#### PREDICTING THE INDIVIDUAL EXPOSURE FROM AIRBORNE HAZARDOUS RELEASES BY RANS- CFD MODELS

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#### INTRODUCTION

One of the key problems in coping with deliberate or accidental atmospheric releases is the ability to reliably predict the individual exposure during the event. Due to the stochastic nature of turbulence, the instantaneous wind field at the time of the release is practically unknown. Therefore, for assessing possible consequences and applying the optimal countermeasures in the least possible interval, a more realistic option is to rely on the maximum expected dosage rather than actual one.

Here, 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 the interval.

$$D_{\max}(\Delta\tau) = \left[\int_{0}^{\Delta\tau} C(t) \cdot dt\right]_{\max} = C_{\max}(\Delta\tau) \cdot \Delta\tau$$
(1)

The key question is whether the available models today, can predict reliably the quantity  $C_{\max}(\Delta \tau)$  fulfilling the needs of every decision maker facing this problem. It is obvious that the ideal model able to perform this task has to be valid for any time interval selected ranging from the inhalation time (i.e. a few seconds) to rather long times (e.g. hours, days, years). For time intervals one hour and longer the models predicting the mean field concentrations are sufficient especially when the source release time is long enough. A variety of models ranging from simple empirical models to complex CFD models are giving such predictions with a good degree of reliability in many cases.

The problem arises when the releases are short and/or the concentrations are high and it is required to estimate either the individual exposure in relatively short times or the exposure times in which health related exposure limits are exceedeed.

### THE PRESENT APPROACH

Recently *Bartzis et al* (2007) have proposed an empirical model that correlates the peak timeaveraged concentration with the mean concentration, the fluctuation intensity and the turbulence integral time scale.

$$\frac{C_{\max}(\Delta \tau)}{\overline{C}} = 1 + b \cdot I \cdot \left(\frac{\Delta \tau}{T_L}\right)^{-n}$$
(2)

where  $C_{\text{max}}(\Delta \tau)$  is the peak time averaged concentration and  $\Delta \tau$  is the time interval. Parameters n and b have the following indicative values: 0.3 and 1.5 respectively.

The fluctuation intensity I corresponds to 1Hz signal is defined as :

$$I = \frac{\sigma_c^2}{\overline{C}^2} \tag{3}$$

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

$$T_L = \int_0^\infty R(\tau) d\tau \tag{4}$$

All model parameters have been calibrated with 1Hz concentration signals representing the instantaneous approximation due to the fact that this frequency is expected in most cases to fall well within the inertial range of concentration spectra (*Mylne K.R.*, 1991).

The fundamental question that is posed in the present study is whether Eq. (2) can be utilized in RANS CFD modelling to predict peak time averaged concentrations for any time range The ideal RANS CFD model in which Eq (2) can be utilized is the one that reliably predict the mean concentration and its variance as well as the integral time scale  $T_L$ . Such modelling approaches hardly exist today.

In the present study an attempt has been made to develop such a model based on the existing ADREA model. The key turbulence parameterization is obtained by the two equation k- $\zeta$  model applicable to neutral and non –neutral atmospheric flows (*Bartzis*, *J. G., 2006*) and (*Bartzis*, *J. G., 2005*). The integral time scale has been estimated from the asymptotic length scale of the k- $\zeta$  model and the mean local velocity applying Taylor's hypothesis. The concentration and its valiance are calculated from the relevant transport equations (*Andronopoulos et al, 2002*).

### **RESULTS AND DISCUSSION**

The model has been applied to the FLADIS T16 field experiment in which ammonia was released near the ground horizontally as a flashing jet. The concentration signal sensors selected for comparison were the ones passed the stationarity test (*Bartzis et al*, 2007)



Fig. 1; Mean concentration



Fig. 2; Standard deviation of concentration

In Fig.1 and Fig. 2 the mean concentration and its standard deviation are compared with the relevant experimental data. Given the uncertainties on the boundary conditions the results are judged quite satisfactory. The discrepancies are higher at the edge of the plume reflecting mainly model uncertainties in diffusion modelling.



Fig 3; Estimated peak concentrations at (a) 1 s and (b) 5 s

In Fig 3a and 3b the peak concentrations averaged over 1s and 5s are presented as estimated by Equation (2). It can be observed that the majority of the data lie within a factor of two from the experimental values. Given the uncertainties of all relevant calculations the results seem very satisfactory suggesting that the method is a promising one in estimating individual dosage at any time interval.

# CONCLUSION

The present work represents the first attempt to estimate peak mean concentrations utilizing RANS CFD models. The obtained results are quite encouraging.

The models will require in the future to be more refined and robust in estimating concentration variance and turbulent integral scales.

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