18th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
9-12 October 2017, Bologna, Italy

ANALYSIS OF SIMULATION RESULTS ISSUED BY A LATTICE BOLTZMANN METHOD IN COMPLEX URBAN ENVIRONMENTS – APPLICATIONS TO PARIS AND HAMBURG

Patrick Armand [1], Christophe Duchenne [1], Boris Fechner[2], Erwan Le Loc'h[2] and Frédéric Gille[2]

[1]CEA, DAM, DIF, F-91297 Arpajon, France
[2]Exa Corporation, Le Madeleine, 76 Route de la Demi-Lune, 92057 Paris La Défense, France

Abstract: This paper presents the main features and results of 3D numerical simulations in an urban environment. The city centre of Hamburg has been chosen to run these simulations, and a Lattice-Boltzmann CFD solver has been used to compute both the flow field of the wind and the plume propagation in the street network after the release of a tracer in the air. The objective of such simulations is to establish response scenarios to accidental or provoked gas / chemical release in urban areas.

Key words: *CFD, Lattice-Boltzmann, simulation, flow, passive scalar, urban environment, concentration.*

INTRODUCTION

In general, advanced flow simulations in built-up (urban or industrial) environment are carried out using "conventional" CFD codes, most of them based on RANS solvers (Reynolds-Averaged Navier-Stokes) or LES solvers (Large-Eddy Simulation). Alternative methods presented for instance in Duchenne *et al*. (2016) or in Armand et al. (2017) are less time consuming as they rely on a simplified 3D diagnostic or RANS flow modelling coupled to a Lagrangian Particle Dispersion Model (LPDM).

This study is dedicated to the presentation of an approach that is still not much used in the environmental CFD. It is based on a Lattice-Boltzmann solver for modelling of both the fluid flow and the tracer (gas or fine particles) dispersion. This approach has several characteristics that significantly differ from classical CFD methods. One main difference is the unsteadiness of the Lattice-Boltzmann solver which notably enables to capture the transient behaviour of the flow, thus of the plume propagation. References to this method can be found in Chen *et al.* (2004), Chen *et al.* (2003), Chen *et al.* (1992) and Teixeira (1998).

The software used in this study is PowerFLOW which has been developed by Exa Corporation for twenty years. PowerFLOW is extensively used in the transportation industry, especially the automotive one. In the field of environment, some large scale simulations have been performed in the past (e.g. to study wind forces on buildings for architectural purposes), but they are not the core application of PowerFLOW.

Since March 2014, PowerFLOW has been equipped with a module adapted to the computation of passive scalar variables in the flow field. The dispersion of a tracer represented by a passive scalar is computed in parallel with the flow variables (pressure, velocity, etc.) using PDE (Partial Differential Equations). The passive scalars may be gases or fine aerosol particles associated to chemical pollutants, radionuclides or pathogenic biological agents, etc.

Last year, the Lattice-Boltzmann approach was applied to a fictitious dispersion in two large urban simulation domains: "La Défense" business district located west of Paris and Hamburg city centre (Boisseranc *et al*., 2016). These simulations were carried to assess the ability of PowerFLOW software to tackle such applications. As the outcome seemed encouraging and the results sensible, we decided in this year's study to correlate the Hamburg city centre case against experimental data and to further analyse the "La Défense" case by considering transient post-processing. The present paper describes the case of Hamburg with some details while for the case of "La Defense" not all the post-processing is completed.

In the case of Hamburg, we discuss how the environmental conditions are taken into account, and how the simulation is set-up. Then, a statistical analysis of the results is performed to validate / correlate the PowerFLOW results versus the experimental results from the CUTE trials (Complex Urban Terrain Experience) performed in the framework of the COST ES1006 Action (Baumann-Stanzer *et al*., 2015). CUTE trials were carried out in the wind tunnel of the Hamburg University over the mock-up of a Central Europe city, and at full-scale downtown the same city. These experiments implied the release of tracer gases towards the complex urban environment of the city centre.

PRESENTATION OF THE "HAMBURG CASES"

In this study, three test-cases were simulated:
* CASE 1: in-field test, continuous gas release from a boat on the river crossing the city for 45 minutes;
* CASE 3 – continuous: wind tunnel test, continuous gas release for 1 hr at a constant rate of 0.5 kg/sec;
* CASE 3 – puff: wind tunnel test, quasi-instantaneous gas release (puff) of 50 kg in 31 seconds.

Hereafter, we consider the continuous and puff releases conducted downtown Hamburg. The purpose of the study is to model this trial using PowerFLOW Lattice-Boltzmann code with its passive scalar module.

