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BEST PRACTICE GUIDE ON POLLUTANT DISPERSION SIMULATIONS WITH THE COMMERCIAL TOOL "ANSYS FLUENT" AT CERN

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Abstract: Large Eddy Simulations (LES) are of raising interest for numerous engineering applications in which an accurate flow prediction is necessary. This paper searches for the optimum mesh resolution in numerical simulations reliably predicting dispersion of pollutants in the lower part of the Atmospheric Boundary Layer (ABL). For the dispersion of pollutants, turbulent quantities have been assessed at several distances from the release point and compared to each other. Areas close to release points located at low altitudes are given a particular importance, because air pollutant concentrations can be too high for people present at such places. To achieve a realistic prediction of the flow and pollutant concentrations close to populated areas, LES are preferred over the Reynolds-Averaged Navier Stokes (RANS) models (Vita et al, 2020). A mesh resolution of 0.5 m is recommended at distances from the release point shorter than 40 m. Near the release point, physical effects like building downwash and horizontal plume enlargement due to the downstream wake region of buildings have a direct impact on pollutant concentrations and particle trajectories. In built-up areas at intermediary distances where the dispersion of the plume is directly influenced by buildings in their given constellation and where the energy production is high, a mesh resolution of 1.5 m is suggested. In areas where the plume is already dispersed and geometrical obstacles are rare, a mesh resolution of 3 m and more is sufficient. In these areas, the dissipation of energy and the transport of particles (mean quantities) that determine the flow are less affected by the mesh size.

Key words: *Large Eddy Simulation (LES), neutral Atmospheric Boundary Layer (ABL), Synthetic Turbulence Generator (STG), Monin-Obukhov similarity theory, pollutant dispersion, discrete phase model (DPM), Computational Fluid Dynamics (CFD).*

INTRODUCTION

Simulating an atmospheric boundary layer (ABL) flow with Large Eddy Simulations (LES) is a challenging and demanding task considering the high turbulent Reynolds number (Re) of these flows and the need of short time steps. For pollutant dispersion simulations, the accurate prediction of ground level velocity and their fluctuations are essential. Both a large domain and a small cell size of the ground level mesh are necessary to resolve obstacles and the turbulence of the flow. The alternative approach of using LES is mainly found in research (Vasaturo R et al 2018), but best practice guides (BPGs) do not exist at present (Vita et al, 2020). To encourage practitioners to use LES and to harmonise LES for ABL flows in the future, turbulence characteristics are investigated for five different grid resolutions in a pollutant release scenario.

At CERN (Conseil Européen pour la Recherche Nucléaire), a project called FIRIA (Fire-Induced Radiological Integrated Assessment) was launched in 2018 to develop a risk assessment methodology that aimed at predicting radiological consequences of fires potentially developing inside some of the Organisation's research facilities. This paper presents a part of the studies carried out for outdoor dispersion pollutant modelling.

Many studies on pollutant dispersion simulations for neutral ABL flows have been carried out for simplified scenarios (i.e., cob arrays, simplified urban roughness arrays, Michelstadt scenario, etc.) showing that LES are performing well in terms of hazmat dispersion modelling (COST ES1006, April

2015). However, the price for the evident gain in model performance compared to Reynolds-Averaged Navier Stokes (RANS) models is a higher computational effort.
Local-scale pollutant dispersion in built-up areas does not only depend on the structure (topographical and geometrical) of the immediate surrounding area, but also on topographical variations and presence of buildings far upwind of the release point. To use the same computing domain for different wind directions and release scenarios, an extended domain has to be modelled.
In this work, simulations have been performed with ANSYS Fluent. The flow is solved with LES and Lagrangian particles are injected to track the pollutant using the Discrete Phase Model (DPM). The paper analyses cases with two different wind directions with two different flow features.

METHODOLOGY

In this chapter, the geometrical setup, meshing, boundary conditions, and numerical methods are described.

