DE LA RECHERCHE À L'INDUSTRIE

COMPARISON OF SIMPLIFIED AND FULL CFD MODELLING OF ACCIDENTAL DISPERSION – APPLICATION TO THE 2013 MICHELSTADT EXPERIMENTAL TRIALS

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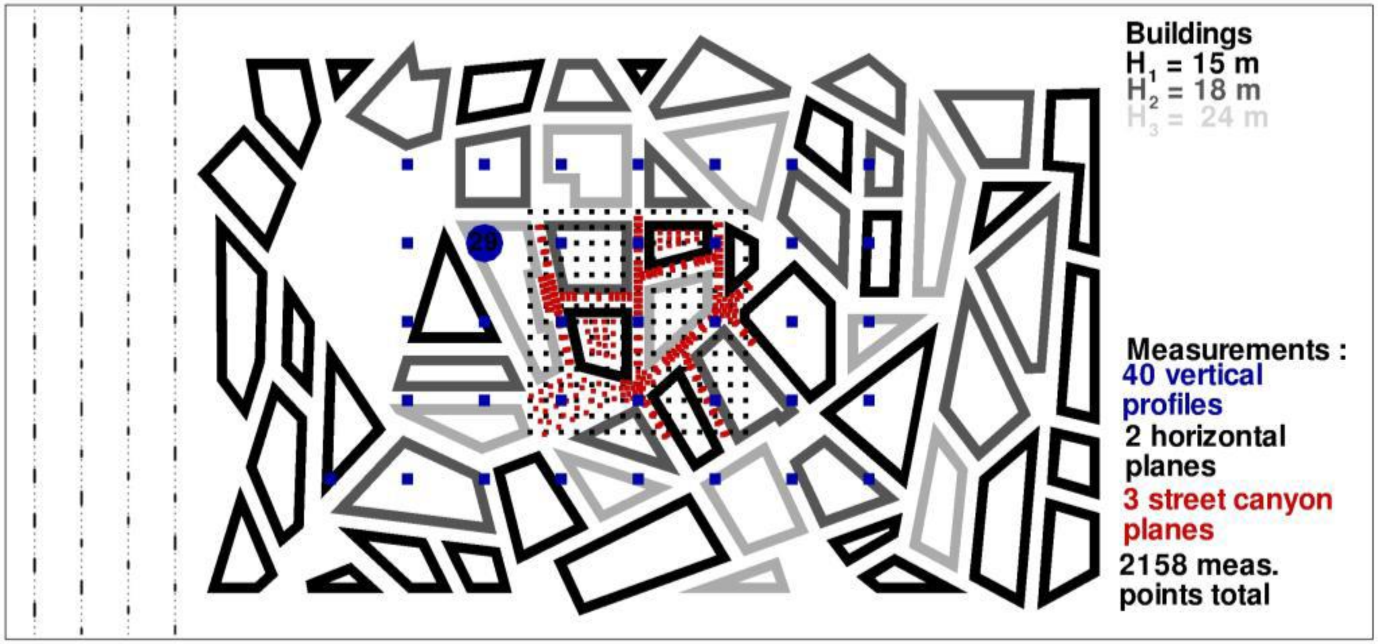
Introduction – Context and aim of this work

- Both accidental and malevolent situations may imply hazmat atmospheric releases
- Consequences on health and environment of these incidents have to be assessed (even if fortunately, all are not as serious as Fukushima, Chernobyl, Seveso, Bhopal...)
- In this domain, both risk studies for regulatory purpose and 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 releases performed around the Michelstadt mock-up in the wind tunnel of the Hamburg University
- In this work, the results of Parallel-Micro-SWIFT-SPRAY (PMSS) and Code_SATURNE are presented and a discussion is proposed about the differences between the results and what should be improved in the models to try to reduce them

Description of Michelstadt experimental trials (1)

- In the frame of COST Action ES1006, trials were carried out 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 represents at 1:225 scale an idealized Central European urban mock-up, called Michelstadt, placed in the ABL modelled by roughness elements

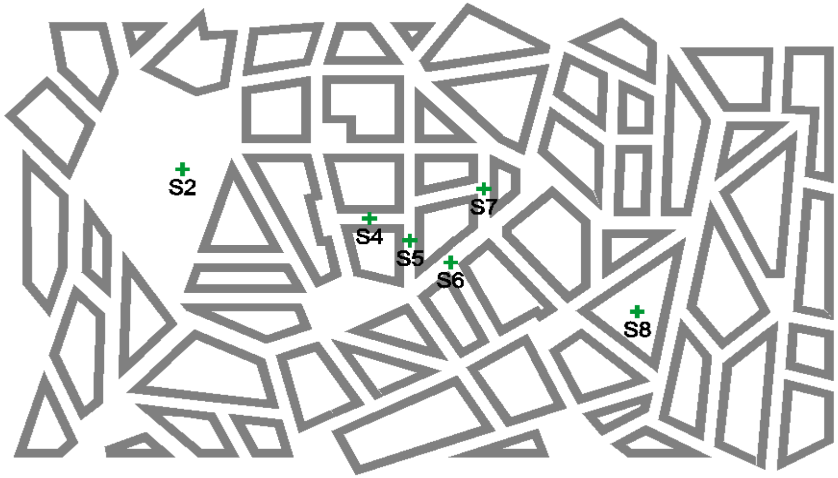
Computational domain with buildings and wind velocity measurements



Description of Michelstadt experimental trials (2)

- Measurements
  - Two-component velocity data time series collected with LDV in 40 vertical profiles, 2 horizontal planes and 3 street canyon planes
  - Concentration data for continuous and short term release modes collected with fast FID in many points downwind, in a 7.5 meter-height plane, and in some vertical profiles, up to 110 meters height
- During the measurements, 5 point sources were used non-simultaneously in continuous and short term release mode, and two opposite wind directions were investigated

Sources positions



- In this presentation, results reported for continuous releases and both wind directions
  - The 1st one is non-blind case with three source locations (S2, S4 and S5)
  - The 2nd one is blind case, with four source locations (S5, S6, S7 and S8)

Flow and dispersion models description

- 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 the flow zones modified by 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)

- 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 a 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 was used (turbulence model can take account of the production / destruction rate due to buoyancy)

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 works on a structured mesh of 3.6 million nodes with a regular horizontal grid of 451 x 301 nodes and a 3 m resolution, and a vertical grid of 27 nodes from the ground to a height of 200 m with a regular grid inside the urban canopy and log. progression above
- Code_SATURNE works on an unstructured mesh of about 6.6 million of tetrahedrons; smallest meshes are near buildings with a size of 2-3 m; mesh is coarser in the middle of streets with a size of 5 m and many more above the urban canopy
- Input data are an experimental inflow vertical profile given between 10 and 150 m height (standard deviation is associated with each wind component)
- As in the wind tunnel, isotherm temperature profile and neutral conditions are considered

Computational parameters (2)

- 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

  N.B. z_0 *is chosen to keep the same surface stress between the value computed by PMSS and the value deduced from the standard deviation measurements using Stüll formula*
- For the Lagrangian model PSPRAY, we deal with about 4.6 million of numerical particles for each release to describe low concentrations with a sufficient number of particles

Typical duration of a computation

Model	CPU time	Number of cores	Computation time
PMSS	6 h 30 min	8	50 min
Code_SATURNE	652 h	240	2 h 40 min

Results – General statistical performance

- To compare the predictions of PMSS and Code_SATURNE with observations, statistical performance measures and criteria recommended by Chang *et al*. (2004) are used
  [- 0.3 < FB < 0.3 ; 0.7 < MG < 1.3 ; NMSE < 4 ; VG < 1.6 ; FAC2 > 0.5]

Statistical performance measures for U and V wind components and concentrations

Results	Model	FB	MG	NMSE	VG	R	FAC2
U wind component	PMSS	-0.046		0.170		0.895	0.688
V wind component	PMSS					0.489	0.265
Concentrations (non blind)	PMSS	0.105	1.095	2.154	3.936	0.602	0.635
	SATURNE	-0.272	1.395	2.878	24.719	0.833	0.625
Concentrations (blind)	PMSS	0.358	1.714	9.014	8.501	0.372	0.451

