
CFD application for impact & risk assessment in
the Industrial Areas-Case Studies
Fluidyn-PANEPR for local scale short-term

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Air Quality Assessment in Industrial Areas

- Impact and risk related to dispersion of contaminants
- CFD for Assessment
 - Objectives
 - Quantities
 - Physical Processes
 - Methods
- Case Studies

This lecture focuses on the use of 3D, transient CFD based methods in air quality assessment.

Air Quality

Air quality means the state of the air in terms of its composition. It is a measure of the pollutants in the air.

Examples:

- Carbon dioxide and hydrocarbons emitted from the automobiles
- Hydrogen sulphide spread from the water treatment plants
- Toxic gases released from the chemical, nuclear and petrochemical industries
- Dust particles dispersed from cement industries and open cast mines
- Plumes of water droplets and aerosols from the thermal and nuclear power plant chimneys



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Air Quality Assessment

The air quality is indicated by various quantities. These are either in terms of the direct measures of quantities or in terms of their impact.

Some of these are:

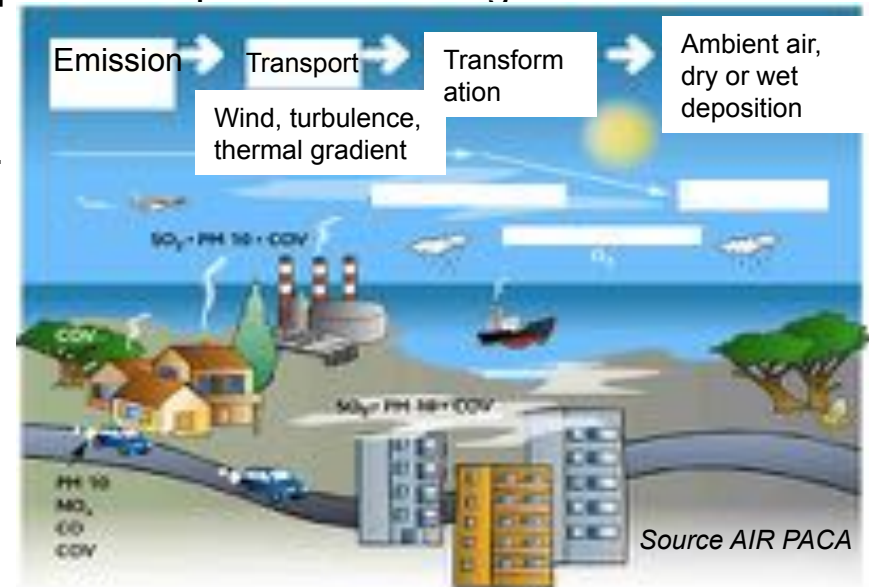
- Mass or volume fraction of pollutant species
- Concentration of the dust, droplets and aerosols in mg/m^3 or ppm
- Cumulative dose for a period
- Visibility

Physical Processes

Selection of the proper method for air quality assessment, either measuring sensors or computational models, for a specific scenario requires identification of the relevant physical processes involved in the dispersion of pollutants through the ambient air.

In general, the processes involve:

1. Emission of pollutants at the sources.
2. Transport of these pollutants
 - a. Bulk convection,
 - b. Molecular diffusion,
 - c. Turbulent dispersion,
 - d. Deposition due to gravity, and
 - e. Settling on the surfaces due to other forces and factors, such as adhesion, recombination reactions and electrostatic precipitation.
3. Transformation of the pollutants while moving through the air. Some examples are the evaporation of water droplets, intensification of fog due to condensation, coalescence of aerosols, and decay of the radio-active species.

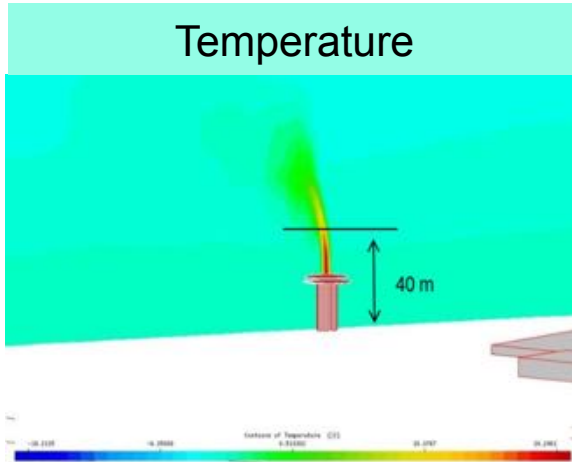


Physical Processes

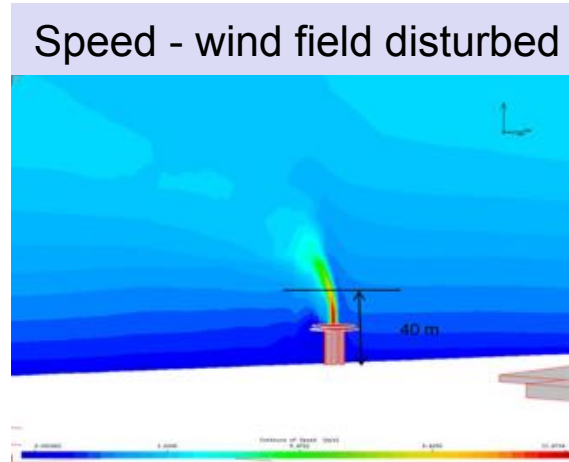
Atmospheric wind field may be affected by

1. Natural convection induced by the emissions which are at a different temperature than the ambient
2. Penetration of high momentum emission sources
3. Condensation and/or evaporation of steam and/or water droplets in the emissions

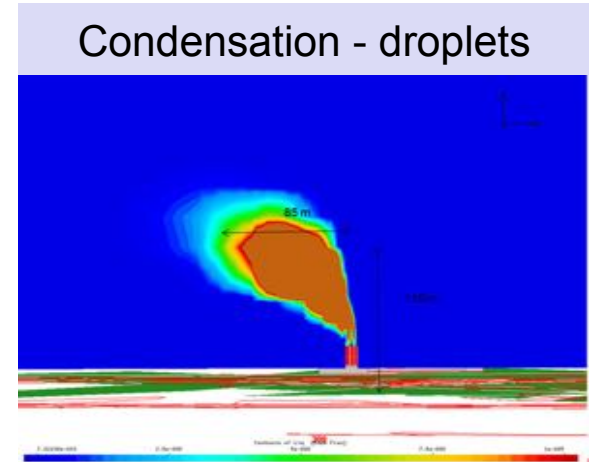
Temperature



Speed - wind field disturbed



Condensation - droplets



Air Quality Assessment - Methods

Air quality assessment methods include:

1. Measurements,
2. Estimations using Gaussian plume model,
3. Integral model for heavy gas jets, and
4. Solution of three dimensional Navier-Stokes equations and pollutant transport equations

In addition to their separate uses, the measurements and predictive methods can be combined to quickly identify the sources of pollutants after their presence is sensed.

Remaining part gives some details of the air quality assessment using 3D transient computational fluid dynamics (CFD) methods.



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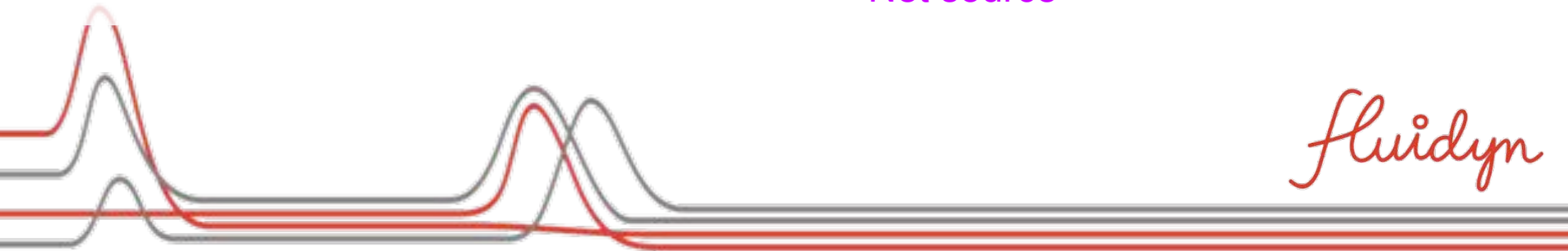
Mathematical Model

The mathematical model is formed using the governing equations formulated based on the assumption of conservation of

1. Mass
2. Momentum
3. Energy, and
4. Pollutant species.

These conservation equations have the following generic form:

$$\begin{aligned} \text{Rate of change of a quantity} &= \text{Net flow rate due to convection} \\ &+ \text{Net flow due to diffusion} \\ &+ \text{Net source} \end{aligned}$$



Primary Results or Solution Variables

 \vec{V}

air velocity from the momentum equations

 ρ

density of air from the mass conservation or equation of state

 p

pressure from equation of state or mass conservation

Equation of state

$$p = RT \sum_n \frac{\rho_n}{W_n}$$

 T

air temperature from conservation of energy

 Y

Pollutant species mass fractions from conservation of species

If pollutant mass fraction is high, it may affect the flow field. Then the equation of state for air should take into account the pollutant composition.

If pollutant mass fraction is very small, then it can be ignored in equation of state.

Temporal and spatial variations are obtained by solving these equations simultaneously.