Geometry setup

The CERN Meyrin site, which houses many experimental facilities and auxiliary buildings (grey in Figure 1), was selected for two pilot studies of the FIRIA project: ISOLDE (red building in Figure 1) and ATLAS Detector (blue building in Figure 1).
The topography was modelled using the digital terrain model data in ASCII format with a grid resolution of 0.5 m, which are publicly accessible from the Geneva SITG website. To reduce initial backflow issues on pressure outlets of the domain and to define the inlet profile correctly, a relaxation or correction of the elevation of the domain on the sides was needed. A horizontal relaxation size from the edges of the domain of 500 m was chosen. A function, which elevates the terrain to a relaxed altitude of depending on the position relative to the edge, was implemented in Python. The original altitude of the edge, ranging from 390 m to 520 m, is then changed to an averaged value of the Meyrin site of 460 m altitude. The correction of elevation was implemented with a cosine function, which is equal to one on the edges and equal to zero in 500 m distance. The modified ASCII data were facetted and converted into facetted STL format using Python to import the topography into ANSYS Fluent (olive and dark green coloured ground in Figure 1).

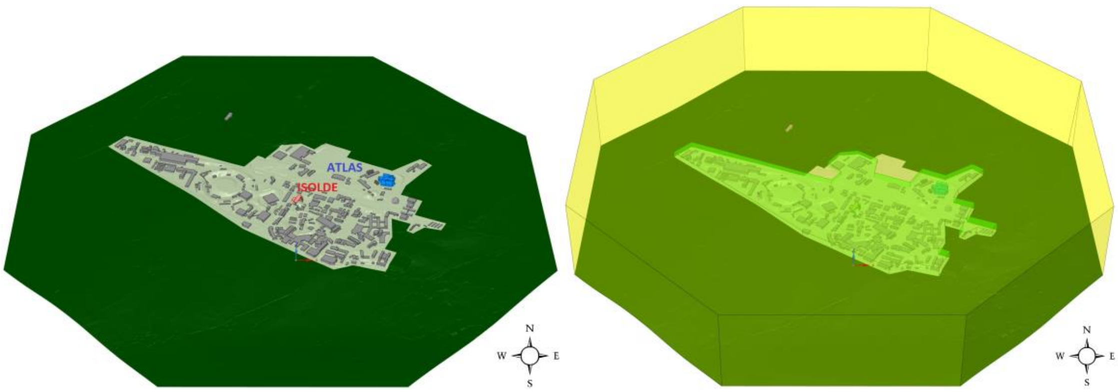

Figure 1. Polyhedral shaped domain including topography model (olive and dark green ground), CAD buildings (grey, red and blue buildings), body of interest (transparent light green volumes) and walls (transparent yellow walls).

The domain has a size of 3×3 km^2 with a height of 500 m, which is large enough to generate a smooth inflow and outflow without an unnatural flow due to the domain relaxation, which could otherwise lead to non-physical solutions. Only pollutant concentrations at distances shorter than 400 m from sources located at low heights were evaluated (no tall stacks). Under such conditions, the pollutants stay close to the ground, below about 50 to 100 m, and a domain height of only 500 m is sufficient to be modelled instead of the full ABL height of about 1000 m.
The computer-aided design (CAD) software ANSYS SpaceClaim was used for constructing the model. The grey buildings were modelled in a simplified way, keeping their shapes sharp without adding details

to them. Bodies of interest around the ISOLDE and ATLAS facilities as well as the full Meyrin site were CAD modelled and used for mesh refinements (light green bodies in Figure 1).
Five perpendicular planes into the most probable and critical wind directions, which are wind blowing into northeast and south, at distances of 40 m, 100 or110 m, 200 m, 300 m, and 400 m from the release points with the widths and heights indicated Table 1 have been defined.

Table 1. Perpendicular planes used for evaluating locally mean velocity and turbulent kinetic energy.

