

# Large Eddy Simulation of concentration fluctuations in an urban street canyon

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**ABSTRACT:** We examine some statistical properties of the concentration field, developing from the steady release of tracer gas at street level in an urban street canyon. To that extent, detailed time-resolved numerical simulations of coupled flow and dispersion are conducted. The numerical model was extensively validated by comparing the predicted time-averaged concentrations to wind tunnel measurements. In this paper, we employ the validated model to assess the time-averaged concentration, the variance and the probability density function (PDF) at various locations in the urban street canyon. The PDF in the mid-plane of the street canyon was found to be wider and more uniform at near-ground locations close to the leeward wall, and narrower and more pronounced at locations higher above the ground and closer to the windward wall. A wider PDF implies that both the mean concentration and the variance are higher, and that longer time periods are needed to determine these quantities at a given confidence level. This observation has an immediate impact on the sensor location and averaging time for siting monitoring networks, and affects the assessment and planning of pollutant mitigation strategies.

**KEYWORDS:** Computational Fluid Dynamics (CFD), Large Eddy Simulation (LES), dispersion, statistical analysis, average, variance, probability density function (PDF).

## 1 INTRODUCTION

Thus far, pollutant dispersion studies have mainly focused on mean concentrations and their spatial distribution for a wide range of configurations and emission scenarios. Studies providing statistical information on air pollutant concentration are rare. Nevertheless, their significant added value was demonstrated in a wind tunnel study by Pavageau and Schatzmann (1999), and discussed again in e.g. Schatzmann and Leitl (2011). They showed that statistical information can help to improve our understanding of dispersion mechanisms, and can assist to suggest specifications regarding e.g. sensor location and averaging time for siting monitoring networks. Compared to wind tunnel studies, performing numerical simulations has the advantage that full-field data of all quantities of interest are available over the considered period of time.

In Moonen et al. (2012a), we assessed the performance of a numerical model to accurately simulate pollutant dispersion in an urban street canyon with tree planting. Detailed time-resolved numerical simulations of coupled flow and dispersion were conducted and compared to corresponding wind tunnel measurements (Gromke and Ruck 2007, 2009). The model performance was assessed in several steps, ranging from a qualitative comparison to measured concentration

profiles, over statistical data analysis by means of scatter plots and box plots, up to the calculation of objective validation metrics, and was found to be excellent.

The goal of the current study is to employ the validated model to assess the statistical properties of the concentration field. We focus on an isolated urban street canyon with near-ground released traffic emissions, under perpendicular approach flow. The numerical model is described in Section 2. Section 3 summarizes the main conclusions of the validation study. In Section 4, the statistical properties of the concentration field are analyzed. We concentrate on three quantities of interest, namely the time-averaged concentration field, its variance and corresponding probability density function.

## 2 NUMERICAL MODEL

### 2.1 Domain dimensions

We perform detailed unsteady simulations of a dispersion experiment, conducted in the atmospheric boundary layer wind tunnel of the University of Karlsruhe, Germany. We focus on a 1:150 scaled isolated street canyon under perpendicular approach flow conditions. The street canyon consists of two parallel buildings of  $0.12 \times 0.12 \times 1.2$  m ( $L_x \times L_y \times L_z$ ), and positioned 0.12 m apart in streamwise direction ( $x$ ). In this way, a street canyon with  $W/H = 0.12/0.12 = 1$  and  $L/H = 10$  is formed ( $H = 0.12$  m), see Figure 1. The cross sectional dimensions of the numerical domain are taken equal to the dimensions of the wind tunnel, namely 2 m wide by 1 m high, hereby accurately reproducing the experimental blockage ratio of 7.2%. The total streamwise length of the domain is  $25 H$  (3 m), and consists of an approach flow region of  $7 H$  (0.84 m), a model region of  $3 H$  (0.36 m) and a wake region of  $15 H$  (1.8 m). The position of the upstream domain boundary coincides with the entrance of the wind tunnel test section, i.e. where velocity profiles have been measured. The downstream distance is chosen in accordance with the best practice guidelines, formulated as outcome of COST Action 732 (Franke et al. 2011).

