ClubU Code_Saturne - NUMTECH

Implementation of Code_Saturne 3.3 for industrial atmospheric dispersion studies

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EDF R&D, Chatou, France

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Summary

- Introduction
  - Industrial dispersion studies in compliance with regulatory requirements
  - Challenges and issues

- Methodology implemented at NUMTECH
  - The approach
  - Achievement steps

- Comparison with other methods and models
  - A "true" unsteady CFD simulation as the standard reference
  - A Gaussian model (ADMS)

- Overview of CFD activities

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Introduction

Industrial dispersion studies in compliance with regulatory requirements

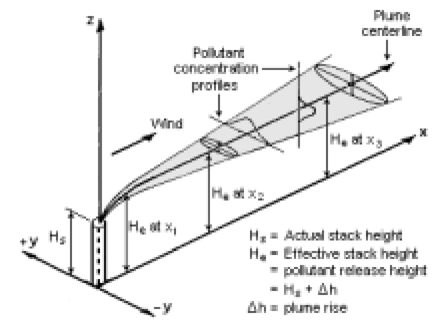
- The concentrations of some pollutants and deposits are subject to administrative rules. The standards set compulsory averages and percentiles to follow.

- To comply with these standards, one should simulate the past **one to five years**, taking into account the specific characteristics of the site:
  - The local weather ;
  - The variation of emissions ;
  - The topography (relief, buildings, land uses).

- In addition to these regulatory constraints comes usually a **Health Risk Assessment (HRA)** study.

[1] See INERIS recommendations for France

Chalenges and issues



The models commonly used to solve these problems :

- Gaussian
- Lagrangian with linearized Navier-Stokes equations

Performances :

- Able to simulate a full year hour by hour (8760 hourly conditions)
- Computation time under one second[1] per iteration
- Not able to meet very local issues and do not take into account fine geometry

CFD models :

- Fine resolution of the geometry
- Too greedy in computing resources (4h[1] per condition)

Statistics :

- Averages : weighting of most common weather conditions
- Percentiles : the calculation of all the conditions should be done.

[1] Order of magnitude based on a 4M cells mesh and with a 12 CPU server (INTEL X5675 @ 3.07GHz)

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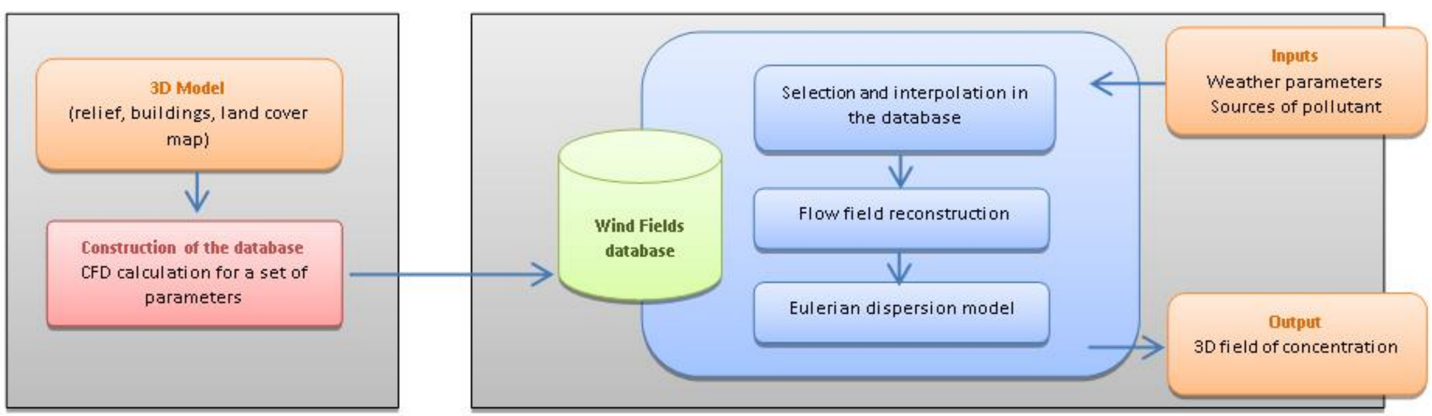
Methodology

The approach

We notice that in frozen-flow mode, we may realize a calculation dispersion based on a pre-calculated wind field within 5 minutes[1]. Thanks to this method, we should simulate a full hourly year calculation in less than 15 days[1] of CPU time.

A flow database should be created beforehand to reproduce all weather conditions. For this purpose, we use the “Nondimensionalization flows” method (Florian Vendel thesis, 2011).



