H14-181
MODELING INDIVIDUAL EXPOSURE FROM AIRBORNE RELEASES

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Abstract: The capability to predict short time individual exposure, i.e. the pollutant concentration integral over a specified small time interval, is very important for several applications that have to do for example with deliberate/accidental hazardous releases, odour fluctuations, material flammability level exceedances, etc. The challenge is to build such a capability in models as simple models as possible dealing with geometries as complex as possible. Along this direction, Bartzis et al. (2008) have inaugurated a simple approach relating maximum individual exposure to parameters such as the fluctuation intensity and the concentration integral time scale. The present methodology has been validated until now only with field measurements. The proper validation needs true stationary cases that in the real atmosphere hardly exist. For this reason and for a first time a wind tunnel experiment was used for the validation of the methodology. The results verify the validity of the methodology. Further improvements are suggested in terms of model parameters. The model improvements are also suggested for application of the model to relatively large time integrals.

Key words: *Dosage; Individual exposure; Turbulence integral time scale, Wind tunnel measurements*

INTRODUCTION

The capability to predict short time individual exposure i.e. the pollutant concentration integral over a specified time interval ranging from inhalation time up to several minutes, is very important in dealing with deliberate air borne hazardous releases. Such a quantity is of a stochastic nature and practically unpredictable especially for very small time intervals since the instantaneous conditions of the atmosphere are unknown at the time of the release. However, what it is more important in emergency management, and predictable at the same time, is the maximum expected individual exposure which is defined as a dosage over a specified time interval $\Delta\tau$:

$$D_{\max}(\Delta\tau) = (\int_{\Delta\tau} \mathrm{C(t)dt})_{\max} = C_{\max}(\Delta\tau)\cdot\Delta\tau \qquad (1)$$

where C(t) is the instantaneous concentration at a receptor point and $C_{max}(\Delta\tau)$ is the maximum time average (peak) concentration over $\Delta\tau$.

The usual methodology to predict the maximum expected concentration/dosage is to assume a probability density function (pdf) as a function of the mean concentration, concentration variance and intermittency factor (e.g. Lung et al. 2002; Yee, 1990). The peak concentration can be estimated from the above pdf with an assumed confidence limit (CL). It is obvious that such a probabilistic approach is very sensitive to the CL selected value. Theoretically if CL tends to unity the peak concentration tends to infinity. However, in reality the peak concentration is finite and is expected to dilute downstream (Bartzis and Efthimiou, 2010).

THE INDIVIDUAL EXPOSURE MODEL

Despite the above mentioned difficulties the challenge remains to build an individual exposure prediction capability in air dispersion models as simple as possible dealing with geometries as complex as possible. Along this direction, Bartzis et al., (2008) have proposed a relatively simple model based on the hypothesis that key parameters in defining maximum dosage are the concentration fluctuation intensity (I) and the autocorrelation time scale T_C i.e.

$$D_{max}(\Delta\tau) = \overline{C}\left[1 + \beta I\left(\frac{\Delta\tau}{T_C}\right)^{-n}\right]\Delta\tau \qquad (2)$$

$$I = \frac{\sigma_c^2}{\overline{C}^2} \qquad (3)$$

where σ_c^2 is the concentration variance and $\overline{C}$ is the mean concentration. The above quantities can be derived by the CFD RANS modeling by solving the relevant transport equations for the mean concentration and its variance. The concentration time scale (T_C) is estimated as a function of the turbulence modeling parameterization and the concentration travel time (Efthimiou and Bartzis, 2011). The β and n are constants derived from experimental evidence. An indicative value for the parameter n = 0.3 has been considered as reasonable based on past experience especially for ground releases. The power law best fit analysis of the FLADIS experiment concentration signals has verified the above n value (Bartzis et al, 2008). Concerning the value of the parameter β, an extensive analysis of the MUST field concentration data of various stability classes have suggested an indicative value of β = 1.65 with an uncertainty of a factor of four (Bartzis and Efthimiou, 2010).