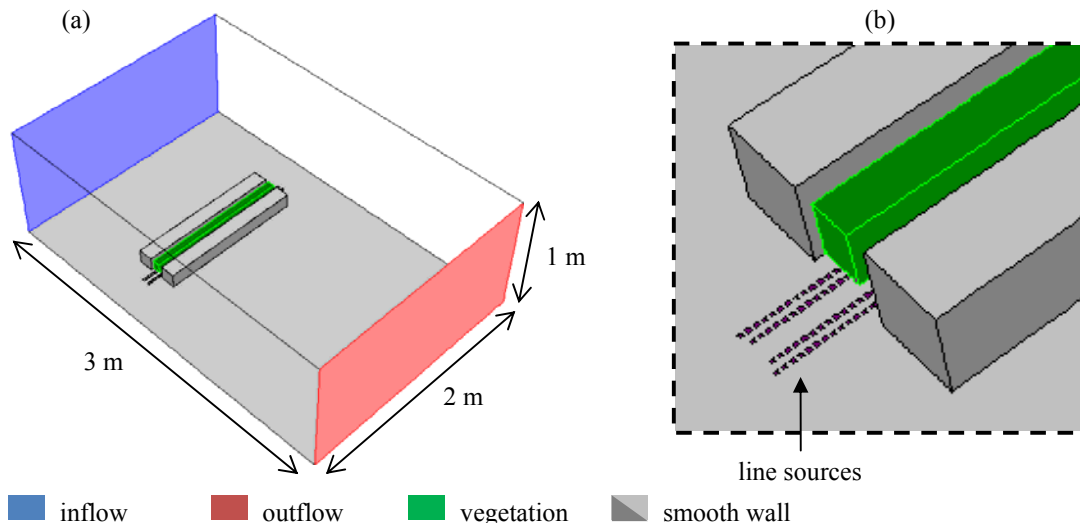


Figure 1. Layout of the computational domain.

## 2.2 Boundary conditions

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No-slip conditions are imposed along the *top, bottom and lateral boundaries* of the domain, corresponding to flow along the smooth wind tunnel walls. The same BC is applied for the surfaces of the canyon model. All walls are considered impermeable for species transport.

At the *inflow boundary*, the measured vertical profiles of mean flow speed  $u(y)$  and turbulence intensity  $I(y)$  can be well approximated by power-law correlations with exponents  $k_u = 0.3$  [-] and  $k_I = 0.65$  [-], respectively (Moonen et al. 2012a):

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$$\frac{I(y)}{I(y_H)} = \left( \frac{y + y_d}{y_H} \right)^{k_I} \quad (2)$$

with  $u(y_H) = 4.65$  m/s the mean flow speed and  $I(y_H) = 16.3\%$  the turbulence intensity at reference height  $y_H = H$  and  $y_d = 0.02$  m a parameter representing the peak in turbulence intensity at the top of the roughness elements. Time-dependent inlet conditions are generated from the measured mean profiles by means of Ansys' inbuilt spectral synthesizer (Ansys Inc. 2009). In this method, the fluctuating velocity components are computed by synthesizing a divergence-free velocity-vector field from the summation of (100) Fourier harmonics. The inflowing fluid is dry air at 293.15 K with zero background tracer concentration.

On the *outflow boundary*, a zero diffusive flux is imposed for all flow variables in the direction normal to the exit plane. This means that the conditions of the outflow plane are extrapolated from within the domain and have no impact on the upstream flow. This assumption is valid for fully-developed flows.

The *line source* is modeled as a series of equidistantly-spaced point sources at ground level, as in the experiment. The individual hypodermic tubes have been approximated by square inflow boundaries, each  $0.005 \times 0.005$  m<sup>2</sup>. The imposed flow rate and concentration are equivalent to the experimental conditions, namely a mixture of 7000 cm<sup>3</sup>/min dry air ( $\rho = 1.225$  kg/m<sup>3</sup>,  $\mu = 1.7894 \cdot 10^{-5}$  kg/(m·s), molecular weight of 28.966 kg/kgmol) and 6.5 cm<sup>3</sup>/min SF<sub>6</sub> ( $\rho = 6.164$  kg/m<sup>3</sup>,  $\mu = 1.42 \cdot 10^{-4}$  kg/(m·s), molecular weight of 146.05499 kg/kgmol). The properties of air are taken from the inbuilt material database (Ansys Inc. 2009). The ones of SF<sub>6</sub> are compiled from various literature sources. SF<sub>6</sub> is considered as an inert gas (i.e. chemical reactions are not modeled). Because of the larger surface area of the individual point sources in the CFD model, the exhaust momentum is lower than in the experiment. This is compensated by adding a source term to the vertical momentum equation in the cells in direct contact with the source. Note that other researchers (Gromke et al. 2008, Salim et al. 2011a,b) proposed more simplified modeling strategies for the line source and reported a qualitatively good agreement with the experimental results. Since SF<sub>6</sub> is about 6 times heavier than air, gravitational effects need to be included in the model.

## 2.3 Computational grid

In LES, the computational grid acts as a filter. The turbulent structures larger than the grid size (i.e. the large eddies) are resolved, while the smaller ones are modeled. Small eddies are more isotropic. Cubic elements have an equal filter length in the three principal directions, and are

thus the -optimal element type for resolving turbulent structures with LES. The grid employed in this study is therefore entirely built up with this element type.

Since uniform grid refinement rapidly results in a prohibitively large number of elements for grids consisting of cubic elements, we developed and validated an algorithm that systematically refines the grid – in all three dimensions – towards regions of interest (Moonen et al. 2012b). The final grid consists of 1'226'062 perfectly cubic elements. The element size gradually reduces from  $H/3$  ( $= 0.04$  m) in the bulk up to  $H/24$  ( $= 0.005$  m) in the region of interest. The employed element size in the region of interest is about 2 times smaller than the one obtained by sensitivity analysis (Salim et al. 2011a) and about 2.5 times smaller than the recommended maximal grid size for isolated buildings (Franke et al. 2011) and street canyons (Bartzis et al. 2004).

## 2.4 *Solution method*

The three-dimensional Navier-Stokes equations, the continuity equation and the species transport equation were solved using the commercial CFD code Ansys Fluent 12.1 that employs the control-volume technique. The staggered pressure-based solver was selected. For the unsteady LES simulations, closure was obtained by means of the dynamic Smagorinsky-Lilly subgrid-scale model (Lilly 1992). The subgrid-scale turbulent Schmidt number was dynamically updated, obviating the need to prescribe a default value. Near-wall modeling was performed using the law-of-the-wall. It was verified that the instantaneous  $y^+$  values in the region of interest did not exceed 60, i.e. the limit of validity of the selected near-wall modeling approach (Ansys Inc. 2009). Pressure-velocity coupling was taken care of by the SIMPLEC algorithm (Vandormaal and Raithby 1984). Pressure interpolation was performed by means of the PRESTO! scheme (Peyret 1996). Green-Gauss cell-based gradient evaluation was employed. The third-order MUSCL discretization scheme (Van Leer 1979) was used for the convection terms of the governing equations. By default, second-order accuracy is used for the viscous terms. Second order implicit time integration is employed.

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The simulations were initialized from a preliminary RANS simulation. An LES time step of 0.00125 s was selected, resulting in cell Courant numbers below 2.5. Typically 100 iterations were required per time step, until the desired level of convergence was reached, i.e. constant residuals of  $10^{-4}$  or less for all equations (Franke et al. 2011). The residuals are defined as the imbalance of the conservation equations, summed over all elements. These values are scaled and the scaled values are used in the code as a measure of the iteration convergence (Ansys Inc. 2009). We reached  $10^{-4}$  for the species transport equation,  $10^{-9}$  for the continuity equation and machine precision ( $<10^{-12}$ ) for the three momentum equations.

