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Validation of a LPDM against the CUTE experiments of the COST ES1006 Action

Comparison of the results obtained with the diagnostic and RANS versions of the flow model

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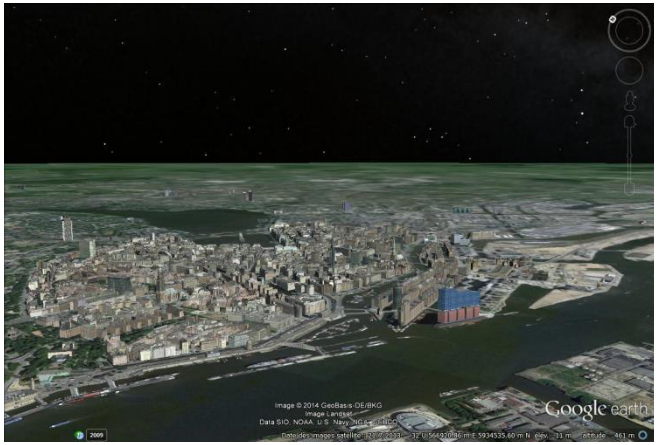
Introduction – Context and aim of this work

- Both accidental and malevolent situations may imply hazmat atmospheric releases
- In this domain, risk studies for regulatory purpose as real-time evaluation carried out for rescue teams and stakeholders make a large use of AT&D modelling / simulation
- If the Gaussian approach seems definitely not adapted to complex environments such as urban districts and industrial sites, « simplified CFD » models offer an alternative approach to « full CFD » which is in principle the reference solution
- Thus, it is essential to compare the advantages and drawbacks of existing models, especially in the case of well-documented experimental campaigns like the Complex Urban Test Experiment (CUTE) performed in the framework of COST ES1006 Action
- In this work, the results of PMSS (Parallel-Micro-SWIFT-SPRAY) with a mass-consistent diagnostic flow model, PMSS with the RANS version of the flow model and Code_SATURNE, a finite volume CFD code, are presented and the differences are discussed

Description of CUTE experimental trials (1)

- In the frame of COST Action ES1006, trials were carried out in a European city and in its mock-up at 1:350 scale, reproduced in the WOTAN atmospheric boundary layer wind tunnel at the Environmental Wind Tunnel Laboratory (EWTL) in Hamburg to provide data for the validation of local scale emergency response models

- The mock-up is placed in the ABL modelled by roughness elements



City centre of Hamburg (left) and its mock-up in the WOTAN wind tunnel (right)

Description of CUTE experimental trials (2)

- For the field trial:
  - The source is located on a boat
  - The tracer is released for 45 minutes with a constant flow rate of 2 g/s
  - The tracer is detected by 20 measurement devices
  - The concentrations are 10-minute averaged

- For the wind tunnel trial:
  - The source is located in the city centre
  - Continuous release: the tracer is released with a constant flow rate of 0,5 kg/s and detected by 34 sensors
  - Puff release: 50 kg of tracer are released during 31 s and detected by 17 sensors
  - Concentration data are measured with fast Flame Ionization Detector (FID)

Flow and dispersion models description (1)

- PMSS (Oldrini, 2011) system includes parallelized models PSWIFT and PSPRAY
  - PSWIFT is a 3D analytically modified mass consistent interpolator over complex terrain and urban areas, able to derive diagnostic turbulence parameters (TKE and dissipation rate) to be used by PSPRAY (especially in flow zones with obstacles)
  - PSPRAY (Tinarelli, 2013) is a LPDM able to take into account the presence of obstacles, derived from the SPRAY code (Tinarelli, 2007) and based on a 3D form of the Langevin equation for the random velocity (Thomson, 1987)
  - A simple model of the momentum conservation equation has been introduced as an option in PSWIFT and this RANS version of the flow uses a zero equation turbulence model based on a mixing-length-based closure

Flow and dispersion models description (2)