The estimation of β based on field data analysis includes uncertainties due to the fact that the concentration time series are not long enough and turbulence stationarity hardly exists. Such drawbacks are expected to be removed if we replace the field data with wind tunnel data. For this reason and for a first time a wind tunnel experiment was used for the validation of the methodology. In addition, the utilization of a number of wind tunnel data will give the opportunity for a more reliable estimation of model uncertainties.

THE WIND TUNNEL MEASUREMENTS

Flow and dispersion experiments were conducted in the boundary layer wind tunnel “WOTAN” at the Environmental Wind Tunnel Laboratory of the University of Hamburg. The 18m long and 4m wide test section of the tunnel is equipped with an adjustable ceiling that allows the modeling of zero-pressure gradient atmospheric boundary layers and flows within and above urban geometries. The test case is the wind and concentration field within and above a 1:225-scale wind-tunnel model of a semi-idealized urban complexity (‘Michel-Stadt’) that is part of the online validation data base CEDVAL-LES (www.mi.uni-hamburg.de/CEDVAL-LESV.6332.0.html). This building structure comprehends distinct characteristics of typical central European cities (Figure 1). With sharp building corners, characteristic courtyards, and complex intersection structures the model was designed to pose a challenge to numerical models while still being an approximation of a genuine urban roughness. Whereas the street canyon width was kept constant, the height of the flat-roof buildings varied between 15, 18, and 24m fullscale.

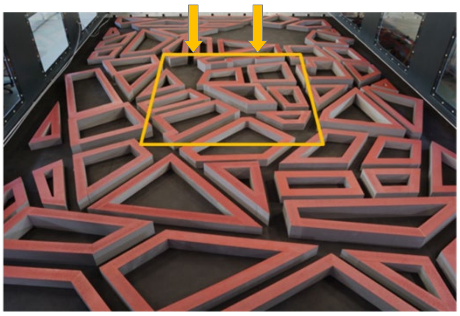

Figure 9. Wind-tunnel model of semi-idealized complexity. The rectangle encompassed the model region of densely spaced flow measurements. The arrows indicate the inflow direction.

MODEL REFINEMENT AND UNCERTAINTIES

Data description and manipulation

All the available data of the wind tunnel experimental series ‘Michel-Stadt’ has been exploited. The relevant dataset includes 1 trial which cover the neutral stability class and one atmospheric condition and contains high resolution concentration time series with time resolution $\Delta\tau = 0.005$s from 196 fast Flame Ionization Detectors (FIDs) sensor measurements. Each sensor contains 55,000 concentration measurements (i.e. $1.078 \cdot 10^7$ data points for all sensors) and each sensor includes data for a time period T = 275s. The min/max values found for I and C_{max}/C_{mean} were 0.077/15.57 and 16.55/8.82 respectively. Following Yee and Biltoft (2004) the autocorrelation time T_C is calculated from autocorrelation function $\rho(\tau)$ as the value at $\rho(\tau) = 0.1$. The min/max values of T_C were found 0.041s/1.001s which correspond to a normalized time range T/T_C = 275 - 6707. These values were long enough to assume turbulence stationarity.

Estimation of the parameter β

For the model refinement only the high resolution ($\Delta\tau = 0.005$s) data has been utilized. For the estimation of the parameter β following the same procedures as in Bartzis and Efthimiou (2010), the exponent n was kept constant (=0.3) whereas the parameter β was varied from signal to signal. In this case the imperfectness of the model as well the possible errors on measurements are going to be reflected to β value variability. The indicative value of constant β is obtained from best fit analysis of parameter A vs I where:

$$A = \left[\frac{C_{max}(\Delta\tau)}{\overline{C}} - 1 \right] \Bigg/ \left(\frac{\Delta\tau}{T_C} \right)^{-n} \qquad (4)$$

as shown in Figure 2. This analysis produces an indicative value β equal to 2.88. This value is higher than the value of 1.65 derived from the field data which was expected. The upper bound of β for the wind tunnel data was found 10 that corresponds to $\beta_{max} \approx 3.5x\beta$. It is reminded that for the field data the relationship was $\beta_{max} \approx 4x\beta$. In Figure 3 the probability density function of the parameter β is presented with its mean value and the variance. It is clear from the histogram that the indicative value of 2.88 lies in the neighborhood of the most probable β-value. On the other hand, the vast majority of β-data lie below 6.6 i.e. 2.3xβ. The latter value is more representative of the β uncertainty in this case. What is more interesting the value of 6.6 is practically the same with the one (6.9) found in the field data analysis. So both wind tunnel and field data analysis point out to an upper bound rounded value of 7.