Wind Direction	Properties					
North-east Azimuth 45°	Distance (m)	40	110	200	300	400
	Width (m)	200	200	200	300	300
	Height (m)	100	100	100	150	150
South Azimuth 180°	Distance	40	100	200	300	400
	Width (m)	200	200	300	300	300
	Height (m)	100	100	100	150	150

Meshing

An unstructured polyhedral mesh was used to adapt the mesh to the geometry, to resolve buildings, and to refine regions of interest or regions with high Reynolds number. For a mesh refinement study, five different meshes were created with ANSYS Fluent Meshing module: very coarse (2.2 M cells), coarse (4.3 M cells), medium (9.8 M cells), fine (16.1 M cells), and very fine (21.6 M cells). Depending on the coarseness level, several parameters vary with sizing functions. The maximum global size for the polyhedral cells ranges between 50 m and 100 m, and the minimum global size and the size function for special buildings is set to 0.5 m to resolve the buildings of interest and their surrounding areas finely enough.
Sizing functions have been defined for several surfaces:

- Inner part of the domain – “ground-inner” (olive surface in Figure 1)
- Outer part of the domain – “ground-outer” (dark green surface in Figure 1)
- Ground close to special buildings, i.e. ATLAS – “ground-special” (turquoise surface in Figure 1)
- Common buildings at the CERN Meyrin site – “buildings” (grey buildings in Figure 1)
- Special buildings, e.g. ATLAS – “special-buildings” (blue building in Figure 1)

Volume size functions have been applied to body-of-interests (transparent light green bodies in Figure 1). A summary of all types of mesh size functions used, their properties (minimum and maximum values), and their growth rates from certain surfaces/volumes can be found in Table 2.

Table 2. Mesh size functions used for the mesh refinement study. All values are in meters. Cell growth rates are constant from each surface or body of interest and they are chosen differently for each mesh refinement.

Refinement level	properties	global sizing	ground-special	ground-inner	ground-outer	special-buildings	common buildings	BOI-special	BOI-buildings
1: very coarse	min.	0.5	-	-	-	-	3.0	-	-
2.2M cells	max.	100	0.5	5.0	10.0	0.5	10.0	0.5	10.0
2: coarse	min.	0.5	-	-	-	-	3.0	-	-
4.3M cells	max.	100	0.5	3.0	6.0	0.5	6.0	0.5	6.0
3: medium	min.	0.5	-	-	-	-	1.5	-	-
9.8M cells	max.	50	0.5	1.5	3.0	0.5	3.0	0.5	4.0
4: fine	min.	0.5	-	-	-	-	1.5	-	-
16.1M cells	max.	50	0.5	1.0	3.0	0.5	3.0	0.5	3.0
5: very fine	min.	0.5	-	-	-	-	1.0	-	-
21.6M cells	max.	50	0.5	1.0	3.0	0.5	3.0	0.5	3.0

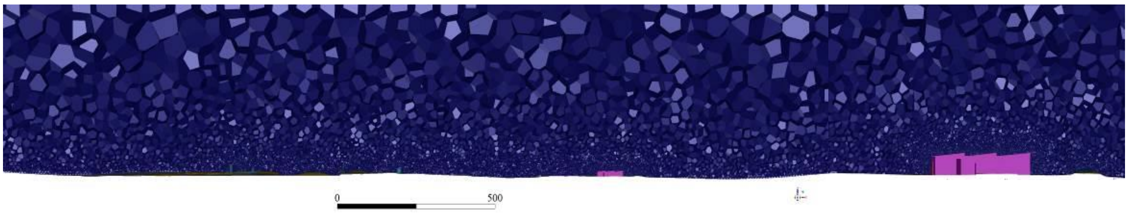

Figure 2. Polyhedral cells display in a cut-plane through the full domain for the very coarse refinement level.

Boundary conditions

Monin-Obukhov similarity theory as described in Dyer (1974) was used to define the velocity profile of the neutral ABL. The terrain roughness value of $z_0 = 1$ m was chosen for suburbs, villages and forests (Stull, 2000). An ultrasonic anemometer located close to CERN at a height of 10 m was used to measure wind data for several years and data statistics were available. The most probable and critical wind directions with wind blowing into northeast and into south were chosen for the simulations. A wind speed of 1 m/s at a height of 10 m above the ground was used.

