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MODELLING OF TOXIC CONTAMINANTS DISPERSION DURING A REAL INDUSTRIAL ACCIDENT USING LARGE EDDY SIMULATION AND RANS MODELS

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Abstract: The paper presents a Computational Fluid Dynamics (CFD) approach based on a finite volume technique for the modelling of pollutant dispersion from a real industrial accident, by applying a Large Eddy Simulation (LES) model for the turbulence-related quantities while the sub-grid scale (SGS) modelling is achieved by the classic Smagorinsky model based on the eddy viscosity hypothesis. The proposed methodology was incorporated into the in-house code ADREA-HF. Numerical simulations were conducted with the use of the ADREA/SIMPLER algorithm for the decoupling of pressure and velocity equations. A number of scenarios were examined and the results obtained were compared with available measurements recorded by sensors of Accidental Gas RelEase (AGREE) data set. We also use a Reynolds-Averaged Navier Stokes (RANS) modelling approach, for comparison reasons. The performance of the models are dependent on the incident wind direction and speed and it varies based on the position of the AGREE sensors. Good agreement between results and measurements was obtained.

Key words: *industrial accident, pollutant dispersion, LES, RANS, CFD*

INTRODUCTION

The rapid rate of industrialisation in the developed countries and the continuous economic growth have significantly improved the standard of living of the population, transportation, large-scale production of goods and modern communications. However, the developed countries are at the same time associated with relatively high levels of industrial accident risk on a daily basis. Major industrial accidents involving the release of toxic airborne contaminants are continuously reported worldwide, with significant impacts on environment, economy and human health. Experience has shown that the transport of contaminants by a wind-blown plume can distribute potentially hazardous material over long distances, resulting in possible serious environmental and health problems that are difficult to address. Therefore, it is important to be able to predict the concentration of the contaminants and the direction of the plume trajectory over a wide range of meteorological conditions.

Markatos et al. (2009) studied the pollutant dispersion of fire plumes and the environmental consequences from large fuel-tank fires using a CFD approach, based on the finite volume method. The proposed model solves the governing equations of flow incorporating turbulence and radiation effects, along with the use of advanced treatment for the convective terms (i.e. MUSCLE and CUPID schemes) of the equations. More specifically, a discrete transfer radiation model was selected for taking into account the radiation effects from the tank walls, while for the turbulence modelling a modified RNG k-ε (Yakhot and Orszag, 1986) was employed with the appropriate modifications for buoyancy effects. The comparison of the numerical results with earlier works (Argyropoulos et al., 2008a, 2008b) do not differ by more than 7-8%, with a maximum of 10% for enthalpy. Extension to the above mentioned studies is the research of Argyropoulos et al. (2010), who presented an improved and integrated version of the previous studies including also the case of Tank 12, according to the accident at BOSD in Buncefield. In addition, the anticipated consequences to the environment and the identification of risk zones for the first respondents were investigated using the safety limit of Immediately Dangerous to Life and Health (IDLH). The numerical results were compared with available semi-empirical data (Fisher et al., 2001) and weather satellite observations. Similar studies for industrial accidents using CFD and Lagrangian models may be found in the works of Sklavounos and Rigas (2012), Sun and Gao (2013), Leelossy et al. (2013), and Shie and Chan (2013), among others.

Recently, Efthimiou et al. (2017) performed CFD simulations, based on RANS models, for the prediction of pollutant dispersion from a hazardous airborne release during a real industrial accident. The numerical results obtained were compared with available measurements from AGREE data set for 30°, 60°, and 90° wind directions, presenting encouraging agreement taking into account the complexity of the problem and the uncertainties associated with the meteorological conditions and emission rate.

The purpose of the present effort is to predict the dispersion of a toxic release during a real industrial accident close to the plant facilities. A LES model (Argyropoulos and Markatos, 2015) was selected and implemented in the in-house CFD code ADREA-HF (Venetsanos et al., 2010). Moreover, we simulated the pollutant dispersion using a RANS approach according to the work of Efthimiou et al. (2017). Various scenarios were examined and the results obtained from both models were compared with available real measurements recorded by sensors of AGREE data set. More details regarding the AGREE test case and model's results can be found in COST ES1006 (2015).