- Code_SATURNE (Archambeau et al., 2004) is a 3D CFD model adapted to atmospheric flow and pollutant dispersion, which can handle complex geometry and physics
  - Based on a finite-volume approach for co-located variables on an unstructured grid
  - Time discretization through a fractional step scheme with prediction-correction step
  - Two approaches of the turbulent flows: RANS with two closure models as well as LES
  - In the present work, RANS approach with k–epsilon turbulence closure (turbulence model can take account of the production / destruction rate due to buoyancy)
  - Code_SATURNE is combined with PSPRAY to model atmospheric dispersion

Computational parameters (1)

- Experimental measurements have been converted to full scale using similarity laws; for calculations, we consider the full scale and digital mock-ups are built at this scale

- PMSS and Code_SATURNE run on a structured mesh of 8.7 million nodes with a regular horizontal grid of 625 x 525 nodes and a 4 m resolution, and a vertical grid of 26 nodes from the ground to a height of 200 m with a regular grid inside the urban canopy and a log. progression above

- Input data are an experimental inflow vertical profile given between 10 and 150 m height (standard deviation is associated with each wind component)

- In the wind tunnel, isotherm temperature profile and neutral conditions are considered

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Computational parameters (2)

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- In PMSS, turbulence is diagnosed using parameterizations as the sum of local turbulence, due to the presence of buildings and evaluated with a mixing length method, depending on the distance to the nearest building and « background » turbulence

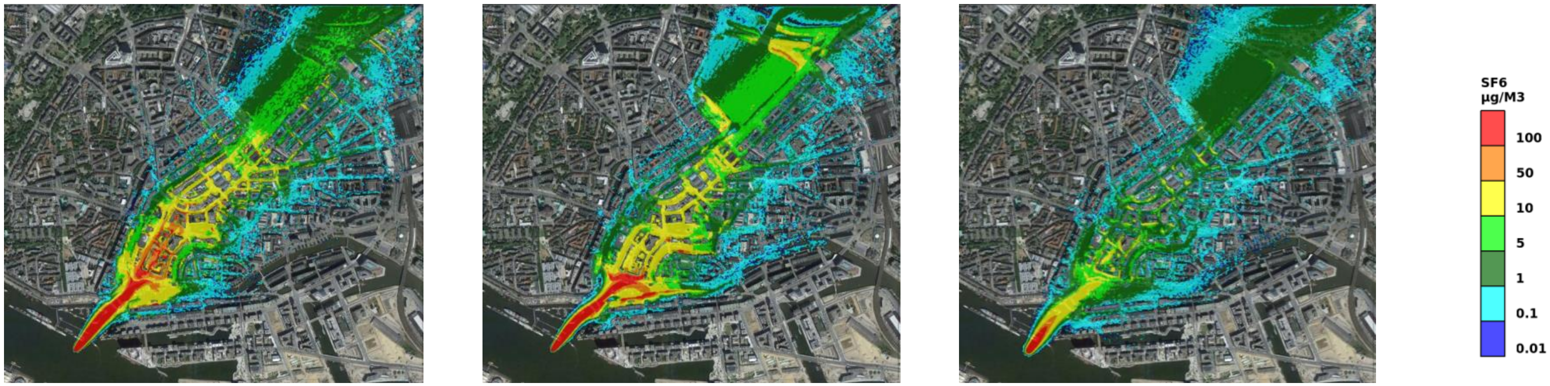
- Background turbulence is estimated with Hanna parameterization (Hanna et al., 1982) and depends, among others, on friction velocity u* which is computed from roughness z_0 and wind speed near the ground

- PMSS momentum model uses a zero equation turbulence model with a mixing-length closure