Dispersion results – Statistical performance

- For concentration results in the non-blind case, a good agreement between the results of both models and observations is obtained as all the defined criteria are satisfied
  - Geometric variance for SATURNE is the single value outside the limits, but as some values are computed equal to zero to represent low concentrations, this parameter loses its full meaning
  - Results are even better if we consider only the release from source S2, with a parameter FAC2 growing up to 0.684; more generally, agreement with observations is better when release occurs on an open place, like source S2, rather than in the middle of a street canyon like sources S4 and S5

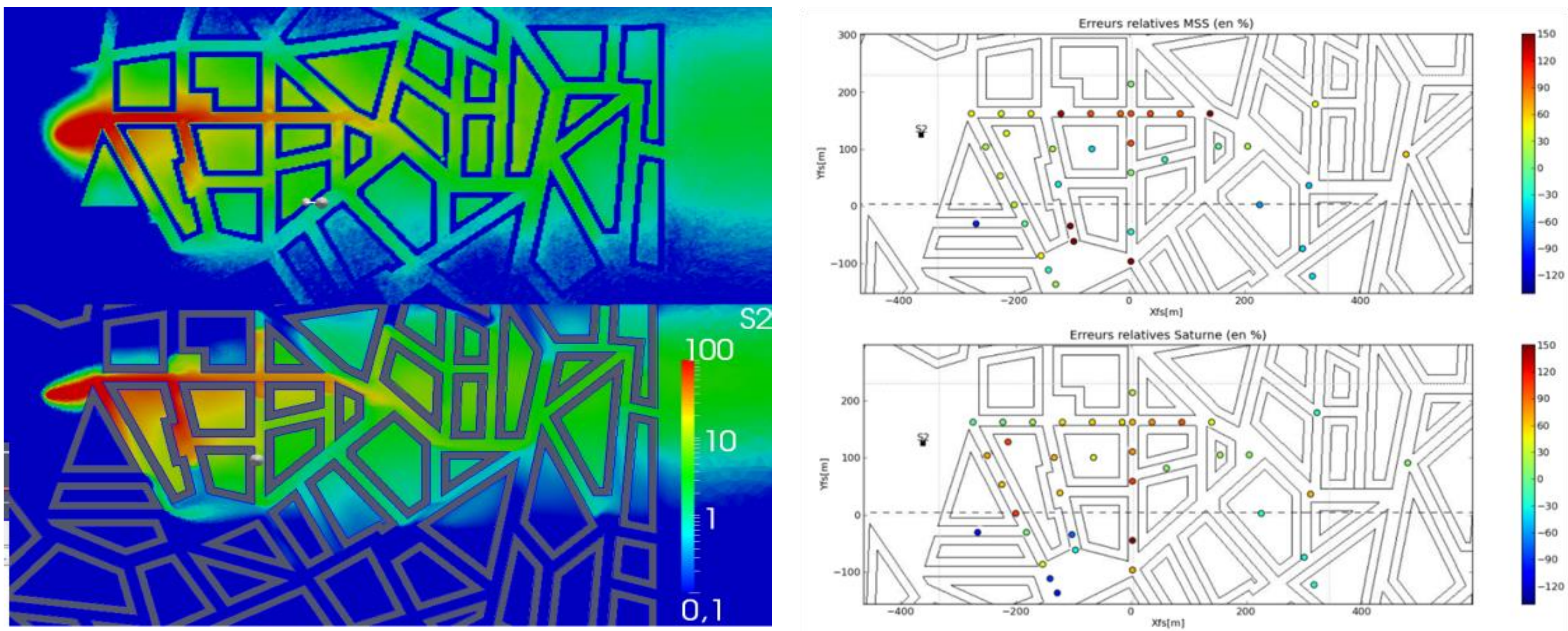
- For concentration results in blind case, statistical numbers are less good because releases occur in more complex environments, at a crossroads (sources S6 and S7) or inside an enclosed courtyard (source S8)