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Mathematical Model

Rate of change of a quantity = Net flow rate due to convection + Net flow due to diffusion + Net source

Mass conservation:

$$\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho \mathbf{V} \phi) = S_m$$

Momentum conservation:

$$\frac{\partial (\rho \mathbf{V} \phi)}{\partial t} + \nabla \cdot (\rho \mathbf{V} \mathbf{V} \phi) = \nabla \cdot \phi \mathbf{\tau} - \phi \nabla p + \mathbf{f}$$

Energy conservation:

$$C_p \left[\frac{\partial (\rho T \phi)}{\partial t} + \nabla \cdot (\rho \mathbf{V} T \phi) \right] = -\nabla \cdot \phi \mathbf{q} - \left[\frac{\partial (\ln \rho)}{\partial (\ln T)} \right]_p \left[\frac{\partial \rho \phi}{\partial t} + \mathbf{V} \cdot \phi \nabla p \right] + S_T$$

Species conservation:

$$\frac{\partial (\rho Y_j \phi)}{\partial t} + \nabla \cdot (\rho \mathbf{V} Y_j \phi) = -\nabla \cdot \phi \mathbf{J}_j + S_{Y,j}$$



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Diffusion Fluxes

 τ

Momentum diffusion flux; function of viscosity and velocity gradients

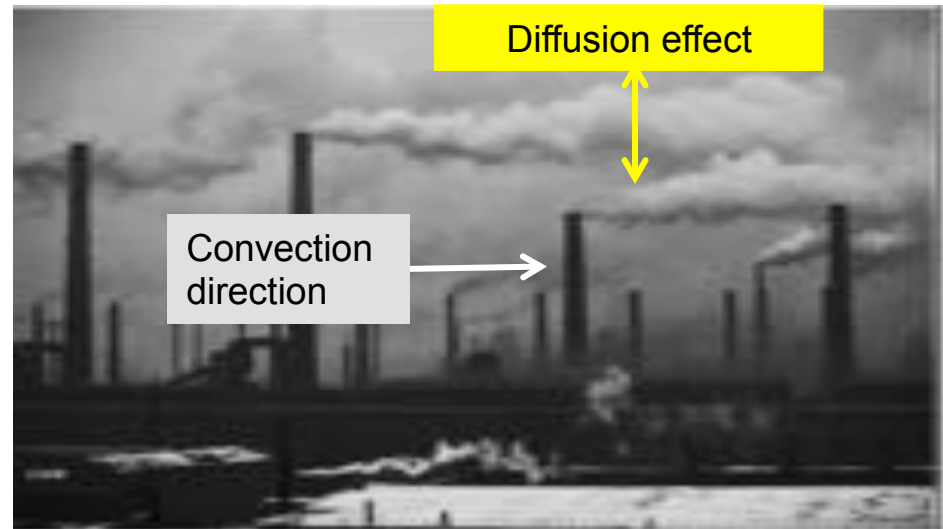
 q

Heat flux by conduction; function of thermal conductivity and temperature gradients

 J

Pollutant species flux due to molecular diffusion; function of mass diffusivity and concentration gradients

The viscosity, thermal conductivity and mass diffusivity are modified using turbulent exchange coefficients to take into account the turbulent dispersion.



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Turbulence Model

- The effect of turbulence can be characterised by the turbulent kinetic energy, k and its dissipation rate ε .
- One commonly used model to compute k and ε is the two-equation k - ε model.

Equation for the turbulent kinetic energy, k :

$$\frac{\partial(\rho k)}{\partial t} + \nabla_{\mathbf{g}}(\rho \mathbf{V} k) - \operatorname{div}\left(\frac{\mu}{P_{rk}} \nabla(k)\right) = -\frac{2}{3} \rho k \nabla_{\mathbf{g}}(\mathbf{V}) - \rho \varepsilon + \text{sources}$$

Equation for the dissipation rate, ε , of the turbulent kinetic energy:

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \nabla_{\mathbf{g}}(\rho \mathbf{V} \varepsilon) - \nabla_{\mathbf{g}}\left(\frac{\mu}{P_{r\varepsilon}} \nabla(\varepsilon)\right) = -\left(\frac{2}{3} c_{\varepsilon_1} - c_{\varepsilon_2}\right) \rho \varepsilon \nabla_{\mathbf{g}}(\mathbf{V}) + \frac{\varepsilon}{k} \left(c_{\varepsilon_1} \mathbf{\sigma} : \nabla(\mathbf{V}) - c_{\varepsilon_2} \rho \varepsilon\right)$$

Effective viscosity:

$$\mu = \mu_{air} + \frac{c_{\mu} k^2}{\varepsilon}$$



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Models for Obstacles

Obstacles to air flow:

- Buildings
- Walls
- Industrial installations such as chimneys, pipe lines etc.
- Flyovers
- Forest cover
- Trees

Ground roughness → Objects very small relative to the domain

Volume porosity (ϕ) → Larger objects

Models for frictional losses (added pressure drop) for different types of surfaces:

- Air flow over water bodies experience less friction
- Air flow through forest cover or urban areas experience larger friction.

Source terms for momentum, turbulent kinetic energy and dissipation rate using coefficient of drag, C_d

$$S_V^v = -C_d A_v |\mathbf{V}| \mathbf{V}$$

$$S_k^v = C_d A_v |\mathbf{V}| \left(C_{pkw} |\mathbf{V}|^2 - C_{dkw} k \right)$$

$$S_\varepsilon^v = C_d A_v |\mathbf{V}| \left(\frac{\varepsilon}{k} C_{p\varepsilon w} |\mathbf{V}|^2 - C_{d\varepsilon w} |\mathbf{V}| \varepsilon \right)$$

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Particle Models

Eulerian Model:

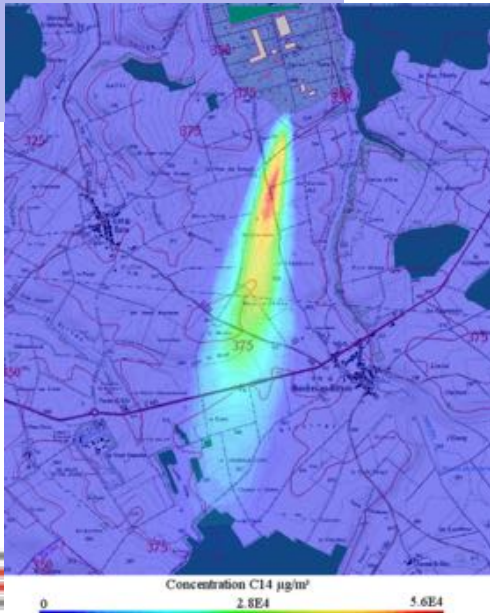
- Solves a scalar transport equation for particle concentration.
- Suitable for
 - large volume fractions with somewhat clear interfaces
 - lighter particles (negligible gravity settling)

Lagrangian Model:

- Tracks individual particles or parcels of particles.
- Suitable for
 - relatively lower volume fractions
 - heavier particles (significant gravity settling)

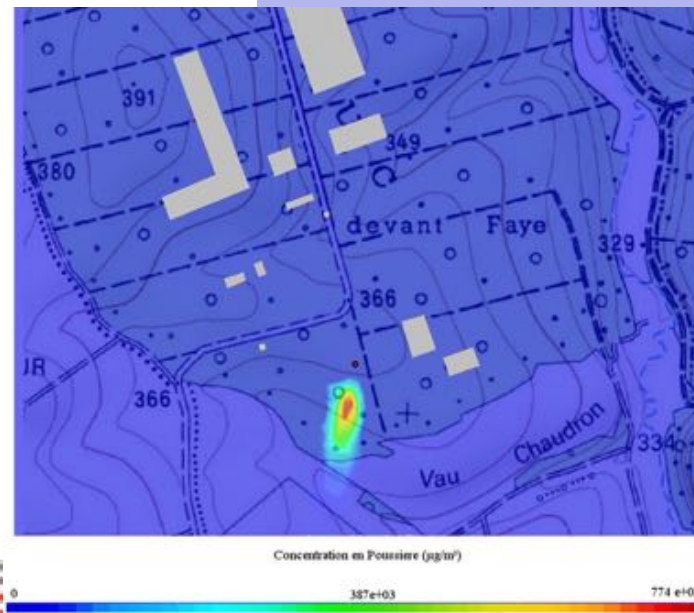
Eulerian → Plume length > 1 km

No settling
due to gravity



Lagrangian → Plume length < 200 m

Settling due to
gravity
considered



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Source Terms

S_m Total mass source:
Emission, phase change

f Momentum source
Emission, buoyancy

S_T Energy source
Emission, phase change, solar radiation

S_Y Pollutant source
Emission, phase change, chemical reaction

In many cases, the turbulence in the emission will also have to be included.

These source terms can be used to model the sources of pollutants from industrial sites, such as chimneys and exhaust pipes.



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Atmospheric Boundary Layer

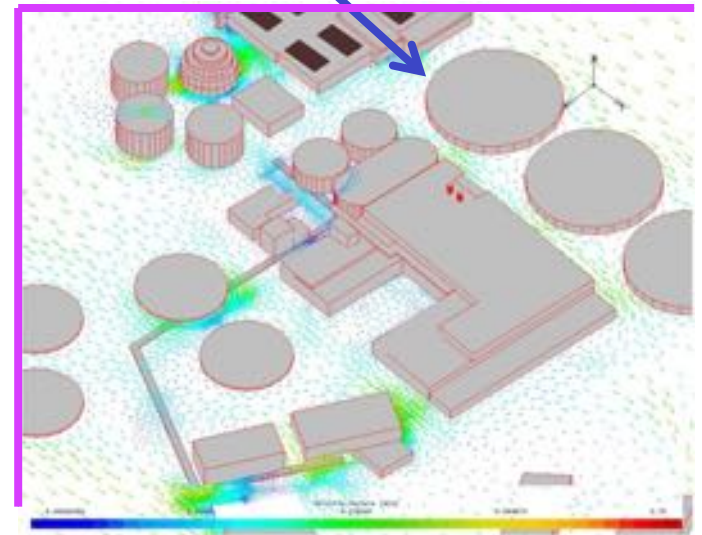
The ABL model serves as the interface between the meteorological observations and the boundary conditions required by the numerical solver for the mathematical model.

- Monin-Obukhov Similarity Theory (MOST)
- Describes the surface boundary layer
- Fundamental physical characteristics:
 - Ground sensible heat flux, Q^h
 - Ground roughness coefficient, z_0
 - Monin-Obukhov length, L
 - Friction velocity, u^*
 - Temperature scale, θ^*

Velocity, temperature and turbulence variations with height at the inflow boundary are calculated using MOST for the appropriate stability class

Inflow Boundary

Wind direction

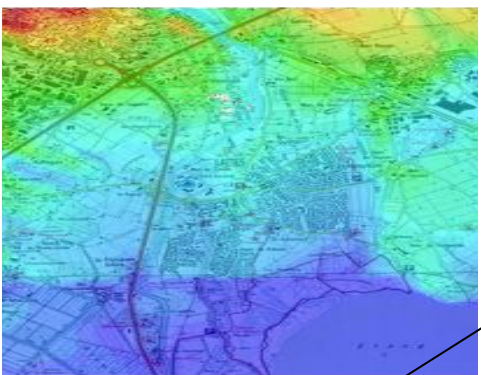


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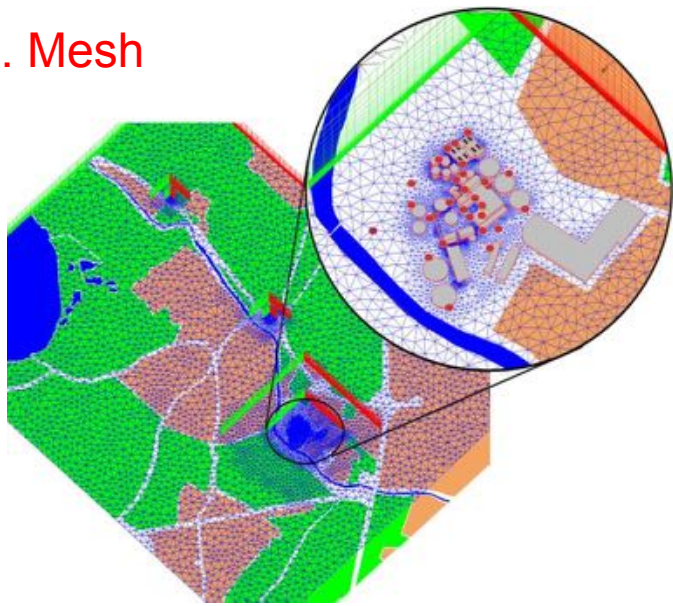
3D CFD impact & risk Assessment: Steps