Simulation set-up

The simulations consider the complex geometry of the buildings, terrain and land-use (ground elevation, river, etc.). During the whole experiment and simulation, the meteorological conditions are considered as constant but they are different for each case. For CASE1, the direction of the wind is 219° (wind from south-west). The wind speed varies with the height above the ground to represent a typical atmospheric boundary layer profile. This wind profile has been recreated considering the velocity at 175 m (equal to 8.9 $m.s^{-1}$) and a neutral atmosphere. The gas source is located on a boat on the river crossing the city (location is shown in **Figure 1**). The tracer gas is released during 45 minutes at a constant mass rate of 2 $g.s^{-1}$. The gas used in the experiment was SF_6 which has a diffusion coefficient D = 1.5 10^{-5} $m^2.s^{-1}$.

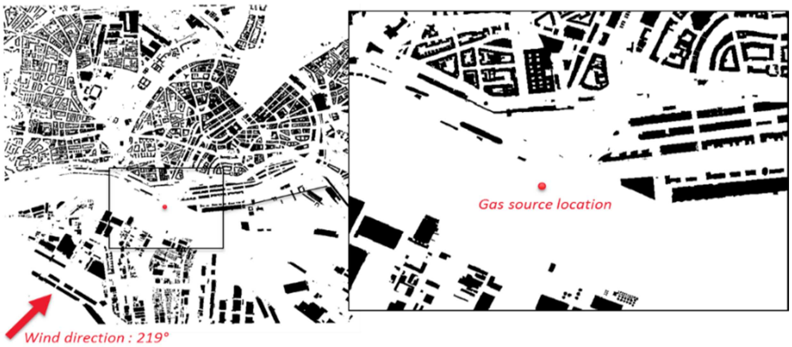

Figure 1: Wind direction and tracer gas source location for CASE1.

For both CASE3 simulations (continuous and puff), the direction of the wind is 235° (wind from south-west). The wind profile has been set up considering the velocity at 49 m (equal to 6 $m.s^{-1}$) and a neutral atmosphere. The gas source is located in the city centre. For the continuous case, the tracer gas is released during 60 minutes at a constant mass rate of 0.5 $kg.s^{-1}$. For the puff case, it is released at the start of the experiment in puffs; 50 kg are released in 31 seconds.

Regarding the numerical resolution, the smallest fluid element size is 0.5 m close to the source of the gas. Except from the source area, the rest of the domain is meshed with a smallest cell size of 2 m. The size of the elements increases gradually away from the geometrical obstacles to optimize the computational cost while guaranteeing the boundary layers as well as the flow phenomena correctly modelled. The largest cell size reaches 64 m far away from any building. As for the computed physical duration, the flow field is simulated during 75 minutes, from t_0 – 15 min to t_0 + 60 min, t_0 being the time at which the tracer starts to be released. The simulation is started 15 minutes before the tracer is released in order to reach a stabilized flow field, this to ensure a steady diffusion of the tracer.

Simulation computational cost

We performed three simulations, one per validation case. Below is the computational cost of each simulation on different clusters:
* CASE1 – 21 hours on 308 CPU, hence 6428 CPU hours (simulation hours multiplied by CPUs);
* CASE3 – continuous – 20 hours on 439 CPU, hence 8897 CPU hours;
* CASE3 – puff – 23 hours on 280 CPU, hence 6464 CPU hours.

RESULTS AND ANALYSIS OF THE "HAMBURG CASES"

Averaged flow field analysis

Figure 2 shows the time-averaged velocity field over the tracer release period using streamlines at 10 m above the ground level for CASE1 and CASE3 (wind direction and velocity being the same for CASE3 simulations, the flow field is the same for these simulations).

In both cases, several areas can be distinguished (see **Figure 2**) and are commented:

1. As the city centre is densely built-up, the velocities in this area are low (blockage effect).
2. Areas with no building or sparsely built-up have higher velocities (over the river and the lake).
3. Some local accelerations of the wind ("Venturi effects") are due to narrowing between buildings.
4. "Wind corridors" are present around the city centre.

If the averaged flow field shows the same specific areas, the overall direction of the wind is of course different and the velocity is slightly higher for the CASE3 simulations. This is particularly true in the corridors areas (zone 4), where the velocity is much higher for CASE3.