All simulations were run on the ETH Brutus cluster (17'000 cores, peak performance 180 TF). Typically, one time step (0.00125 s) required 1.6 hours of CPU time. A stable flow pattern is reached after 10 s (8000 time steps), corresponding to more than 15 domain flow-through times. Statistics were collected during the subsequent 8000 time steps (10 s). In section 4, we will show that the considered time period (10 s in the reduced-scale model, or 25 minutes in full scale) is sufficient to obtain converged statistics in the largest part of the domain. We will show that, for specific locations and applications, even longer averaging times are required.

### 3 MODEL VALIDATION

The model performance was analyzed in detail in Moonen et al. (2012a). In this section, we only summarize the main conclusions of the comparison between the results, based on the model described in Section 2, and the corresponding wind tunnel measurements by Gromke and Ruck (2007, 2009). The comparison focused on the mean near-wall pollutant concentration, normalized according to:

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with  $c$  [-] the measured concentration,  $u_H$  [m/s] the mean streamwise flow velocity at height  $H$  [m] in the undisturbed approach flow and  $Q/\ell$  [m<sup>2</sup>/s] the tracer gas source strength per unit length, with  $Q$  being 6.5 cm<sup>3</sup>/min SF<sub>6</sub> mixed with 7000 cm<sup>3</sup>/min dry air and  $\ell = 1.42$  m.

Figure 2a and b depict scatter plots of the mean normalized concentration at the leeward and windward wall of the street canyon, respectively. Predicted and observed data have been paired in space and are plotted against each other. Information on the spatial location is retained, and is represented by the different marker types (\*, x, + and . for  $z/H = 0, \pm 1.25, \pm 3.75$  and  $\pm 4.9$ , respectively). Points on the diagonal indicate a perfect match between simulations and measurements. The two dotted lines bound the region where measured and simulated data differ by less than a factor two.

Figure 2a shows a good degree of correlation between model results and measurements at the leeward wall. A detailed analysis of the different datasets reveals that the simulated mean normalized concentration in the center of the street canyon (\*;  $z/H = 0$ ) is consistently higher than the observations, while the simulated concentrations at the edges of the street canyon (.;  $z/H = \pm 5$ ) are consistently lower than the observations. The mean normalized concentrations at the windward wall are significantly lower than at the leeward wall, and are systematically over-predicted by the model (Figure 2b). Note that this discrepancy does not necessarily imply poor model performance. As will be shown in the next section, the specific temporal flow features in the areas where the largest discrepancies occur necessitate the acquisition of extremely long time series in order to arrive at statistically relevant quantities. The latter condition applies both to measurements and to time-resolved simulations.

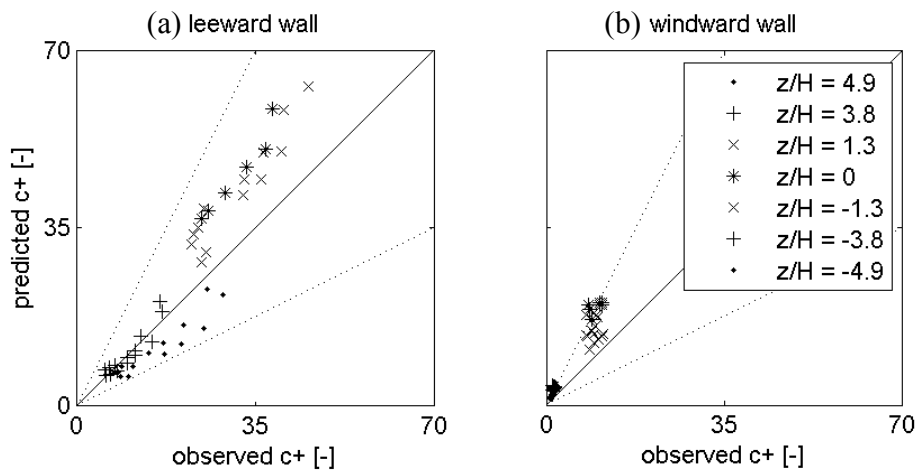


Figure 2. Predicted versus observed mean normalized concentration near (a) the leeward wall and (b) the windward wall of a street canyon. Marker types indicate the spatial location.

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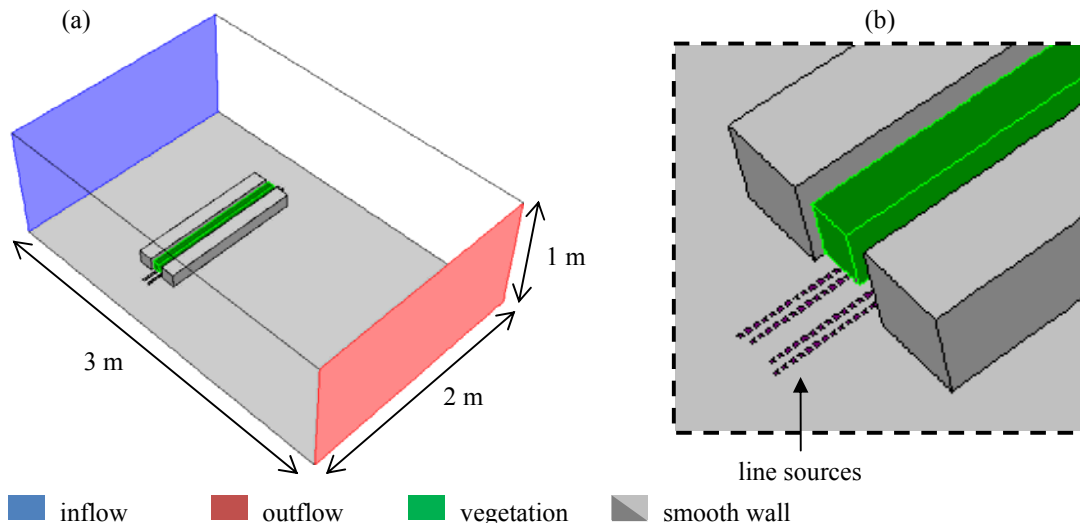


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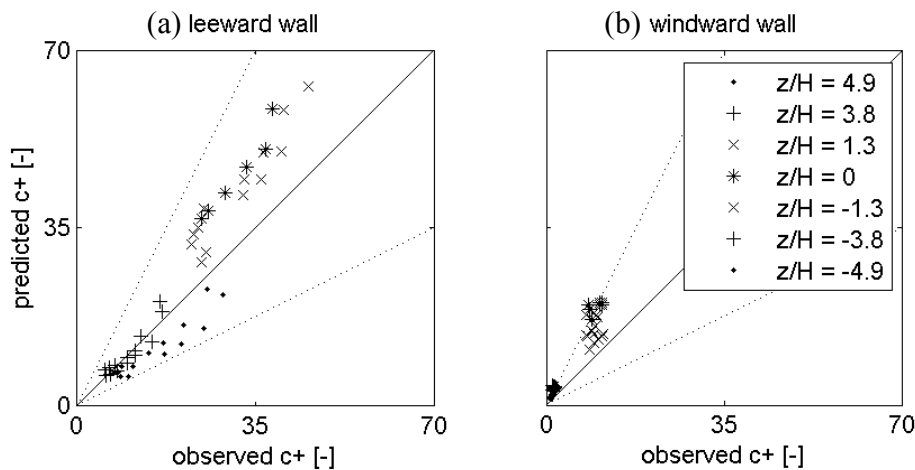


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## 4 ANALYSIS OF TEMPORAL FLOW FEATURES

### 4.1 Time series

Figure 3 depicts the temporal evolution of the normalized concentration at a typical near-ground location in the street canyon (solid line). Periods characterized by a relatively low scalar concentration alternate with sudden peaks of high concentration. The short duration of these peaks, i.e. on the order of a few milliseconds, necessitates employing small time steps in the simulation (in this case  $\Delta t = 0.00125$  s). The intermittent time between two high-concentration events does not seem to follow a regular pattern. The concentration history at a specific point is the result of the contaminated fluid parcels that reach that point over time. The peak concentrations originate from fluid parcels whose trajectory passed through the scalar source. The lower intermediate concentration is representative for the background concentration after mixing.

Two additional statistical quantities are shown on Figure 3, namely the cumulative mean (dashed line) and the cumulative standard deviation (dotted line). The cumulative mean is calculated according to:

$$c_{avg}^+(t) = \frac{1}{t - t_0} \int_{t_0}^t c^+(t) dt \quad (4)$$

and the cumulative standard deviation is obtained as:

$$c_{std}^+(t) = \sqrt{\frac{1}{t - t_0} \int_{t_0}^t (c^+(t) - c_{avg}^+(t))^2 dt} \quad (5)$$

where the onset of the averaging period ( $t_0$ ) is taken 10 s after the start of the simulation, to avoid including transitional affects.

From Figure 3, it is clear that both quantities gradually strive towards a constant value. The true mean and standard deviation theoretically require considering an infinitely long time series. In practice however, it can be noticed that their magnitude hardly changes after  $t = 16$  s. The considered time interval of 10 s (25 min in full scale) is therefore sufficiently long to study the concentration fluctuations at this spatial location. As will be shown in Section 4.3, points at different spatial locations have different requirements regarding the time period to reach representative statistical quantities. Considering higher order moments generally also implies acquiring longer time series.

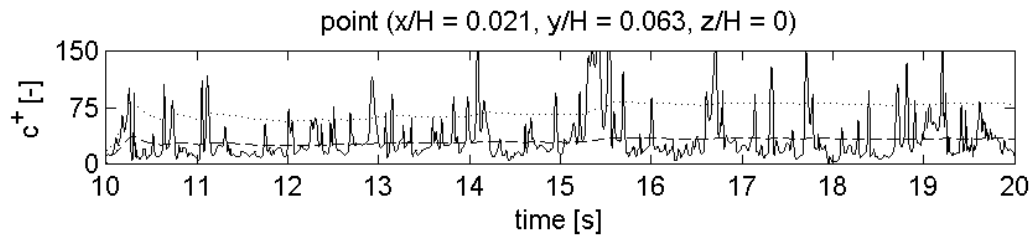


Figure 3. Temporal evolution of the mean normalized concentration at a point in the street canyon (solid line) and the corresponding cumulative mean (dashed line) and cumulative standard deviation (dotted line).

#### 4.2 Mean and standard deviation

Figure 4 depicts the ten-second mean (left) and standard deviation (right) of the normalized concentration in every cell along the mid-plane ( $z/H = 0$ ) of the urban street canyon. The flow direction of the standing vortex is schematically indicated as well. The tracer sources are pairwise clustered around  $x/H = \pm 0.2$ , leading to a locally increased mean normalized concentration in the cells above the sources. The tracer sources around  $x/H = -0.2$  receive already contaminated air from the tracer sources around  $x/H = +0.2$ , explaining the location of the maximum tracer gas concentration. The concentration rapidly decreases with increasing distance from the tracer sources (along a streamline) due to mixing and dilution. The highest mean normalized concentrations are found near the ground and at the lower part of the leeward wall.

Although the source strength is uniform in time, the standard deviation of the concentration fluctuations in the air above the sources is larger than at any other place in the considered cross section (Figure 4). This clearly demonstrates the unsteadiness of the flow. Since the line source is composed of a series of point sources, turbulent fluctuations can easily cause a fluid parcel to travel either above the source or immediately next to it. The local instantaneous concentration therefore varies between zero and the source strength, resulting in a high standard deviation.

