Atmospheric CFD modelling for environmental applications at local scale

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Outline

• Objectives
• Focus: concentration fluctuations
• Overview: other activities
Objectives

- Develop an integrated modelling tool for studies of the atmospheric environment at local scale
- Dispersion of pollutants and its impact on population and environment in urban and around industrial areas.
- Other impact studies: reactive pollutants, particle formation and dispersion, noise propagation …
- Accidental releases,
- Population comfort (wind and turbulence prediction), extreme winds, wind energy …
The model: Mercure_Saturne

- Developed by CEREA
- 3-D model adapted to atmospheric flow and dispersion simulation
- Core of the model: CFD model Code_Saturne (EDF) which can handle complex geometry and complex physics
- Unstructured grid, finite volumes
- Simulations:
  - Full scale, fine resolution, complex terrain
  - Large scale meteo. conditions taken into account
  - $k-\varepsilon$ turbulence closure model
  - neutral gaz releases, point source, continuous releases
  - Chemistry, aerosols …
Concentration time series (wind tunnel measurements)

At 300 m
High fluctuations near the source

At 1000 m
Focus: concentration fluctuations

• Two approaches:
  • Hybrid RANS / PDF  
    (PhD Thesis A. Radicchi)
  • Pure RANS  
    (PhD Thesis M. Milliez)
Hybrid approach
RANS/PDF

RANS
(\(k-\varepsilon\))

\(\langle u_i \rangle, \langle P \rangle\)

\(k, \varepsilon\)

PDF
(SLM\(^1\))

\(f(\phi)\)

(PDF Eulérienne de la concentration)

\(^1\) Simplified Langevin Model
Résolution des EDS pour la trajectoire d'un échantillon de particules de fluide,

\[ dx_{p,i} = u_{p,i} dt \]
\[ du_{p,i} = -\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_i} dt - \frac{u_{p,i} - \langle u_i \rangle}{T_L} dt + \sqrt{C_0 \varepsilon} dW_i \]

\[ \langle u_i \rangle, \langle P \rangle, \varepsilon \rightarrow \text{Champs moyens (RANS)} \]
\[ x_{p,i}, u_{p,i} \rightarrow \text{Champs instantanés (EDS)} \]
\[ W_i, T_L \rightarrow \text{Proccessus de Wiener, Temp caracterisitique de la turbulence} \]
[ RANS / PDF ]

- Résolution de l'équation pour le mélange de la concentration transportée par chaque particule de fluide,

\[
d\phi_p = -\frac{\phi_p - \langle \phi \rangle}{\tau_m} dt + S(\phi) dt
\]

\[\langle \phi \rangle \rightarrow \text{Conc. moyenne}\]

\[\phi_p \rightarrow \text{Conc. instantanée particule } p\]

\[\tau_m \rightarrow \text{Temp de mélange}\]
Figure 6.18: Vertical profiles of mean concentration and scalar fluctuation, normalized on $\theta_*$ for plane source release. Lines are model results and symbols are measured profiles. Measurement stations are $x_L = 0.53$ m (continuous, $\circ$), $x_L = 1.06$ m (dashed, $\square$), $x_L = 1.54$ m (dotted, $\diamond$) and $x_L = 2.03$ m (dash-dotted, $\triangle$).
Pure RANS approach:

**Concentration mean:**

\[
-\rho \left( \frac{\partial C}{\partial t} + U_j \frac{\partial C}{\partial x_j} \right) = \frac{\partial}{\partial x_i} \left( D \frac{\partial C}{\partial x_j} \right) - \rho \frac{\partial (u'_j c')}{\partial x_j} \\
- \rho u'_j c' = \frac{\mu_t}{Sc_t} \left( \frac{\partial C}{\partial x_j} \right) \quad \mu_t \text{ turbulent viscosity} \quad \mu_t = \frac{-\rho C_{\mu}}{\varepsilon} \\
Sc_t \text{ Schmidt number}
\]

**Concentration variance:**

\[
-\rho \left( \frac{\partial \overline{c'^2}}{\partial t} + U_j \frac{\partial \overline{c'^2}}{\partial x_j} \right) = \frac{\partial}{\partial x_i} \left( D \frac{\partial \overline{c'^2}}{\partial x_j} \right) - \rho \frac{\partial (u'_j c'^2)}{\partial x_j} - 2 \rho u'_j c' \frac{\partial C}{\partial x_j} - 2 D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j} \\
- \rho u'_j c'^2 = \frac{\mu_t}{Sc_t} \left( \frac{\partial \overline{c'^2}}{\partial x_j} \right) \quad 2 D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j} = \rho \varepsilon_c = \frac{\rho}{R_f} \overline{c'^2} \frac{\varepsilon}{k}
\]
The Mock Urban Setting Test (MUST)

- Yee and Biltoft (2004).
- Near full scale experiment in the U.S. Army Dugway Proving Ground (Utah), conducted for the DTRA (Defense Threat Reduction Agency)
Simulations with Mercure