Step 1 : Creation of the wind field database

Step 2 : Hourly calculation of dispersion

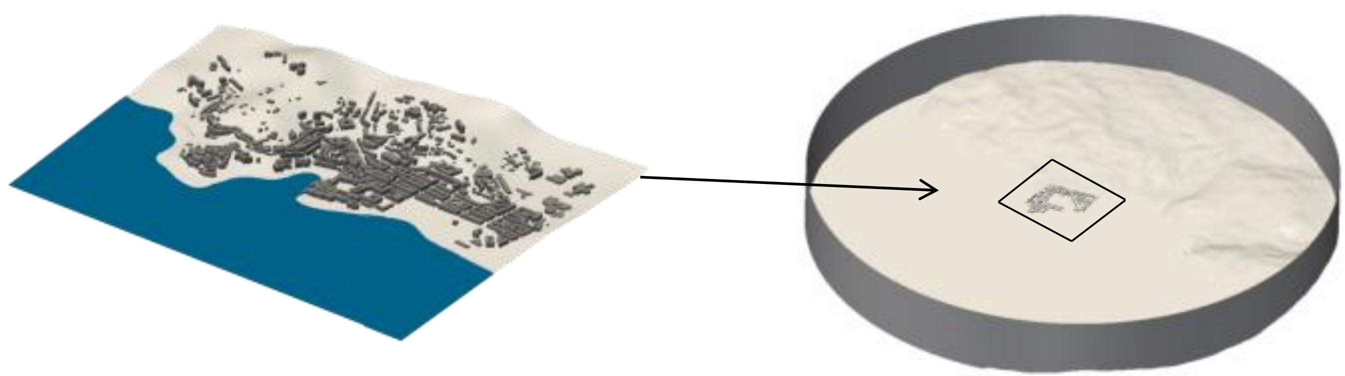
[1] Order of magnitude based on a 4M cells mesh and with a 12 CPU server (INTEL X5675 @ 3.07GHz)

Step 1 : 3D numerical model

We will choose a cylindrical CFD model in order not to favour any direction.

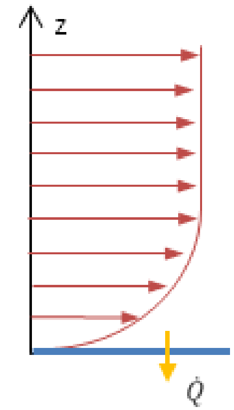
The numerical model is cut into two domains:

- A close area including the detailed geometry of the site and of the land ;
- A far area, coarsely meshed, that allows to take into account the influence of the nearby environment including land use (water, forest, city, agricultural land) and relief.



Models and meshes are generated by “Salome_platform” scripts.

Step 1 : Setup of the flow field

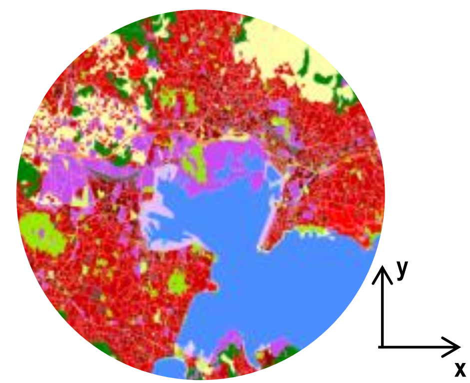


Wind rose weather conditions are defined with:

- A wind magnitude[1] (m/s)
- A direction[1] (°)
- An atmospheric stability (1/Lmo)

These conditions combined with surface elevation and land use maps are used to build speed, turbulence and temperature profiles, which will be the boundaries conditions on atmosphere and the heat flux condition at ground level.

$$\bar{u}(z) = \frac{u_*}{\kappa}\left[\ln\left(\frac{z}{z_0}\right) - \Psi_m(\zeta)\right]$$



Land cover map

The heat flux in each face of the ground is calculated to ensure the maintenance of a constant Lmo in the field.

[1] Usually measured at a height of 10 m in synoptic condition

Step 1 : CFD modeling assumptions

Model:

- Module Atmo : Dry atmosphere
- Turbulence model : k-ϵ linear production
- Wall function : Two Scale model
- Radiative model : Disable

Equation parameters:

- Velocity-Pressure algorithm : SIMPLEC
- Scheme : UPWIND

Step 1 : Wind field database & Sensitivity

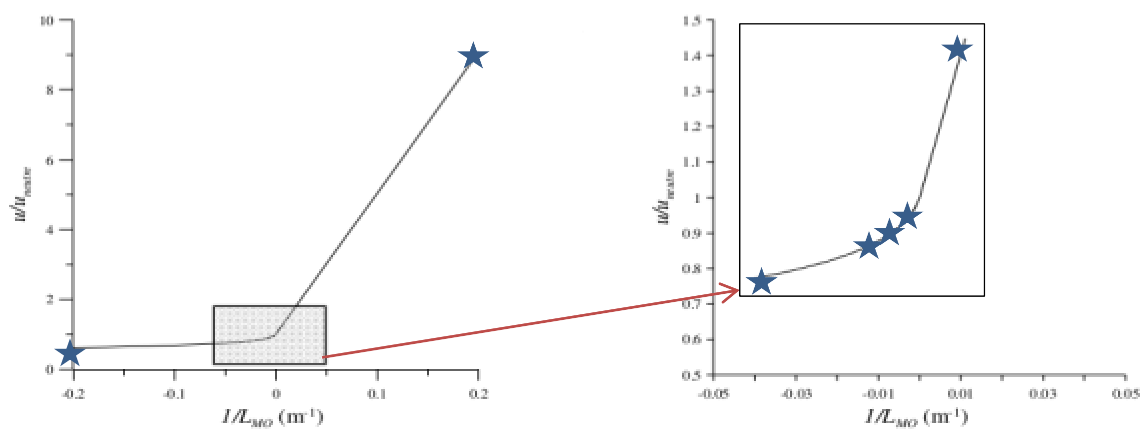
The number of weather conditions that should be used for flow calculation is based on the accuracy of the input data available at the station :

- **36 wind directions**
- 7 stabilities
- 1 wind intensity

$$\tilde{u} = \frac{u\kappa}{u_*} = f\left(\frac{\vec{x}}{L_{MO}}, \frac{z_0}{L_{MO}}, \gamma\right) = F\left(\vec{x}, \frac{1}{L_{MO}}, \gamma\right)$$

All quantities are nondimensionalized -> Sensitivity tests as shown a good reconstruction[1]

The only sore point in this method is the choice of the stability criterion.