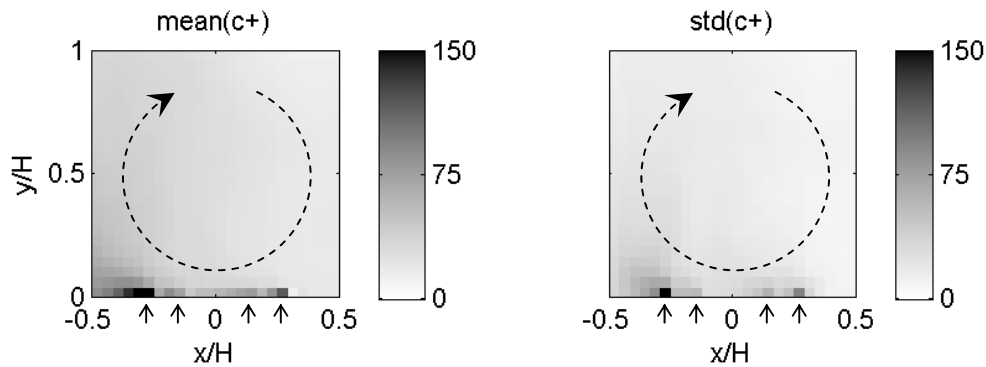


Figure 4. Mean and standard deviation of the normalized concentration in the mid-plane of the street canyon ( $z/H = 0$ ). The standing vortex and the position of the tracer sources are schematically depicted as well.

#### 4.3 Probability density function

Time-resolved simulations can offer interesting information beyond first order statistics. Figure 5 depicts probability density functions (PDFs) at 9 locations in the center plane of the urban street canyon ( $z/H = 0$ ). The PDF gives the relative likelihood that a certain normalized concentration is found at that specific location. From Figure 5, it is clear that the shape of the probability density function is highly location-dependent. Distributions near the leeward wall are consistently wider than distributions near the windward wall, and the width of the PDF decreases with increasing height above the ground. Moreover, the normalized concentration with the highest likelihood is higher for wider distributions. These observations are in agreement with the observed patterns of mean concentration and standard deviation (see Section 4.2, Figure 4).

Statistical principles state that the width of the PDF, or more precisely the variance, is proportional to the required sampling time for determining a statistical quantity such as the mean, with a given level of confidence. In other words, a long time period needs to be considered at locations where the variance is high. The observed spatial variability of the variance of the PDF im-

plies that very long time series are required at locations near the ground and near the leeward wall, while locations higher above the ground and closer to the windward wall require shorter time series for the same level of accuracy. These observations have important consequences when comparing CFD results to full-scale field data: the turbulent time scales governing dispersion might exceed the time period over which quasi-stable conditions can reasonably be expected to occur in the field. Measurement sensor locations should therefore be selected with care, preferentially avoiding regions characterized by a high variance.

