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

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**Abstract**: In the frame of the European COST Action ES1006, this paper presents the comparison of PMSS and Code_ SATURNE results with trials corresponding to various source locations and release conditions, carried out on the mock-up representing the idealized urban city of Michelstadt. Results of the codes show a good agreement with the experiments of both codes and, as computation time for PMSS is very short, give credence to the use of simplified CFD models to deal with emergency situations, when they occur in a complex environment.

***Key words:*** *COST Project ES1006, Michelstadt experiment, AT&D modelling, CFD, numerical and experimental comparison.*

## INTRODUCTION

Numerous accidental situations as malevolent activities imply the atmospheric release of hazardous materials. Even if all events are not as serious as Chernobyl or Fukushima nuclear accidents and Seveso or Bhopal chemical disasters, consequences on health and environment of all kinds of incidents on industrial sites or during transport operations have to be assessed. In this domain, experience feedback on past events, risk studies for regulatory purpose, or real-time evaluation carried out for rescue teams and stakeholders make a large use of AT&D modelling and simulation. Many models are available from the simplest to the most advanced and detailed ones with very different computational resources requested. 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 continuous or short tracer releases performed around the Michelstadt mock-up in the wind tunnel of the Hamburg University. In this context, two codes were used: Parallel-Micro-SWIFT-SPRAY (PMSS), a simplified CFD model, and Code_SATURNE, a full CFD model. This paper presents the Michelstadt experimental trials, a short description of the two models, flow field and atmospheric dispersion results which are compared to measurements, and finally, a discussion about observed differences and what should be improved in the models to try to reduce them.

## DESCRIPTION OF THE MICHELSTADT EXPERIMENTAL TRIALS

In order to provide data for the validation of local scale emergency response models 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. The mock-up represents at 1:225 scale an idealized Central European urban environment model, called Michelstadt, placed in the atmospheric boundary layer modelled by roughness elements. For measurements, two-component velocity data time series were collected with Laser Doppler Velocimetry (LDV) in 40 vertical profiles, 2 horizontal planes and 3 street canyon planes (see Figure 1). Concentration data for continuous and short term release modes were collected with fast Flame Ionization Detector (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. In the present paper results are reported for continuous release mode and both wind directions. The first one corresponds to a non-blind case *i.e.* where observations are known, with three different source locations (S2, S4 and S5), the second one to a blind case, with four different source locations (S5, S6, S7 and S8).

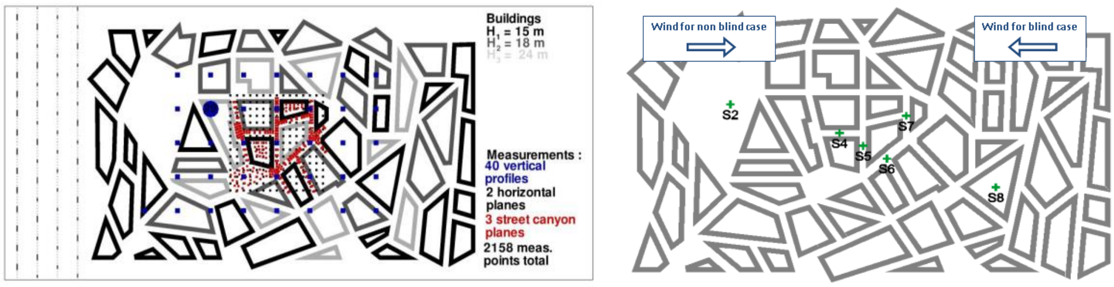


**Figure 1.** Computational domain with buildings, wind velocity measurement positions and sources positions.

## MODELS DESCRIPTION

The PMSS modelling system (Oldrini *et al.*, 2011) includes parallelized models PSWIFT and PSPRAY. PSWIFT is an analytically modified mass consistent interpolator over complex terrain and urban areas. Given topography, meteorological data and building geometry, a mass consistent 3-D wind field is generated. It is also able to derive diagnostic turbulence parameters (namely the Turbulent Kinetic Energy, TKE, and its dissipation rate) to be used by PSPRAY especially inside the flow zones modified by obstacles. PSPRAY is a Lagrangian particle dispersion model (LPDM) able to take into account the presence of obstacles. It is directly derived from the SPRAY code (Tinarelli *et al.*, 2007 and 2013) and based on a 3D form of the Langevin equation for the random velocity (Thomson, 1987).