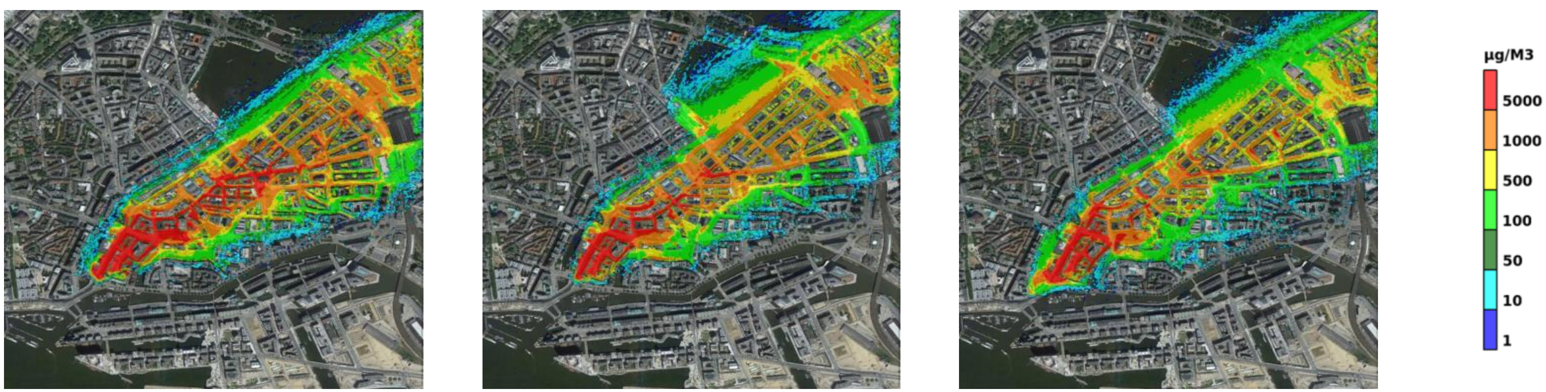
- In Code_SATURNE, turbulence is computed with the k-epsilon model

- For the Lagrangian model PSPRAY, we deal with about 2000 numerical particles per second to describe low concentrations with a sufficient number of particles

PMSS and Code_Saturne concentration fields (1)