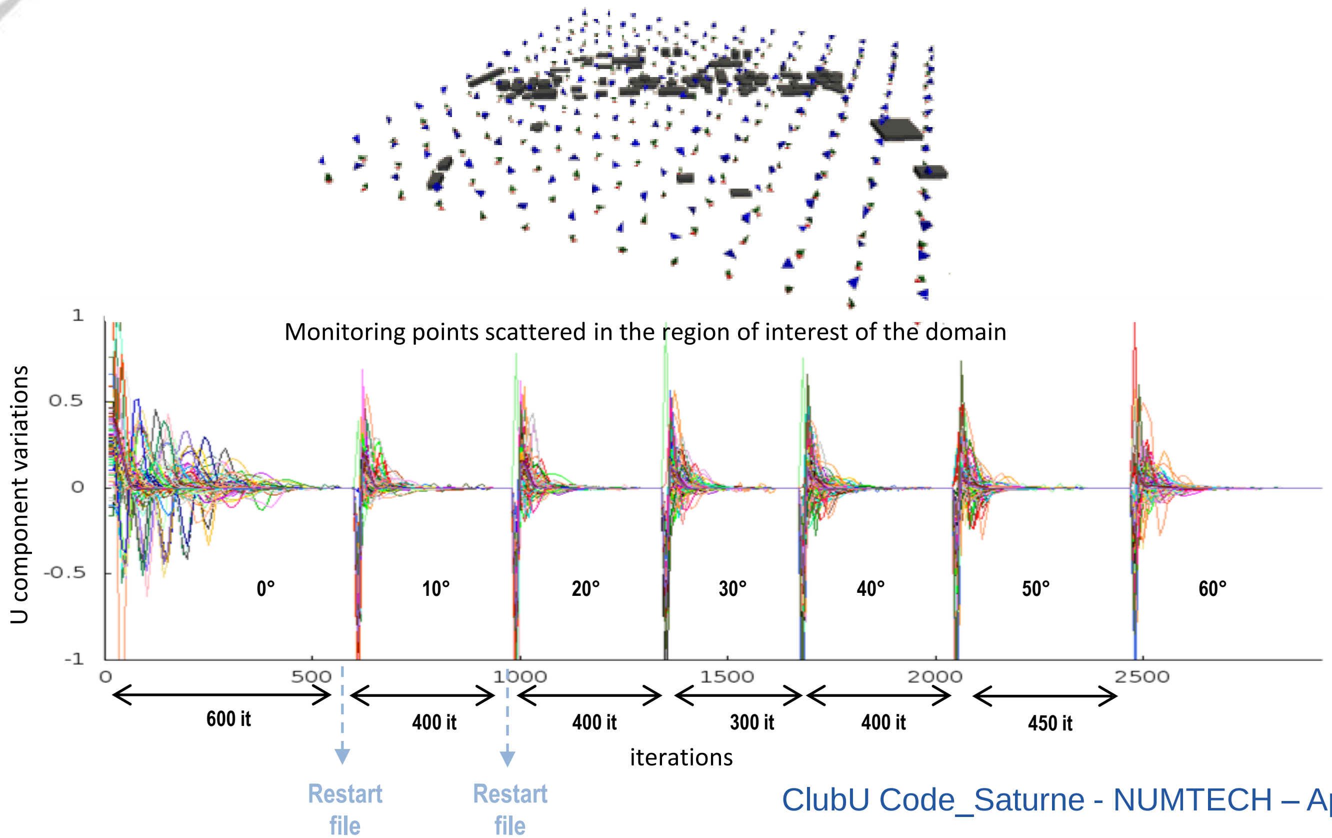


[1] reverse procedure of nondimensionalization

Step 1 : Workflow & Convergence detector

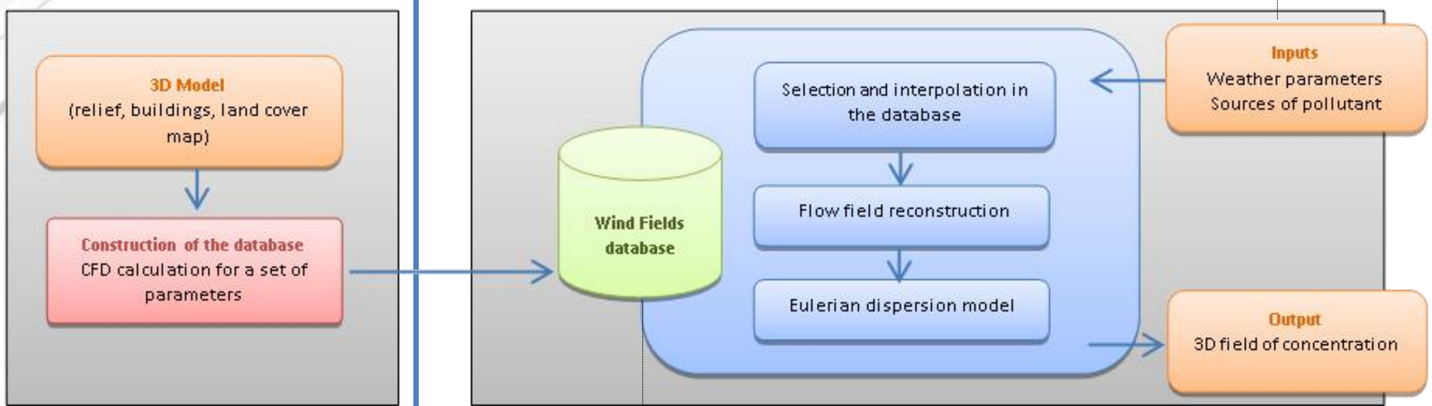
We have developed a first set of user scripts allowing to:

- Run each of desired conditions one after the other ;
- Automatically detect the good steady convergence of calculations;
- Generate RESTART files.



Step 2

8760 conditions per year



Step 1 : Creation of the wind field database

Step 2 : Hourly calculation of dispersion

7 x 36 = 252 wind fields

Step 2 : Interpolation and reconstruction[1]

"Lecamp.f90" routine has been adapted to be able to read simultaneously several "RESTART" files.

	U	Phi	Lmo^{-1}	T0
1	6.1680	200.0000	.0017	8.2000
2	6.1680	200.0000	.0017	8.1000
3	5.6540	200.0000	.0018	8.1000
4	4.1120	240.0000	.0026	8.1000
5	4.1120	210.0000	.0036	8.2000
6	3.5980	220.0000	.0041	8.5000

→ Select in DB

Phi	Lmo^{-1}
200.0	**0.01**
200.0	**0.001**

Code_Saturne performs interpolations and reconstruction operations:

- **Linear interpolation** of the values on Lmo^{-1} between the RESTART files
- **Reconstruction[1]** variable to the desired wind intensity:

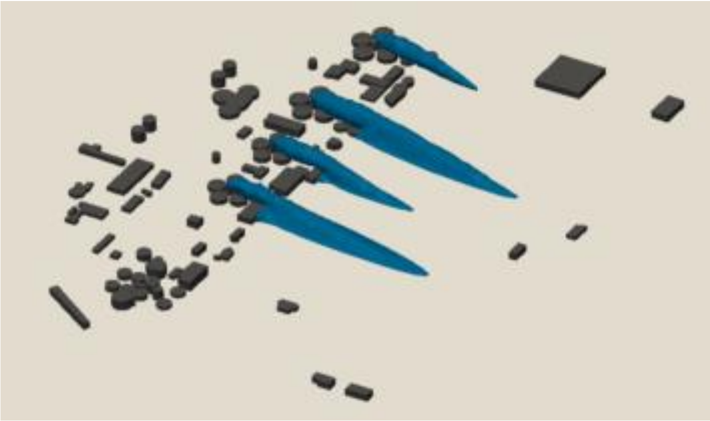
$$\tilde{u}_1 = \frac{u_1 \kappa}{u_{*1}} = \tilde{u}_2 = \frac{u_2 \kappa}{u_{*2}} \qquad \tilde{k}_1 = \frac{k_1 \sqrt{C_\mu}}{u_{*1}^2} = \tilde{k}_2 = \frac{k_2 \sqrt{C_\mu}}{u_{*2}^2} \qquad \tilde{\varepsilon}_1 = \frac{\varepsilon_1 \kappa z}{u_{*1}^3} = \tilde{\varepsilon}_2 = \frac{\varepsilon_2 \kappa z}{u_{*2}^3}$$

$$\tilde{t}_1 = \frac{t_1 \kappa}{u_{*1}} = \tilde{t}_2 = \frac{t_2 \kappa}{u_{*2}} \qquad \tilde{p}_1 = \frac{p_1 \kappa}{u_{*1}} = \tilde{p}_2 = \frac{p_2 \kappa}{u_{*2}}$$

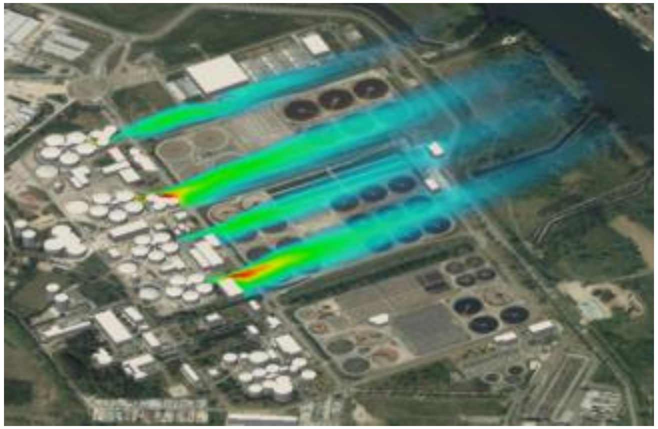
[1] reverse procedure of nondimensionalization

Step 2 : Hourly calculation of dispersion

- Steady calculation in frozen-flow mode;
- Dispersion calculation by using passive eulerian scalars or drift-flux eulerian scalars;
- Particles dry deposition;
- Wet deposition;
- Exportation of desired clips only;
- Calculation of statistics.



