17th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
9-12 May 2016, Budapest, Hungary

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 MODELS

Christophe Duchenne[1], Patrick Armand[1], Maxime Nibart[2], and Virginie Hergault[3]

[1]CEA, DAM, DIF, F-91297 Arpajon, France
[2]Aria Tecnologies, F-92100 Boulogne-Billancourt, France
[3]Alten, F-92100 Boulogne-Billancourt, France

Abstract: In the frame of the European COST Action ES1006, this paper presents the comparison of PMSS diagnostic, PMSS momentum, and Code_SATURNE results with trials carried out in the city of Hamburg and in its mock-up. The results comparison highlights the impact of the modelling approaches on the atmospheric dispersion and the importance of taking into account the momentum equation. For the field experiment, some of the statistical measures are larger than the acceptance limits due to the low values of the concentrations and the high degree of variability and uncertainty of the real field data. The metrics for the wind tunnel experiment are better and meet the acceptance limits. Finally, the sensitivity tests show the importance of having access to appropriate meteorological input data for modelling in order to achieve more reliable simulations of accidental releases.

Key words: *Diagnostic flow, momentum equation, LPDM, COST ES1006, CUTE experiments, validation.*

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 making use of modelling and simulation. Several 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 Complex Urban Test Experiment (CUTE). The CUTE dataset includes results from field and wind tunnel measurement, carried out in the downtown area of the city of Hamburg and in its mock-up, reproduced in the wind tunnel of the Hamburg University. Measurements of concentration resulting from continuous or short tracer releases were utilized in 2014 as a test-bed for modellers involved in the European COST Action ES1006. In this respect, two codes were used: Parallel-Micro-SWIFT-SPRAY (PMSS), a simplified CFD model combined with a Lagrangian Particle Dispersion Model PSPRAY, and Code_SATURNE, a full CFD code with a RANS k-ε turbulent flow model also combined with PSPRAY. A comparison of PMSS results, obtained on one hand with the diagnostic fast-response version of the flow model (PMSS diagnostic) and with its RANS version on another (PMSS momentum), has been performed. Results of the codes are compared together and with the experiments using the methods and metrics proposed in the frame of the project. This paper presents the CUTE experimental trials, a short description of codes, atmospheric dispersion results which are compared to measurements, and finally, a sensitivity analysis on the initial conditions.

DESCRIPTION OF THE CUTE EXPERIMENTAL TRIALS

In order to provide data for the validation of local scale emergency response models in the frame of COST Action ES1006, the CUTE dataset includes results from field and wind tunnel measurement, carried out in the downtown area of the city of Hamburg and in its mock-up at 1:350 scale, reproduced in the WOTAN atmospheric boundary layer wind tunnel at the Environmental Wind Tunnel Laboratory in Hamburg (see Figure 1). For the field trial, the source was located on a boat and the tracer (SF_6) was released continuously for 45 minutes with a constant flow rate of 2g/s. The tracer was detected by 20 measurement devices and each recorded concentration represents a 10-minute average concentration. For the wind tunnel dataset, concentration time series of tracer from continuous and puff releases were measured with fast Flame Ionization Detector (FID). The source was located in the city center. Firstly, the tracer was released continuously with a constant flow rate of 0.5kg/s and detected by 34 sensors. Then, 50kg of tracer were released during 31s and detected by 17 sensors.

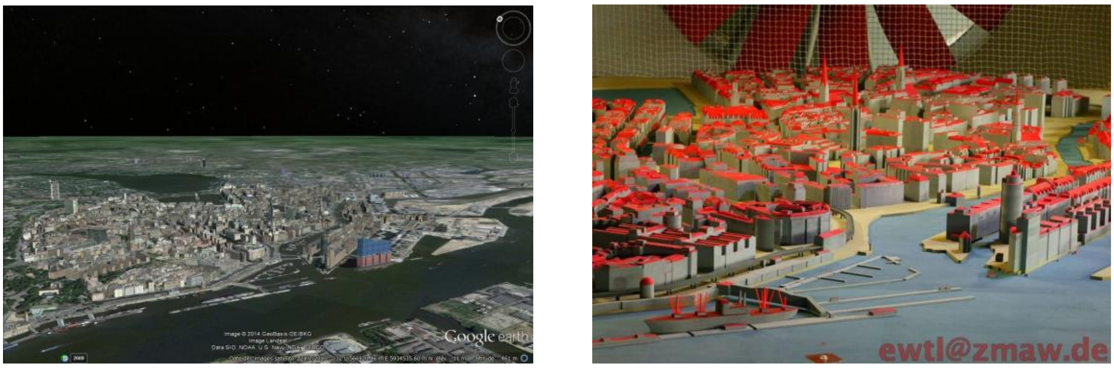

Figure 1. City centre of Hamburg (left) and its mock-up in the WOTAN wind tunnel (right)

