ATMOSPHERIC DISPERSION AND INDIVIDUAL EXPOSURE OF HAZARDOUS MATERIALS. VALIDATION AND INTERCOMPARISON STUDIES.

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Abstract: Recently, new approaches have been introduced in the CFD-RANS modeling, where the concentration time scales are estimated as a function not only of the flow turbulent time scales but also of the pollutant travel times. The new approaches have been implemented for the calculation of the concentration fluctuation dissipation time scale and the maximum individual exposure at short time intervals using the *k-ζ* model for turbulent parameterization. The purpose of this study is to implement and validate again the new methodology using the standard *k-ε* model. The validation is performed using selected trials of the MUST experiment under neutral conditions. Special emphasis is given on the selection of the constant value of the concentration fluctuation dissipation time scale when the *k-ε* model is used. An intercomparison of the results between the two turbulence models is performed also with a view of identifying model strengths and limitations.

Key words: *standard k-ε, k-ζ, turbulent integral time scales, pollutant travel time, individual exposure.*

INTRODUCTION

In the recent years, the increasing likelihood of a deliberate or accidental atmospheric release of a hazardous material in an urban (built-up) area has focused the attention of researchers to the understanding of the dispersion of these hazardous materials in such complex environments. Health effects are not dependent only on the magnitude of the pollutant concentration, but also on the duration that the individual is exposed to the high concentration. Therefore, for the assessment of health effects, it is more appropriate to use the dosage, defined as the product of the concentration times the time duration, rather than to use just the concentration itself. For this reason, it is very important to be able to reliably predict the maximum individual dosage during the event. 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. Recently Bartzis, J. G. et al. (2008) have introduced an approach relating maximum dosage $D_{max}(\Delta\tau)$ during a time interval $\Delta\tau$, to parameters such as the concentration fluctuation intensity I and the turbulent integral time scale T_C:

$$D_{\max}(\Delta\tau) = \left[1 + \beta I\left(\frac{\Delta\tau}{T_C}\right)^{-n}\right]\overline{C}\Delta\tau\,, \quad \left(I = \frac{\overline{C'^2}}{\overline{C}^2},\ T_C = \int_0^\infty R_C(\tau)d\tau\right) \tag{1}$$

where $\overline{C}$ is the mean concentration, β and n are constants that are derived from experimental evidence, $\overline{C'^2}$ is the variance and $R_C(\tau)$ is the autocorrelation function.

The need for the estimation of such parameters poses new challenges to Computational Fluid Dynamics (CFD) models. The simplest and most practical CFD models are the Reynolds Averaged Navier Stokes (RANS) models based on the concept of eddy viscosity/diffusivity. In this case, the conservation equation for the concentration variance is usually expressed in terms of the following Partial Differential Equation (PDE) (e.g. Milliez, M. and B. Carissimo, 2008):

$$\frac{\partial\rho\overline{C'^2}}{\partial t} + \frac{\partial\rho\overline{u_i}\overline{C'^2}}{\partial x_i} = -2\rho K_C\left(\frac{\partial\overline{C}}{\partial x_i}\right)^2 + \frac{\partial}{\partial x_i}\left[\rho D\frac{\partial\overline{C'^2}}{\partial x_i} + \rho K_C\frac{\partial\overline{C'^2}}{\partial x_i}\right] - \rho\frac{\overline{C'^2}}{T_{dc}} \tag{2}$$

where $\overline{u_i}$ is the mean velocity in the i-direction and D is the molecular mass diffusivity.

The estimation of the eddy diffusivity K_C and the dissipation time scale T_{dc} is based on the selected turbulent closures scheme. In the two equation turbulence modeling, turbulent closure is obtained by utilizing two additional transport equations corresponding to two different turbulent parameters. Concerning the selection of the first turbulent parameter, it has been almost unanimously accepted to be the turbulent kinetic energy (k). For the selection of the second turbulent parameter, several choices have

appeared in the literature (e.g. Wilcox, 1998). In such models, if ξ is the second selected parameter, any other turbulent parameter φ_t needed to obtain closure is estimated by the dimensional analysis i.e. $\varphi_t \propto k^m \xi^n$.

The application of the equation for finding φ_t in CFD-RANS for the dispersion near the source could be questionable, due to the fact that full mixing is implied, which is not a valid assumption in this case. From a theoretical point of view, the diffusion and turbulent characteristics are always affected by the travel time of the pollutant, especially near the source. According to the literature, the effect of the travel time in the complex Eulerian CFD-RANS modeling has been taken into consideration only by Yee, E. et al. (2009) by using the physical law x/U, where x is the distance from the source and U the mean local wind velocity. Recently, Efthimiou, G. C. and J. G. Bartzis, (2011) have introduced the 'radioactive tracer method' for the estimation of the pollutant travel time in CFD-RANS modeling. This new method has allowed the estimation of the concentration time scales near and far from the source. In the same study the turbulent parameterization was based on the k-ζ model.

It is well known that the standard k-ε model (Launder, B. E. and D. B. Spalding, 1974) is one of the widely used turbulence models for atmospheric flows and has been applied successfully in a number of local scale problems such as street canyons, complex terrains etc. For this reason the purpose of this study is to incorporate this model to the new methodology for the estimation of the concentration time scales.

THE INTEGRAL TIME SCALES

The new approach is based on experimental evidence (Efthimiou G. C. and J. G. Bartzis, 2011) that the concentration autocorrelation time scale, T_C, is highly correlated with the pollutant travel times especially near the source. The proposal is:

$$T_C = \min(c_c T_{travel}, T_{C\infty}),\ c_c = 0.11 \tag{3}$$

where T_{travel} is calculated by the 'radioactive tracer method' as has been introduced in Efthimiou G. C. and J. G. Bartzis (2011). $T_{C\infty}$ is the autocorrelation time scale under fully mixed conditions. When the k-ζ or k-ε model is implemented, the time scale $T_{C\infty}$ is parameterized with k and ζ or ε respectively as follows:

$$\textbf{\textit{for k-}}\boldsymbol{\zeta}\textbf{\textit{ model:}}\ T_{C\infty} = c_h k^{-1/2} \zeta^{-1},\ c_h = 1.0 \tag{4}$$

$$\textbf{\textit{for k-}}\boldsymbol{\varepsilon}\textbf{\textit{ model:}}\ T_{C\infty} = k\varepsilon^{-1} \tag{5}$$

Concerning the dissipation time scale T_{dc} appearing in Equation 2 the following relationship is used:

$$T_{dc} = c_{dc} T_C \tag{6}$$

For the k-ε model the constant c_{dc} is equal to 0.8 based on Milliez, M. and B. Carissimo (2008). For the k-ζ model the equivalent value for c_{dc} (based also on the parameterization between ε and ζ) is 3.05.

It should be noted that in the previous study (Efthimiou G. C. and J. G. Bartzis, 2011) the new methodology for the estimation of the concentration time scale T_C (Eq. 3) using the k-ζ model (Eq. 4) and the value of c_{dc}=3.05 for Eq. 6 produced good results for the concentration standard deviation and the individual exposure for two selected trials of the MUST field experiment under neutral conditions. In the present study, the simulations of the same trials are repeated using the standard k-ε model i.e. Eq. 3, Eq. 5 and Eq. 6 by giving special emphasis on the selection of the c_{dc} value.

RESULTS AND DISCUSSION

The Trials 11 and 12 of the MUST field experiment have been considered for the validation of the methodology. The experiment, the selected trials and the numerical simulations have been described analytically in Efthimiou, G. C. and J. G. Bartzis, (2011). It is reminded that the simulations are performed in two steps. The first step concerns the simulation of the oncoming boundary layer. The results of the 1D calculation for the horizontal velocity $SU = \sqrt{U^2 + V^2}$ and k (normalized by the reference velocity U_{ref}) and the corresponding experimental results are presented in Fig. 1 (only the results of Trial 11 are presented). As expected, the results for the horizontal velocity SU/U_{ref} are similar for both turbulence models while the turbulent kinetic energy profile of the k-ε model is underestimated in comparison with the profiles of the k-ζ model and the experiment. Similar results have been derived also for Trial 12. It should be noted that the numerical results of the 1D simulations are used as inlet boundary conditions for the 3D simulations. The second computational step consisted of performing the full three-

dimensional flow and dispersion calculations using as initial and boundary conditions the profiles obtained from the first step.

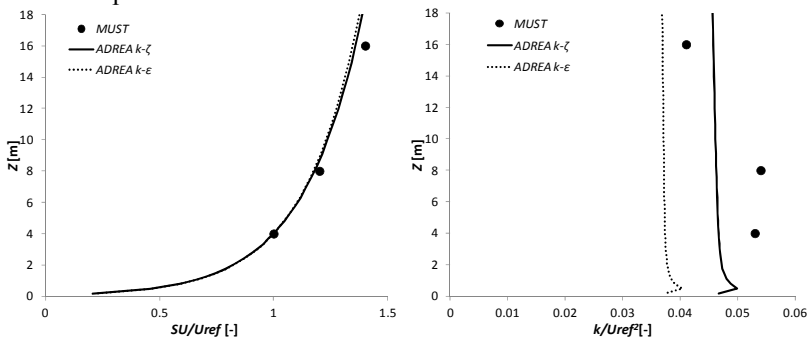

Figure 1. Inlet profiles of the horizontal velocity SU/U_{ref} (left) and the turbulent kinetic energy k/U_{ref}^2 (right) as determined from the experiment and calculated by the 1D ADREA precursor simulations for Trial 11.

Mean concentration results

Figure 2 displays the scatter plots for the mean concentrations for Trial 11 and Trial 12 of the 3D simulations. The comparison is performed between the predictions of the *k-ε* model and the *k-ζ* model and includes all the concentration sensors. A distinct underprediction of the results is observed for the *k-ε* model especially near the source where the mean concentration values are expected to be higher.

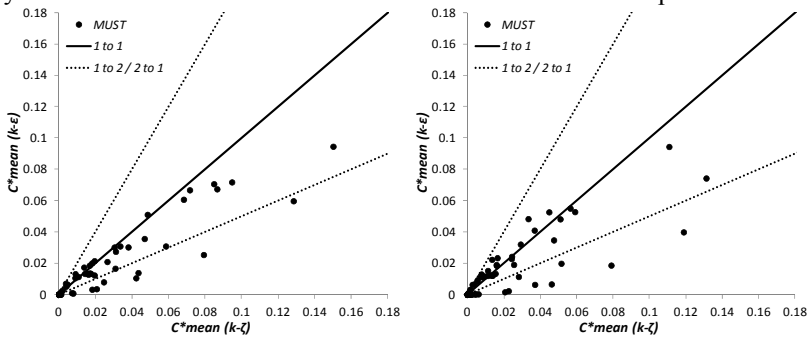

Figure 2. Scatter plots for the normalized mean concentrations in case of Trial 11 (left) and Trial 12 (right) of the MUST experiment. The comparison is performed for the predictions between the *k-ε* and *k-ζ* model.

In order to evaluate the performance of the mean concentration model with the experimental values, validation metrics have been used. These are the fractional bias (FB), the normalized mean square error (NMSE) and the factor of two of observations (FAC2). The results for both trials are presented in Table 1. Concerning the model performance with regards to metrics, the COST 732 guidelines require the following quality acceptance criteria: FAC2 > 50%, |FB| < 0.3 and NMSE< 4 for mean concentrations.

Table 1. Validation metrics for the mean concentration of Trial 11 and Trial 12 of the MUST experiment. The results have been grouped in near ground measurements and total measurements.

	Validation metrics		
	FAC2	FB	NMSE
Near ground measurements			
Trial 11 (*k-ζ* / *k-ε*)	0.60 / 0.43	-0.08 / 0.52	0.35 / 0.77
Trial 12 (*k-ζ* / *k-ε*)	0.89 / 0.52	-0.22 / 0.39	0.33 / 0.53
Total measurements			
Trial 11 (*k-ζ* / *k-ε*)	0.48 / 0.44	-0.24 / 0.11	0.69 / 0.73
Trial 12 (*k-ζ* / *k-ε*)	0.70 / 0.46	-0.19 / 0.12	0.42 / 0.53

In case of Trial 11, the FAC2 of the *k-ε* model is lower than the FAC2 of the *k-ζ* model for the near ground measurements, indicating that the *k-ζ* model predicts better the observed mean concentrations. Also the higher values of FB and NMSE of the *k-ε* model indicate that the model gives a high underprediction and scatter of observations respectively. Overall all the metrics of the *k-ζ* model for the

near ground measurements fulfil well the quality acceptance criteria while only the NMSE of the *k*-*ε* model fulfills the criteria (NMSE < 4). Concerning the total measurements, it is obvious that the FAC2 for both models is below the limit, while acceptable values for the NMSE and the FB have been calculated. In case of Trial 12, the results of the *k*-*ζ* model are much better than the *k*-*ε* model's results, both for the near ground measurements and the total measurements. It is worth to notice for the near ground measurements that the FAC2 of the *k*-*ζ* model is equal to 89% while for the *k*-*ε* model is very close to the limit of acceptance (52%). The scatter and the underprediction of the *k*-*ε* model's results are lower in comparison to Trial 11. Totally for all the measurements the *k*-*ζ* model predicts the observations better than the *k*-*ε* model based on the FAC2 and the NMSE while the absolute value of the FB is common for both models. Overall for *k*-*ζ* model all the metrics of Trial 12 fulfil the quality acceptance criteria while *k*-*ε* model's metrics fulfill only the limits of FB and NMSE.

Concentration standard deviation results

The selection of the parameter c_{dc} in Eq. 6 is essential regarding the results. A sensitivity study on the influence of this parameter to the results has been performed for both Trials using the *k*-*ε* model. In the first simulation, where the value of c_{dc} was equal to 0.8, the concentration standard deviation was underpredicted very much (e.g. for Trial 11 and for all sensors: FAC2 = 5.7%, NMSE = 2.49, FB = 1.03). By increasing c_{dc} the underestimation was decreasing and a value of c_{dc} equal to 1.7 gave the best overall performance of the model.

Figure 3 displays the scatter plots for the concentration standard deviation for both trials. Similar to Figure 2 the comparison is performed between the predictions of the *k*-*ε* model and the *k*-*ζ* model for all sensors. Similar to the mean concentration, a distinct underprediction of the results is observed for the *k*-*ε* model especially near the source.

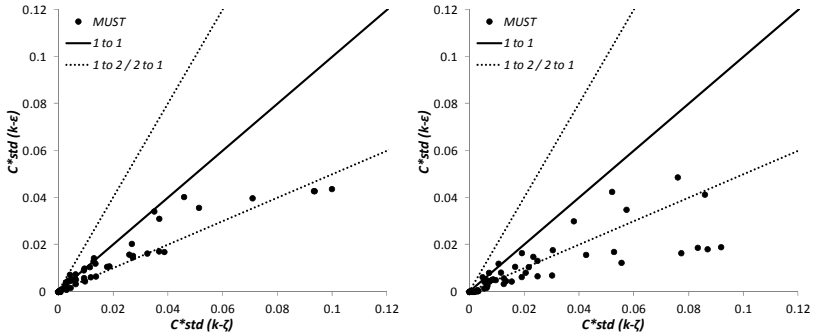

Figure 3. Scatter plots for the normalized concentration standard deviation in case of Trial 11 (left) and Trial 12 (right) of the MUST experiment. The comparison is performed for the predictions between the *k*-*ε* and *k*-*ζ* models.

The validation metrics for the concentration standard deviation are presented in Table 2. The results have been grouped in a similar way as the mean concentration results (i.e. near ground and total measurements). It should be noted that the same state-of-art values have been used to validate the model.

Table 2. Validation metrics for the concentration standard deviation of Trial 11 and Trial 12 of the MUST experiment. The results have been grouped in near ground measurements and total measurements.

	Validation metrics		
	FAC2	FB	NMSE
Near ground measurements			
Trial 11 (*k*-*ζ* / *k*-*ε*)	0.63 / 0.60	0.21 / 0.37	0.22 / 0.35
Trial 12 (*k*-*ζ* / *k*-*ε*)	0.82 / 0.67	0.075 / 0.19	0.088 / 0.17
Total measurements			
Trial 11 (*k*-*ζ* / *k*-*ε*)	0.59 / 0.69	-0.33 / 0.12	1.39 / 0.26
Trial 12 (*k*-*ζ* / *k*-*ε*)	0.76 / 0.68	-0.35 / -0.047	1.20 / 0.34

For the near ground measurements it is obvious that the FAC2 of *k*-*ζ* and *k*-*ε* models is comparable for Trial 11, while *k*-*ζ* presents a higher FAC2 for Trial 12. Also the FB values indicate that both models underpredict the near ground measurements. The values of NMSE indicate a smaller scatter in the data for

k-ζ model. Concerning the total measurements in Trial 11, the k-ε model predicts better the observations than the k-ζ model by giving higher values for the FAC2 and smaller, absolute, values for the NMSE and the FB. For Trial 12, the k-ζ model gives a better performance for the FAC2, but it overpredicts more and presents a higher scatter of the results than the k-ε model. It is obvious also that the metrics of k-ζ and k-ε models fulfil the quality acceptance criteria for all measurements, except the FB of the total measurements for the k-ζ model and the FB of the near ground measurements for the k-ε model and Trial 11 which are slightly higher from the limits.

Individual exposure results

Modeled peak dosages have been estimated for the time intervals $\Delta\tau$ = 0.02, 0.2, 1.0, 2.0, 5.0 and 10s utilizing Eq. (1) as obtained by the present models and for β = 1.65. The results of the arc-maximum peak dosages for Trial 11 are presented in Fig.4 (the concept of arc-maximum values and how the experimental peak dosages have been estimated, are described in Efthimiou, G. C. and J. G. Bartzis, 2011). The predictions of peak dosages for both models lie all inside the fraction of two of the observations for all distances away from the source and all the time intervals strengthening further the robustness of the model (1). An underprediction of the dosages is obvious for the k-ε model and this originates mainly from the underprediction of concentration mean and variance. The results of Trial 12 are similar to Trial 11 (not presented here).

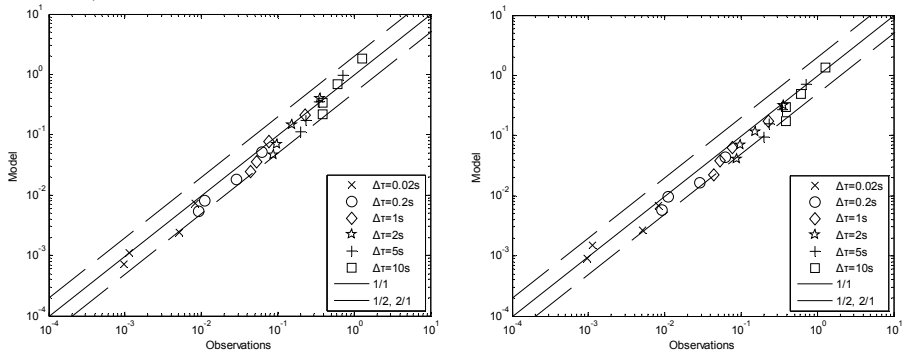

Figure 4. Scatter plots for the normalized maximum arc dosages for the k-ζ model (left) and the k-ε model (right) in case of Trial 11 of the MUST experiment for various time intervals $\Delta\tau$ = 0.02, 0.2, 1.0, 2.0, 5.0 and 10s.

CONCLUSIONS

The proposed approach on concentration time scale dependency on pollutant travel time seems to be a valid approximation in predicting plume dispersion from a point source in CFD RANS modeling using the k-ζ and standard k-ε turbulence models. In case of k-ε model, the concentration standard deviation results revealed their sensitivity to the parameter c_{dc} used to model the dissipation time scale. The choice of a new value 1.7 for c_{dc} allowed a good insight into the fluctuation results. The validation study was performed against MUST field experimental data under neutral conditions. An overall better performance for concentration mean and standard deviation was observed when the k-ζ model was used. Finally the present approach expands the capability of the relatively simple two equation CFD RANS models to predict short time exposures.

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