Dynamics results – Statistical performance

- Statistical numbers for PMSS are inside defined criteria for the longitudinal component of wind, but not for the transverse component; nevertheless, consequences on dispersion are limited because the transverse component of wind is low and transverse dispersion is mainly due to turbulent diffusion
- Measurements of standard deviation show the anisotropy inside streets canyon between the horizontal components of wind (with a standard deviation in the axis of the street more important than the standard deviation perpendicular to the axis of the street); PMSS diagnosed only a horizontal and a vertical standard deviation, so that standard deviation for U and V components are equal everywhere in the computation domain
- In PMSS, parameterizations which modify the interpolated wind field around buildings are defined for a single building or between two buildings in case of a street canyon; rules are established to deal with places where there are several wind modified zones but they certainly do not cover every cases of urban configurations

PMSS and SATURNE concentration fields (S2)

- Although statistical numbers are similar for both models, concentration fields are slightly different for source release S2; transverse diffusion appears to be more important with PMSS as with SATURNE, but both models overestimate concentrations inside the street parallel to the mean flow, and underestimate concentrations on the sides of the plume

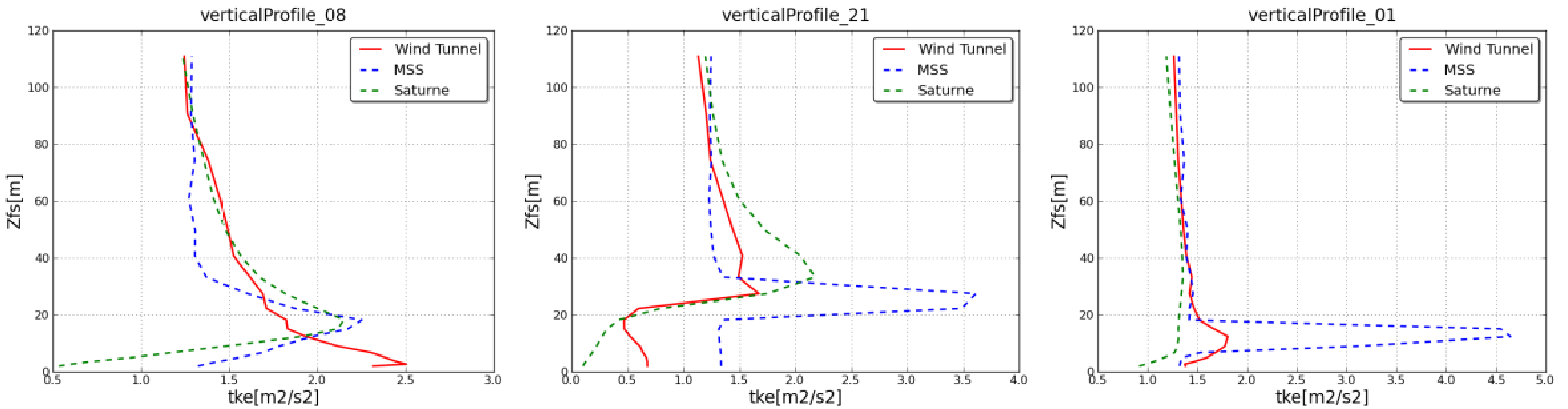


Concentration field at a height of 7.5 m and relative errors compared to observations for continuous release from source S2 (PMSS at the top and SATURNE at the bottom)

PMSS and SATURNE TKE vertical profiles (S2)

- Mean TKE is well diagnosed or assessed by both models, particularly above 40 m; however, SATURNE underestimates TKE near the ground quite everywhere in the domain while PMSS overestimates TKE at a height corresponding to the roofs of buildings
- As PSWIFT does not conserve momentum, the transition between urban canopy and the atmosphere above may be brutal with strong local wind shears; TKE is thus overestimated and boosts the tracer transfer from the urban canopy to the atmosphere above roofs with higher advection limiting the fall of the plume inside streets far away from the release point