MODELS DESCRIPTION

The Parallel-Micro-SWIFT-SPRAY (PMSS) modelling system (Tinarelli et al., 2013; 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 3D 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., 1994 and 2007). It is based on a 3D form of the Langevin equation for the random velocity (Thomson, 1987).

A simplified model of momentum equation has been introduced as an option in PMSS and this RANS version of the flow uses a zero equation turbulence model with a mixing-length-based closure.

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-ε turbulence closure. The turbulence model can take into account the stratification of the atmosphere through the production or destruction rate due to buoyancy. In this paper, Code_SATURNE is combined with PSPRAY to model atmospheric dispersion.

COMPUTATIONAL PARAMETERS

Wind tunnel measurements have been converted to full scale using similarity laws. For calculations, we consider that we are at the full scale and digital mock-ups are built at this scale. PMSS (diagnostic and momentum) and Code_SATURNE work on a structured mesh with a regular horizontal grid of 625x525 nodes and a 4-meters resolution, and a vertical grid of 26 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 8.7 million nodes.

Input data consist of an experimental inflow vertical profile. A standard deviation is associated with each wind component. We consider an isotherm profile for temperature and therefore, neutral conditions. In PMSS diagnostic model, turbulence is diagnosed using parameterizations. We consider turbulence as the sum of the local turbulence due to the presence of buildings, evaluated with a mixing length method depending on the distance to the nearest building, and the background turbulence depending on the atmospheric conditions we have supposed (here, neutral). Background turbulence is estimated with Hanna parameterization (Hanna et al., 1982) and depends, among others, on surface stress u*. PMSS computes u* from roughness z0 and wind speed near the ground. We decide to fix z0 in 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.

Unlike Code_SATURNE, where turbulence is performed with the k-ε model, PMSS momentum model uses a zero equation turbulence model with a mixing-length-based closure.

For the Lagrangian model PSPRAY, we deal with about 2000 numerical particles per second, so that we can describe low concentrations with a sufficient number of numerical particles.

All cases were run as blind tests, having minimum input information available for the model simulations, as it would be the case during a real accident.

RESULTS

Figure 2 and Figure 3 show concentrations near the ground obtained with PSPRAY from the three flow models (PMSS diagnostic, PMSS momentum and Code_SATURNE) for the field and wind tunnel experiment respectively. 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). Furthermore, there is a significant channeling effect towards the east for models with momentum resolution. Indeed, momentum enables to take into account global effects due to obstacles like channeling or Venturi effects. Besides, the plume modelled with Code_SATURNE is shorter than those obtained with both PMSS versions (diagnostic and momentum) due to stronger wind fields calculated with Code_SATURNE and a stronger turbulence in the case of the field experiment.

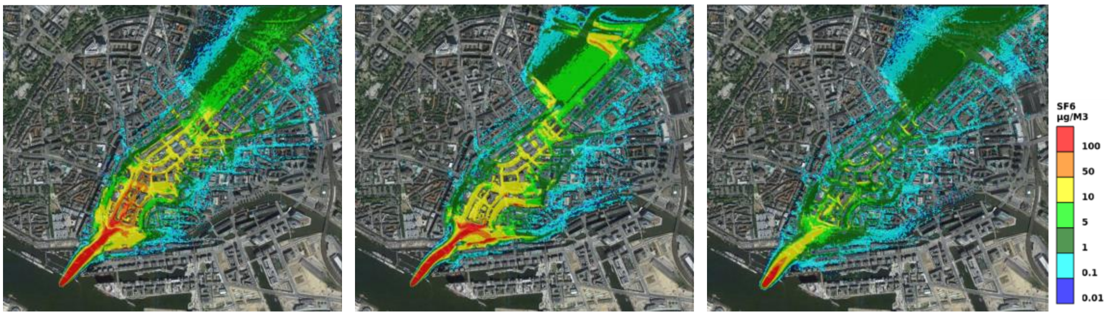

Figure 2. Field experiment / continuous release – Concentration field – Cross-section near the ground
PMSS diagnostic (left) / PMSS momentum (centre) / Code_SATURNE (right)

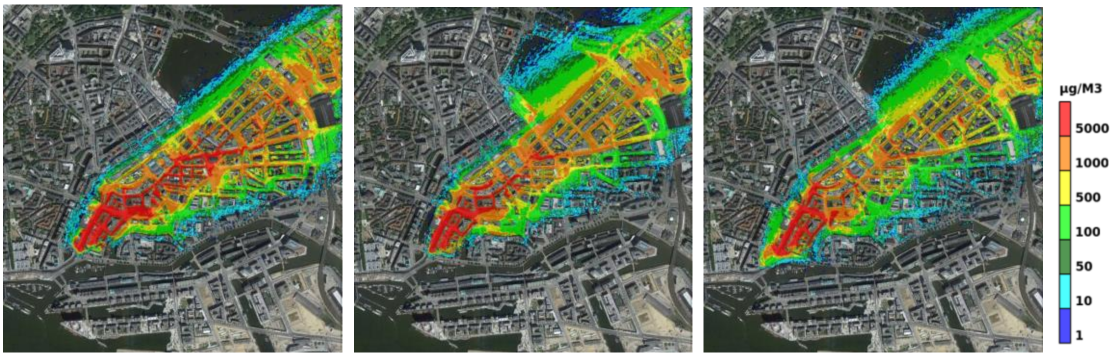

Figure 3. Wind tunnel experiment / continuous release – Concentration field – Cross-section near the ground
PMSS diagnostic (left) / PMSS momentum (centre) / Code_SATURNE (right)

In order to evaluate the predictions of models (here, PMSS and Code_SATURNE) against observations, Chang et al. (2004) recommend the use of statistical performance measures, which include the fractional bias (FB), the normalized mean square error (NMSE), and the fraction of predictions within a factor of two of the observations (FAC2). These statistical measures have to be compared with the following criteria to assess if there is a good agreement between computational results and observations for the concentrations.

-0,67 < FB < 0,67 ; NMSE < 6 ; FAC2 > 0,3

For the field-experiment, the continuous release results are shown considering ten-minute averaged concentration and for the wind tunnel experiment, five-minute averaged concentration.

In Table 1, the summarized statistics for continuous and puff releases are reported. In the case of the field experiment, the statistical measures indicate biased FB and NMSE, larger than the acceptance limits. In contrast, a FAC2 within the 0.3 acceptance criterion can be noticed. Observations and predictions mainly show small concentration values, in a range from 10^{-6} to 10^{-2} ppmv. Consequently, the comparison of concentration values is quite severe since even small differences between the paired values produce a relatively large scatter. The metrics for wind tunnel experiment are better and meet the acceptance limits.

Table 1. 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

The initial conditions and input data are among the key items, and their related uncertainty which is assumed to be relatively high in case of accidental release, strongly controls the model results. Sensitivity analysis was run for different turbulence conditions and wind data needed as input for models (see the companion paper by Tinarelli et al., 2016).

A sensitivity test was performed to verify the change in model output to different driving wind data. Two different simulations were carried out. In the first one, a vertical wind profile was calculated starting from the only available measurement at 175 m. The wind direction was kept constant with height. In the second one, the data measured at a weather mast 8 km away was used to build a wind profile with wind directions varying with height by following the available measurements.

In Figure 4, the effect of the different wind input conditions is visible as the plume disperses in slightly different directions and the affected areas are substantially different. The sensitivity test highlights the importance of having access to appropriate meteorological input data for modelling, characterizing, for example, the vertical variability of wind direction, in order to achieve more reliable simulations of accidental releases. While, in general, it is not easy to provide such kind of observed data, in case of known sensitive sites such as for instance industrial plants, a proper planning of a net of sensors becomes essential for optimum support in the use of emergency response tools.