3D iso-contours of concentration



contours of concentration

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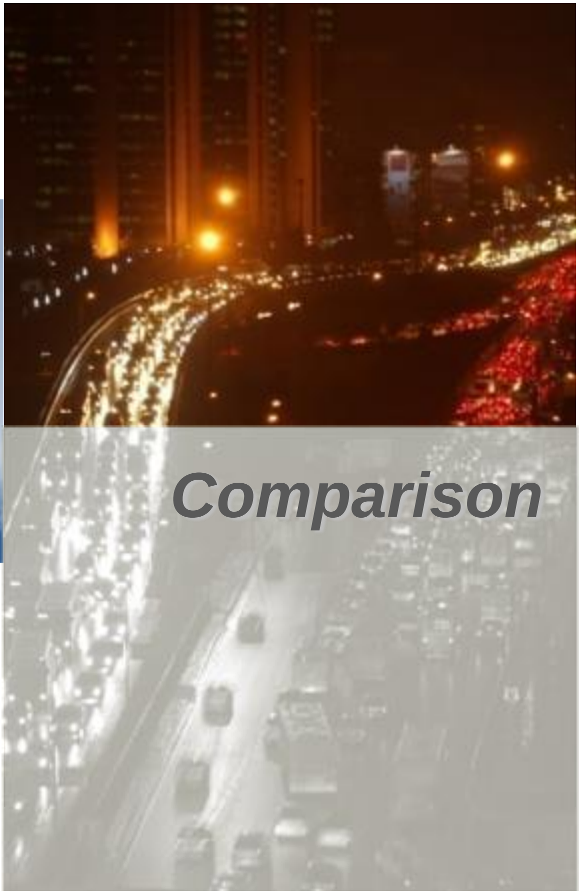


Comparison

Presentation of the benchmark

Softwares and models used:

- CFD frozen-flow (Code_Saturne 3.3.1)

  Methodology previously described

- « True » unsteady CFD (Code_Saturne 3.3.1)

  - CFL 20
  - Weather conditions defined with:
    - A wind magnitude (m/s)
    - A direction (°)
    - An atmospheric stability (1/Lmo)

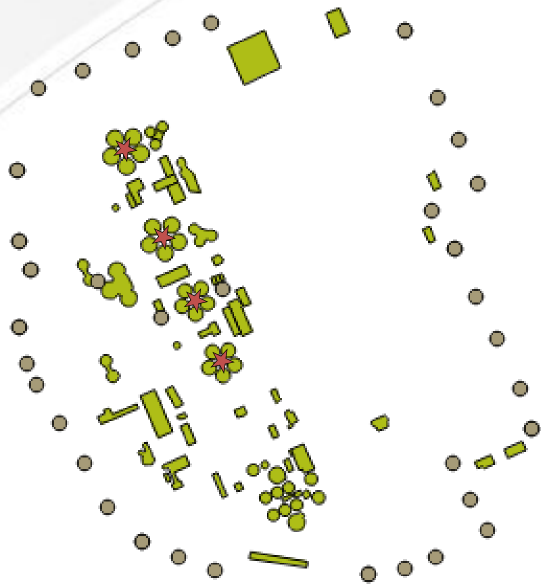
  -Linear interpolation of parameters between hours was performed.

- Gaussian model (ADMS 5.0)

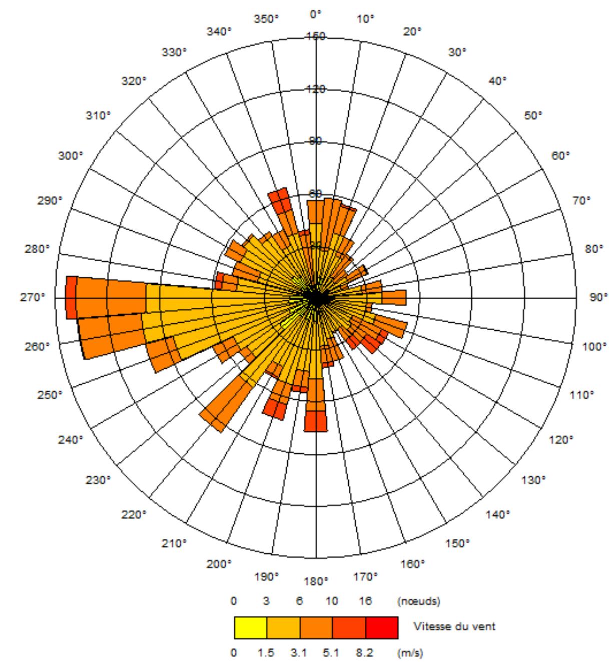
  The simulation was performed according to the state of the art and best practices "ADMS" :
    - Only the main buildings were modelled
    - The output grid resolution is 100x100