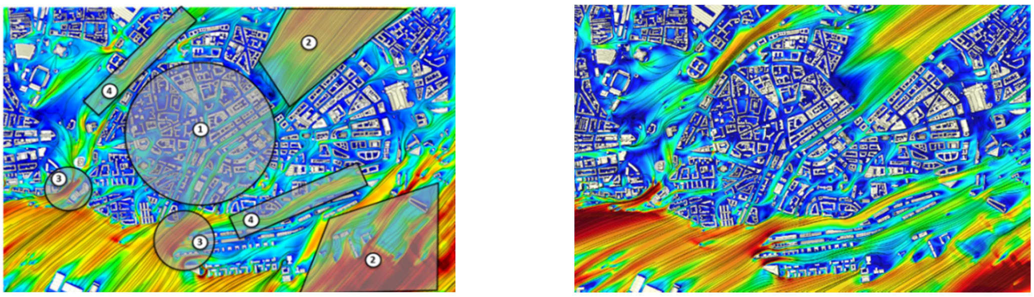

Figure 2: Time-averaged velocity at 10 m above the ground level. Left: CASE1 with zone definition, Right: CASE3.

Figures 3 & 4 show the averaged concentration field over the 60 min. of stabilized flow field simulation for CASE1 and CASE3-cont, over 5 minutes periods for CASE3-puff (presented at 2 m above the ground level with a logarithmic scale). This enables to visualize the propagation of the tracer along with the wind. For each simulation, the plume follows the wind direction. Thus, the concentration plots look alike with the higher concentration areas contained in the densely-constructed areas where the blockage due to the buildings prevents the tracer to dissipate efficiently. For CASE3-puff, high concentration levels show fast decay.

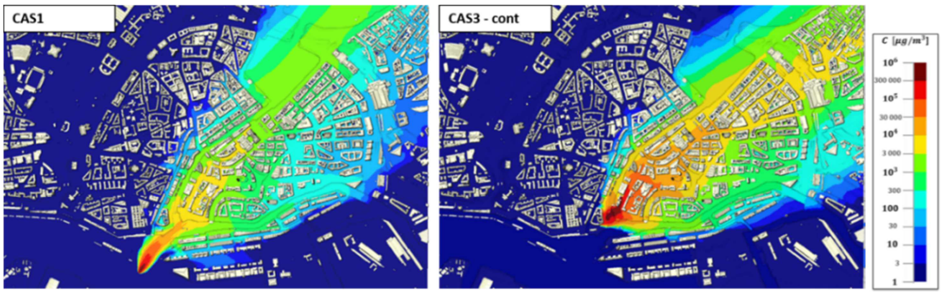

Figure 3: CASE1 and CASE3-continuous – Time-averaged concentration field at 2 m above the ground level.

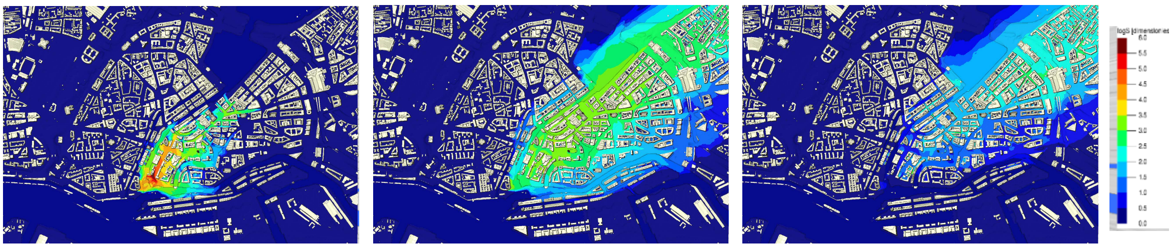

Figure 4: CASE3-puff – Averaged concentration field (over 5 minutes) at 2 m above the ground level. Left: 0-5 minutes, centre: 10-15 minutes, right: 25-30 minutes.

Statistical analysis

In this section, we compare punctual measurements in the experiments and the CFD simulations. For CASE1 and CASE3-continuous, we use the averaged gas concentration measured at each probe while for CASE3-puff, we use the averaged dosage which is the integral of the concentration over time. Dosage is calculated for one puff for CFD while averaged over a large number of puffs (~250) in the experiments.

Statistical correlation is evaluated using the 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 $|FB| \leq 0.67$, $NMSE \leq 6$ and $FAC2 \geq 0.3$.

In this paper, we focus on the FAC2 values, displayed in the scatter plots below (**Figures 5 & 6**).