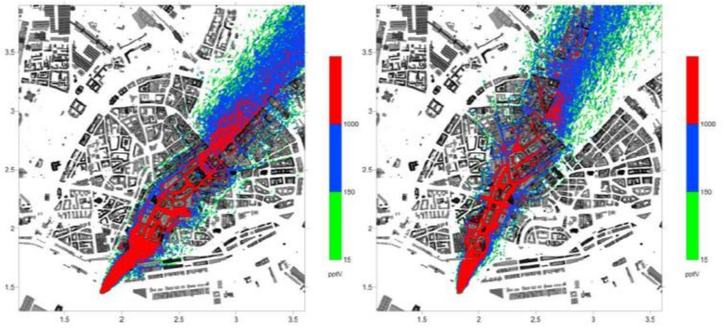

Figure 4. Field experiment / continuous release – Cross-section near the ground (PMSS diagnostic) Comparison of concentration field with two wind inlet profiles

CONCLUSIONS

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 the city of Hamburg and its mock-up, reproduced in the wind tunnel of the Hamburg University. Simulations to reproduce 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. A comparison of results highlights the impact of the flow model on the atmospheric dispersion and the importance of taking into account the momentum equation.

Methods and metrics (FB, NMSE, FAC2) proposed in the frame of the project, were used to compare results of codes with field and wind tunnel experiments. In the case of 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 characterizing this case, the differences between observed and predicted data are small, but they have a large relative importance. Moreover, real field data are characterized by a much higher degree of variability and uncertainty with respect to the carefully controlled, quasi-stationary wind tunnel conditions, and this has a consequence in evaluating the performances of the models. Results for the wind tunnel experiment are in a good agreement with measures, as all metrics satisfy defined criteria.

Compared with the results of other modellers involved in the COST Action ES 1006, performances of PMSS and Code_SATURNE are similar to equivalent models in their categories.

Finally, the sensitivity tests highlight the importance of having access to appropriate meteorological input data for modelling in order to achieve more reliable simulations of accidental releases. In case of known sensitive sites, a proper planning of a net of sensors becomes essential for optimum support in the use of emergency response tools.

REFERENCES

Archambeau F, N. Mechitoua and M. Sakiz, 2004: Code_SATURNE: a finite volume code for the computation of turbulent incompressible flows - industrial applications. *Int. Journal on Finite Volumes*, **1**, 1-62

Chang J. C. and S. R. Hanna, 2004: Air quality model performance evaluation. *Meteorology and Atmospheric Physics*, **87**, 167-196

Hanna, S. R., G. A. Briggs and R. P. Hosker Jr: 1982, ‘Handbook on Atmospheric Division’, *U.S. Dept. of Energy report DOE/TIC-11223*, Washington, DC.

Oldrini O., C. Olry, J. Moussafir, P. Armand and C. Duchenne, 2011: Development of PMSS, the parallel version of Micro-SWIFT-SPRAY, *14th International Conference on Harmonisation within Atmospheric Dispersion Modelling fir Regulatory Purposes*, Harmo’14, Kos (Greece), Oct. 2-6, 2011.

Thomson D.J., 1987: Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *J. Fluid Mech.*, **180**, 529-556

Tinarelli G., D. Anfossi, G. Brusasca, E. Ferrero, U. Giostra, M.G. Morselli, J. Moussafir, F. Tampieri and F. Trombetti, 1994: Lagrangian particle simulation of tracer dispersion in the lee of a schematic two-dimensional hill. *Journal of Applied Meteorology*, **33**, N. 6, 744-756

Tinarelli G., G. Brusasca, O. Oldrini, D. Anfossi, S. Trini Castelli and J. Moussafir, 2007: “Micro-Swift-Spray (MSS) a new modelling system for the simulation of dispersion at microscale. General description and validation”. *Air Pollution Modelling and its Applications XVII*, C. Borrego and A.N. Norman eds., Springer, 449-458

Tinarelli, G., L. Mortarini, S. Trini-Castelli, G. Carlino, J. Moussafir, C. Olry, P. Armand, and D. Anfossi, 2013: Review and validation of Micro-SPRAY, a Lagrangian particle model of turbulent dispersion. *Lagrangian Modeling of the Atmosphere, Geophysical Monograph, Volume 200, AGU*, pp. 311-327, May 2013.

Tinarelli G., M. Nibart, P. Armand and S. Trini Castelli, 2016: A sensitivity analysis for a Lagrangian particle dispersion model in emergency-response test cases, *17th International Conference on Harmonisation within Atmospheric Dispersion Modelling fir Regulatory Purposes*, Harmo’17, Budapest (Hungary), May 9-12, 2016. *To be published.*