The implementation of Code_Saturne 3.3 for industrial atmospheric dispersion studies was presented in April 2015 by Florian COHN at EDF R&D, Chatou, France.
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
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
Challenges 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.

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

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

\[
\bar{u}(z) = \frac{u_s}{\kappa} \left[ \ln \left( \frac{z}{z_0} \right) - \Psi_m(z) \right]
\]

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

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.
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.

Monitoring points scattered in the region of interest of the domain

U component variations

600 it 400 it 400 it 300 it 400 it 450 it

0° 10° 20° 30° 40° 50° 60°
Step 1: Creation of the wind field database

3D Model
(relief, buildings, land cover map)

Construction of the database
CFD calculation for a set of parameters

Step 2: Hourly calculation of dispersion

Selection and interpolation in the database
Flow field reconstruction
Eulerian dispersion model

Inputs
Weather parameters
Sources of pollutant

Output
3D field of concentration

8760 conditions per year

7 x 36 = 252 wind fields
Step 2 : Interpolation and reconstruction

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

<table>
<thead>
<tr>
<th>U</th>
<th>Phi</th>
<th>Lmo⁻¹</th>
<th>T0</th>
<th></th>
<th>Phi</th>
<th>Lmo⁻¹</th>
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<tbody>
<tr>
<td>1</td>
<td>6.1680</td>
<td>200.0000</td>
<td>0.0017</td>
<td>8.2000</td>
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<td></td>
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<td>0.0018</td>
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<td>8.1000</td>
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<td>220.0000</td>
<td>0.0041</td>
<td>8.5000</td>
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</tr>
</tbody>
</table>

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:

\[
\tilde{u}_1 = \frac{u_1 \kappa}{u_{*1}} = \tilde{u}_2 = \frac{u_2 \kappa}{u_{*2}}
\]

\[
\tilde{t}_1 = \frac{t_1 \kappa}{u_{*1}} = \tilde{t}_2 = \frac{t_2 \kappa}{u_{*2}}
\]

\[
\tilde{k}_1 = \frac{k_1 \sqrt{C_{\mu}}}{u_{*1}^2} = \tilde{k}_2 = \frac{k_2 \sqrt{C_{\mu}}}{u_{*2}^2}
\]

\[
\tilde{\epsilon}_1 = \frac{\epsilon_1 K z}{u_{*1}^3} = \tilde{\epsilon}_2 = \frac{\epsilon_2 K z}{u_{*2}^3}
\]

\[
\tilde{p}_1 = \frac{p_1 \kappa}{u_{*1}} = \tilde{p}_2 = \frac{p_2 \kappa}{u_{*2}}
\]

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
ClubU Code_Saturne

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

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.

Wind Rose

- Channeled sources
- Buildings
- Monitor points located on the site boundaries
Presentation of the benchmark

- 1 million cells
- 3 prism layers in the first 2 meters
## Performances

<table>
<thead>
<tr>
<th>Model/Condition</th>
<th>CPU time per condition</th>
<th>Nb of conditions</th>
<th>Total CPU time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian model</td>
<td>0.45 sec</td>
<td>X 2000</td>
<td>14 min</td>
</tr>
<tr>
<td>Frozen-Flow dispersion</td>
<td>4 min per condition</td>
<td>X 2000</td>
<td>5 days</td>
</tr>
<tr>
<td>« Real » CFD unsteady simulation</td>
<td>Real-Time 2 h CPU per hour</td>
<td>X 2000</td>
<td>164 days</td>
</tr>
<tr>
<td>Steady Weather Condition</td>
<td>1h</td>
<td>X 252</td>
<td>10 days</td>
</tr>
</tbody>
</table>
Results – unsteady simulation

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

<table>
<thead>
<tr>
<th>Probes</th>
<th>Gaussian</th>
<th>Unsteady</th>
<th>Frozen-Flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>North</td>
<td>P100 : 49.85 Avg : 1.49</td>
<td>P100 : 69.22 Avg : 1.40</td>
<td>P100 : 61.13 Avg : 1.38</td>
</tr>
<tr>
<td>West</td>
<td>P100 : 28.8 Avg : 1.26</td>
<td>P100 : 50.5 Avg : 1.10</td>
<td>P100 : 48.1 Avg : 1.01</td>
</tr>
<tr>
<td>South</td>
<td>P100 : 33.0 Avg : 6.6</td>
<td>P100 : 50.6 Avg : 6.2</td>
<td>P100 : 44.3 Avg : 6.5</td>
</tr>
<tr>
<td>Middle</td>
<td>P100 : 117.5 Avg : 4.3</td>
<td>P100 : 330.8 Avg : 6.9</td>
<td>P100 : 400.1 Avg : 7.3</td>
</tr>
</tbody>
</table>
ClubU Code_Saturne

Overview of CFD activities
Overview of CFD activities at NUMTECH

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

Ventilation and air quality within Professional and public premises

Vector fields and stream lines

NO₂ concentration contours