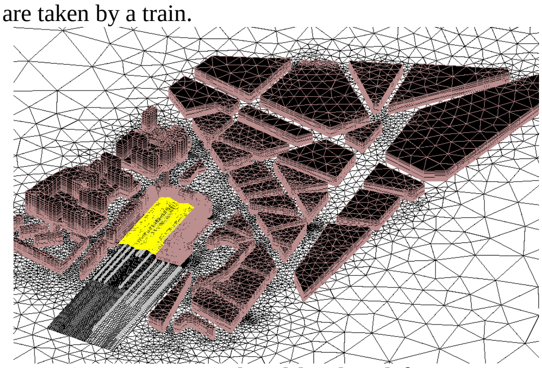


Figure 1: Numerical model and mesh for source reconstruction testing

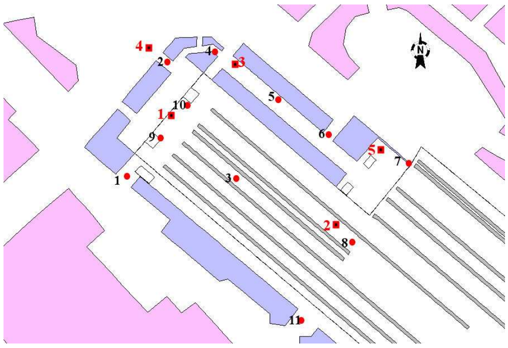


Figure 2: Sensor locations

In this study, 63 different release locations has been selected to build the concentration database.

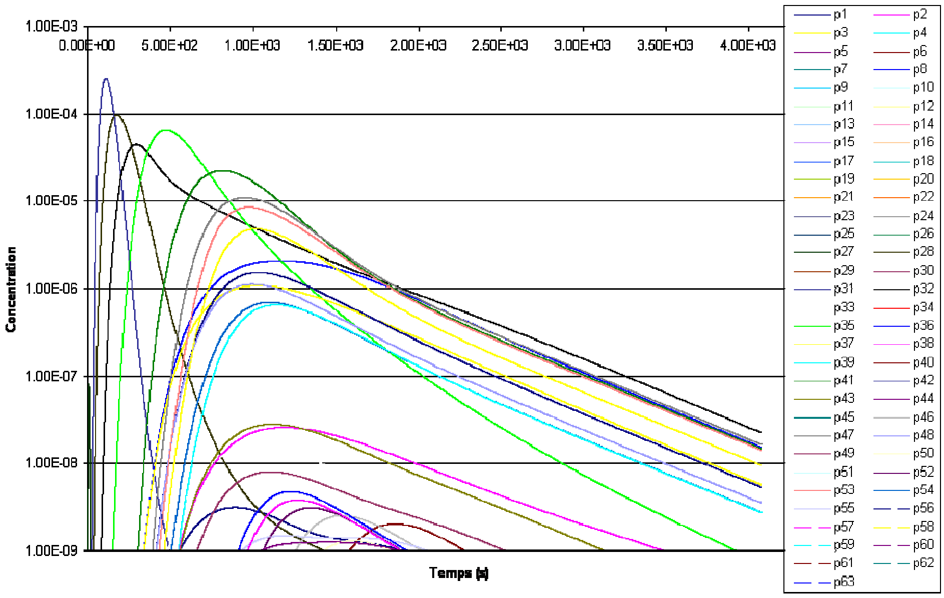
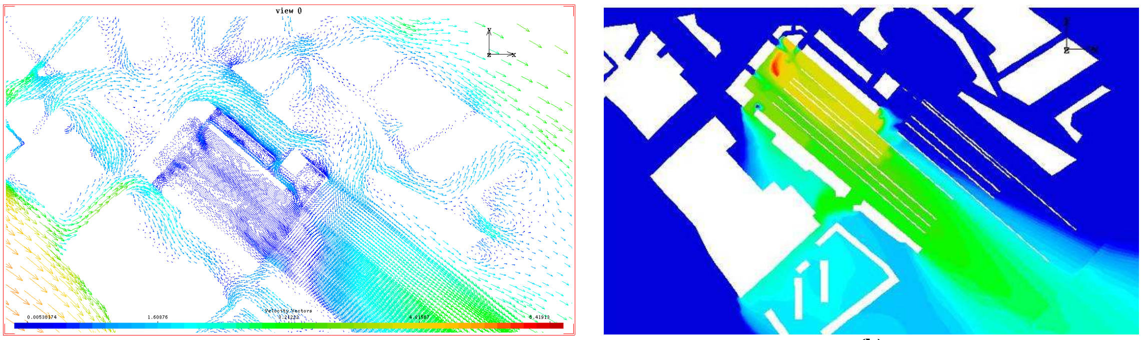


Figure 3 : Concentration plots for a unit puff from all potential sources at sensor n°1 (case 100°N – V_{10}=1m/s)