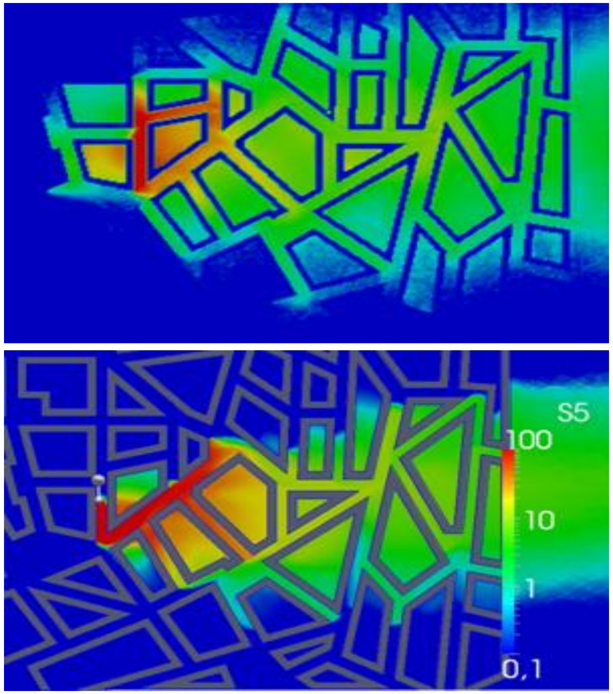
  $\Rightarrow$ Most of points far away from sources have under-predicted concentrations (FB > 0)

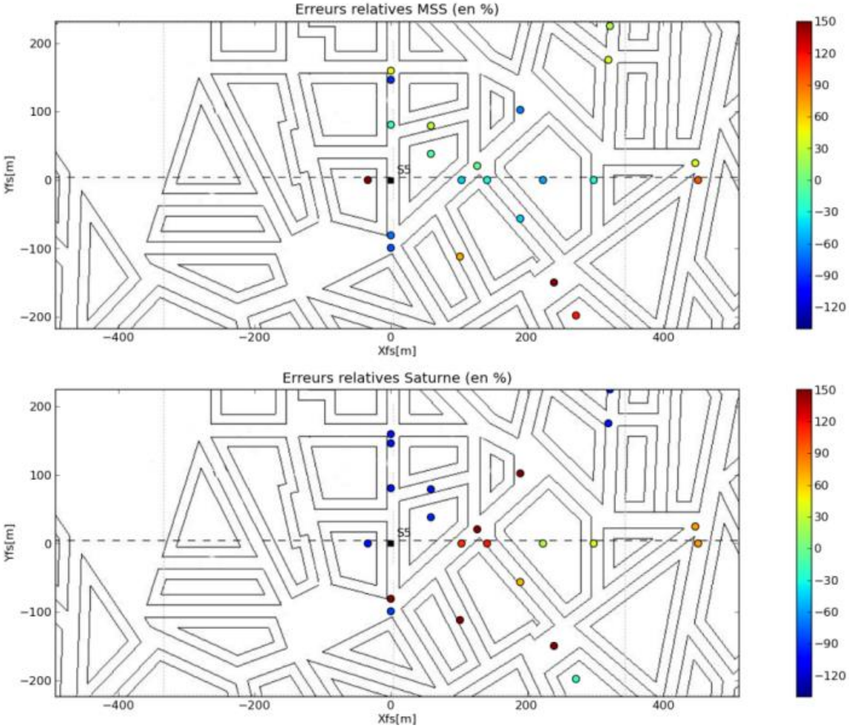


Vertical profiles of TKE upwind a building (left), inside a street canyon (middle) and downwind (right)

PMSS and SATURNE concentration fields (S5)

- Results for source release S5 highlight the underestimation of TKE by Code_SATURNE (especially for the points located in the North of S5)
- Release occurs inside a street canyon and plume moves only to the South of the street

