H13-28
MAXIMUM INDIVIDUAL EXPOSURE ESTIMATION USING CFD RANS MODELLING

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Abstract: One of the key problems in coping with deliberate or accidental atmospheric releases is to estimate the maximum individual exposure in short times. Recently Bartzis, *et al.*, (2007) have inaugurated an approach relating maximum dosage to parameters such as the fluctuation intensity and the concentration integral time scale. The fluctuation intensity can be derived by the CFD RANS modelling by solving the relevant transport equations for the mean concentration and its variance. The concentration time scale is estimated as a function of the turbulence modeling parameterization and the concentration travel time (Efthimiou, G.C. and J.G. Bartzis, 2010). The present methodology has been validated until now only for neutral flows. The purpose of this study is to validate the methodology for various atmospheric stability classes. For this reason the extensive dataset of MUST experiment (Yee, E. and C. Biltoft, 2004) has been used. This dataset includes 81 trials which cover practically all stability classes and various atmospheric conditions and contains in total 4004 non zero concentration sensor data with time resolution 0.01 – 0.02 s. The results verify the validity of this methodology. Another important output is the estimation of the methodology uncertainty involved. This work contributes to the better estimation of maximum individual exposure studies in short time intervals.

Key words: *Individual exposure; Dosage; Concentration fluctuations; Turbulence integral time scale.*

BACKGROUND

One of the key problems in coping with deliberate or accidental atmospheric releases of hazardous materials in urban (built-up areas) is to estimate the individual exposure over a certain time interval. In many cases the releases are short and/or the concentrations are high and there is a need to estimate the individual exposure in relatively short times. Due to the stochastic nature of turbulence, the instantaneous wind field at the time of the release is practically unknown. For that reason the short time actual exposure at a certain receptor point is also unknown. To assess however the consequences and countermeasures, one needs to predict the maximum expected exposure rather the actual one. It is reminded that the maximum exposure over a time interval $\Delta\tau$ can be expressed in terms of the maximum dosage $D_{max}(\Delta\tau)$:

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

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

It is evident that a desirable prediction model should be able among others to predict $C_{max}(\Delta\tau)$. Thus the real problem in the present work is posed as follows. A hazardous air pollutant is released from a point source. The release could be instantaneous or finite and it is characterized by its peak release rate. If the rate of release is constant then the peak release rate coincides with the constant release rate. We need to predict at a certain receptor point downstream the concentration $C_{max}(\Delta\tau)$. The basic assumption here is that the turbulence field within the time range from the start time of the release to the ending time of the plume passage from the receptor is stationary. Is it possible for a CFD RANS model to be able to predict such a quantity? The selection of RANS models is justified from the fact they are the simplest and most practical CFD models to cope with a complex environment such as the urban environment.

THE APPROACH

Since the key target is the prediction of $C_{max}(\Delta\tau)$, the whole modeling approach can be reduced to a simplified problem as follows. The source is replaced by a continuous source of constant release rate equal to the real peak release rate. The abovementioned stationarity assumption on turbulence is extended for an infinite time. It is expected that the extreme value of $C_{max}(\Delta\tau)$ of the simplified problem is expected to be at least equal to that of the real problem as defined above. This can be explained from the fact that in the simplified problem the $C_{max}(\Delta\tau)$ value is expected to be greater or equal of the one in the real problem. It should be noted in addition that the introduction of the simplified problem is a plausible approach for all prediction models including DNS and LES due to the fact that the atmospheric turbulence is stochastic and it is practically impossible to know exactly the turbulence field at the time of the start of the release.

Before discussing the modeling of $C_{max}(\Delta\tau)$ it should be clear from the beginning that its value is finite and is expected not to be higher than the concentration of the release material. Then $C_{max}(\Delta\tau)$ is expected to dilute downstream. For example in Figure 1 $C_{max}(\Delta\tau)$ measured during MUST Experiment Trial No 11 (Yee, E. and C. Biltoft, 2004) is plotted against plume downwind distance. The dilution of $C_{max}(\Delta\tau)$ as the pollutant moved downstream is clear.