1. Site Data

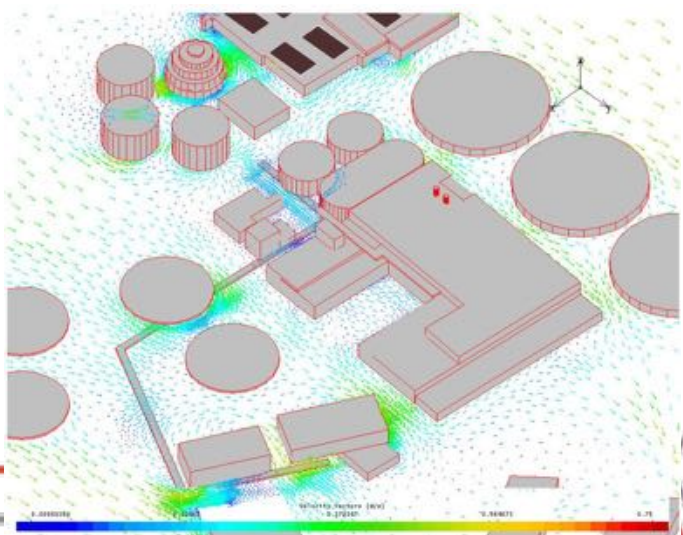
Terrain Map + altitude contours + geographical features + human constructions + weather data + source



2. Mesh



3. Wind field



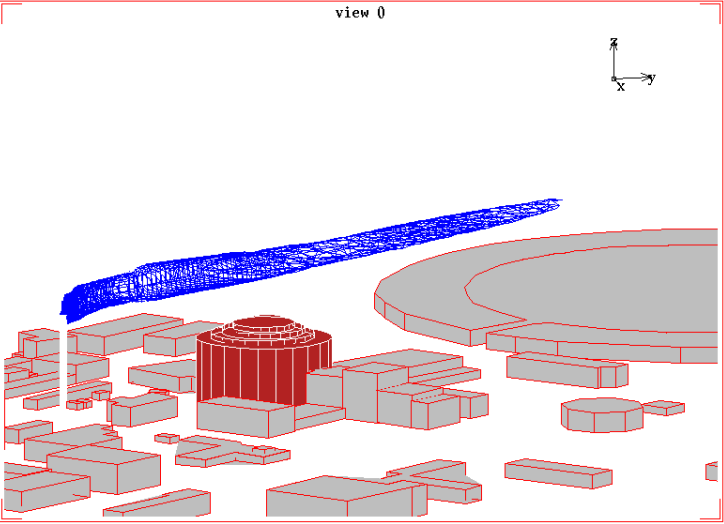
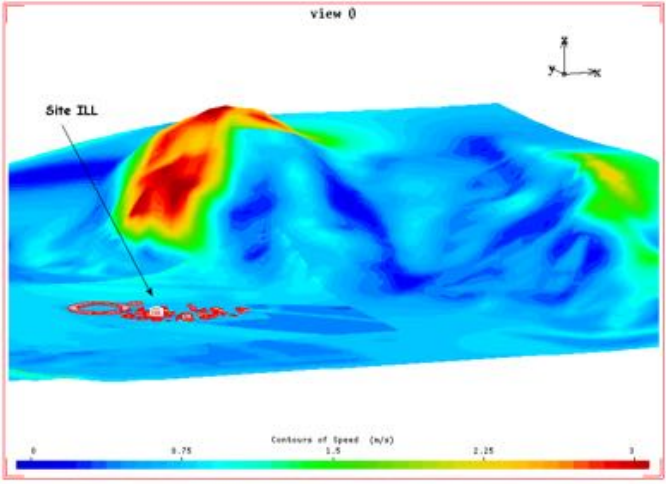
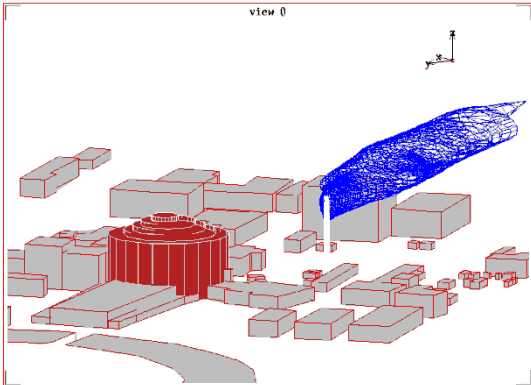
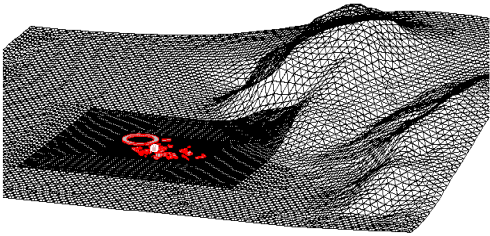
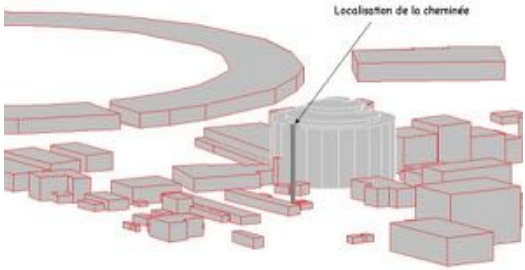
4. Pollutant plume



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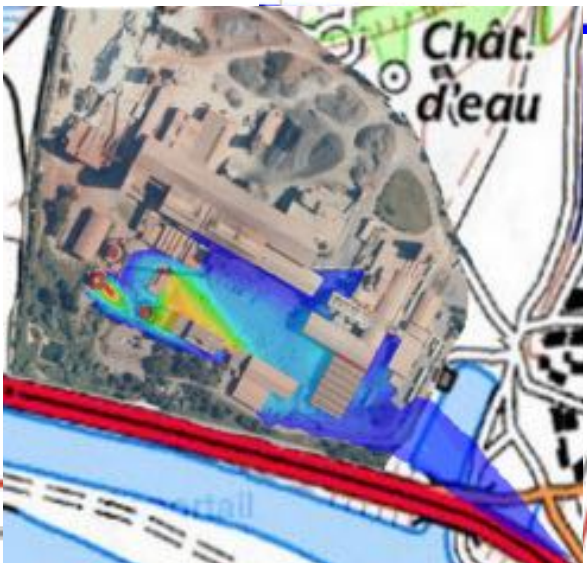
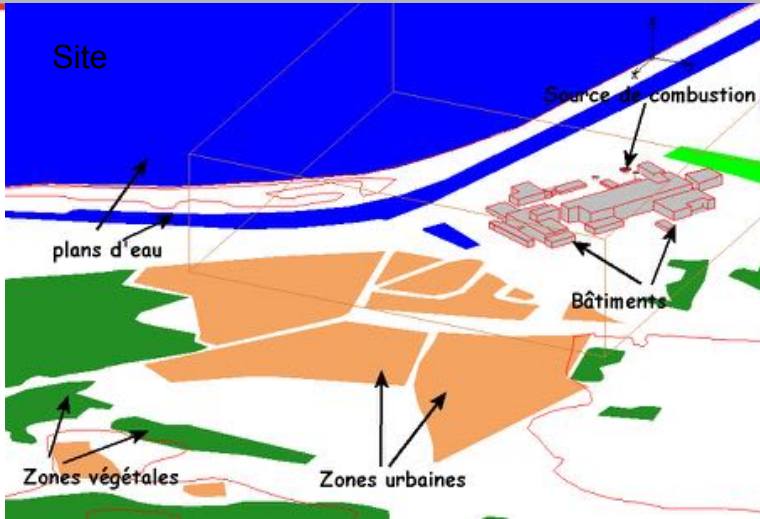
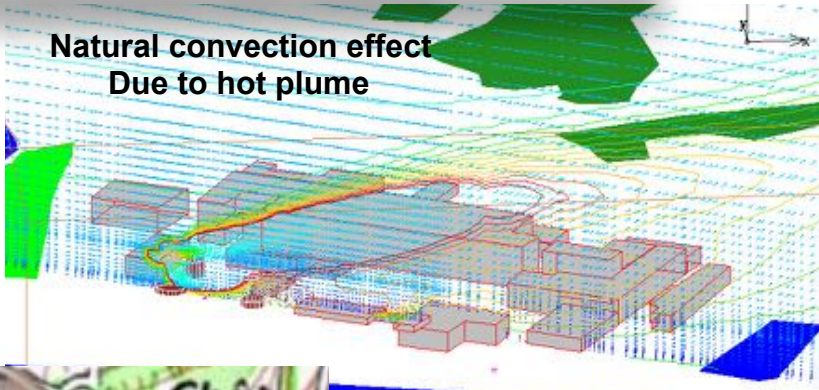
Dispersion from an exhaust stack

- ILL Nuclear site in Grenoble
- Exhaust in case of accidental release of H2
- Influence of nearby reactor building

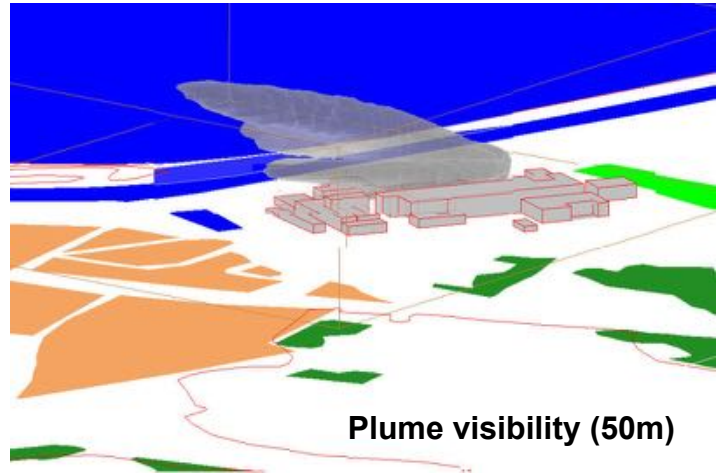


DISPERSION OF HOT GASES FOLLOWING A FIRE

- Software : fluidyn-PANEPR
- Tank fire on a petrochemical site
- Natural convection and visibility