Code_SATURNE (Archambeau *et al.*, 2004) is a three-dimensional CFD model adapted to atmospheric flow and pollutant dispersion, which can handle complex geometry and complex physics. The numerical model is based on a finite-volume approach for co-located variables on an unstructured grid. Time discretization of the Navier–Stokes equations is achieved through a fractional step scheme, with a prediction-correction step. In Code_SATURNE, two approaches can be used to deal with turbulent flows: the Reynolds averaged Navier–Stokes method (RANS) with the choice between two closure models, as well as the large-eddy simulation (LES) method. In the present paper, we use a RANS approach with a k–epsilon turbulence closure. The turbulence model can take account of the stratification of the atmosphere through the production or destruction rate due to buoyancy.

## COMPUTATIONAL PARAMETERS

Experimental measurements have been converted to full scale using similarity laws. For calculations with both codes, we consider that we are at the full scale and digital mock-ups are built at this scale. PMSS works on a structured mesh with a regular horizontal grid of 451x301 nodes and a 3-meter resolution, and a vertical grid of 27 nodes, from the ground to a height of 200 meters, with a regular grid inside the urban canopy and a logarithmic progression above. It leads to a computational grid with about 3.6 million nodes. 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 meters; mesh is coarser in the middle of streets with a size of 5 meters and many more above the urban canopy.

Input data consist of an experimental inflow vertical profile, given between 10 and 150 m height. Associated with each wind component is given the standard deviation. As we are in a wind tunnel, we consider an isotherm profile for temperature and therefore, neutral conditions. Unlike Code_SATURNE, where turbulence is performed with the k-epsilon model, with PMSS, turbulence is diagnosed using parameterizations. We consider here turbulence 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, depending on the neutral atmospheric conditions we have supposed. Background turbulence is estimated with Hanna parameterization (Hanna *et al.*, 1982) and depends, among others, on surface stress u*. PMSS computes u* from roughness $z_0$ and wind speed near the ground. We decide to fix $z_0$ in the order 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, so that we can describe low concentrations with a sufficient number of numerical particles. Despite this, computation times remain short compared to those of Code_SATURNE, as it is shown in Table 1.

**Table 1.** Duration to compute all non-blind releases.

| 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

In order to evaluate the predictions of PMSS and Code_SATURNE with observations, Chang *et al.* (2004) recommend the use of statistical performance measures, which include the fractional bias (FB), the geometric mean bias (MG), the normalized mean square error (NMSE), the geometric variance (VG), the correlation coefficient (R), and the fraction of predictions within a factor of two of observations (FAC2). For the Michelstadt test case, we compare these statistical measures with the following criteria to assess if there is a good agreement between computational results and observations, for both dynamic quantities and concentrations [-0,3 < FB < 0,3 ; 0,7 < MG < 1,3 ; NMSE < 4 ; VG < 1,6 ; FAC2 > 0,5 ].

For concentration results in the non-blind case, table 2 shows a good agreement between results of both codes and observations, as all the defined criteria are satisfied. Geometric variance for Code_SATURNE is the single value outside the limits we have fixed, 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 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). In PMSS, parameterizations which modify the first 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, as configuration of buildings varying a lot in realistic urban environments, they cannot cover every case.

Regarding dynamic results for PMSS, statistical number are inside defined criteria for the longitudinal component of wind, but not for the transverse component. Nevertheless, consequences on dispersion are limited because, in the transverse direction, the component of wind is low and transverse dispersion is mainly due to turbulent diffusion. Moreover, measures of standard deviation shows anisotropy inside streets canyon between the two 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 of wind are considered equal everywhere on the computation domain.

**Table 2.** Statistical performance measures for dynamic (U and V wind components) and concentrations.

| Results | Model | FB | MG | NMSE | VG | R | FAC2 |
|---|---|---|---|---|---|---|---|
| Dynamic U | PMSS | -0.046 | | 0.170 | | 0.895 | 0.688 |
| V | PMSS | | | | | 0.489 | 0.265 |
| Concentrations (non blind) | PMSS | 0.105 | 1.095 | 2.154 | 3.936 | 0.602 | 0.635 |
| | Code_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 |

Although statistical numbers are similar for both codes, concentration fields are slightly different, as shown in figure 2 for source release S2. Transverse diffusion appears to be more important with PMSS as with Code_SATURNE, but both codes slightly overestimate concentrations inside the street parallel to the mean flow, and underestimate concentrations on the sides of the plume.