The Monin-Obukhov similarity theory was implemented at the inlets of the domain. The Synthetic Turbulence Generator (Shur and Spalart et al, 2014) was used to add fluctuations to the mean velocity terms. A precursor method was not applicable due to the quickly changing terrain in all directions around the CERN site. In the west, the Jura Mountains are reaching heights up to 1800 m, in the Southwest and Northeast, farms, vineyards and forests dominate the terrain. Since there is no constant roughness on the ground, a terrain roughness of $z_0 = 1$ m was assumed.

For the top of the domain and the sides of the domain pointing in the wind direction, velocity inlets were defined to improve convergence and reduce backflow issues. The distance to the release points is far enough to make sure that the flow on the sides would not influence the flow in the centre of the domain. At the outlets, simple pressure outlets have been defined. At all the walls (ground and buildings), a no-slip condition was applied.

Numerical methods

The in ANSYS Fluent implemented LES with second-order implicit time-dependent solution formulation and the Wall-Adapting Local Eddy-viscosity (WALE) model, with $C_W = 0.325$, was used (Nicoud and Ducros, 1999). A time step between 0.1 s and 0.2 s was chosen to make sure that the Courant-Friedrichs-Lewy (CFL) condition of CFL < 1 is satisfied. Due to the increasing mesh size and velocity from ground level to higher parts of the atmosphere, the CFL condition can be met in the whole domain. The standard bounded-central-differencing method was chosen for the momentum equation to reach better stability and convergence of the solution.

In the first step, the flow field was solved with RANS model with enhanced wall treatment. In the second step, fluctuations were added to the flow field depending on mean velocity and Turbulent Kinetic Energy (TKE). Afterwards the LES was started and the domain was flushed during approximately 30 min of the simulated time before starting the pollutant release. As typical release durations are between 20 min and 60 min for the accident scenarios at CERN, the total simulated time is shorter than two hours.

RESULTS

Five different mesh resolutions have been analysed in two wind directions on five perpendicular planes with wind blowing into northeast (NE) and into south (S). Mean velocity magnitude (Figure 3) and TKE (Figure 4) have been calculated from the exported time dependent velocities in each Cartesian coordinate and time step. The finer the mesh, the more data points are available. The atmospheric flow is mainly disturbed close to buildings where velocity layers are separated. The air is moving faster, and the flow is less disturbed with increasing altitude.

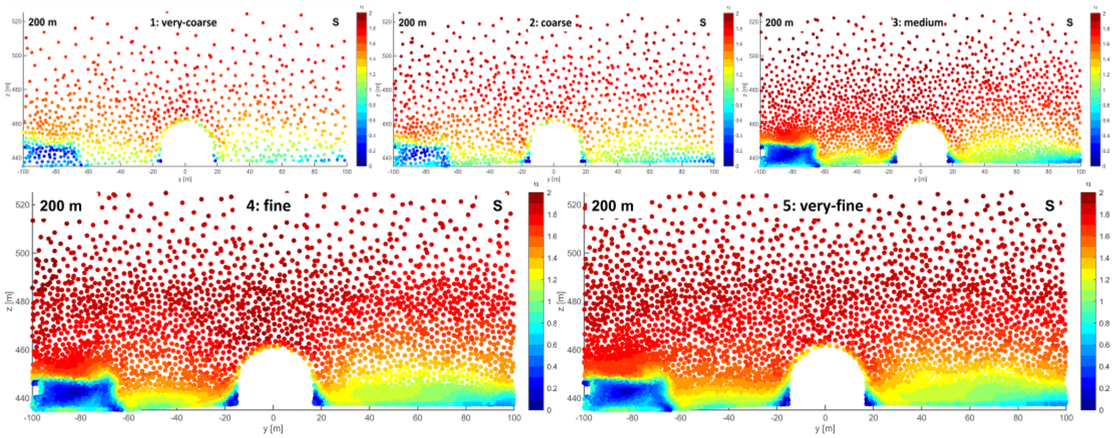

Figure 3. Mean velocity magnitude coloured on perpendicular planes. Example for all mesh sizes in south wind direction at 200 m distance from the release point.