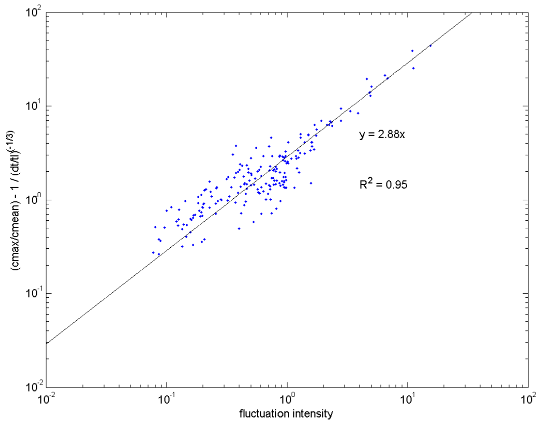

Figure 2. Correlation of the quantity A to fluctuation intensity. The data follow a linear relationship with slope 2.88 and R^2 = 0.95.

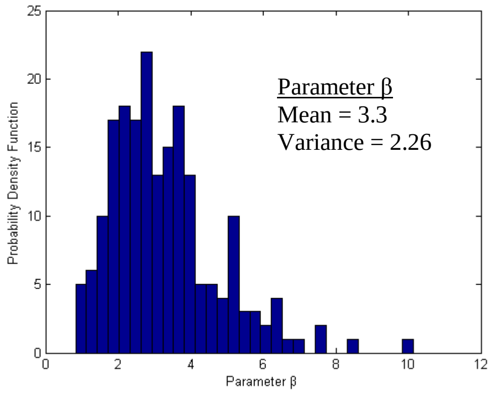

Figure 3. The probability density function of the parameter β data.

Model performance for $\Delta\tau = \Delta\tau_0$

In Table 1 the factor of two of observations (FAC2) and the percentage not exceeding the experimental value multiplied by a factor of two (FACx2) are presented using the two values for the parameter β as have been estimated until now from the corresponding experiments i.e. 1.65 (field data) and 2.88 (wind tunnel data). As expected the the value of β=2.88 has improved considerably the results.

Table 1. Wind field data : C_{max} model vs observation performance for $\Delta\tau = \Delta\tau_0$.

β	FAC2	FACx2
1.65	80.1%	80.1%
2.88	95.41%	98.98%

THE MODEL OVERALL PERFORMANCE ($\Delta T \geq \Delta T_0$)

In this study except of the estimation of the parameters of the model (equation 2), there is a need also to test the performance of the model for large and small time intervals. Thus the model performance is tested with the wind tunnel data for time intervals ranging from $\Delta\tau_0$ to 10s ($\Delta\tau/\Delta\tau_0$ = 1 – 2000).

In Table 2 the factor of two of observations (FAC2) and the percentage not exceeding the experimental value multiplied by a factor of two (FACx2) are presented for $\Delta\tau$ ranging from $\Delta\tau_0$ to 10s using the two values for the parameter β.

Table 2

Parameter β		FAC2	FACx2
ORIGINAL MODEL	1.65	97.24%	98.45%
PRESENT MODEL	2.88	95%	99.95%

In this case the original value of 1.65 gives better results for large Δτ values >It is surprising that FAC2 is slightly smaller for b=2.88. In Figure 3 all $C_{max}(\Delta\tau)$ data are compared with the model equation (2) with β = 2.88. . It is noticed that the model predicts rather well the experimental values at small integral times, while a model overprediction occurs for the large time intervals. It is obvious that there is a need for model improvement with the following two characteristics:

1. For small time integrals the results of the model should be the same as before.
2. For large time integrals the results of the model should be decreased.