Looking at turbulent kinetic energy (TKE) profiles, as shown in figure 3 at different places in the domain (upwind or downwind a building, or inside a street canyon), explains the shape of plumes. Mean TKE is well diagnosed or assessed by both codes, particularly above a height of 40 meters. However, Code_ SATURNE underestimates TKE near the ground almost everywhere on the domain. On another hand, PMSS overestimates TKE at a height corresponding to the roofs of buildings. In PMSS, TKE is the sum of a ground turbulence which is about constant on the domain, and a local turbulence diagnosed from wind shear with parameterizations based on a mixing length method. As PSWIFT computes a mass consistent 3D wind field, without conserving momentum, the transition between urban canopy and the atmosphere above may be brutal so that important wind shears are performed locally. TKE is also locally important and overestimated. As a consequence, it boosts transfer of the tracer from the urban canopy where it has been emitted, to the free atmosphere above roofs where advection is higher, and it avoids the fall of the plume inside streets far away from the release point. Then, most of points far away from sources have under-predicted concentrations and fractional bias FB is positive, indicating a mean under-estimation of concentrations.

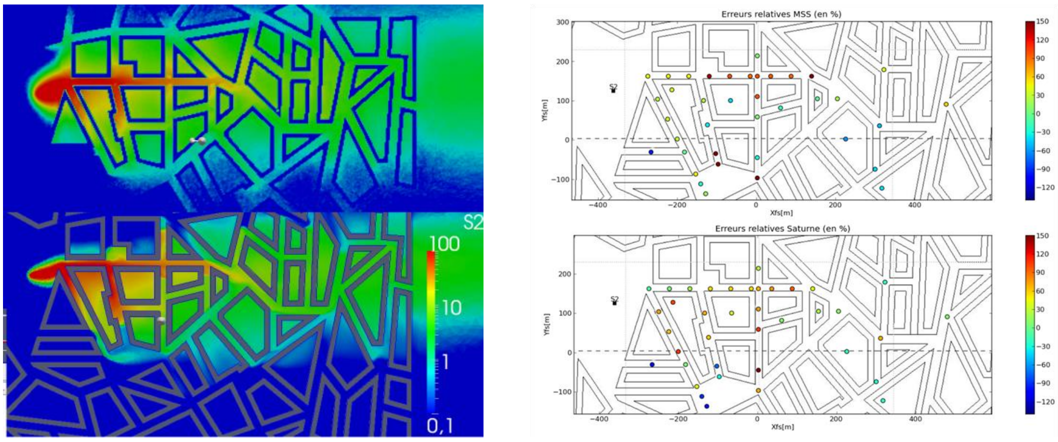


**Figure 2.** Concentration field at a height of 7.5 m and relative errors compared to observations for continuous release from source S2 (PMSS at the top and Code_SATURNE at the bottom).

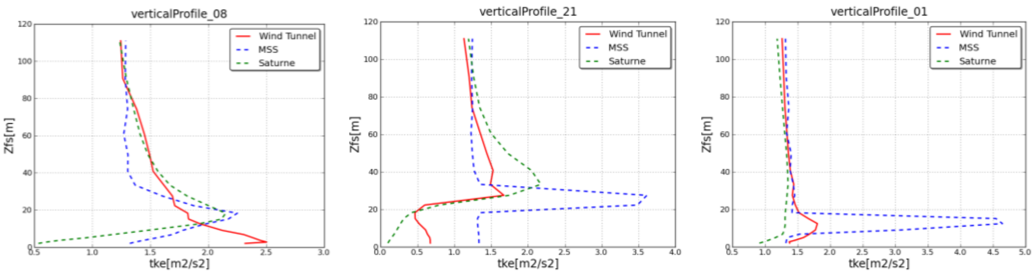


**Figure 3.** Vertical profiles of TKE upwind a building (left), inside a street canyon (middle) and downwind (right).

Results for continuous release source S5 presented in figure 4, highlight the underestimation of TKE by Code_SATURNE. In this case, observed concentrations at points located in the north of the release point S5 are largely under-estimated by the model. The release occurs inside a street canyon and plume moves only to the South of the street. Looking at wind field inside the urban canopy (figure 5) confirms that wind simulated by Code_SATURNE blows to the South inside that street and, as very low TKE values are assessed near the ground, the motion of the plume near the release point S5 is only due to advection.