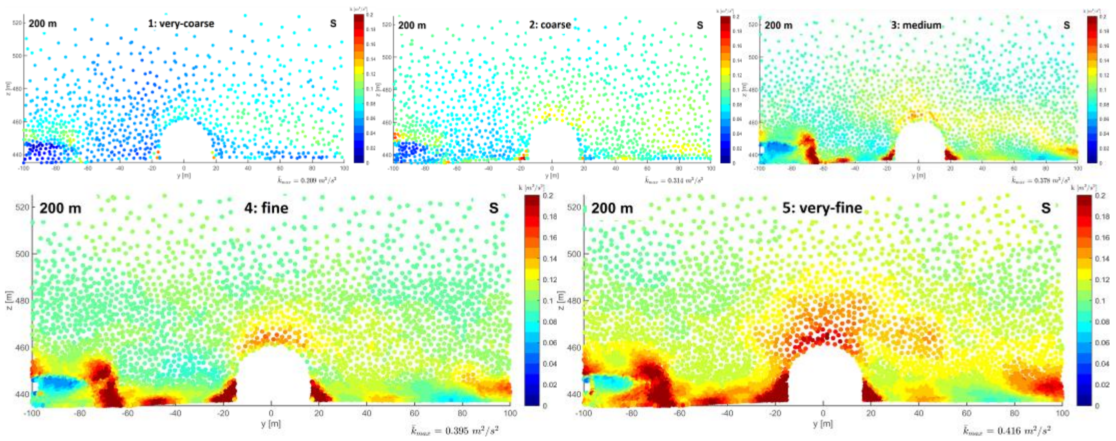

Figure 4. TKE coloured on perpendicular planes. Example for all mesh sizes in the wind direction towards south at 200 m distance from the release point.

It was observed that values for TKE were changing drastically with the mesh resolution: With the finer mesh, the resolved fluctuations and therefore the TKE increase. In LES, eddies smaller than the grid size are sub-grid modelled and only the part which can be resolved is seen in the figures due to its fluctuations in the time dependent velocity values.

To simplify a comparison of the plots for all wind directions and distances, averaged and maximum values extracted from the planes are compared, namely the averaged mean velocity magnitude, averaged TKE, and the maximum TKE (Figure 5 and Figure 6).

DISCUSSION AND CONCLUSION

To predict the movement and dispersion of pollutants through the air in the ABL, two quantities are of major importance: The mean velocity, which affects the resting duration of particles in certain areas, and TKE, which has an impact on the plume size.

In Figure 5, results for the mean velocity averaged over the whole plane are shown. Analysing the results for both wind directions, two trends can be found: (1) when increasing the distance from 200 m to 300 m, the values are increasing due to the increasing size of the plane. The plane heights change from 100 m to 150 m. This behaviour corresponds to the velocity increasing logarithmically with the height; (2) the medium, fine, and very fine mesh predict similar values for each distance from the release point (green bars in Figure 5). For the wind direction towards NE, this behaviour can be described with the sizing function "ground-outer", which is set to 3 m for each refinement level and only the cell growth rate is changing. The cell growth rate has nearly no impact on the mean velocity predictions. For wind blowing towards S, similar values are obtained not only for medium, fine, and very-fine meshes but also for the coarse mesh. Increasing the mesh size with the sizing function “ground-inner” from coarse 3 m to medium/fine 1.5 m to very fine 1 m does not significantly change the results for averaged mean velocity (Figure 3).

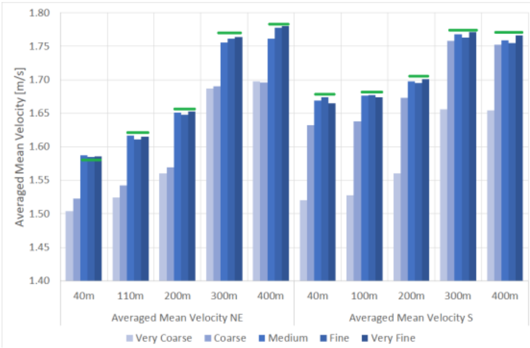

Figure 5. Normalized averaged mean velocity plots showing the differences of the values for each plane and wind direction.