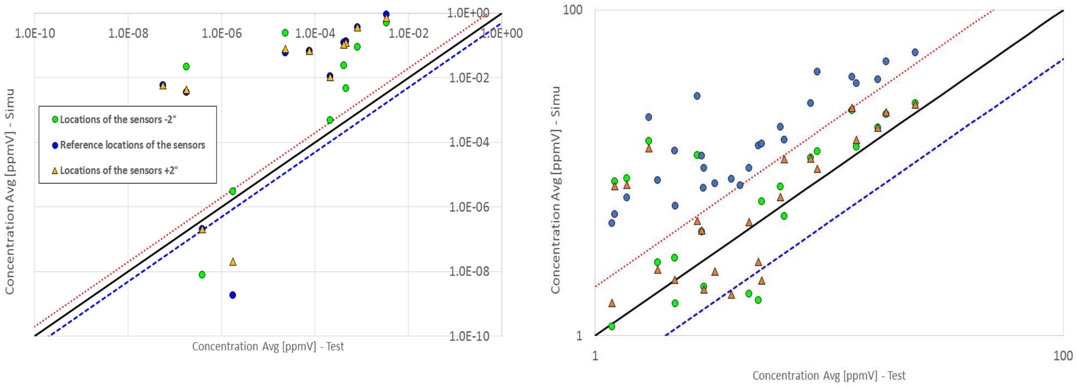

Figure 5: Scatter plot of the mean tracer gas concentration for CASE1 (left) & CASE3-cont (right).

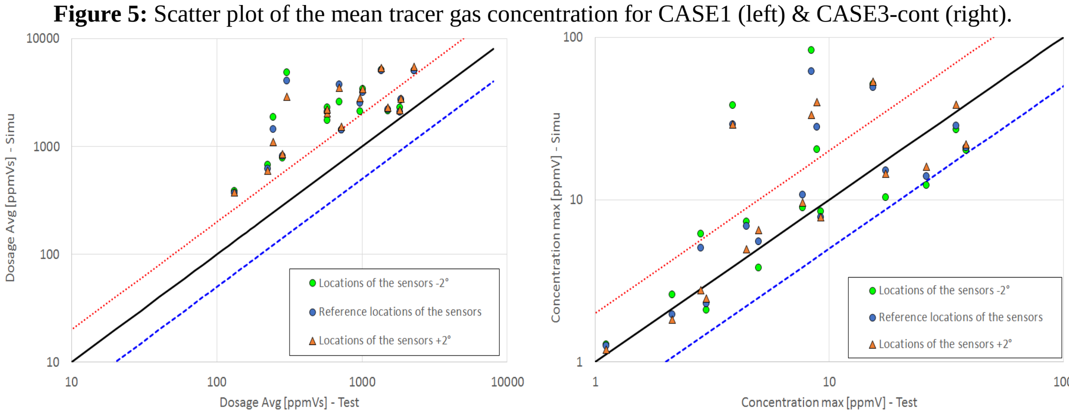

Figure 6: Scatter plots of the mean dosage (left) and peak concentration (right) for CASE3-puff.

On the above plots, we figured the domain of acceptance for FAC2, materialized by the two dotted lines. The results for CASE1 and CASE3-continuous are very poor as very few of the measurement probes correlate between experiment and CFD. The results for CASE3-puff are more encouraging as FAC2 for the mean dosage is higher (0.25) and the FAC2 peak concentration would validate PowerFLOW (0.75).

Given such initial results, we questioned the numerical model of the city and the wind direction as, following the given coordinates of the probes, some of them seem to be either within buildings or over the river. We then decided to conduct an equivalent wind direction sensibility study (within the same simulation) by assessing the sensitivity of the results to the probe location. We also recorded tracer concentration at locations rotated from the city centre model by -2° and +2° (shown on **Figures 5 & 6**). This showed different effects on each CASE:

- CASE1: no effect as the FAC2 of the mean tracer gas concentration remains almost null;
- CASE3-continuous: FAC2 is now within acceptation range (0.5 for -2°, 0.53 for +2°);
- CASE3-puff: no effect for -2°, slight negative effect for +2° (0.25 to 0.19).

This study shows a strong dependence of the results to the wind direction: for CASE3-continuous as a +/-2° rotation of the probes can make PowerFLOW predictions acceptable given the Hanna and Chang criteria whilst the correlation was very poor with the original wind direction.

As for the poor correlation in the full-scale experiment CASE1, there could be other explanations:

- Environmental conditions: we assumed in our simulation a constant wind direction and intensity. This is a strong hypothesis as in real life, the meteorological conditions are not constant for such a period of time (we simulated a 45 minute long gas release).
- Low measured and simulated values of the concentration: the gas release in this test is much lower than in the CASE3 experiments and a large number of probes is outside of the higher concentration area. Thus, the measured values are very small leading to large relative errors.
- Geometry differences: our simulation model was based on the wind tunnel model and there are differences between the numerical model and the real field.