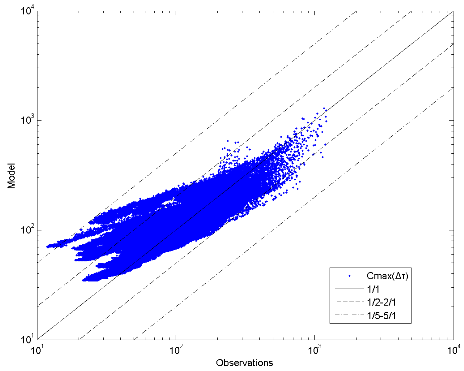

Figure 4. Peak concentration comparisons ($\Delta\tau/\Delta\tau_0$ = 1– 2000).

MODEL IMPROVEMENTS

A plausible approach to remove the above mentioned model behavior is to allow *β* parameter to be a function of $\Delta\tau/\Delta\tau_0$ instead of being a constant. i.e.

$$\beta = \beta\left(\frac{\Delta\tau}{T_c}\right) \tag{5}$$

The model behaviour at small Δτ suggests:

$$\beta_0 = 2.88 \tag{6}$$

After an extensive data analysis in order to identify a proper *β* – function, the following correlation for the parameter β is suggested:

$$\beta\left(\frac{\Delta\tau}{T_c}\right) = \beta_0 e^{-a\frac{\Delta\tau}{T_c}} \tag{7}$$

The best fit analysis of β versus $\Delta\tau/\Delta\tau_0$ suggest the following value for *a*:

$$\alpha = -0.012 \tag{8}$$

Thus, the improved model for $C_{max}(\Delta\tau)$ estimation is given as follows:

$$C_{max}(\Delta\tau) = \overline{C}\left[1 + \beta e^{-a\frac{\Delta\tau}{T_c}} I\left(\frac{\Delta\tau}{T_c}\right)^{-n}\right] \tag{9}$$

with *β* = 2.88, *n* = 0.3 and *a* = –0.012. The improved $C_{max}(\Delta\tau)$ model results are presented in Figure 5.

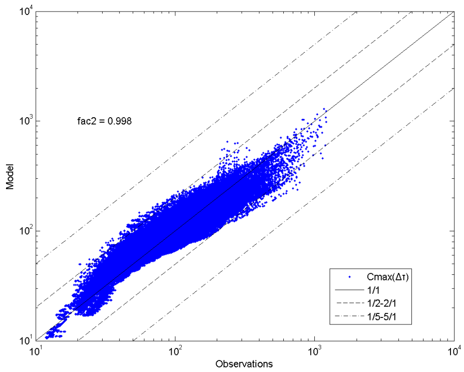

Figure 5. Peak concentration comparisons using the improved model (9) ($\Delta\tau/\Delta\tau_0$ =1 – 2000).

It is obvious by comparing Figure 4 and Figure 5 that the improved model is considerably better than the original one. An indicator for this is FAC2 that has been increased to the value of 0.998.

CONCLUSIONS

The present work is focused on the validation of Bartzis, et al., (2008) empirical model for $C_{max}(\Delta\tau)$ to predict reliably the individual maximum exposure in case of deliberate or accidental atmospheric releases of hazardous substances. For the first time concentration data from a wind tunnel experiment has been utilized for this purpose. The extensive dataset of the 'Michel Stadt' was analyzed which included 1 trial of neutral stability class and contained in total 196 concentration sensor data with time resolution of 0.005 s. From the data analysis the parameter β was estimated equal to 2.88. For the estimated value of the parameter β, the $C_{max}(\Delta\tau)$ model predicts very well (FAC2 ≈ 0.95 and FACx2 ≈ 0.99) the maximum individual exposure. Concerning the large time intervals an exponential correction term has been introduced to β-value based on experimental evidence. The new model is capable of predicting all time intervals giving an overall FAC2 ≈ 1.

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