Presentation of the benchmark

Input data and modeling assumption



- Channeled sources
- Buildings
- Monitor points located on the site boundaries



Wind Rose

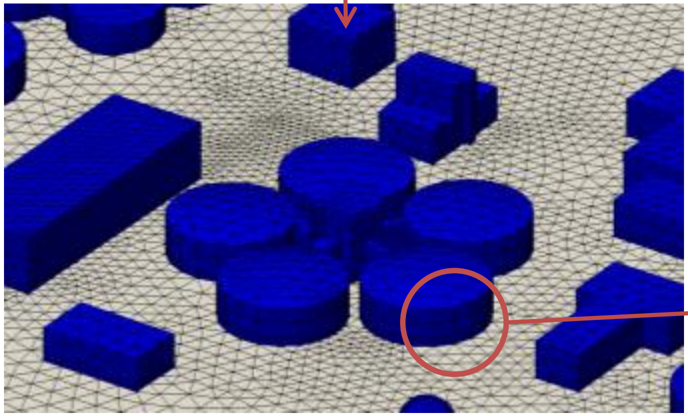
In this benchmark, the ground is flat and the roughness (land use) is constant and uniform throughout the study area

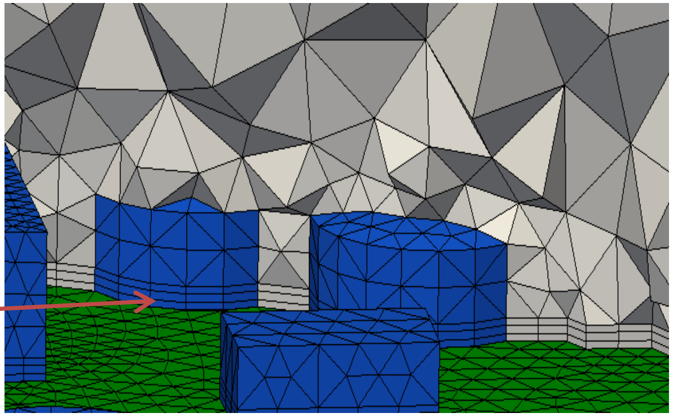
The emission of pollutant is constant

Presentation of the benchmark

CFD Model

- 1 milion cells
- 3 prism layers in the first 2 meters



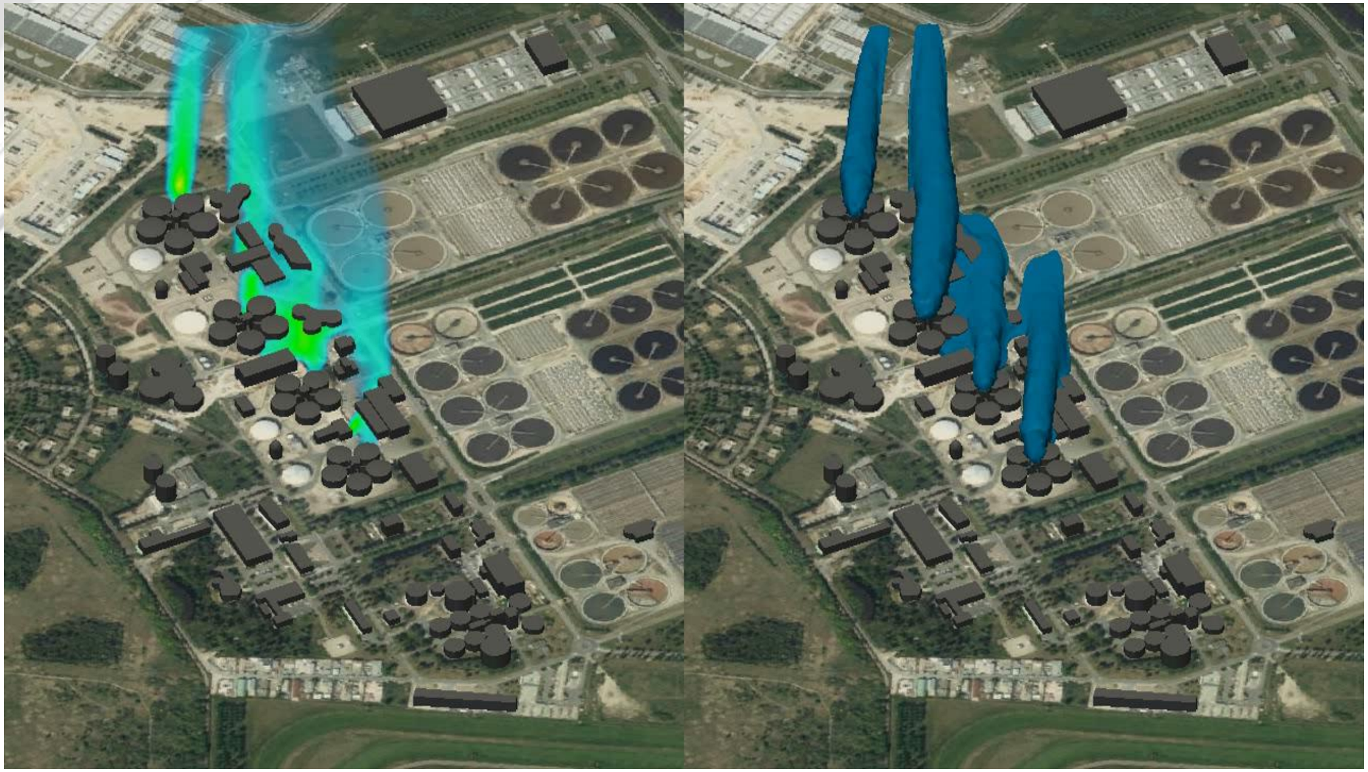


Performances

	CPU time per condition	Nb of conditions	Total CPU time
Gaussian model	0.45 sec	X 2000	14 min
Frozen-Flow dispersion	4 min per condition	X 2000	5 days