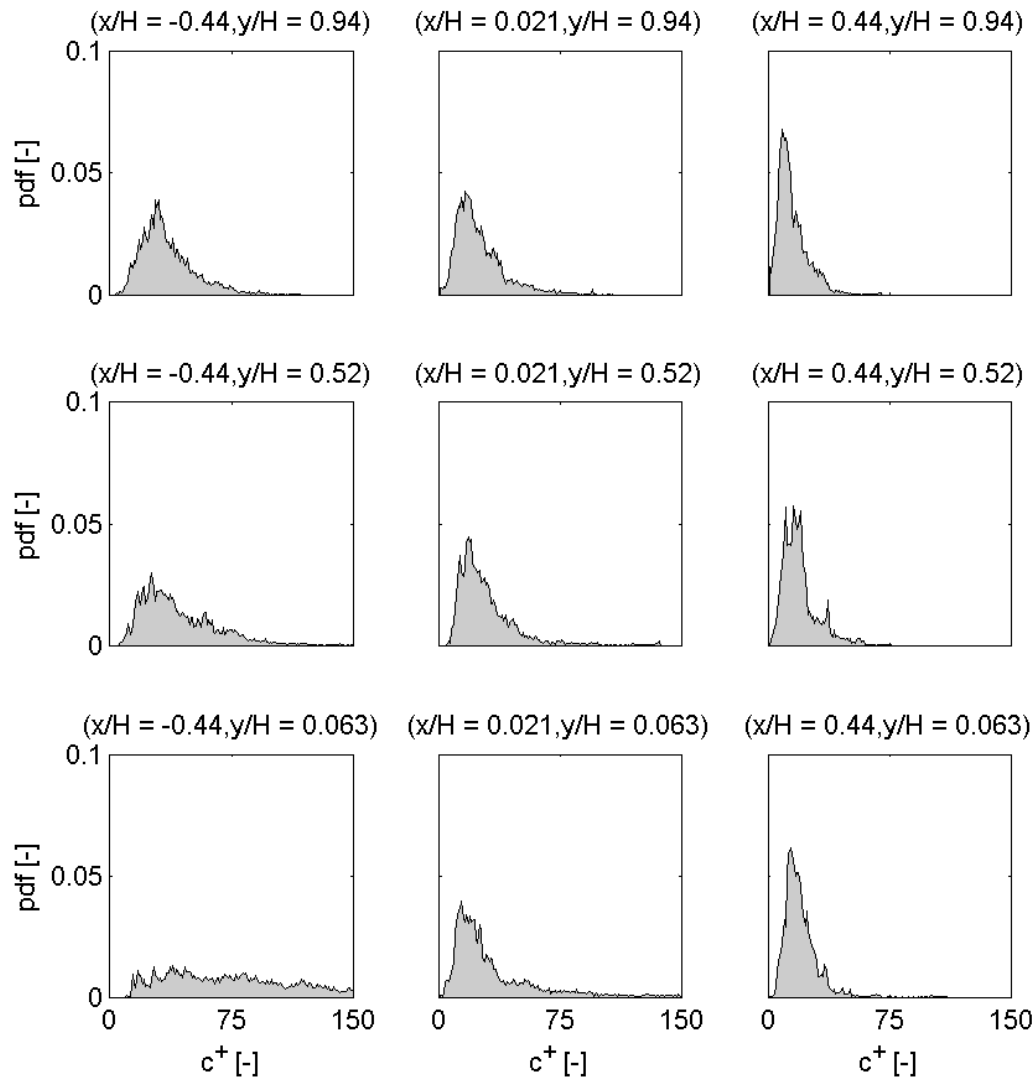


Figure 5. Probability density function (PDF) of normalized concentration at several location along the mid-plane of the street canyon ( $z/H = 0$ ). Bin size is one unit of normalized concentration.

## 5 CONCLUSIONS

Unsteady simulations of coupled flow and dispersion inside a street canyon were performed and some statistical properties of the concentration field were analyzed. We focused on the time-averaged concentration, the variance and the probability density function (PDF) at various locations in the urban street canyon. The following observations were made:

- The region in the immediate neighborhood of the pollutant source is not only characterized by a high mean concentration, but also by a large variance.
- The PDF in the mid-plane of the street canyon was found to be wider and more uniform at near-ground locations close to the leeward wall, and narrower and more pronounced at locations higher above the ground and closer to the windward wall.
- At locations characterized by a wide PDF, long time periods are needed to determine statistical quantities, such as the mean and the variance, at a given confidence level.

We have shown that carefully conducted numerical simulations are capable to provide accurate and detailed information on concentration fluctuations in urban street canyons, at high spatial and temporal resolution. The results in this paper clearly illustrate the need for sufficiently long averaging times in unsteady numerical simulations, and, by analogy, also in wind tunnel tests and during field campaigns. We believe these observations are relevant to all modelers and experimentalists, involved in pollutant dispersion research.

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