VALIDATION OF LATTICE BOLTZMANN METHOD IN COMPLEX URBAN ENVIRONMENT – HAMBURG & LA DEFENSE

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Agenda

1. Introduction
2. Validation Cases: Hamburg
3. Exploration Case: La Défense
Introduction to LBM Methods and PowerFLOW

**Real Fluid**
Free molecules in continuous space

**Physics governed by Kinetic Theory (Boltzmann)**

**Molecular Level**

Navier-Stokes equations can be recovered from kinetic theory

**Mesoscopic Level**

Lattice-Boltzmann methods (PowerFLOW)

Discrete formulation of kinetic theory & Numerical integration
Solve the Lattice Boltzmann equations on a given lattice

Simple conversion of microscopic variables to fluid dynamic quantities

**Macroscopic Level**

Fluid considered as a continuous medium
Physics governed by Navier-Stokes equations (PDE)

Discrete approximation & Numerical integration
Solve the PDE equations on a given mesh

**Classical CFD**

**Results:**
Fluid dynamic quantities at discrete points in space and time
pressure, velocity, density...
Turbulence in PowerFLOW:

- Only statically anisotropic eddies outside the Kolmogorov range are computed.

Passive scalar are used to represent small particle field:
- Pollutant gases, pathogenic agent, radioactive agent, etc.
- Closed or open environments
- Up to 64 different scalars in the same simulation
- PDE is solved for each scalar in addition of the flow field variables.

Only statically anisotropic eddies outside the Kolmogorov range are computed.
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Hamburg Validation Cases

- Three different validation cases available from COST ES1006 (see next slides)

- All based on the same Simulation Model and Global Setup

- Surface Mesh:
  - Ground + buildings (4000 x 4000 m)
  - Triangular mesh, 9M elements

- Volume Mesh:
  - Cubic cells
  - Variable resolution (finest: 0.5m)

- Simulation Parameters:
  - Isothermal Simulation
  - Turbulence intensity: 10%
  - Time step: 7ms
  - Physical time simulated: 75min
Hamburg Case 1

Wind direction and intensity are constant in time.
Velocity profile reconstructed based on the Velocity 8.9 m/s at z=175m
Neutral atmospheric stability

Gaz:
- Punctual source; from a boat on the river
- Q = 2g/sec (45min)
- Gas: SF6; C_d=1.5e-05 m²/sec
Hamburg Case 3 Continuous

Wind direction and intensity are constant in time
Velocity profile reconstructed based on the Velocity 6 m/s at z=49m
Neutral atmospheric stability

Gaz :
- Punctual source (1m diameter cylinder)
- Q = 0.5 kg/sec (60min)
- Gas: SF6; Cₐ=1.5e-05 m²/sec
Hamburg Case 3 Puff

Wind direction: 235°

Wind direction and intensity are constant in time
Velocity profile reconstructed based on the Velocity 6 m/s at z=49m
Neutral atmospheric stability

Gaz:
- Punctual source (1m diameter cylinder)
- Initial release 50 kg in 31 sec
- Gas: SF6; $C_d=1.5\times10^{-5}$ $m^2/sec$
Validation Criteria

- CASE 1 and CASE 3 Continuous: time averaged gas concentration
- CASE 3 Puff: dosage (integral of the concentration over time)
- As mean of statistical correlation, we calculate the usual metrics: fractional bias (FB), geometric mean bias (MG), normalized mean square error (NMSE) and fraction of predictions within a factor of 2 of observations (FAC2).

- We used the reference acceptance criteria for atmospheric dispersion modelling of accidental releases in built environments defined by Hanna & Chang, which are:
  - $|FB| \leq 0.67$
  - NMSE $\leq 6$
  - FAC2 $\geq 0.3$
The results for this case are disappointing as no Probe lies within the acceptance range (materialized by the 2 dotted lines).

We conducted a sensibility test to Probe location; we also recorded data for a Model rotated by -2° and +2° (*)
  - These tests also gave almost no correlated Probe

There are disputable reasons for this poor match:
  - Geometry delta between our WT Model and the actual city
  - Hypothesis of constant meteorological conditions during the experiment

(*) Typically, a 4m variation compared to the reference location
The results for this case are also disappointing as no Probe lies within the acceptance range.

We can note though a clear trend for the Simulation to over-predict the Experiment measurements.