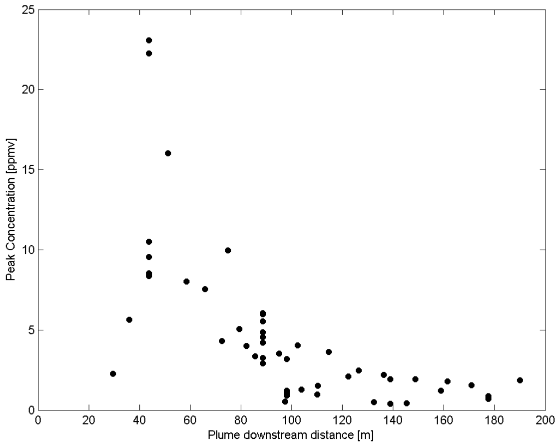

Figure 1. Plume downstream distance of the peak experimental concentration for Trial No 11 of the MUST experiment.

The fact that $C_{max}(\Delta\tau)$ is a finite quantity makes the deterministic models more attractive than the probabilistic ones. Recently Bartzis, *et al*., (2007) have inaugurated an approach relating the parameter $C_{max}(\Delta\tau)/\overline{C}$ to the fluctuating intensity I and the $\Delta\tau/T_L$ ratio:

$$\frac{C_{max}(\Delta\tau)}{\overline{C}} = f\left(I, \frac{\Delta\tau}{T_L}\right) \qquad (2)$$

where T_L is the turbulence integral time scale derived from the autocorrelation function $R(\tau)$:

$$T_L = \int_0^\infty R(\tau)d\tau \qquad (3)$$

The fluctuation intensity I is defined as:

$$I = \frac{\sigma_C^2}{\overline{C}^2} \qquad (4)$$

where σ_C^2 is the concentration variance.

Bartzis, *et al*., (2007) based on past efforts to estimate maximum time averaged concentrations from Gaussian plume at different averaging times came to the following proposal:

$$\frac{C_{max}(\Delta\tau)}{\overline{C}} = 1 + \beta \cdot I \cdot \left(\frac{\Delta\tau}{T_L}\right)^{-n} \qquad (5)$$

Where β and n are constants derived from experimental evidence. The indicative values given, have as follows:

$$\beta = 1.5; \quad n = 0.3 \qquad (6)$$

The experience up to now has shown that this model seems to give reasonable results within a factor of two (Efthimiou, G.C. and J.G. Bartzis, 2010; Efthimiou, *et al*, 2008; Bartzis, *et al*, 2007). This approach requires besides the prediction of the mean concentration $\overline{C}$, the predictions of σ_C^2 and T_L. Concerning CFD-RANS modeling a considerable experience has been built in predicting σ_C^2 (e.g. Milliez, M. and B. Carissimo, 2008; Andronopoulos, *et al*, 2002). With respect to T_L a plausible estimation has been proposed recently (Efthimiou, G.C and J.G. Bartzis, 2010) as a function of the turbulence local characteristics of the flow and the pollutant travel time.

MODEL REFINEMENT AND UNCERTAINTIES

It should be noted that model (5) has been calibrated by a limited number of field data from neutral flows. There is a need to expand the application to more data including non neutral flows as well. In addition, the utilization of a large number of data will give the opportunity for a more reliable estimation of model uncertainties.

For this purpose all available data of the field experimental series MUST has been exploited. The relevant dataset includes 81 trials which cover practically all stability classes and various atmospheric conditions and contains high resolution concentration time series ($\Delta\tau$ = 0.01 – 0.02s) from 5832 sensor measurements. A total number of $1.36 \cdot 10^8$ concentration measurements have been processed.

A detailed description of the MUST experiment is given in Biltoft, C., (2001) and Yee, E. and C. Biltoft, (2004). A total of 120 standard size shipping containers of width 12.2 m, length 2.42 m and height 2.54 m were set up in a nearly regular array consisting of 12 rows of 10 obstacles. The MUST experiment, is a well established experiment with high quality concentration and meteorological measurements. The dataset includes 81 trials which cover practically all stability classes and various atmospheric conditions. The tracer gas (propylene) was measured from 48 fast-response photoionization detectors (DPIDs) with time resolution of 0.02s and 24 Ultraviolet Ion Collectors (UVICs) with time resolution of 0.01s. These sensors were located at various heights and distances from the corresponding sources.

The purpose of the data assessment was to select the time series that are appropriate for the present analysis. For each trial specific time periods (e.g. 200s, 900s, 450s) were selected for the calculation of statistical measures (mean, variance, maximum and integral time scale). These periods were originally chosen by Yee, E. and C. Biltoft, (2004) and were primarily based on the stationarity (i.e., speed and direction) of the wind over the period. The total number of sensor concentration data for all trials is (48 DPID + 24 UVIC sensors) x 81 trials = 5832 data. From this population only the 4004 non zero concentration sensor data have been found.