For CASE3-puff, given that peak concentration correlation is very good whilst mean dosage correlates poorly, we considered comparing CFD mean dosage to 95th percentile dosage from experiments as shown in **Figure 7**. In this test, FAC2 is significantly improved as it is equal to 0.75.

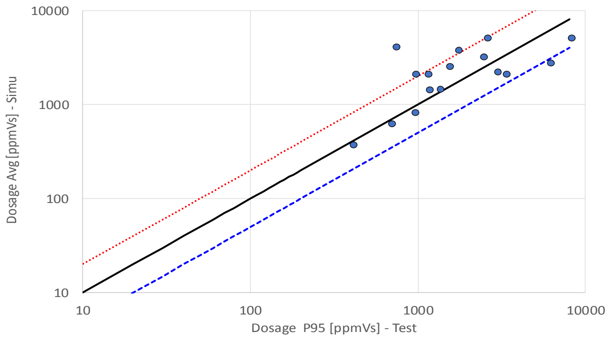

Figure 7: Scatter plot of the 95th percentile dosage for CASE3-puff.

CONCLUSIONS

CFD simulations in the urban or industrial environment can bring insights into the complexity of the flow and associated dispersion phenomena, something that is a more difficult or impossible to achieve either with a simpler modeling or an experimental approach. To illustrate this purpose, the Lattice-Boltzmann simulations presented in the paper enlighten a high-concentration area on the east side of the source, not located in the main flow direction and thus, not intuitive for emergency responders.

This first attempt at validating the Lattice-Boltzmann Method (LBM) highlights a strong dependency to the environment control and modelling. In the CUTE test-cases of COST ES1006 Action, PowerFLOW shows correct and encouraging predictions for the wind tunnel experiments while only a poor correlation is obtained for the full-scale experiment.

In Hamburg simulations, we used constant tracer gas release and environmental setup. Note that in the forthcoming “La Défense” simulation, we use time-dependent conditions which are a natural extension of the LBM. In these computations, we will study in more detail the transient tracer concentration field.

Finally, this study was performed on a relatively small cluster which allowed for a 24-hour turn-around time for a single simulation. As the solver has a good scalability, a larger cluster could be used in the case of an emergency to allow for a quick response. In addition, these simulations can be used for building databases or response surfaces to qualify in advance multiple scenarios that could be then interrogated in such an event.

REFERENCES

Armand, P., C. Duchenne, O. Oldrini, and S. Perdriel. EMERGENCIES Mediterranean, a prospective high-resolution modelling and decision-support system in case of adverse atmospheric releases applied to the French Mediterranean cost. Proceedings of the 18th Harmo Conference, October 9-12, 2017, Bologna, Italy.

Baumann-Stanzer, K., S. Andronopoulos, P. Armand, E. Berbekar, G. Efthimiou, V. Fuka, C. Gariazzo, G. Gasparac, F. Harms, A. Hellsten, K. Jurcacova, A. Petrov, A. Rakai, S. Stenzel, R. Tavares, G. Tinarelli, and S. Trini Castelli. COST ES1006 Model Evaluation Case Studies: Approach and results. COST Action ES1006, April 2015.

Boisseranc, F., P. Armand, C. Duchenne, and G. Douarre. Analysis of simulation results issued by a Lattice Boltzmann Method in complex urban environments – Applications to Paris and Hamburg. Proceedings of the 17th Harmo Conference, May 9-12, 2016, Budapest, Hungary.

Duchenne, C., P. Armand, M. Nibart, and V. Hergault. Validation of a LPDM against the CUTE experiment of the COST ES1006 Action. Comparison of the results obtained with the diagnostic and RANS version of the model. Proceedings of the 17th Harmo Conference, May 9-12, 2016, Budapest, Hungary.

Chen, H., S. Chen, W. H. Matthaeus. Recovery of the Navier–Stokes equations using a lattice-gas Boltzmann method. Phys. Rev. A 45, R5339, 1992.

Chen, H., S. Kandasamy, S. Orszag, R. Shock, S. Succi, and V. Yakhot. Extended Boltzmann kinetic equation for turbulent flows. Science, Vol. 301, 2003, pp. 633–636.

Chen, H., S. Orszag, I. Staroselsky, and S. Succi. Expanded analogy between Boltzmann kinetic theory of fluid and turbulence. Journal of Fluid Mechanics, Vol. 519, 2004, pp. 307–314.

Teixeira, C. M. Incorporating turbulence models into the Lattice-Boltzmann Method. International Journal of Modern Physics C, Vol. 9, 1998, pp. 1159–1175.