Figure 6 shows the averaged mean TKE on the left side and the maximal mean TKE on the right side. The averaged mean TKE is decreasing in the wind direction towards NE (dark green line in Figure 6). The energy dissipation is higher than the energy production in this case because there are no buildings on the ground. For the wind blowing towards the S direction, the light green line indicates roughly equal energy dissipation and production because buildings are present up to and beyond 400 m from the release point. This leads to similar values for averaged mean TKE at all considered distances. For each distance, the averaged mean TKE is increasing proportionally with the mesh size (red and orange lines in Figure 6). This means that turbulent fluctuations are better resolved, and less sub-grid modelled with finer meshes.

Values obtained for the maximum mean TKE are plotted right in Figure 6. They are nearly equal close to the release point (violet lines). This can be explained by the small mesh size of only 0.5 m chosen for the surface of the building, ground, and volumes of the body-of-interest around the area of concern, which ensures a good prediction close to the release point. At longer distances, the modelled maximum mean TKE strongly increases when changing to the medium mesh, while remaining roughly the same for the finer meshes – medium, fine, and very fine (brown and grey lines in Figure 6). This means that the medium resolution is needed as a minimum to obtain self-consistent results.

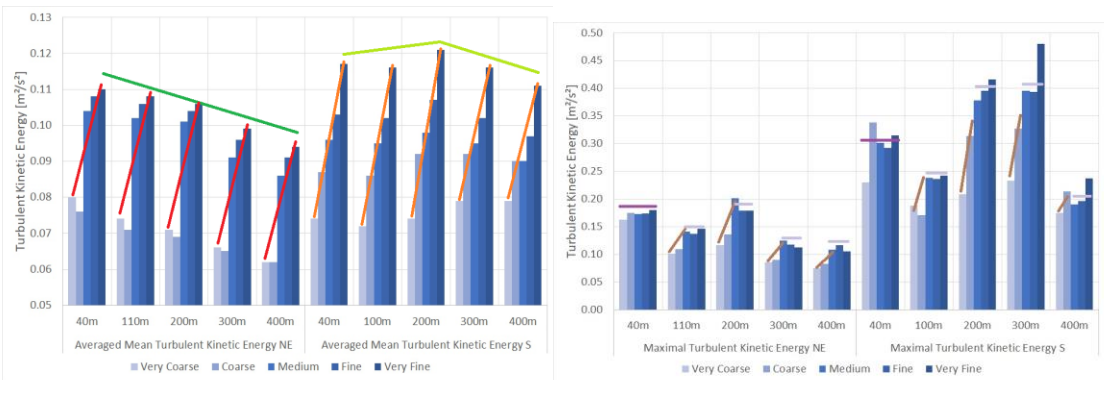

Figure 6. Averaged (left) and maximum (right) mean TKE graph shows the difference of the values for each plane and wind direction.

Note that with decreasing cell size the plume size increases as well due to the generally larger turbulent fluctuations, which leads to lower pollutant concentrations. If local pollutant concentrations are important for the pollution impact, e.g. inhalation of hazardous materials, finer mesh shall be used if safely conservative results are required. Coarser mesh can be used in cases when the exposure to the hazardous materials is less point dependent, e.g. polluted agricultural land with crops collected from larger areas.

The result for the maximum mean TKE confirms the necessity of local refinements. Areas close to the release point shall be resolved satisfactorily due to their direct impact on the plume dispersion. Generally, the finer the mesh resolution is, the better the prediction is. At distances far from the release point, the mesh size is not that important because the initial shape of the plume is already well resolved in a finer mesh.

More studies that have been performed within the FIRIA project at CERN will be published soon. One of them will concentrate on the sensitivity analysis on boundary conditions for pollutant dispersion simulations and how to select the boundary conditions to be conservative or realistic.

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