« Real » CFD unsteady simulation	Real-Time 2 h CPU per hour	X 2000	164 days

Steady Weather Condition	1h	X 252	10 days

Results – unsteady simulation



concentration at 1.5 m above ground level and 3D iso-contours (NOx)

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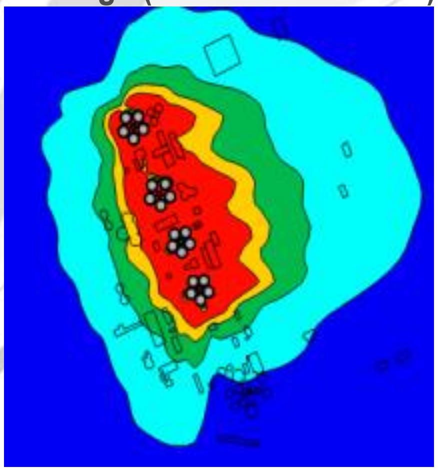
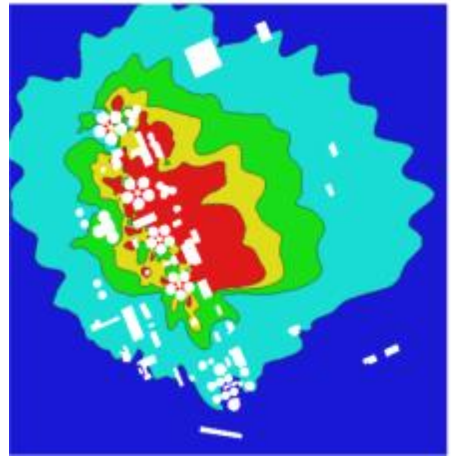
Results (1,5 m)

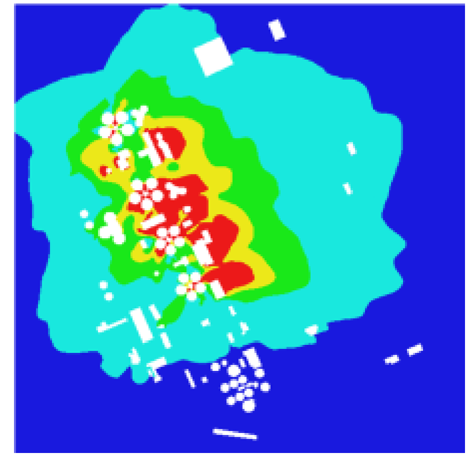
Average (NOx concentration)



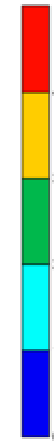
Gaussian simulation



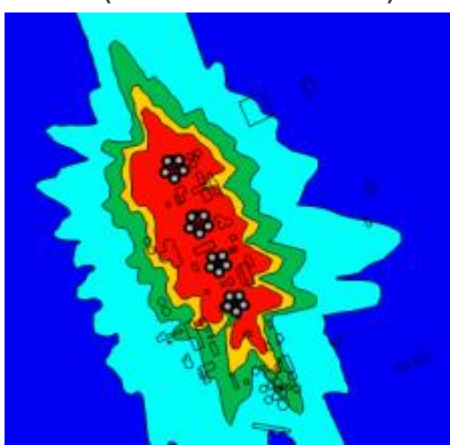
CFD unsteady simulation



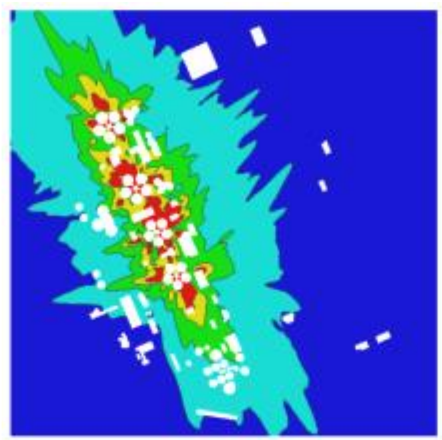
CFD frozen-flow simulation



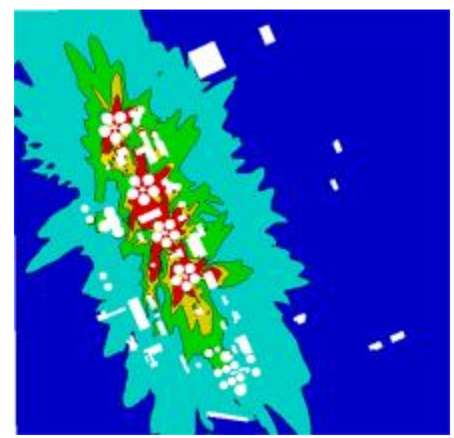
P100 (NOx concentration)