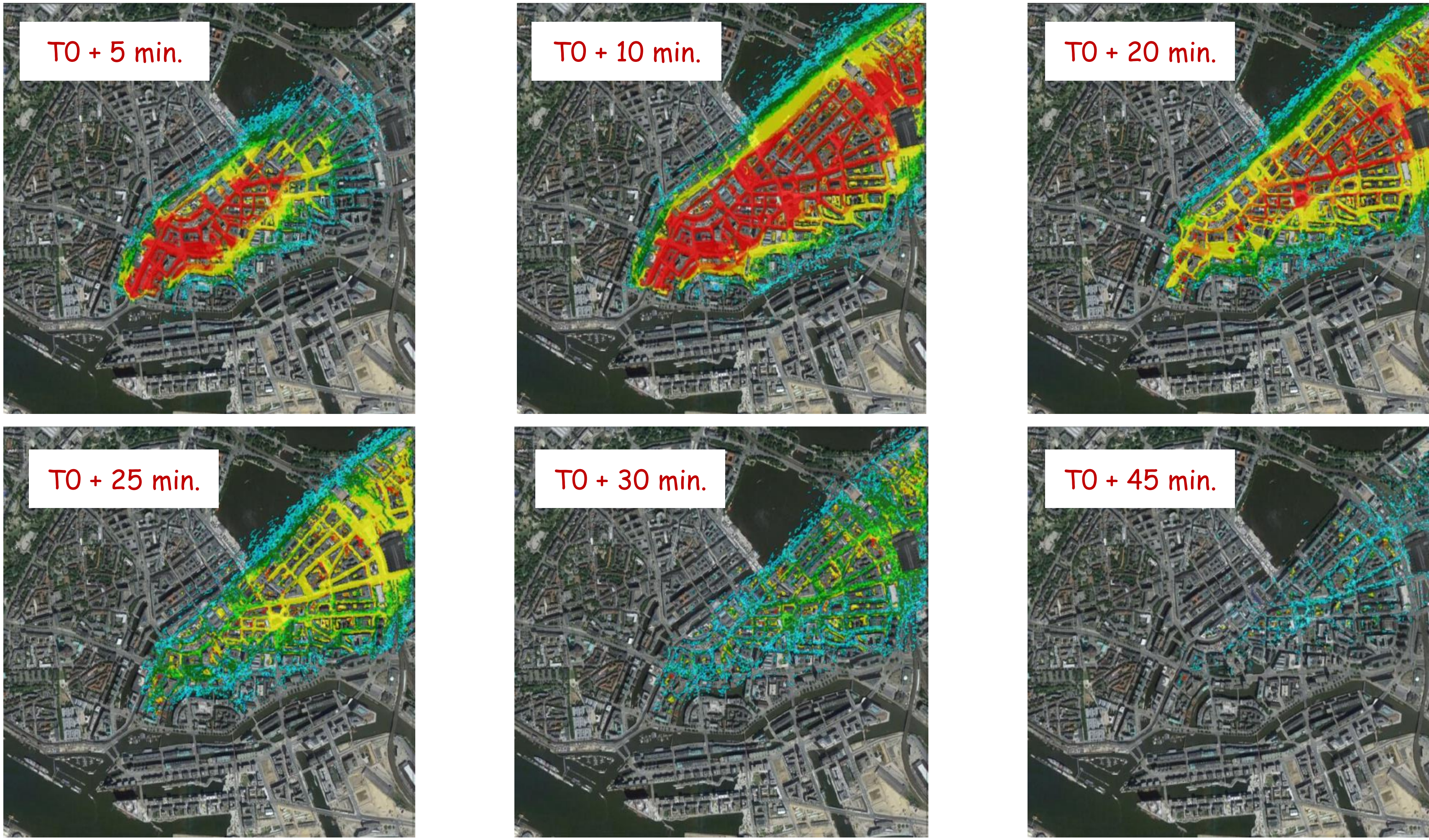


Field experiment / continuous release – Concentration field – Cross-section near the ground
PMSS diagnostic (left) / PMSS momentum (centre) / Code_SATURNE (right)



Wind tunnel experiment / continuous release – Concentration field – Cross-section near the ground
PMSS diagnostic (left) / PMSS momentum (centre) / Code_SATURNE (right)

PMSS and Code_Saturne concentration fields (2)



Wind tunnel experiment / puff release – Concentration field – Cross-section near the ground
PMSS with the flow diagnostic model - Six successive times (in minutes)

PMSS and Code_Saturne concentration fields (3)

- Some areas of the plume obtained with PMSS diagnostic present null or low concentrations contrary to models resolving momentum conservation (PMSS momentum and Code_SATURNE)

- Significant channeling effect towards the east for models with momentum resolution as global effects due to obstacles like channeling or Venturi effects are taken into account

- The plume modelled with Code_SATURNE is shorter than those obtained with both PMSS versions (diagnostic and momentum) due to stronger wind calculated with Code_SATURNE and stronger turbulence in the case of the field experiment

Dispersion results – Statistical performance (1)

- To compare the predictions of PMSS and Code_SATURNE with observations, we use statistical performance measures and criteria recommended by Chang et al. (2004)

[$-0.67 < FB < 0.67$; $NMSE < 6$; $FAC2 > 0.3$]

Statistical performance measures for mean concentrations

Results	Model	FB	NMSE	FAC2
Field experiment / Continuous release	PMSS diagnostic	0.03	6	0.35
	PMSS momentum	-1.08	23	0.31
	Code_SATURNE	1.43	40	0.31
Wind tunnel experiment / Continuous release	PMSS diagnostic	-0.35	1.9	0.38
	PMSS momentum	-0.10	2.2	0.47
Wind tunnel experiment / Puff release	PMSS diagnostic	-0.42	2.6	0.38

Dispersion results – Statistical performance (2)

- For the field experiment:
  - PMSS Diagnostic has (surprisingly) a better score (FB, NMSE, FAC2) than PMSS Momentum and Code_SATURNE
  - FB and NMSE are larger than the acceptance limits
  - FAC2 is within the 0,3 acceptance criterion

  → The Wind direction was not as expected: a relatively small number of sensors was hit by the plume, hence the scores are based on a small number of pairs of measured and computed values where concentrations are significant. Observations and predictions mainly show small concentration values (in a range from 10^{-6} to 10^{-2} ppmv)

  → The comparison of concentration values is quite severe since even small differences between the paired values produce a relatively large scatter.