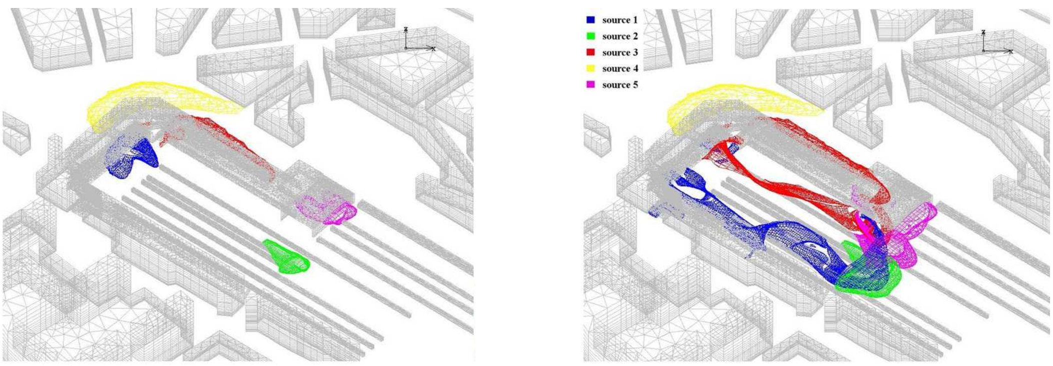
Before testing the methodology of the source reconstruction, four forced wind conditions have been modeled by Fluidyn-PANEPR to produce steady flows inside/outside the station ([100°N;1m/s and 4.5m/s]; [300°N;1m/s and 4.5m/s]).

Initially, different releases from 5 locations in the domain with 1 kg/s continous mass flow rate have been run for the 4 wind conditions.



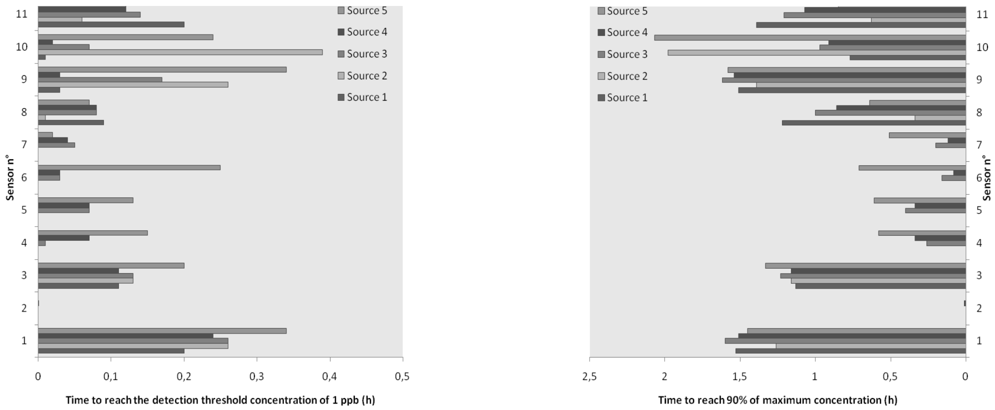
(a) **(b)**

Figure 4: (a) Internal and external flow pattern and (b) Horizontal concentration contours generated in and around the railway station by forward simulation for a synthetic case (source 1)



T=5 min T=16 min

Figure 5: 3D plumes in and around generated in and around the railway station by forward simulation for the 5 synthetic cases simultaneously at different times



(a) (b)

Figure 6: Time to reach (a) detection threshold concentration (1 ppb) – (b) 90% of maximum concentration at sensor (h) (case 300°N – V_{10}=4.5m/s)

The above results give valuable information on the time transfer of toxic compound from different source locations (1 kg/s continuous release). It shows that the detection threshold concentration is reached before 24 min but the longer time to reach 90% of the maximum concentration is more than 2 hours. Even for moderate meteorological conditions, the time transfer from the release point can be really long in some areas of the station and could give additional time for emergency planning in case of a quick release parameters determination.

CONCLUSIONS

A stochastic event reconstruction method for chemical or biological agent dispersion is presented. A probability model is suggested to take into account the concentration fluctuations and the zero concentration measurements that can be recorded from a sensor network due to threshold detection limit.

The proposed method is based on Bayesian inference with Markov Chain Monte-Carlo sampling.The complex flow fileds a 3D confined environnement need a specific approach with an high fidelity CFD code. In the event reconstruction, the dispersion models are typically executed for many times within the MCMC algorithm in order to samplpe the posterior distribution. A forward CFD model used is not adapted to an emergency response because of the important time computation which constiture a real burden. That is why, a concentration database which store the unit transfer functions between potential sources and sensors network is build in order to get significant improvement in computational cost and a possible fast response operational action.

Early detection of the biological or chemical agents with quick and accurate reconstruction of the dispersion events is critical in organizing an emergency response. Once the release event is characterized according the observations at sensors, forward projections can be performed to analyze the extent of exposure to the contamination.

The developed MCMC algorithm framework will be now tested on the synthetic cases modeled by a CFD code in the railway station. The expected performances would provide elements for pratical applications in environment and for a emergency numerical platform development.

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