Before deciding on the validation strategy one should keep in mind the coefficients β and n show some variation when trying to fit the experimental data (Bartzis, *et al.*, 2007). This could be attributed not only to the model imperfectness but also to the fact that perfect stationarity does not exist especially for long times and the measured signals are often ‘contaminated’ by non local large scale disturbances. For the same reasons the estimated time scale T_L shows also sensitivity to the time series length as well as to time resolution.

In order to make the whole validation procedure simple and workable it has been decided to keep the exponent n constant (=0.3) and leave the proportionality factor β to be 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 and its variability/uncertainty.

Applying this strategy to every signal, it has been also clear that for practical reasons it was not realistic to perform a quality assurance of the signals with respect to errors or/and stationarity. Therefore known statistical methods to identify outliers have been applied. More specifically, two well known methods have been applied:
a) The Box Plot method (MATLAB, 2008) which gave 194 outliers and 3810 remaining data with a maximum value 3.92.
b) The Grubbs Test (Grubbs, F., 1969) which gave 45 outliers and 3959 remaining data with a maximum value 5.88.
For conservative reasons the second method has been adapted. Thus, the 45 above mentioned outliers were removed from the population of β. The 3959 β - values have been used in the following analysis.

In Figure 2 the experimental probability density function of the parameter β data is presented. It is interesting to see that the data seem to follow well a Gamma distribution function.

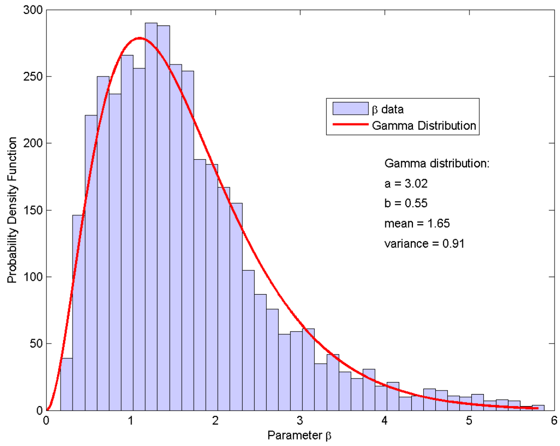

Figure 2. The probability density function of the parameter β data and the fitted Gamma distribution.

It is reminded, that the Gamma probability density function (pdf) is given by the relation:

$$p(x\,|\,a,b) = \frac{1}{b^{a}\cdot\Gamma(a)}\cdot x^{a-1}\cdot e^{-\frac{x}{b}} \tag{7}$$

where α is the shape parameter and b is the scale parameter. The maximum likelihood estimates (MLEs) of the parameters α, b as well as the 95% confidence intervals of their values as derived using MATLAB are presented in Table 1. The mean value of the gamma distribution with parameters α and b is α·b while the variance is $\alpha\cdot b^2$. These values are presented also in Table 1.

Table 2. Parameters α, b of the Gamma distribution with their 95% confidence intervals and the corresponding mean and variance.

Parameters	MLEs	95% confidence intervals	
		Lower bound	Upper bound
α	3.02	2.89	3.14
b	0.55	0.52	0.57
Mean	1.65	1.51	1.8
Variance	0.91	0.79	1.03

These results strengthen further the validity of the equation (5). It should be noted that the mean value 1.65 is well comparable with the indicative value 1.5 given by Bartzis, *et al.*, (2007).

Since the parameter β is expected to have a finite value it is not enough to express its variance only by a pdf in which its extreme value goes theoretically to infinity. There is a need to try to estimate its upper bound. One method of extracting this value is to use Extreme Value Theory (Gumbel, E.J., 1958) one method of which is to take the exceedances over a predetermined parameter threshold β=u (Reiss, R.D. and M. Thomas, 2007). Following by Balkema, A.A. and L. de Haan, (1974) and Pickands, (1975), the pdf of these exceedances can be approximated by the Generalized Pareto Distribution (GPD) (Reiss, R.D. and M. Thomas, 2007). The GPD approach can conclude to a finite extreme value. This value is estimated from the relationship:

$$\beta_{max} = u - \frac{\sigma}{\xi} \tag{8}$$

where ξ is the GPD shape parameter and σ its scale parameter. The threshold value u can be obtained by applying the mean excess plot method (Munro, R.J. *et al*., 2001). The mean excess is the sum of the excesses over the threshold u divided by the number of data points which exceed the threshold u (Gencay, R., 2001). The relevant plot is shown in Figure 3.