- For the wind tunnel experiment, the metrics are better and meet the acceptance limits

Sensitivity test (1)

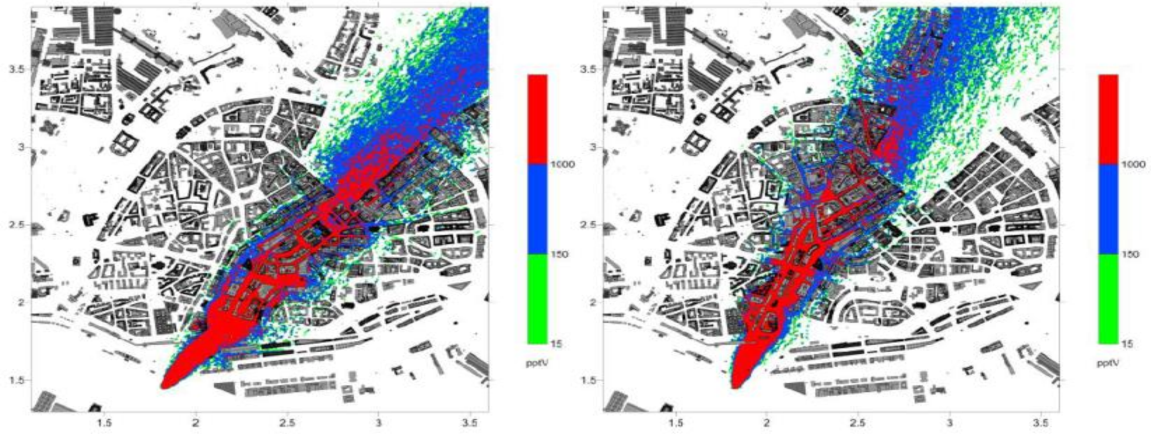
- The initial conditions and their related uncertainty (relatively high in case of accidental release) strongly controls the model results

- A sensitivity test was performed to verify the change in model output to different driving wind data; two different simulations were carried out using:

  - A vertical wind profile calculated starting from the only available measurement at 175 m (the wind direction was kept constant with height)

  - The data measured at a weather mast 8 km away in order to build a wind profile with wind directions varying with height by following the available measurements

Sensitivity test (2)



Field experiment / continuous release – Cross-section near the ground (PMSS diagnostic)
Comparison of concentration field with two wind inlet profiles

- The plume disperses in slightly different directions and the affected areas are different

  → The sensitivity test highlights the importance of having access to appropriate met' input data for modelling in order to achieve more reliable simulations of accidental releases

- It is not easy to provide observed data (in case of sensitive sites)

  → A proper planning of a sensor network is essential in order to increase the support of emergency response tools

Conclusion (1)

- In the frame of the COST Action ES1006, atmospheric dispersion of continuous and puff releases experiments and modelling were carried out in the downtown area of a European city and its mock-up reproduced in the wind tunnel of the Hamburg University

- Simulations to reproduce the flow were performed using PMSS with a mass-consistent diagnostic flow model, PMSS with the RANS version of the flow model, and Code_SATURNE, a finite volume CFD code with a RANS k-epsilon turbulent flow model

- The three flow models are combined with a Lagrangian Particle Dispersion Model

- The comparison of the results highlights the impact of the flow model on the atmospheric dispersion and the importance of taking into account the momentum equation

Conclusion (2)

- Metrics were used to compare the results of codes with field and wind tunnel experiments
  - For the field experiment, the statistical measures indicate biased FB and NMSE, larger than the acceptance limits, but a FAC2 within the 0.3 acceptance criterion
    → Given the low absolute values of the concentrations, the differences between observed and predicted data are small, but they have a large relative importance
    → Real field data are characterized by a higher degree of variability and uncertainty with respect to the carefully controlled, quasi-stationary wind tunnel conditions
  - For the wind tunnel experiment, results are in a good agreement with measures (all metrics satisfy defined criteria)

- The sensitivity tests highlight the importance of having access to appropriate met' input data for modelling in order to achieve more reliable simulations of accidental releases
  → In case of sensitive sites, a proper planning of a sensor network is essential to increase the support of the emergency response tools

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Questions?

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