Gaussian simulation



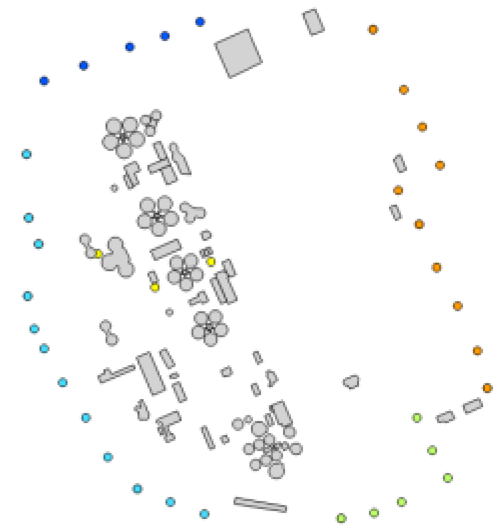
CFD unsteady simulation



CFD frozen-flow simulation

Results

Probes	Gaussian	Unsteady	Frozen-Flow
North	P100 : 49,85 Avg : 1,49	P100 : 69,22 Avg : 1,40	P100 : 61,13 Avg : 1,38
Est	P100 : 20,32 Avg : 1,26	P100 : 31,55 Avg : 1,25	P100 : 31,35 Avg : 1,25
West	P100 : 28,8 Avg : 1,26	P100 : 50,5 Avg : 1,10	P100 : 48,1 Avg : 1,01
South	P100 : 33,0 Avg : 6,6	P100 : 50,6 Avg : 6,2	P100 : 44,3 Avg : 6,5
Middle	P100 : 117,5 Avg : 4,3	P100 : 330,8 Avg : 6,9	P100 : 400,1 Avg : 7,3



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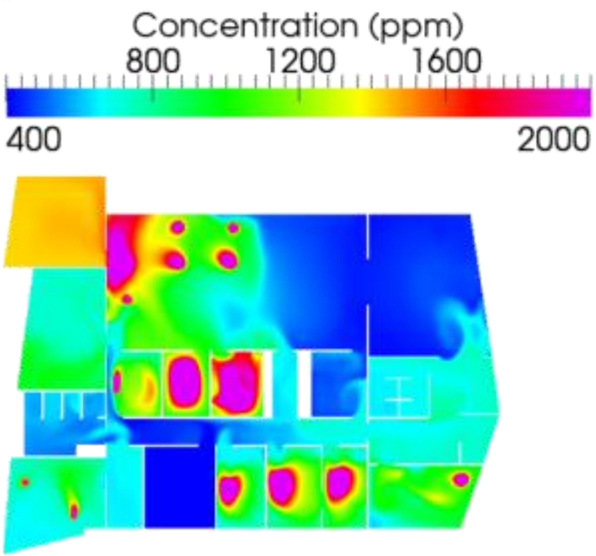
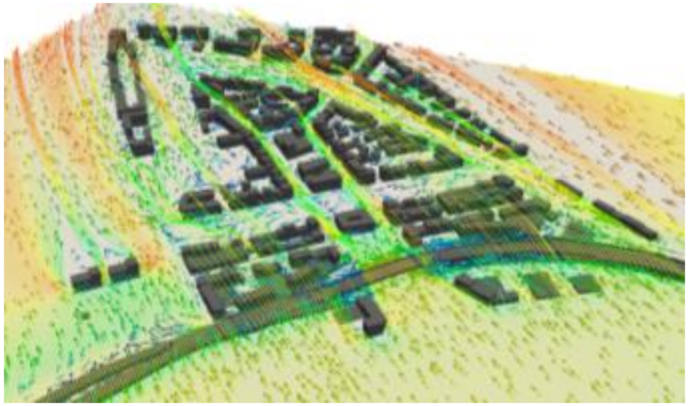
Overview of CFD activities at NUMTECH

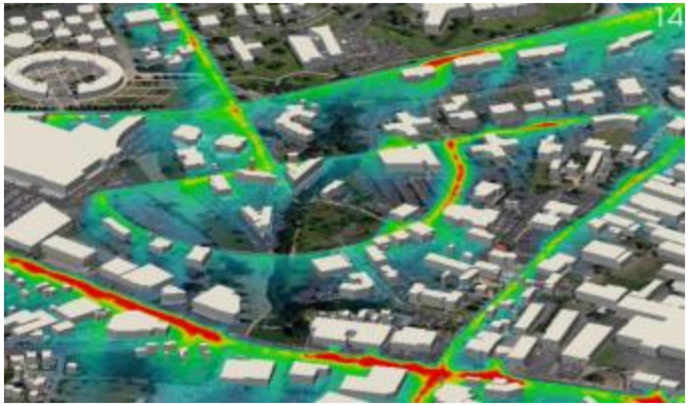
Ventilation and air quality within
Professional and public premises



Modèle CFD - iso-contours CO_2 h=1,5m

Urban Dispersion / traffic / road construction
(bridge, tunnel, interchange)


Vector fields and stream lines


NO_2 concentration contours

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