- **Mesh**: ~800 000 hexahedral elements
- **Dimensions**: 240 m x 233 m x 32m

Horizontal grid: lower levels

Stretched vertical grid

- **MUST**: 20 selected cases
- **Detailed study of dynamics and mean concentration with Mercure** (Milliez and Carissimo, 2006).
Simulations with Mercure

Mean concentration (ppm)  Root mean square of concentration fluctuations (ppm)
Simulations with Mercure

- 20 simulated cases:

![Graphs showing data comparisons between MUST and Mercure]
Simulations with Mercure

20 simulated cases:

Root mean square of concentration fluctuations

<table>
<thead>
<tr>
<th></th>
<th>MG</th>
<th>VG</th>
<th>FAC2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Line1</td>
<td>0.94</td>
<td>3.31</td>
<td>63.5%</td>
</tr>
<tr>
<td>Line2</td>
<td>1.028</td>
<td>1.437</td>
<td>67.2%</td>
</tr>
<tr>
<td>Line3</td>
<td>0.980</td>
<td>1.341</td>
<td>69.2%</td>
</tr>
<tr>
<td>Line4</td>
<td>1.156</td>
<td>1.368</td>
<td>67.0%</td>
</tr>
<tr>
<td>All horizontal</td>
<td>1.05</td>
<td>2.22</td>
<td>66.4%</td>
</tr>
<tr>
<td>Tower T</td>
<td>0.51</td>
<td>2.70</td>
<td>50.3%</td>
</tr>
<tr>
<td>Masts A, B, C, D</td>
<td>0.66</td>
<td>2.56</td>
<td>53.8%</td>
</tr>
<tr>
<td>All vertical</td>
<td>0.61</td>
<td>2.61</td>
<td>52.6%</td>
</tr>
<tr>
<td>All</td>
<td>0.82</td>
<td>2.40</td>
<td>60.1%</td>
</tr>
</tbody>
</table>

- MG = exp (|ln Co| – |ln Cp|)
- VG = exp [(ln Co-ln Cp)^2 ]
- FAC2 = fraction of data that satisfy 0.5<Cp/Co<2

Co = MUST observations
Cp = Mercure predictions
|x| = average over the data set
Simulations with Mercure

- Influence of turbulence and stratification

Root mean square of concentration fluctuations (ppm)

- 10 simulated cases:
  - FAC2 (neutral) = 46.9 %
  - FAC2 (stable) = 53.3 %
  + 6 %
Simulations with Mercure

- Influence of initialisation and emission rate

Root mean square of concentration fluctuations (ppm)

c’(source) = 1% C(source)
Overview : other activities

- Cloud modeling: plume + fog
- Impact of building and complex terrain on dispersion
- Chemistry of reactive plumes
- Aerosols formation (local scale)
- Wind energy
- Radiative effects
- Operational ABL prediction (SIRTA)
- Traffic and tunnel

Following presentations
Panache Bugey
12 mars 1980

Calcul code Mercure
iso-concentration
eau liquide
Fig. 2 Comparison of the in-situ spectra measured by the aircraft with the simulated ones. 

a) Horizontal slice at $z=1320$ m above the ground for case B (- - : iso-LWC and —— : iso-$N_c$). The symbol $*$ shows the maximum of LWC, and the circles are part of the same arc whose center is $*$. 

b) shows the measured spectra (black) 660 m far from the * and the log-normal curves (blue) obtained from the LWC and $N_c$ values given by the code at the position of the shaded circles (located 660 m far from the *).
Évolution de la visibilité

*Nouveau paramètre d’étude : la visibilité*

\[ VIS = -\frac{\ln(0.02)}{\beta} \text{ avec } \beta = 144.7 \left(\frac{\rho_0 q_1}{\beta}\right)^{0.88} \]

Variations spatio-temporelles de la visibilité

3 phases dans l’évolution du brouillard :
La formation, le développement vertical et la dissipation de la couche de brouillard
IV. Résultats

Spectre des gouttelettes à 2m

- Diamètre moyen de l’ordre de 10 µm et 20 µm
- \(Nc\) de l’ordre de quelques centaines de gouttelettes par cm³

Distribution des gouttelettes de nuages (cm-3/µm) à 2m en fonction du diamètre des gouttelettes (µm)
Overview: other activities

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- Wind energy
- Local ABL prediction (SIRTA)
- Traffic and tunnel
- Radiative effects
Résultats pour la situation de vent de Sud (Mercure_Saturne 1.1.3)

Attaque du 1er aéro
Résultats pour la situation de vent de Sud (Mercure_Saturne 1.1.3)
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Near source aerosol modeling (Thesis B. Albriet)
Overview: other activities

- Cloud modeling: plume + fog
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- Chemistry of reactive plumes
- Aerosols formation (local scale)
- Wind energy
- Local ABL prediction (SIRTA)
- Traffic and tunnel
- Radiative effects
Wind energy: turbulence in complex terrain and mask effect for large parks (Thesis L. Laporte)

Askervein Hill: