20th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
14-18 June 2020, Tartu, Estonia

CFD RANS AND LES SIMULATIONS FOR THE VALIDATION OF THE BUILD (BUILDING URBAN AND INDUSTRIAL LAGRANGIAN DISPERSION) MODEL, ON ISOLATED OBSTACLE AND NETWORK OF STREETS CONFIGURATIONS

Mehdi Slimani[1], Lionel Soulhac[2], Guillevic Lamaison[3], Patrick Armand[1], Luc Patryl[1]
Ludovic Donnat[4] and Olivier Duclaux[4]
[1]CEA, DAM,DIF F-91297 Arpajon, France
[2]Univ Lyon, INSA Lyon, Ecole Centrale de Lyon, Université Claude Bernard Lyon I, Laboratoire de Mécanique des Fluides et d'Acoustique UMR 5509, F-69621 Villeurbanne, France
[3]Univ Lyon, Ecole Centrale de Lyon, INSA Lyon, Université Claude Bernard Lyon I, CNRS, Laboratoire de Mécanique des Fluides et d'Acoustique UMR 5509,F-69134 Ecully, France
[4]TOTAL Refining & Chemicals, R&D Division, RC/SDR/R&D/ANA/LQA

Abstract: The atmospheric dispersion of CBRN (Chemical, Biological, Radiological and Nuclear) toxic substances, of accidental or intentional origin, on an urban or industrial complex built area, is a subject of major concern for the safety of people and the protection of infrastructures. In order to face these different types of risks and threats, industrial companies and public authorities need operational simulation tools for assessing, in advance or in emergency, the health consequences of harmful discharges on the population and on first responders.

In this context, a new software called BUILD (Building, Urban and Industrial Lagrangian Dispersion model) has been developed to simulate the atmospheric dispersion of gases and particles in a complex built environment. In order to validate this new model, simulations have been performed on the wind tunnel experimental test case of continuous and instantaneous releases behind a 2D square obstacle (Gamel, 2015) and in a regular network of streets (Cierco et al., 2010, Ben Salem et al., 2015). Results of the operational BUILD model are compared with experimental data and with detailed CFD calculations.

Key words: *Atmospheric dispersion model, street canyon, network of streets, operational and emergency response*

INTRODUCTION

The release of CBRN toxic substances (Chemical, Biological, Radiological and Nuclear) into the atmosphere has become a current issue concerning the safety of people and the protection of the infrastructure, specifically in the case of accidents or criminal acts. We can mention the events of the Chernobyl accident (1986) or most recently, in France, the accident of Lubrizol company near Rouen (2019).

The numerical simulation of the atmospheric dispersion, based on operational simulation tools, is one of the solutions to help the first responders and the decision makers during the crisis management phase. This software must be usable simply, rapidly and provide a reliable estimate of the hazardous plume and of the contaminated area.

The software called BUILD (Building Urban and Industrial Lagrangian Dispersion model) is an operational tool developed by CEA and the Fluid Mechanics and Acoustics Laboratory of the University of Lyon. It uses a SIRANE like parameterization for the flow in the dense part of an urban area (Soulhac et al. 2011, 2012, 2017). Unlike SIRANE, BUILD has an enhance parameterization for the flow to consider the deviation by building and obstacles with the recirculating transverse component of the flow in each street and a three-dimensional diagnostic flow model in the roughness sublayer.

To represent obstacles and buildings in sparse areas (isolated roughness regime), the BUILD model uses an analytical building wake parameterization. Transport and dispersion of pollutants are solved using a

Lagrangian particle stochastic approach coupled with the simplified flow defined above. This new operational model is able to simulate the dispersion from a point source in a complex built area in a computational time less than one minute on a laptop.

This article presents the first case of validation of the BUILD software. In the second section, we describe the experimental case used for the software validation. In the third section, we present the methodology of the CFD simulation. In the last section, we show some results and comparisons between CFD, experiments and BUILD. Finally, we conclude with the next steps in the development and validation of the BUILD model.

EXPERIMENTAL TEST CASE

To validate the BUILD model, we chose to start with academic configurations: isolated obstacles (Gamel, 2015) which will be described below and idealized neighborhood (Cierco et al., 2010, Ben Salem et al., 2015). These experiments were conducted in the wind tunnel of the Fluid Mechanics and Acoustics Laboratory of the University of Lyon.

The isolated obstacle consists in a two-dimensional square-section obstacle (extended on the width of the wind tunnel) placed in a rough boundary layer of neutral stratification. A continuous line source of pollutants is placed downstream of the obstacle. Velocity and concentration measurements were made around the obstacle to characterize the dispersion and the turbulent fluxes of pollutants with different measurement approaches (Marro et al., 2020). Figure 1 shows the experimental setup.