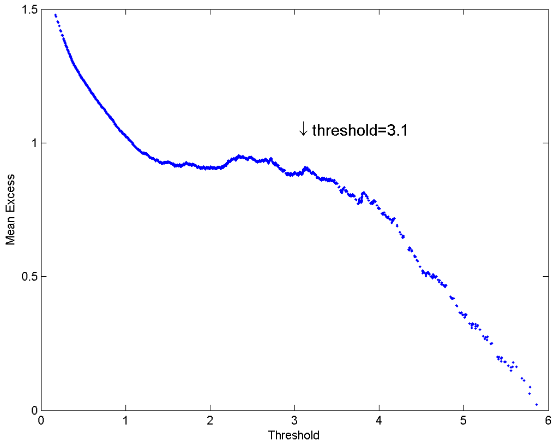

Figure 3. Mean excess plot of the parameter β.

The mean excess parameter as a function of the selected threshold should be approximately linear as the theory of GPD imposes (Reiss, and Thomas, 2007). According to Figure 3 this criterion is fulfilled for an approximate value of threshold above 3.1. In the tail of the distribution (threshold > 3.1) we expect the extreme values of β_{max} to be constant. This value is obtained from equation (8). The ξ and σ parameters are derived by the Maximum Likelihood Estimation (MATLAB, 2008) applied to the data above threshold and their corresponding values are ξ = -0.35 and σ = 1.2. The application of equation (8) gives β_{max} = 6.5. This value appears to be approximately four (4) times higher than the mean β value of 1.65 obtained above. If we adopt the gamma pdf as defined above to describe β variability/uncertainty, this value corresponds to a confidence limit 99.94%.

Trying to summarize we can conclude that the model (5) can be further refined by keeping n = 0.3 and giving to constant β a more probabilistic value with its pdf described by a gamma function with a = 3.02 and b = 0.55 corresponding to mean value β = 1.65. The pdf can be valid up to β_{max} = 4 x (mean β) corresponding to Gamma cdf confidence limit of 99.94%.

In Figure 4 all $C_{max}(\Delta\tau)$ data are compared with the model equation (5) with β = 1.65 and n = 0.3. The experimental data are well predicted within a factor of two. In fact the factor two FAC2 = 82.25% whereas FAC5 = 99.42%. The latter result is expected if one takes into consideration that β_{max} = 4 x (mean β).

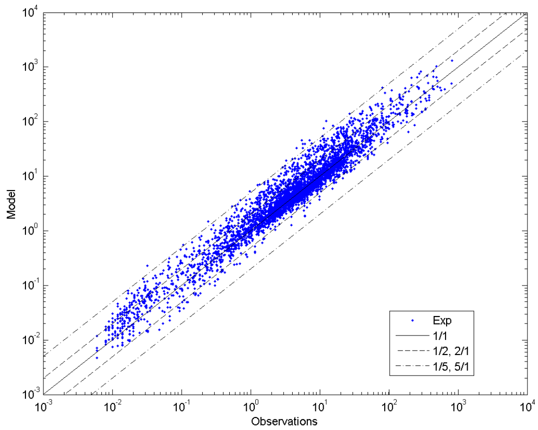

Figure 4. Peak concentration comparisons (Δτ = 0.01 – 0.02 s).

CONCLUSIONS

The present work is addressed on the validation of Bartzis, *et al*., (2007) empirical model (equation (5)) to predict reliably the individual maximum exposure in case of deliberate or accidental atmospheric releases of hazardous substances for various atmospheric stability classes.

For the first time a vast amount of data has been utilized for this purpose. The extensive dataset of the MUST experiment was analyzed which included 81 trials of various stability classes and contained in total 5832 concentration sensor data with time resolution of 0.01 – 0.02 s.

The present analysis of the data strongly supports the validity of equation (5) to predict maximum individual exposure in short time intervals. For this purpose a steady state CFD – RANS model could provide the necessary input parameters (i.e. $\overline{C}$, σ_C^2 and T_L). It is recommended that the nominal value for β to be changed to 1.65.

For the first time the β variation and uncertainty has been systematically studied. It shows very clearly a gamma function variation (equation (7)) with the parameters a = 3.02 and b = 0.55. (Uncertainties for a and b are also given). An extreme value β_{max} = 4 x 1.65 is also estimated based on Extreme Value Theory which corresponds to probability 99.94% of the Gamma pdf.

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