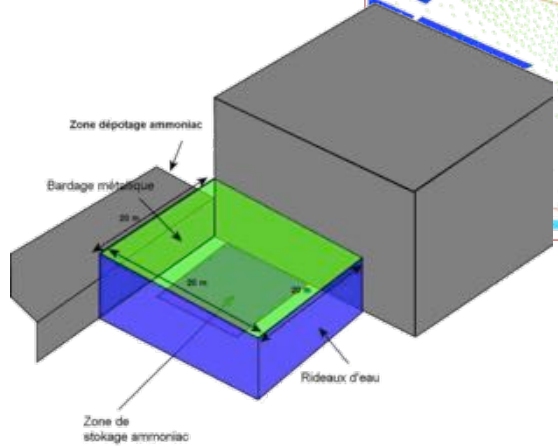
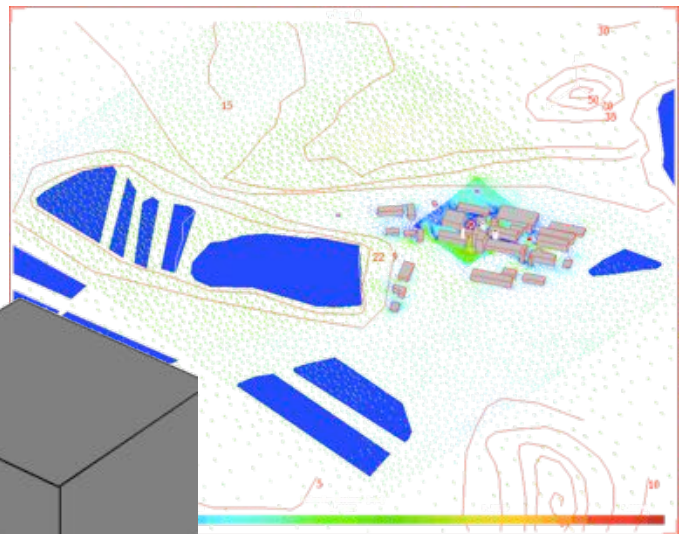
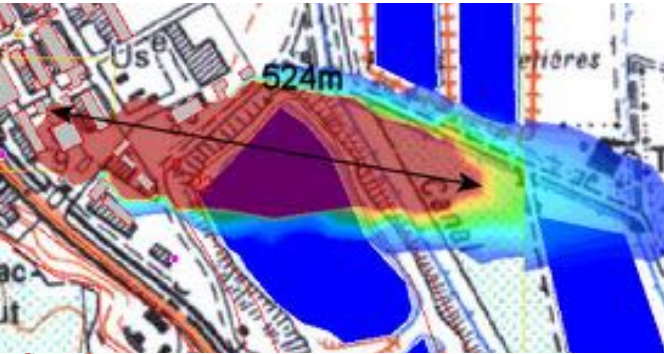
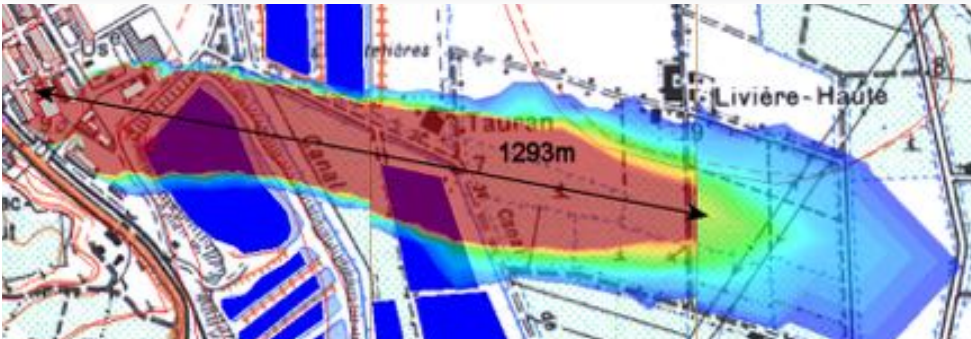
Toxic gas concentration at ground level



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EVALUATION OF THE PROTECTION MEASURES

- Accidental dispersion of HF and NH₃
- Nuclear power plant (AREVA)
- Confinement and water curtain assessment



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Case Study 3: Real Time Monitoring and Warning

- Aim:
 - Sense pollutant presence
 - Locate and quantify the pollutant source
 - Predict short term dispersion
- Uses weather and wind field predictions and real time data from monitor points.
- Calculate source strength, location, time and duration.
- Short term prediction is done using **faster than real time CFD** simulations.
- This information helps to estimate the extent of dispersion of harmful pollutants and helps in executing the mitigation measures.



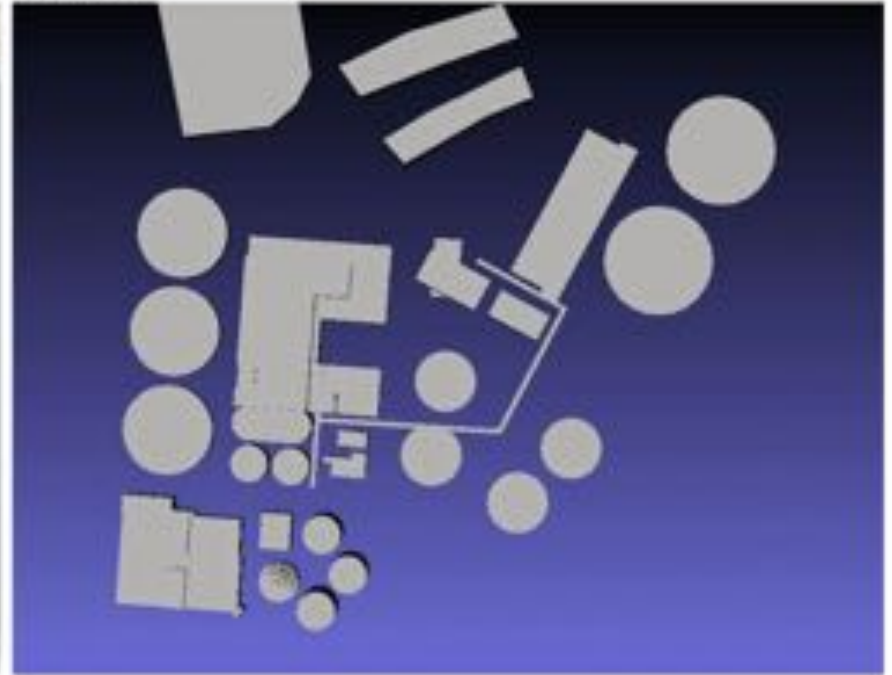
Functioning of the Platform

The objective is to **monitor**, on a industrial site, **the release from accidental or chronic sources** by using a **monitoring network** and an **inversion of CFD modeling** coupled to **measured weather conditions**.

Industrial Site

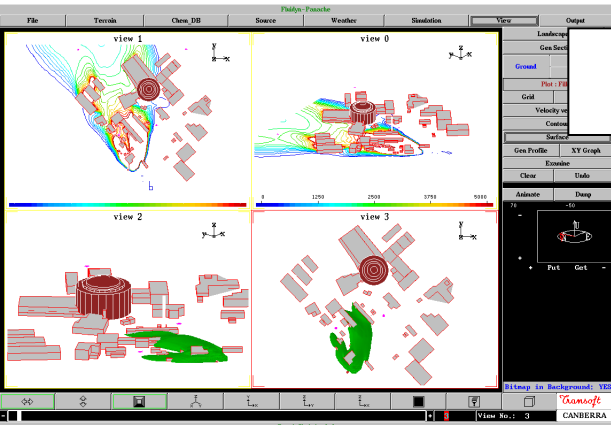
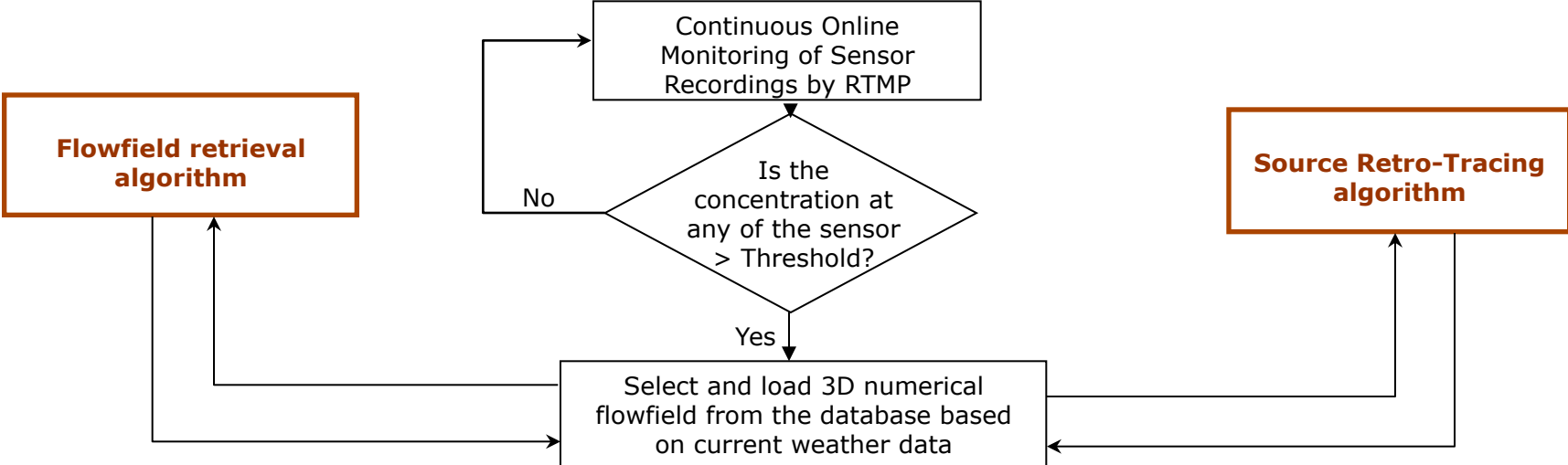


Model



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Predictive Real Time Modeling Platform [RTMP]



Algorithm

- Study the site or system to be installed with the warning module.
- Build models for the behavior of the system.
- Formulate the source vector. E.g., $\mathbf{m} = [\text{location, strength, start time, duration}]$
- Identify the potential sources \mathbf{m} .
- Compute the $P(\mathbf{m})$, the 'prior' probability distribution for \mathbf{m} .
- Sensor mapping; decide the optimum locations of the sensors.
- Build the Bayesian inference model

$$P(\mathbf{m}|C) = P(\mathbf{m}) \times P(C|\mathbf{m}) / P(C)$$

- Validate the module by conducting theoretical tests.
- Install sensors.
- Validate the module by conducting experimental campaigns.