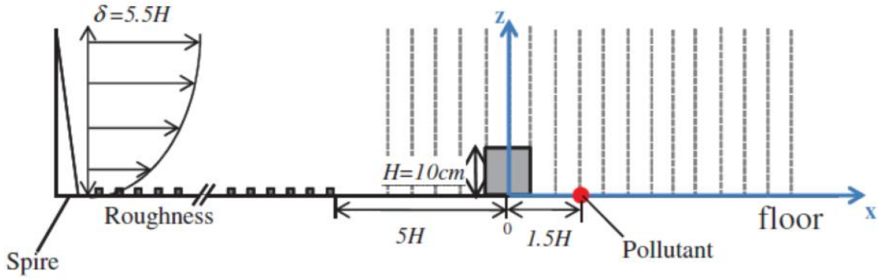

Figure 1. Experimental setup

CFD SIMULATIONS: COMPUTATIONAL SETTING AND PARAMETERS

During this work, we performed comparisons with experimental measurements, CFD results and BUILD. Two numerical simulation have been done: RANS (Reynolds Averaged Navier Stokes) and LES (Large-Eddy Simulations). The RANS and LES simulations provide us a statistical description of the turbulent velocity and concentration fields.

The numeric domain is defined by the following dimensions presented in Figure 2. The width of the domain is similar to the wind tunnel geometry (7 H). The computational domain respects the recommendations from the best practices guidelines (Franke et al., 2004).

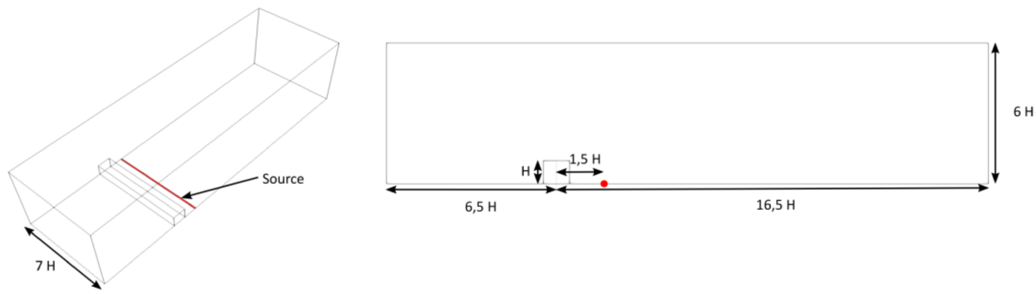

Figure 2. Computational domain

We use a structured and conformed mesh. It is non-uniform toward the flow and in the vertical direction but uniform in the transversal direction. The grid contains 9 million cells for RANS and LES simulations and it is shown in Figure 3.

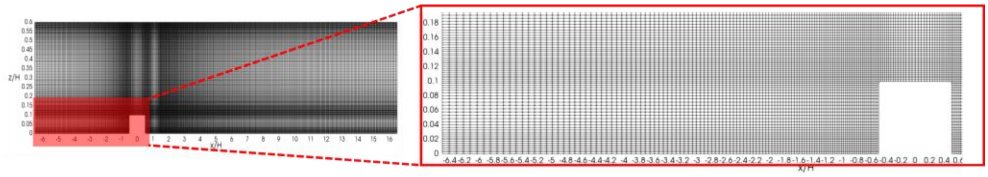

Figure 3. Computational grid

The CFD calculations have been performed with ANSYS Fluent code. For RANS simulations, we choose the realizable k-ε turbulence model and we apply the following boundary conditions: at the inlet, we use the experimental profile of velocity, turbulent kinetic energy and dissipation rate. Symmetry conditions are used on the lateral sides and at the top of the domain. We assume that the ground and the walls of the obstacle are aerodynamically smooth. The source of pollutants is modelled with a velocity inlet from the ground. Pressure velocity coupling is taken into account by the SIMPLEC algorithm. Pressure interpolation is PRESTO!. Second order upwind discretization schemes are used for both momentum, turbulent kinetic energy, turbulent dissipation rate, source term and energy.

For LES simulations, we apply the dynamic Smagorinsky subgrid scale model. At the inlet, we use a synthetic turbulence generation. The top of the domain is a slip wall and the side of the domain are transversally periodic. The time step is computed in such a way that the Courant number is around 0.5. We ensure that the flow does enough domain crossing to reach a good statistical convergence.

