MODELLING THE CONCENTRATION FLUCTUATION AND INDIVIDUAL EXPOSURE IN COMPLEX URBAN ENVIRONMENTS

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Abstract: The concentrations fluctuations of a dispersing hazardous gaseous pollutant in the atmospheric boundary layer, and the hazard associated with short-term concentration levels, demonstrate the necessity of estimating the magnitude of these fluctuations using predicting models. Moreover the computation of concentration fluctuations and individual exposure in case of dispersion in realistic situations, such as built-up areas or street canyons, is of special practical interest for hazard assessment purposes. In order to predict or/and estimate the maximum expected dosage and the exposure time within which the dosage exceeds certain health limits, the knowledge of the behaviour of concentration fluctuations at the point under consideration is needed. In this study the whole effort is based on the 'Mock Urban Setting Test – MUST', an extensive field test carried out on a test site of the US Army in the Great Basin Desert in 2001 (Biltoft, 2001; Yee, 2004). The experimental data that was used for the model evaluation concerned the dispersion of a passive gas between street canyons which have been created by 120 standard size shipping containers. The computational simulations have been performed using the laboratory CFD code ADREA, which has been developed for simulating the dispersion and exposure of pollutants over complex geometries. The ADREA model is evaluated by comparing the model's predictions with the observations utilizing statistical metrics and scatter plots. The present study has been performed in the frame of the Action COST 732 "Quality Assurance and Improvement of Micro-Scale Meteorological Models".

Key words: *Individual exposure; Concentration; Fluctuations; Transport equation; Turbulence integral time scale.*

1. INTRODUCTION

In recent years, the increasing likelihood of a deliberate or accidental atmospheric release of a hazardous material in an urban (built-up) area has focused our attention to the understanding of the dispersion of the gaseous materials in these complex environments and the ability to reliably predict the individual exposure during these events. Due to the stochastic nature of turbulence, the instantaneous wind field at the time of the release in the atmospheric boundary layer is practically unknown. Therefore, for consequence assessment and countermeasures application, it is more realistic to rely on maximum expected dosage rather than actual one. It is reminded that the maximum dosage $D_{\max}(\Delta\tau)$ over a time interval $\Delta\tau$, can be derived from the maximum (peak) time averaged concentration $C_{\max}(\Delta\tau)$ within this interval.

$$D_{\max}(\Delta\tau) = \left[\int_0^{\Delta\tau} C(t)\cdot dt\right]_{\max} = C_{\max}(\Delta\tau)\cdot\Delta\tau \tag{1}$$

A desirable prediction model is the one that can provide estimations not only for mean concentrations but also for peak time averaged concentrations at any time interval. The present work is dealing with the question if CFD RANS models can be further improved to provide such a capability.

Recently Bartzis, et al., (2007) have inaugurated an approach relating the parameter $C_{\max}(\Delta\tau)/\overline{C}$ to the turbulent fluctuating intensity I and the $\Delta\tau/T_L$ where:

$$I = \frac{\sigma_C^2}{\overline{C}^2}, \qquad \sigma_C^2 = \overline{C'^2} \qquad \text{and} \qquad T_L = \int_0^{\infty} R(\tau)\,d\tau \tag{2}$$

T_L is the integral time scale and $R(\tau)$ the concentration autocorrelation function.

It is obvious that the right model needs to provide at least reliable predictions for the mean concentration, the concentration variances and the integral time scales.

2. METHODOLOGY

In the present study a CFD RANS modeling approach is used to meet the above requirements and is evaluated against the MUST – field experiment where a total of 120 standard size shipping containers were set up in a nearly regular array of 10 by 12 obstacles, covering an area of around 200 by 200 m. The terrain of the field site is characterized as 'flat open terrain', an ideal horizontally homogenous roughness. The whole approach has been incorporated into the existing laboratory code ADREA, a 3-D finite volume mesoscale and local scale transport code for complex terrain applications (Bartzis, 1991). In ADREA code the Reynolds averaged fully compressible transport equations of mass momentum and energy can be solved. The key turbulence parameterization is obtained by the two equation k-ζ model applicable to neutral and non-neutral atmospheric flows (Bartzis, 2006; Bartzis, 2005). Concerning pollutant transport the appropriate transport equations for mean concentrations and concentration variance are utilized based on the eddy diffusivity concept.

Formulation of the concentration variance equation
More specifically the transport equation for the concentration variance is expressed as following (Andronopoulos, et al., 2002):

$$\frac{\partial\left(\rho\overline{C'^2}\right)}{\partial t}+\frac{\partial}{\partial x_i}\left(\rho\overline{u_i}\,\overline{C'^2}\right)=-2\rho\overline{u_i'C'}\frac{\partial\overline{C}}{\partial x_i}+\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial\overline{C'^2}}{\partial x_i}-\rho\overline{u_i'C'^2}\right)-2\rho D\overline{\frac{\partial C'}{\partial x_i}\frac{\partial C'}{\partial x_i}} \tag{3}$$

To close Equation 3, the modelling approach for the production term, and the turbulent diffusion term is the more or less standard gradient-transfer approximation (e.g. Andronopoulos, et al., 2002).

For the dissipation term the most common approximation has as follow (Csanady, 1967):

$$D\overline{\frac{\partial C'}{\partial x_i}\frac{\partial C'}{\partial x_i}}=\frac{\overline{C'^2}}{T_{dc}} \tag{4}$$

T_{dc} is a turbulent dissipation time scale expected to be directly related to the integral time scale of turbulence T_L. The most common modelling approach for T_{dc} comes from the assumption that it is proportional to the turbulent kinetic energy (k) to the turbulent energy dissipation ratio (Milliez et al., 2008; Hsieh et al., 2007): (i.e. $T_{dc}\propto k/\varepsilon$) which in the present study turbulent modelling approach is expressed as:

$$T_{dc}=c_{dc}k^{\frac{1}{2}}\zeta^{-1} \tag{5}$$

In the present work the first approach is to utilize the abovementioned relation (5). The need to improve further the model predictions has created second thoughts concerning modelling approaches for T_{dc}. The starting point adopted along this road is to utilize a constant value of T_{dc} that gives the best overall concentration prediction i.e.:

$$T_{dc}=T_{dc0}=constant \tag{6}$$

Formulation of the peak time-averaged concentration equation
Following Bartzis et al., (2007) the following empirical relation has been adopted:

$$\frac{C_{\max}\left(\Delta\tau\right)}{\overline{C}}=1+b\cdot I\cdot\left(\frac{\Delta\tau}{\mathrm{T}_L}\right)^{-n} \qquad \text{b = 1.5} \quad \text{n = 0.3} \tag{7}$$

with the following approximation for T_L:

$$T_L\approx T_{dc0} \tag{8}$$

3. RESULTS AND DISCUSSION

The present modelling approach as described above has been applied to the field data of the 25/09/2001 MUST experiment. The experiment refers to a near ground point source dispersion under nearly neutral conditions. During the release period of interest (200s), the mean horizontal wind speed at the 4-m level of the upwind mast was V_h = 7.934 [ms^{-1}] and the source strength Q = 0.00375 [m^{3}s^{-1}]. The height of the buildings is H=2.54m.

The concentration variance predictions have been obtained by utilizing both models (5) and (6). Sensitivity simulations have led to the following optimum values: $c_{dc}=6.1$ and $T_{dc0}=2.467\ [s]$.

For the comparison of the two models, the statistical metrics for the normalized concentration standard deviation have been estimated using the BOOT software (www.harmo.org/kit). The statistical indices used are the fractional bias (FB), the normalised mean square error (NMSE), the correlation coefficient (R), the fraction within a factor of two (FAC2) and the hit rate (HR). The results are shown in Table 1.

It is clear from this Table that model (6) showed a better overall behaviour. Thus, only the model (6) has been used for the remaining analysis.

Figures 1 and 2 show the scatter plots of the mean normalized concentration and its normalized standard deviation as obtained by the selected model. The peak time averaged concentrations for $\Delta\tau=0.02s$ (the time resolution for most of the measurements) are shown in the form of a scatter plot in Figure 3. The corresponding FAC2 and FAC5 metrics are shown in Figure 4.

Table 1. Statistical metrics for comparison of the concentration fluctuations with the two models of the dissipation decay time T_{dc}

Variable	Metrics	Model for Decay Time (T_{dc})	
		Equation(6) $T_{dc0} = 2.467\ [s]$	Equation (5) $c_{dc} = 6.1$
$\sigma_C^* = 6.1$	FB	-0.407	-0.533
	NMSE	2.43	3.09
	R	0.718	0.635
	FAC2	0.447	0.404
	HR	0.64	0.47

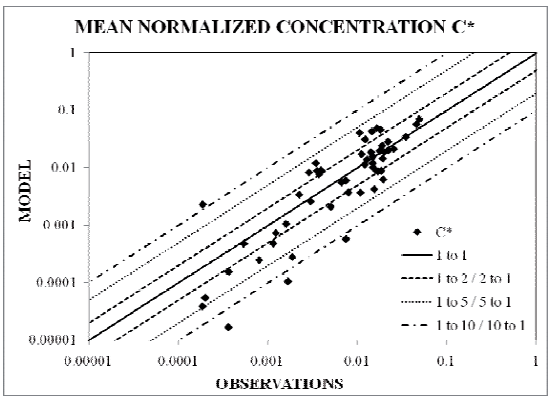

Figure 1. Mean concentration comparisons.

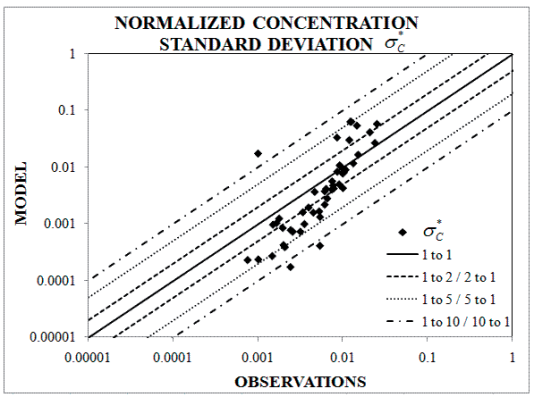

Figure 2. Concentration standard deviation comparisons.

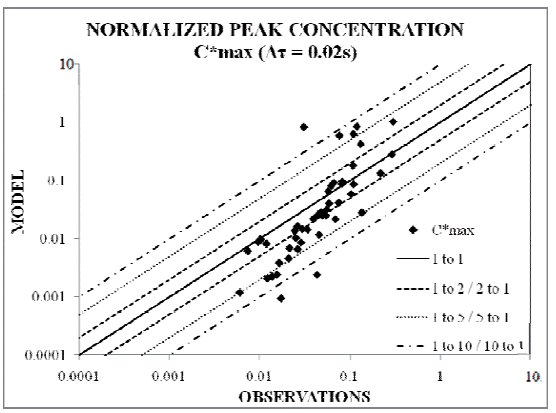

Figure 3. Peak concentration comparisons ($\Delta\tau = 0.02s$).

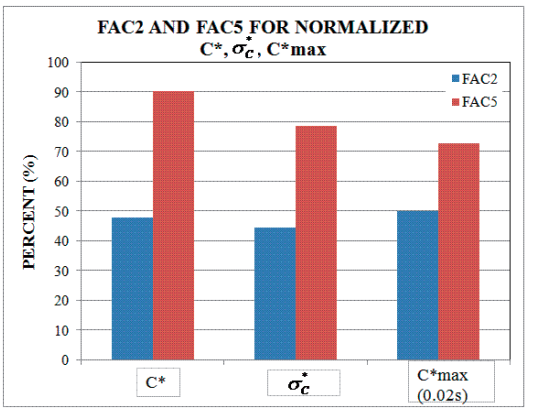

Figure 4. Statistical metrics FAC2 and FAC5 for the present model.

The overall results are quite reasonable. For the mean concentration there is a tendency of model underestimation of the small values. For the concentration fluctuations the model tends to slightly overestimate the high values. This tendency is reversed as we move to the smaller values and near 0.01 ppm the results are closer to the 1:1 line. The discrepancies for peak concentrations seem to come from the errors in estimating concentration mean and variance. This becomes more clear in Figure 5 where the peak concentrations are derived from Equation 7 using for concentration means and variances the experimental ones. Figure 5 supports further the validity of Bartzis, et all. (2007) model to predict peak concentrations within a factor of two.

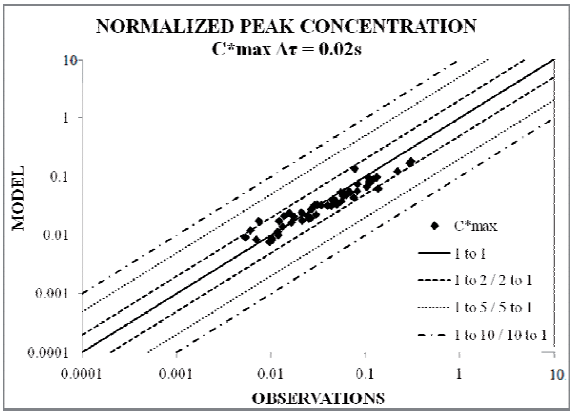

Figure 5. Peak concentration comparisons ($\Delta\tau = 0.02s$). The model results are coming by applying Equation 7 and experimental concentration mean and variance.

4. CONCLUSION

1. In this work a CFD RANS modelling approach has been presented capable of predicting mean concentrations, concentration variances and peak concentrations necessary to estimate pollutant hazard and individual exposure at any time interval.

2. Concerning plume turbulent time scale modelling, the average value approach gave better results compared with the widely used approach of local scale modelling.

3. The Comparisons with the 25/09/2001 MUST experiment have shown satisfactory results although there is still a room for improvements especially in the plume turbulent time scaling.

4. The present results support further the validity of Bartzis, et all., (2007) empirical model to predict peak concentrations within a factor of two.

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DETERMINATION OF CONCENTRATION FLUCTUATIONS WITHIN AN INSTANTANEOUS PUFF THROUGH WIND TUNNEL EXPERIMENTS

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Abstract: The instantaneous release of a dangerous substance in the atmosphere (industrial accident, malicious act) remains a difficult problem of modelling because of the turbulent nature of the atmospheric boundary layer. Indeed, the majority of dispersion models is based on a statistical description of turbulence and provides averages on a whole of possible realization of the flow. These approaches, justified for long releases, become insufficient in the case of short releases, because the transport of the pollutant is then only due to one particular realization of the flow. Consequently, the peaks of concentration affecting the exposed population are likely to be underestimated. It is thus necessary to improve the models of dispersion so they can provide a probability of concentration at each location. The literature offers several approaches to describe the probability density function of the fluctuations of concentration but very few experimental data are available to validate these approaches, in particular in the case of short releases and a fortiori in an urban context, in the presence of buildings. This is why we carried out a series of wind tunnel experiments to characterize the fluctuations of concentration during the passage of an isolated puff transported in a boundary layer flow. The experiments were initially carried out on a flat ground, then in the presence of buildings. A specific experimental methodology was designed to measure the fluctuations of concentration. A FID allows the measurement of the temporal evolution of the concentration during the passage of a puff. For each position of the sensor compared to the source, measurement is carried out for a hundred rejections, in order to be able to estimate and connect the characteristics of the instantaneous puffs to the characteristics of the average puff (position of the centre of mass, standard deviation of the temporal distribution of concentration…). The results obtained made it possible to quantify the relative influence of the various mechanisms which lead to the dispersion of a puff: Dispersion of the position of centre of mass Relative dispersion (around centre of mass) Internal fluctuation Moreover, they led to the quantification and the taking into account of the variability of parameters essential for the modelling of the internal fluctuations. A discussion makes it possible to connect the role of the three phenomena described above to the particular configuration of the boundary layer flow in the wind tunnel (roughness, presence of obstacles).