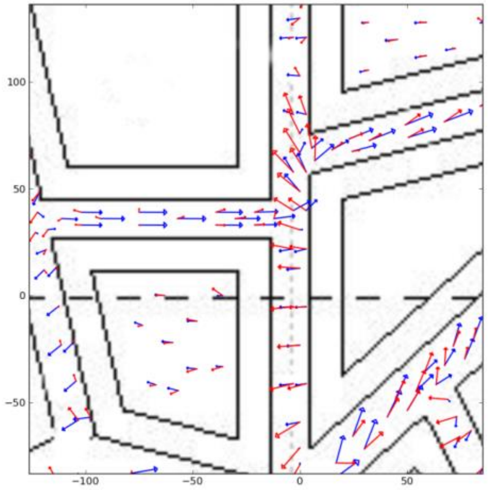


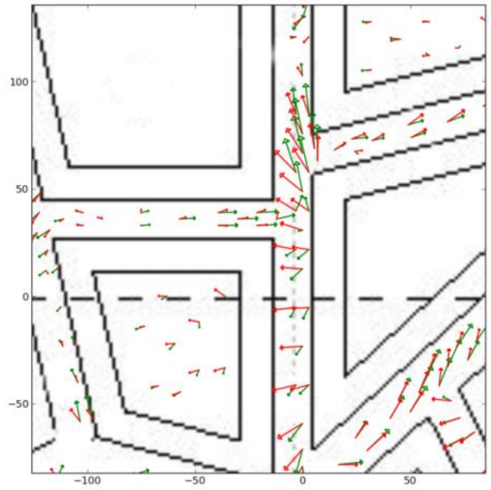


Concentration field at a height of 7.5 m and relative errors compared to observations for continuous release from source S5 (PMSS at the top and SATURNE at the bottom)

PMSS and SATURNE concentration fields (S5)

- Wind simulated by SATURNE blows to the South inside that street and, as very low TKE values are assessed near ground, motion of the plume near S5 is only due to advection
- Near S5, the wind simulated by PMSS agrees with the observations, with a direction perpendicular to the street; in this case, the horizontal motion of the plume inside the street near S5 is primarily due to turbulent diffusion; vertically, an eddy takes place inside the street and allows to a part of the plume to rise up above the canopy





- As seen before, TKE is over-estimated by PMSS at roofs' height so that a larger as expected part of the plume moves inside the enclosed courtyard upwind where PMSS over-estimates the concentration

Wind field at a height of 7.5 m near sources S4 and S5 (PMSS in blue, SATURNE in green and obs. in red)

Conclusion and perspectives (1)

- Flow and dispersion of continuous releases carried out in the Michelstadt mock-up have been performed using Code_SATURNE, a RANS k-epsilon turbulent flow model and an Eulerian approach for dispersion model, and PMSS, a mass-consistent diagnostic flow model combined with a LPDM

- Methods and metrics proposed in the frame of COST ES1006 project have been used to compare results of both models with experiments
  - Results for the non-blind case are in a good agreement with measures, as all metrics satisfy defined criteria
  - For the blind case, as sources are located inside a more complex environment in terms of flow, values assessed for the metrics decrease
  - Compared with the results of other modellers involved in COST Action ES1006, performances of PMSS and Code_SATURNE are similar to equivalent models

Conclusion and perspectives (2)

- A fine analysis of results obtained for dynamic quantities highlights that PMSS gives strong wind shears at roofs' level and then, strong and overestimated TKE, because PSWIFT model does not consider the conservation of momentum

  ⇒ *Introduction in PMSS of a simplified model for momentum conservation is in progress and is going to allow to compute smoother wind profile between the urban canopy and free atmosphere above, and then to diagnose a more realistic TKE profile*

- Although turbulence is well assessed on average in PMSS, standard deviation is a derived variable consisting in vertical and horizontal components, thus cannot consider horizontal anisotropy as it is observed locally, especially inside streets canyon

  ⇒ *This should be a future topic to improve the PMSS model*

- Finally, results show that PMSS, as a simplified CFD approach, can produce realistic and very acceptable results for complex urban environments, and in a very short time, compared to CFD models, compatible to deal with an emergency situation

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Thank you

Questions?

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