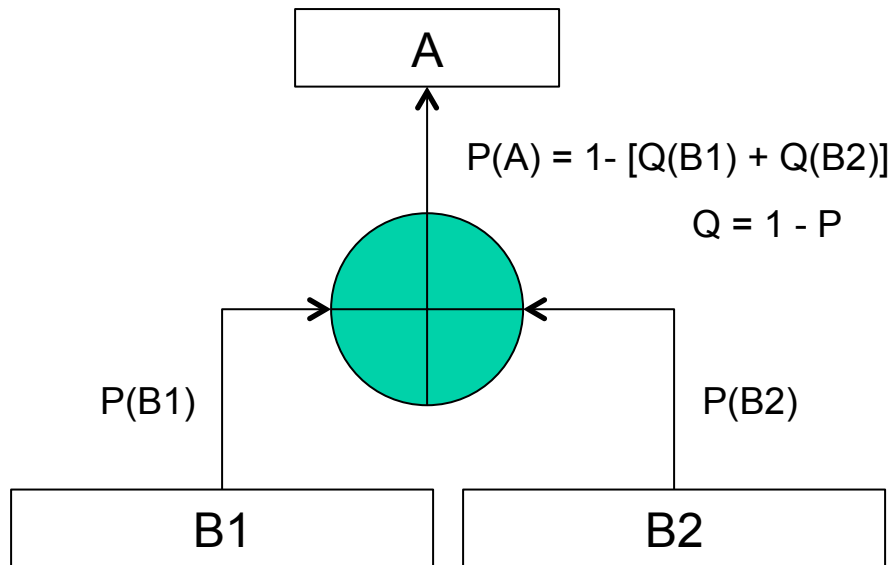
Bayesian Inference

The probabilities and the forward conditional probabilities $P(A|B1)$ and $P(A|B2)$ are given.

If A occurs, what is the probability that it occurred due to B1?

Bayes' * Theorem:

$$P(B1|A) = \frac{P(A|B1) \times P(B1)}{P(A)}$$



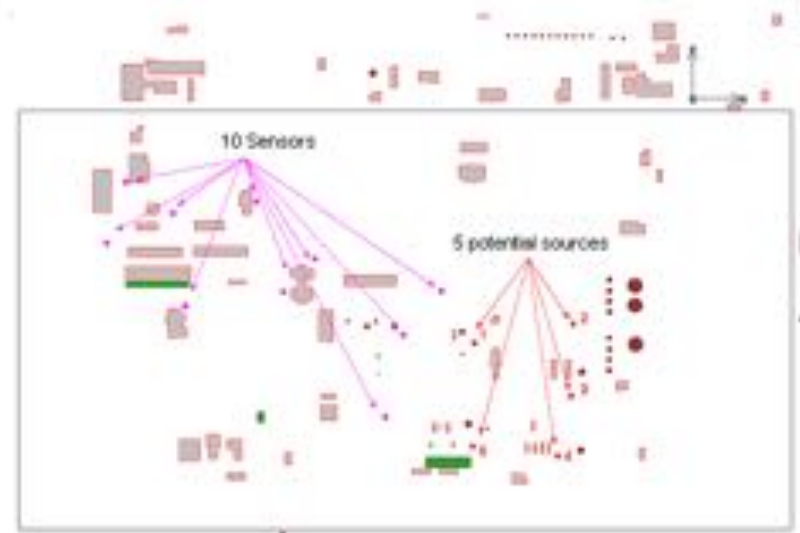
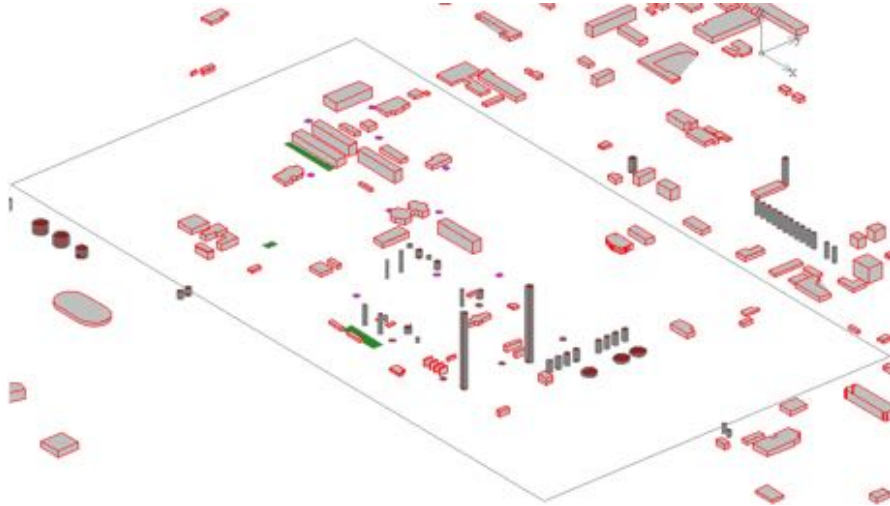
“In the Bayesian framework, how much we believe something after we see the evidence depends not just on what the evidence shows, but on how much we believed it to begin with.”, Jordan Ellenberg, *How Not to be Wrong – The Hidden Maths of Everyday Life*, Penguin Books, p. 179, 2014.

*The Reverend Thomas Bayes (1702-1761)

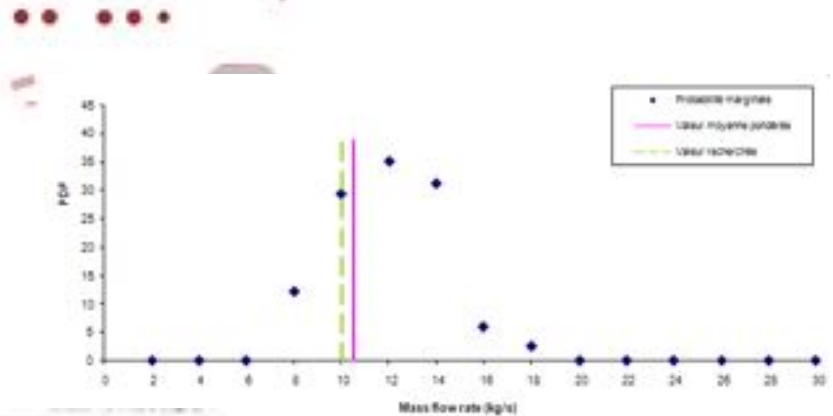
An introduction to Bayes' theorem with simple examples:
(<https://onlinecourses.science.psu.edu/stat414>)

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A Test Case



Number of potential sources = 5
Actual release: 10 kg/s from source 4.

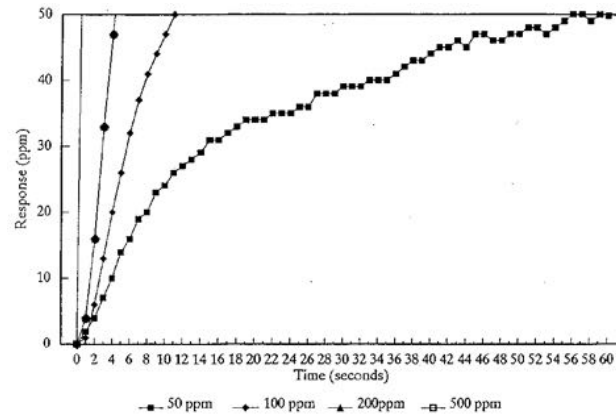
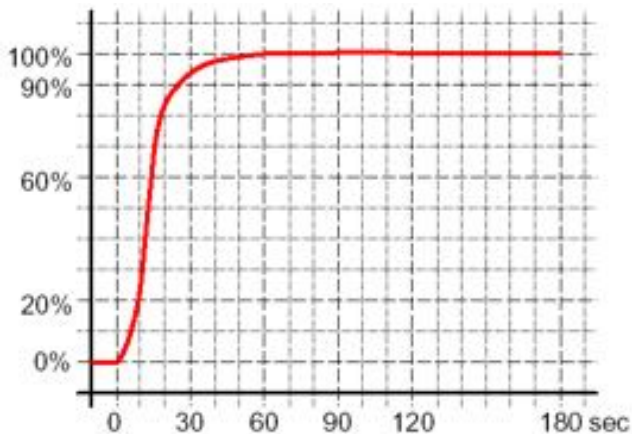


	Mass Flow (Kg/s)	Starting time (s)
Average MCMC samples	11.9	120
Average Weighted value	10.5	121
Target	10	130

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Sensor Characteristics

In the case of toxic sensors, there is no standard. There are many kinds of sensors: electrochemical or semiconductor. In terms of security, a quick detection enables a quick and efficient action. Sensors have a response time before recording the real concentration. This response time should be taken into account in the source identification algorithm.



Response curve of H₂S sensors H₂S ((a): electrochemical sensor, (b): semiconductor sensor (Source : DRÄGER Safety)

More details in ...

SOURCE DETERMINATION IN CONGESTED ENVIRONMENT THROUGH BAYESIAN INFERENCE

Jean-Marie Libre⁽¹⁾, Malo Le Guellec⁽²⁾, Amita Tripathi⁽²⁾, Thibault Maillard⁽²⁾, Stéphanie Guérin⁽¹⁾, Claude Souvrayev⁽²⁾, Aldo Castellari⁽²⁾.

(1) TOTAL E&P, La Défense, FRANCE

(2) Fluidyn-Transoft, Saint-Denis, FRANCE

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ABSTRACT

The quick identification of contaminant plume sources can greatly enhance emergency response efforts. The critical questions are: Where is the leak? What is the release mass flow? How long is the release duration? Accurate estimation of the source term is essential to predict plume dispersion, manage the emergency planning and mitigate consequences in the surrounding area.

Based on limited information provided by a finite and noisy set of transient concentration measurements obtained from real-time gas sensors, the source identification is also complicated by the presence of building obstacles.