RESULTS AND VALIDATION

The analysis of the comparison between different approaches allow us to characterize the ability of the BUILD model to represent the principal features of the dispersion of pollutants, and to identify the main issues for which the model need to be improved. In this section, we will show some comparisons between experiment, CFD simulations and BUILD with vertical profiles along the domain for the flow characteristics and the behaviour of the dispersion.

First, Figure 4 shows the difference between RANS and LES simulations to represent the topology of the flow and the recirculation zones. Indeed, there are a lot of studies on the characteristics of these zones (Hosker, 1985; Schofield and Logan, 1990; Vinçont, 1999). At the foot of the obstacle, the RANS simulation has a detachment point too close to the obstacle, whereas LES simulations provide a position closer to the literature value. Downstream of the obstacle, both give a good distance for the reattachment point.

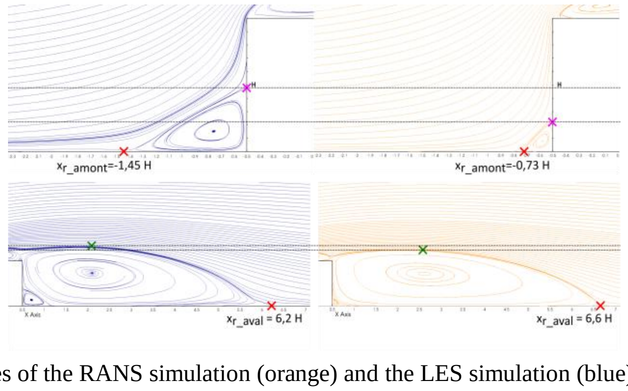

Figure 4. Streamlines of the RANS simulation (orange) and the LES simulation (blue), upstream (left) and downstream (right) of the obstacle

In the Figure 5, we show profiles along the domain of the x-component of the velocity of both simulations. Profiles are very similar downstream of the obstacle. The upstream profile has a noticeable difference due to the gap of the detachment point position.

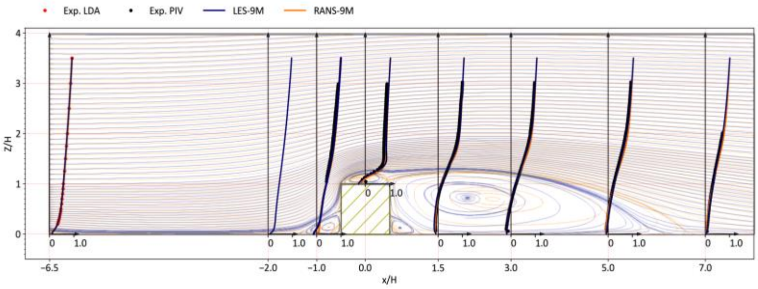

Figure 5. Evolution of U/U_∞ along the domain from the experiment (dot red and black), the RANS simulation (orange line) and the LES simulation (blue line). In the background, streamlines from Figure 3 with the RANS simulation (orange) and the LES simulation (blue)

In the Figure 6, we show profiles along the domain of the turbulent kinetic energy. In LES simulations we distinguish the part of energy modelled and the part resolved. At x = 5 H and 7 H, profiles are like each other. However, in the recirculation zone, there are some differences between the results of simulations. The maximum gap is at the boundary of the recirculation zone, which corresponds to the mixing zone.

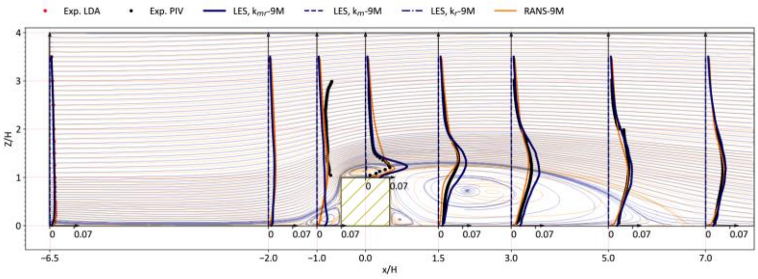

Figure 6. Evolution of dimensionless turbulent kinetic energy (k/U_∞^2) along the domain from the experiment (dot red and black), the RANS simulation (orange line) and the LES simulation (blue line). In the background, streamlines from Figure 3 with the RANS simulation (orange) and the LES simulation (blue)

In the Figure 7, we show profiles from the experiment, LES simulations and BUILD. LES simulation gives a good behavior of the concentration in comparison with the experiment. BUILD provides a good approximation at the end of the recirculation zone. However, the species repartition in the recirculation is not too far from the experiment but it has to be improved next to the limit of the mixing zone. This result is acceptable, taking into account that the computational time is about 12 seconds on a laptop whereas the LES simulation needs few weeks on a supercalculator.