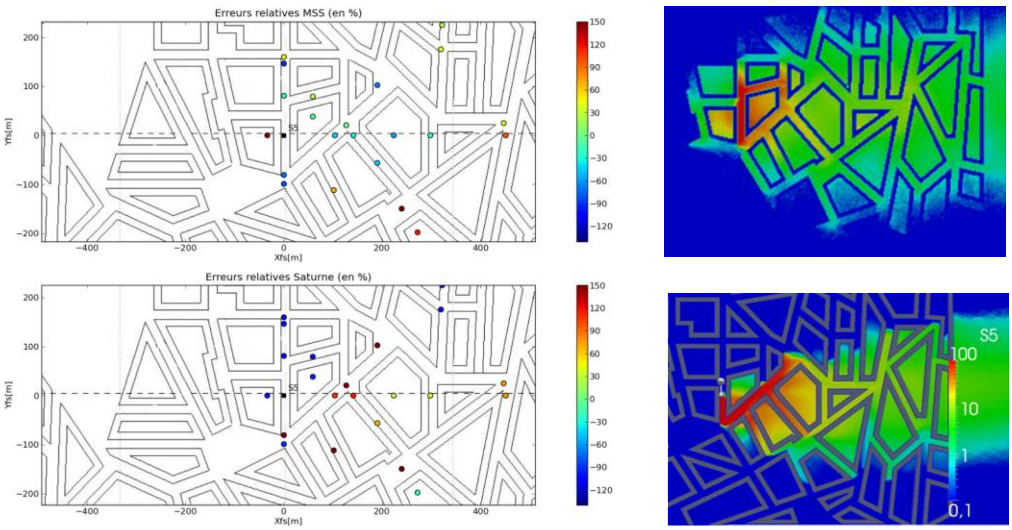


**Figure 4.** Concentration field at a height of 7.5 m and relative errors compared to observations for continuous release from source S5 (PMSS at the top and Code_SATURNE at the bottom).

Near release point S5, wind simulated by PMSS agrees with observations, with a direction perpendicular to the street for both. In this case, the horizontal motion of the plume inside the street near source S5, is primarily due to turbulent diffusion. Vertically, an eddy takes place inside the street and allows to part of the plume to rise up above the urban canopy.

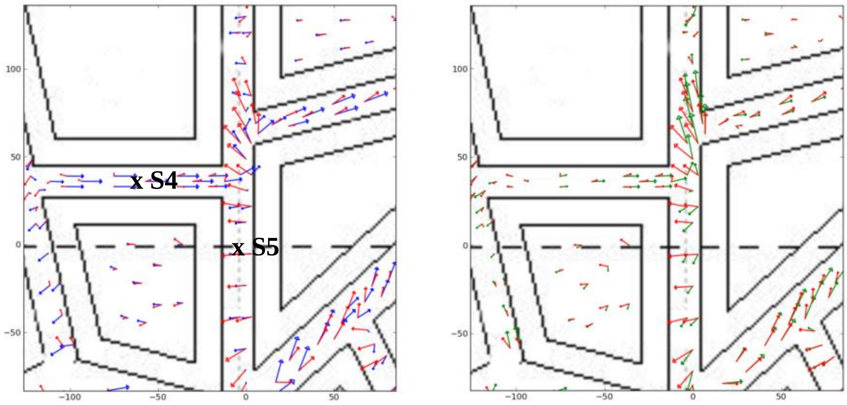


**Figure 5.** Wind field at a height of 7.5 m near sources S4 and S5 (PMSS in blue, Code_SATURNE in green and observations in red).

As seen before, TKE is overestimated at roofs' height so that a larger as expected part of the plume, rising up the street canyon, moves inside the enclosed courtyard upwind, where PMSS code over-estimates concentration, as shown in figure 4.

## CONCLUSIONS

Simulations to reproduce flow and atmospheric dispersion of continuous releases carried out on the mock-up representing the idealized urban city of Michelstadt, were performed using Code_SATURNE, a finite volume CFD code on unstructured meshes with 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 Lagrangian Particle Dispersion Model. The methods and metrics proposed in the frame of COST ES1006 project were used to compare results of both codes 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 modelers involved in COST Action ES1006, performances of PMSS and Code_SATURNE are similar to equivalent models.

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's conservation is a work 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, standard deviation, as a derived variable, consists of a vertical and a horizontal component in PMSS, which 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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