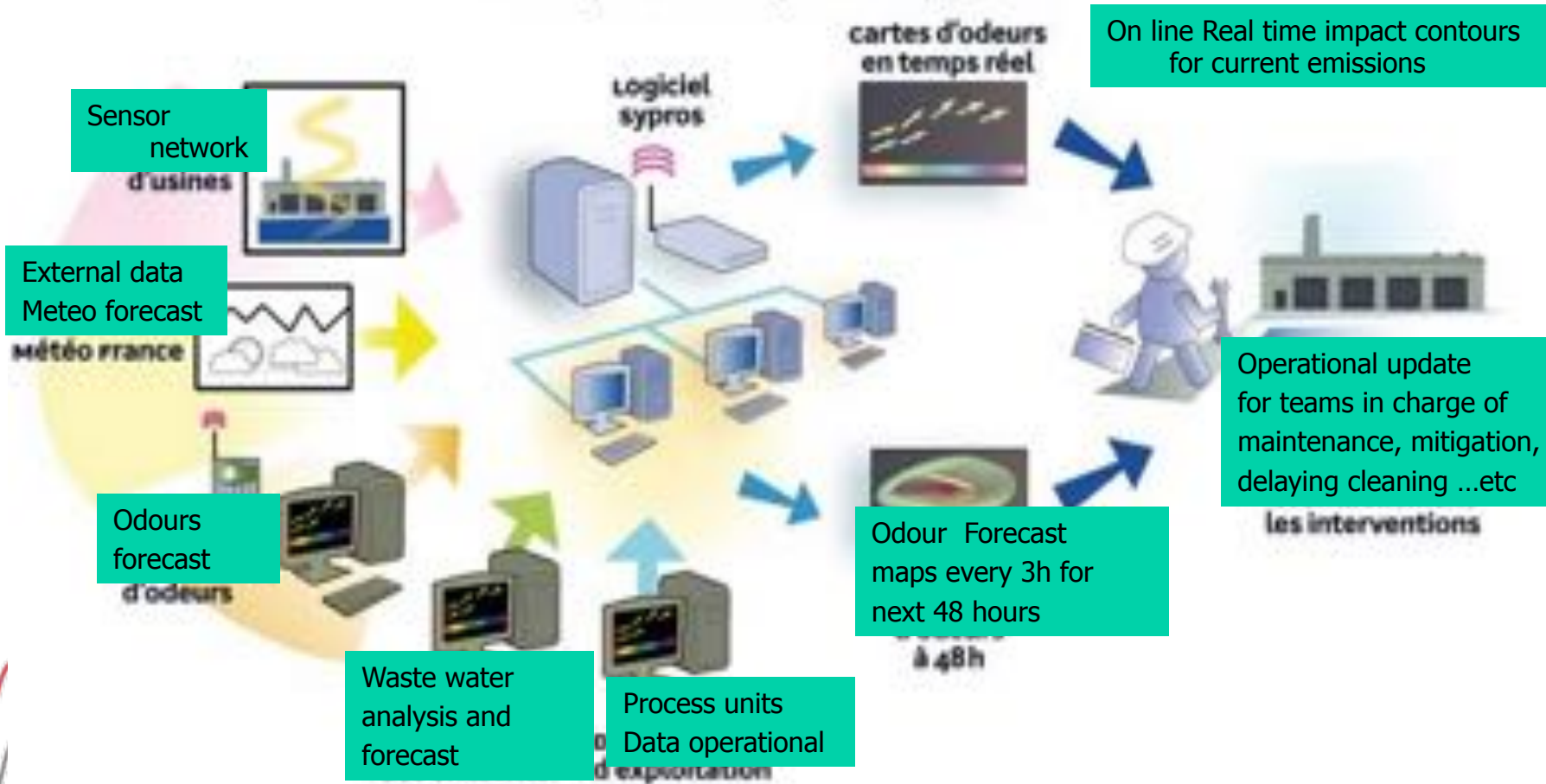
While high-resolution CFD simulations are available for predicting plume evolution in complex geometries, a Bayesian probabilistic inferential method can provide the probability density function of the source parameters (location, mass flow, release duration, etc).



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An Operational Example

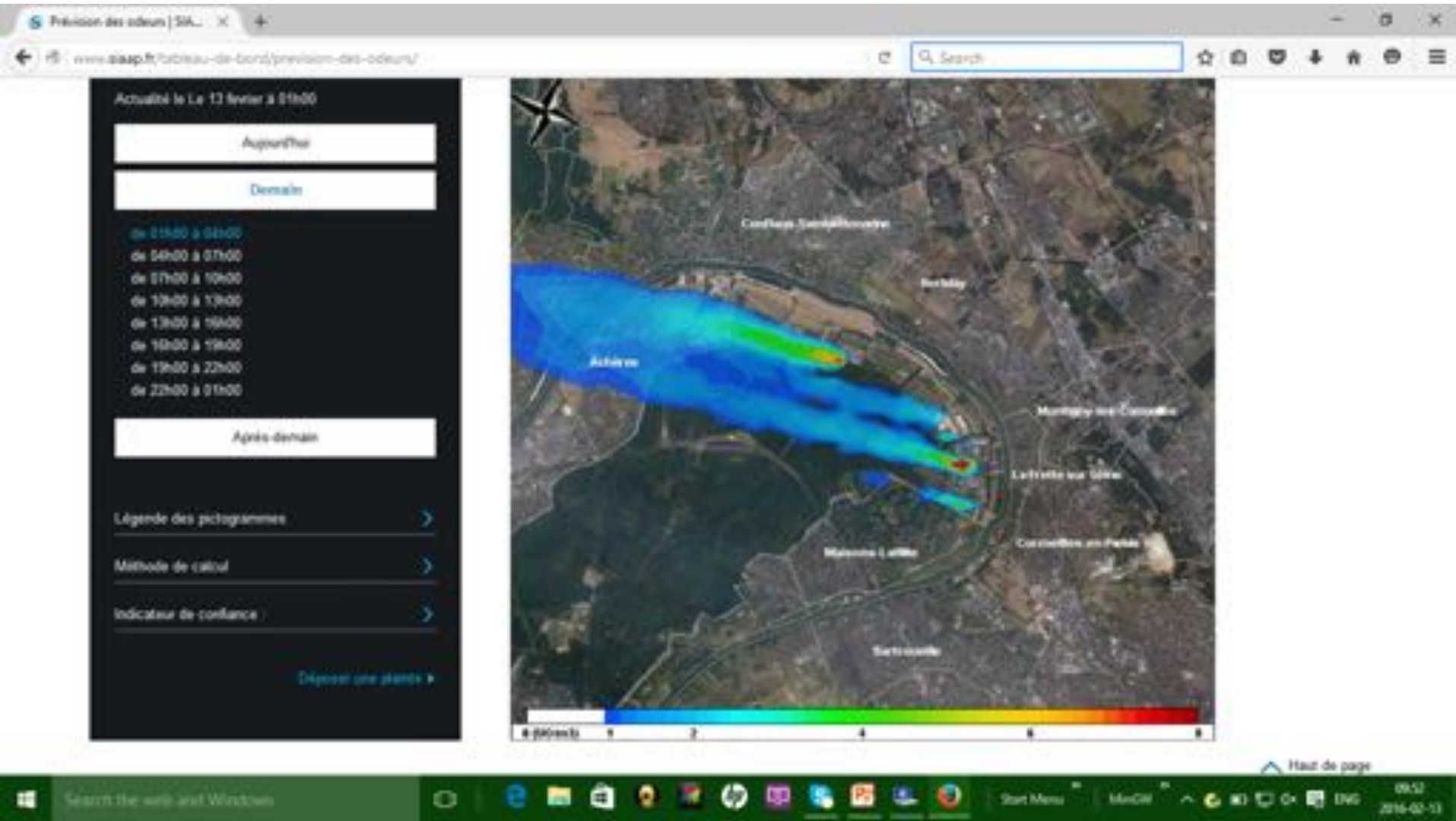
Water Treatment Plant Odour Source Localisation



Working Example: Pollutant Prediction

<http://www.siaap.fr/tableau-de-bord/prevision-des-odeurs/>

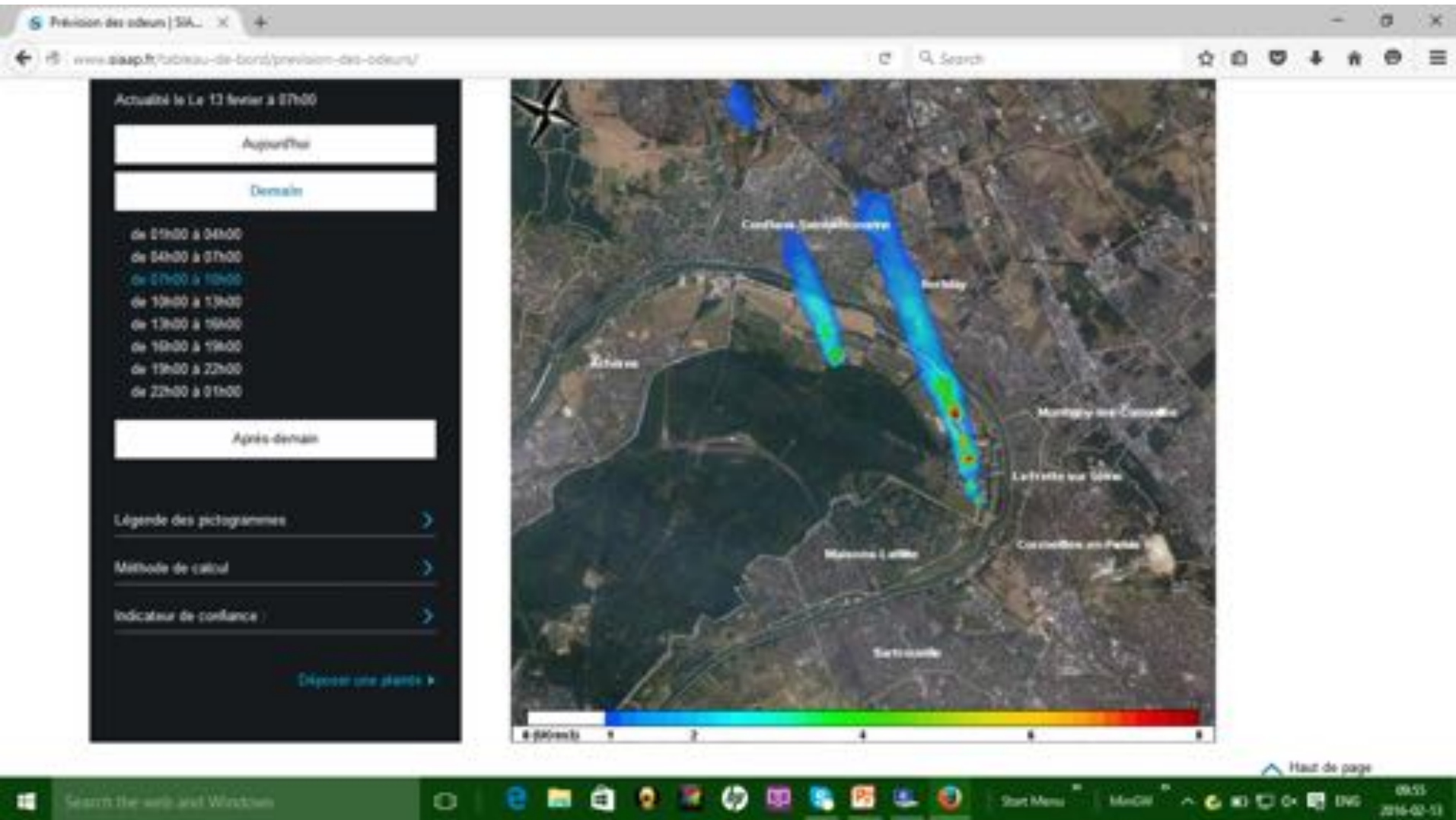
13 February, 2016: 01:00 – 04:00 (LocalTime)