The sensibility test to the Probe location show much improved results:
- The FAC2 jumps to 0.53 for the +2° test
- The FAC2 jumps to 0.50 for the -2° test
The results for Puff case are better as the FAC2 is 0.25.

We note the same clear trend of overpredicting the Experiment measurements.

The sensibility test to the Probe location does not show any improvement:
- FAC2 is 0.25 for the -2° test
- FAC2 is 0.19 for the +2° test
Hamburg Case 3 Continuous – Comments

- In our validation exercise, we averaged the concentration over the whole length of the simulated gas release (60 minutes)

- In this slide, we look at sliding averages over 10 minutes

- Originally, our predictions are OK (FAC2 is 0.38 for 0-10 minutes) but very quickly, we overpredict the Experiment concentrations

- Is there a gas build-up in our Simulations, are we still under resolved?
Hamburg Case 3 Puff – Comments

- As the mean Dosage comparison showed, the Simulation overpredicts consistently the Experiments

- This is reinforced by the scatter plot of the 95 percentile Dosage for which the FAC2 is 0.75

- This could also denote a too coarse resolution so we refined the Grid around the city centre
Increasing the resolution has no impact on the averaged Concentration as all the Probes lie close to the slope 1 curve on the left scatter plot.

As a result, the correlation for the Continuous case remains poor, as shown by the right plot.
The concentration levels are reduced for the increased resolution case

The FAC2 is 0.5, in the acceptance range defined by Hanna & Chang
Hamburg Case 3 Puff – Increased Resolution

- Shown left is the difference of the averaged Velocity fields for the original and the increased resolution Simulations.
- We see here that the Velocity increases in the centre of the model.
- Velocity decreases in the more open areas, around the densely built area.
Hamburg Case 3 Puff – Increased Resolution

0 to 5 minutes Gas Averaged Concentration Fields
Hamburg Cases – Next Steps

- Finalizing the setup in terms of Resolution
  - Puff case is OK, but not the Continuous case
  - Results seem to improve though
  - Test finer resolution scheme(s)

- Investigate on better matching the boundary conditions and possibly the fidelity of our Simulation Model

- Test proof our future BP vs. another Experiment / City?
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La Défense Setup

Wind direction varies in time

Wind speed [m/s]

Boundary conditions in time

Gaz S1:
- Punctual source
- Gas: Amoniac; $C_d = 1.59 \times 10^{-5} \text{ m}^2/\text{s}$
- 1.918 tons for 2 min

Gaz S2:
- Surface source (puddle)
- Gas: Amoniac; $C_d = 1.59 \times 10^{-5} \text{ m}^2/\text{s}$
- Decreases by steps over 45 min

Gas mass flow [kg/s]

Wind direction

Time [min]
Gas S1 Concentration Volume Visualization
Velocity & S1 Concentration Histories in Z plane (Ground +2m)
Dangerous Areas Mapping
# Probe Time Metrics

<table>
<thead>
<tr>
<th>Probe</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean Dosage (mg/m^3)</td>
<td>376</td>
<td>802</td>
<td>9489</td>
<td>2971</td>
<td></td>
</tr>
<tr>
<td>Concentration Peak (mg/m^3)</td>
<td>1.6</td>
<td>2.0</td>
<td>85.6</td>
<td>12.2</td>
<td></td>
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<tr>
<td>Arrival Time</td>
<td>1840</td>
<td>1740</td>
<td>330</td>
<td>1050</td>
<td>2410</td>
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<tr>
<td>Peak Time</td>
<td>1960</td>
<td>3690</td>
<td>330</td>
<td>1050</td>
<td>3050</td>
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<tr>
<td>Leaving Time</td>
<td>5220</td>
<td>5180</td>
<td>920</td>
<td>3420</td>
<td>3650</td>
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<tr>
<td>Ascent Time</td>
<td>120</td>
<td>1950</td>
<td>0</td>
<td>0</td>
<td>640</td>
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<tr>
<td>Descent Time</td>
<td>3260</td>
<td>1490</td>
<td>590</td>
<td>2370</td>
<td>600</td>
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<tr>
<td>Duration Time</td>
<td>3380</td>
<td>3440</td>
<td>590</td>
<td>2370</td>
<td>1240</td>
</tr>
</tbody>
</table>
Probe 3 Location – Health Risks Management – S1

![Diagram of Probe 3 Location with health risks management graph showing concentrations at 1 min, 3 min, 10 min, and 30 min intervals.](image)

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Probe 3 Location – Health Risks Management – S2

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Thank you for your attention

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