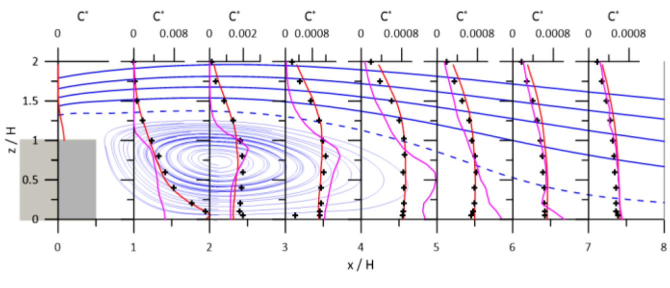

Figure 7. Evolution of the concentration field dimensionless from the experiment (black cross), the LES simulation (red line) and the BUILD simulation (pink line). In the background, streamlines from the LES simulation.

CONCLUSIONS AND PERSPECTIVES

In this article, we presented a first validation of the BUILD model during its development process. The comparison with wind tunnel experiments and RANS/LES simulations on the academic case of an isolated obstacle provides encouraging results, with a computational time less than 15 seconds on a laptop. The BUILD model will be improved in the future, with a focus on the second academic case of an idealized neighborhood (Garbero, 2008; Cierco et al., 2010; Ben Salem et al., 2015).

REFERENCES

Ben Salem, Nabil, V. Garbero, P. Salizzoni, G. Lamaison and L. Soulhac, 2015: Modelling Pollutant Dispersion in a Street Network. *Boundary-Layer Meteorology*, **155-1**, 157-87.

Cierco, F.-X., L. Soulhac, P. Méjean, G. Lamaison, P. Salizzoni and P. Armand. Validation of the SIRANERISK model against a wind tunnel experiment of dispersion of a short release in an idealized urban street network. In *13th Int. Conf. on Harmo. within Atmos. Disp. Modell. for Regul. Purposes*, Paris, France, 2010.

Franke, J., Hirsch, C., Jensen, A.G., Krüs, H.W., Schatzmann, M., Westbury, P.S., Miles, S.D., Wisse, J.A., Wright, N.G., 2004. Recommendations on the use of CFD in wind engineering. In: van Beeck, J.P.A.J. (Ed.), Proceedings of the International Conference on Urban Wind Engineering and Building Aerodynamics. COST Action C14, Impact of Wind and Storm on City Life Built Environment. Von Karman Institute, Sint-Genesius-Rode, Belgium, 5–7 May 2004.

Gamel, H., 2015: *Caractérisation expérimentale de l'écoulement et de la dispersion autour d'un obstacle bidimensionnel*. PhD, École Centrale de Lyon, France.

Garbero, V., 2008: *Pollutant dispersion in urban canopy.* PhD, École Centrale de Lyon, France.

Hosker, R P. , 1985: *Flow around isolated structures and building clusters: A review*. United States.

Marro, M., Gamel, H., Méjean, P. *et al.* High-frequency simultaneous measurements of velocity and concentration within turbulent flows in wind-tunnel experiments. *Exp Fluids* **61,** 245 (2020).

Schofield, W. H., and Logan, E., 1990: *Turbulent Shear Flow Over Surface Mounted Obstacles.* ASME. *J. Fluids Eng*. December 1990; 112(4): 376–385.

Soulhac, L., P. Salizzoni, F.-X. Cierco and R. J. Perkins, 2011: The model SIRANE for atmospheric urban pollutant dispersion; part I, presentation of the model. *Atmospheric Environment*, **45-39**, 7379-7395.

Soulhac, L., P. Salizzoni, P. Mejean, D. Didier and I. Rios, 2012: The model SIRANE for atmospheric urban pollutant dispersion; PART II, validation of the model on a real case study. *Atmospheric Environment*, **49**, 320-37.

Soulhac, L., C. V. Nguyen, P. Volta and P. Salizzoni, 2017: The model SIRANE for atmospheric urban pollutant dispersion. PART III: Validation against NO2 yearly concentration measurements in a large urban agglomeration. *Atmospheric Environment*, **167**, 377-88.

Vinçont, J.-Y., 1999: *Détermination des flux turbulents de masse dans le sillage d'un obstacle : application à l'écoulement à l'intérieur de la canopée urbaine.* PhD, Ecole Centrale de Lyon, France.