Working Example: Pollutant Prediction

<http://www.siaap.fr/tableau-de-bord/prevision-des-odeurs/>

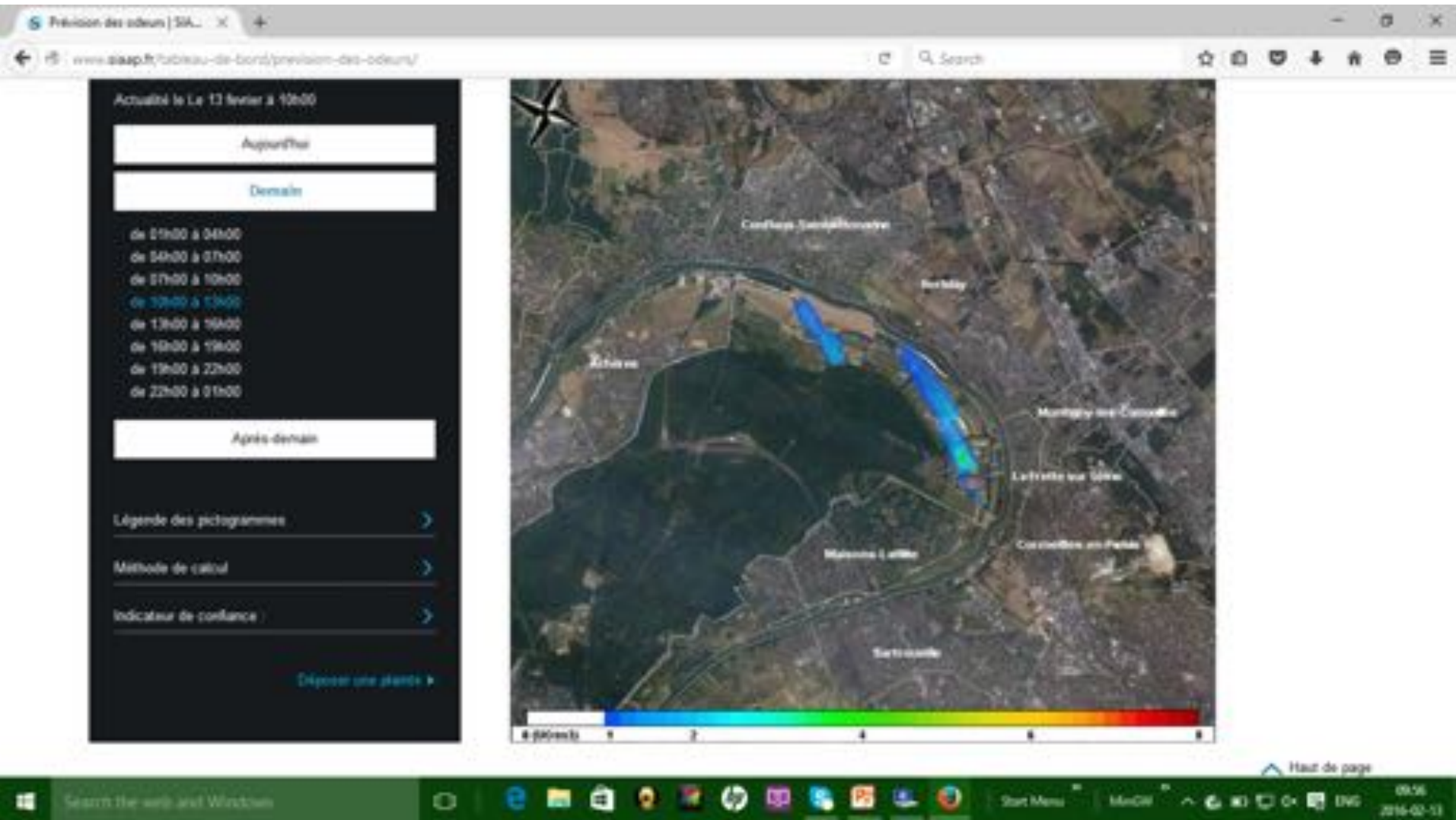
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Working Example: Pollutant Prediction

<http://www.siaap.fr/tableau-de-bord/prevision-des-odeurs/>

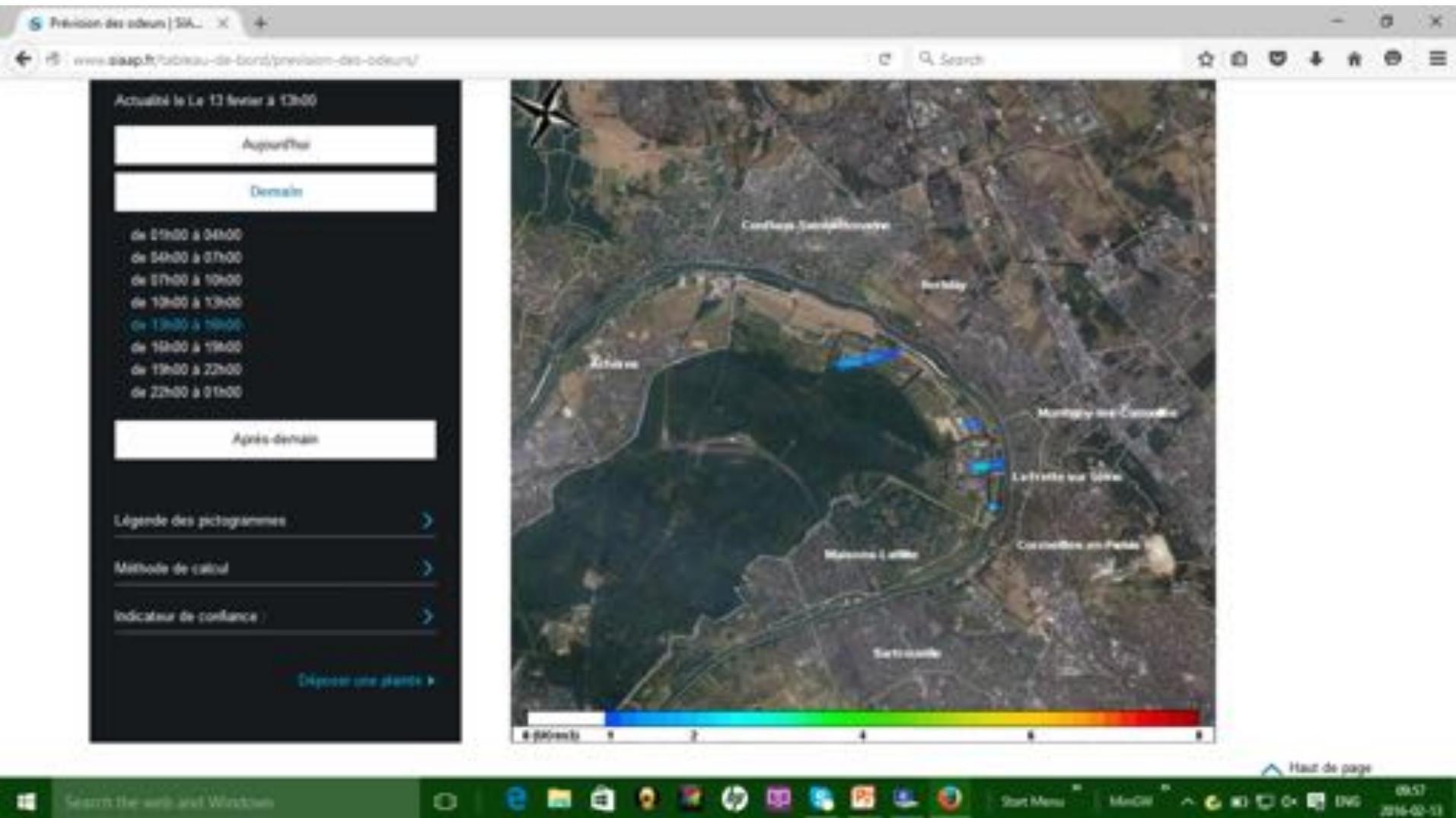
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Working Example: Pollutant Prediction

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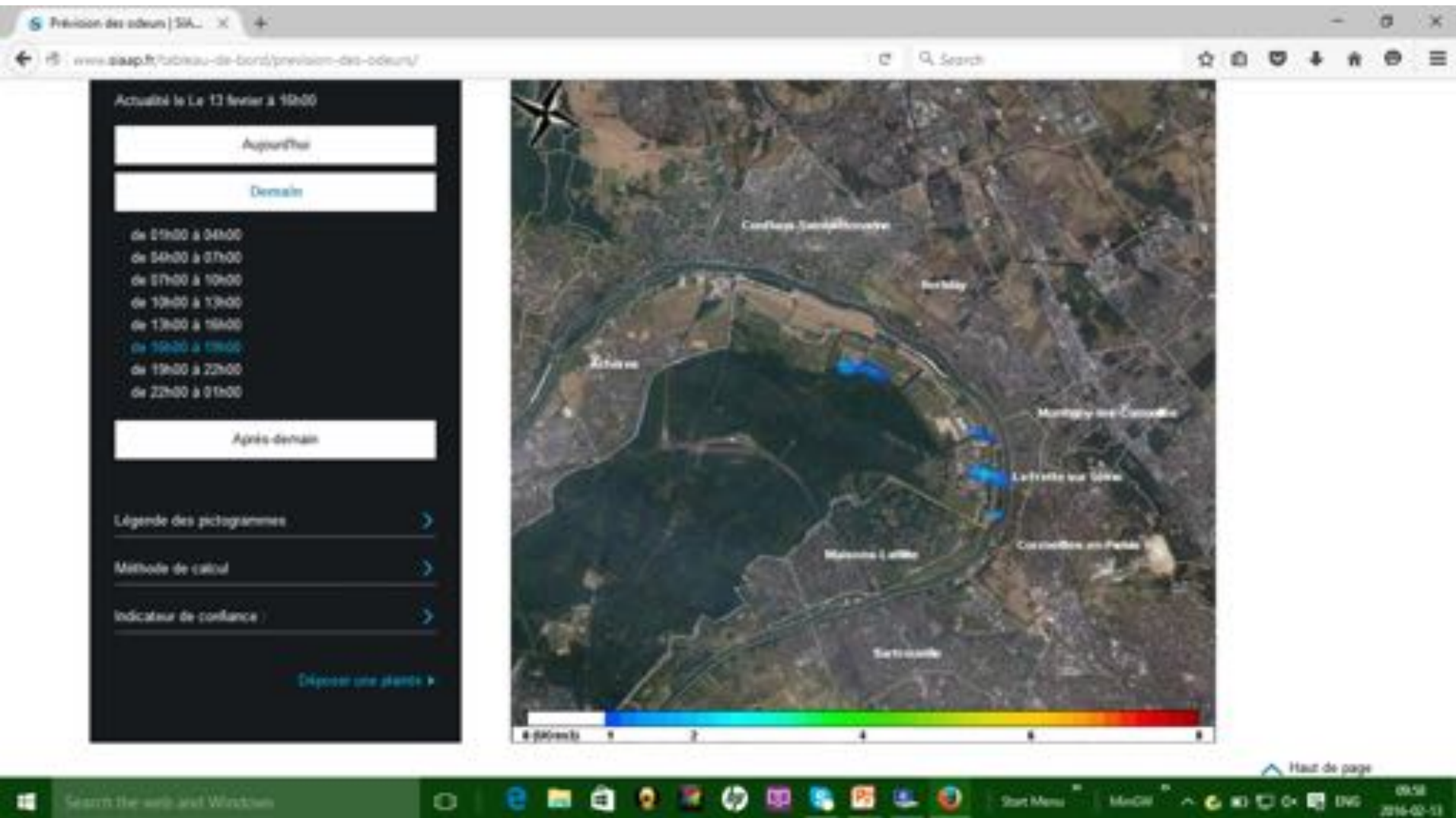
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Working Example: Pollutant Prediction

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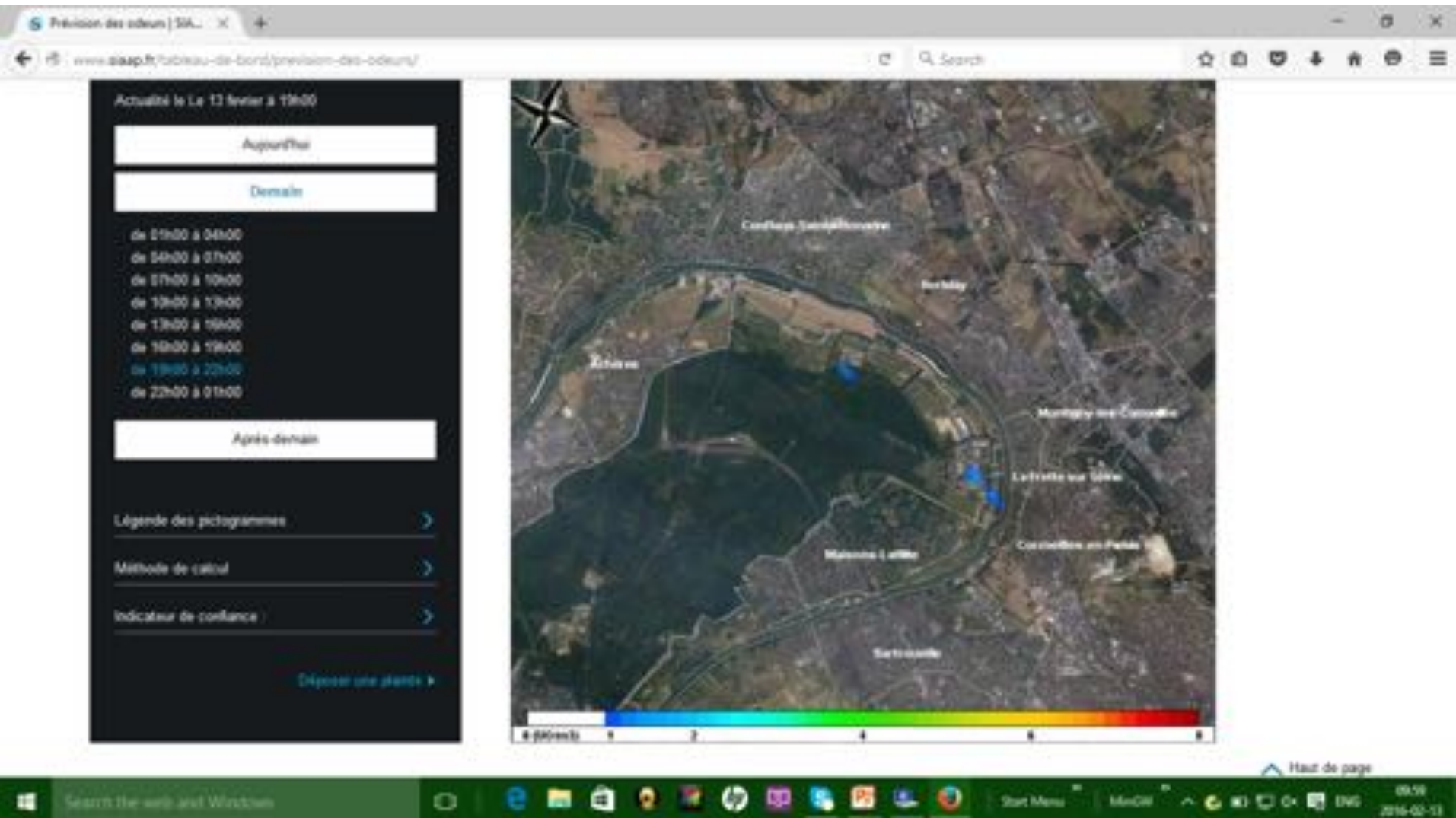
13 February, 2016: 16:00 – 19:00 (LocalTime)



Working Example: Pollutant Prediction

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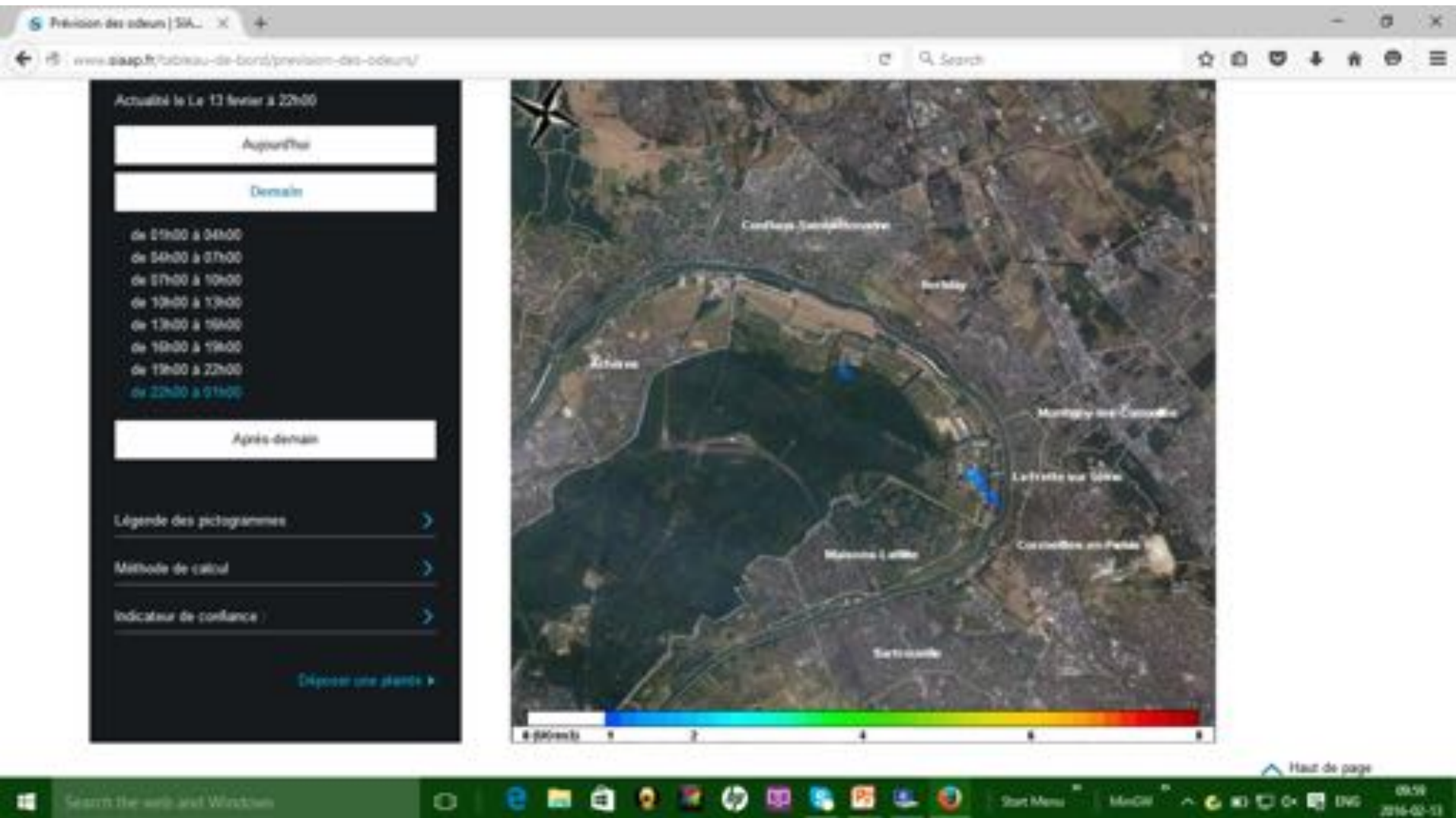
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Working Example: Pollutant Prediction

<http://www.siaap.fr/tableau-de-bord/prevision-des-odeurs/>

13 February, 2016: 22:00 – 01:00 (LocalTime)



Guidelines

Increasing use of 3D CFD modelling for air quality assessment necessitates guidelines. For example, certain requirements stipulated by French Ministry of Environment are:

- Validation of the numerical tool
- Atmospheric stability class conservation over a 2-km domain
- Grid independency (Variation of results $<10\%$ with grid factors of 0.8 and 1.2)
- Proper meshing of obstacles (10 cells)
- Cell aspect ratio less than 10
- Mesh orientation aligned with the wind
- Numerical scheme of at least 2nd order of precision
- Growth factor less than 1.2 between two cells
- Wind profiles as defined by the WG
- Boundary conditions far from zone of interest
- Proper integration of the source term (geometry, temperature)
- Modification of the wind field by the source, if applicable
- Prandtl and Schmidt numbers equal to 0.7
- Proper turbulence model

Thank you for the attention.

For more details, please contact

Claude.souprayen@fluidyn.com

A decorative graphic at the bottom of the slide consisting of several overlapping, wavy lines in red and grey, resembling a signal or waveform.

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