NUMERICAL METHODS

Dispersion modelling using the LES approach

The proposed mathematical model is based on the filtered continuity and filtered Navier-Stokes equations, together with the filter scalar mean transport equation for a passive component of a mixture (Koutsourakis et al., 2012). In the present study, a LES modelling approach is adopted using a classical Smagorinsky sub-grid scale (SGS) model (Smagorinsky,1963) for treating the Reynolds and Cross terms (Argyropoulos and Markatos, 2015), which should be capable of ensuring the accurate transfer of energy between unresolved and resolved turbulent scales (Piomelli, 1999). The Smagorinsky SGS model is based on the eddy-viscosity hypothesis, for which the velocity and length scales are specified and combined with a Boussinesq approximation. The value of Smagorinsky constant, C_s, is taken equal to 0.1. The filtered related Δ is taken as $\Delta = V^{1/3}$, where V is the volume of the computational cell. Near the solid boundaries, we impose Van-Driest Damping function (van Driest, 1956) in order to eliminate the eddy viscosity near to the wall. The turbulent sub-grid scale Schmidt number is set to 0.72. In this work, we select class *D* of atmospheric stability, which represents neutral conditions.

The set of model filtered partial-differential equations, together with the appropriate boundary conditions and the auxiliary relations have been solved by means of the Finite Volume Method (Patankar and Spalding, 1972; Versteeg and Malalasekera, 2007). The developed model is incorporated in the ADREA-HF code. A relatively simplified geometry of the accident's location and buildings is imported in the ADREA HF code and then is reconstructed with the use of porosities, which allows the representation of any solid surface on a structured mesh with good accuracy (Bartzis et al., 1991). The computational domain is constituted by 71 buildings, and had a spatial extent of $28H_{max}$ x $25.2H_{max}$ x $6H_{max}$ (H_{max} is the maximum height of buildings and is taken equal to 40 m) in the West-East, South-North, and vertical directions, respectively (Efthimiou et al., 2017). A grid of 544x469x54 (13,777,344 cells) was selected for the current simulations. The total amount of the emitted hazardous airborne release from the five main openings on two opposite sides of a building is taken equal to 900 kg (Efthimiou et al., 2017).

The treatment of the convective term was achieved by using a second order accurate deferred correction central scheme (Ferziger and Peric, 2002). A second order accurate Crank-Nicolson numerical scheme was also selected for the time advancement, while for the discretization of concentration a second order accurate linear upwind scheme along with a SMART limiter was chosen. The solution was obtained using an iterative algorithm, namely ADREA/SIMPLER (Kovalets et al., 2008). In the present study, the

ADREA-HF LES version with MPI parallelisation was adopted for the current simulations. Hence, the Krylov subspace method BiCGstab is used, with the additive Schwarz preconditioner. Both the preconditioner and the solution of the preconditioner system are done in parallel. Finally, the value of time step is adjusted automatically based on the desired Courante-Friedrichse-Lewy (CFL<1) number and prescribed error bands.

Dispersion modelling using the RANS approach

The proposed model based on the 3-D RANS equations, expressing the conservation of mass, momentum, concentration and two turbulence variables. Energy equation is not considered since neutral conditions are adopted for the accident, according to the available meteorological data (Efthimiou et al., 2017). The turbulence modelling is achieved by using the standard k-ε model (Launder and Spalding, 1974). The boundary conditions are specified as follows. Zero-flux conditions were used for the concentration field, while the momentum flux to the wall obeys to the classical wall-functions of Launder and Spalding (1974). A power-law profile was also used at the inlet boundary for the wind velocity which is in a good agreement with the available measured wind velocity. At the inlet boundary profile for turbulence kinetic energy and dissipation rate of turbulence, the proposed methodology of Mavroidis et al. (2015) was adopted. Finally, at the outlet lateral planes of the domain, zero horizontal gradient boundary conditions were imposed, while for the upper boundary zero gradient conditions are used for all the variables, excluding the case for the vertical velocity where constant pressure is applied.

The set of the aforementioned partial differential equations along with the appropriate boundary conditions have been solved by the means of the FVM (Versteeg and Malalasekera, 2007). The developed model has been employed in the ADREA-HF code. For the convective terms of momentum, turbulence kinetic energy and dissipation rate of turbulence an accurate linear upwind scheme was used. In addition, the time step was automatically adapted based on the desired CFL number, whose maximum value is was set equal to 2. The solution was obtained using the preconditioned Biconjugate Gradient Stabilized Method.

RESULTS

The overwhelming amount of results obtained dictates an indicative choice of them for presentation. Therefore, the numerical results obtained were compared with measurements for only four sensors, namely no. 26, 27, 38 and 64. The sensor no. 64 is located downwind of the release near the plume centre-line, while the sensor no. 38 is located close to the release. Finally, the locations of sensors no. 26 and 27 are in the vicinity of the releases and on the left sides of the plume.

In Figure 1(a), it is observed that the RANS model overpredicts the first measurement at 1498 s, while LES slightly underestimates it. These differences may be explained by the inaccuracy of the assumed emission rate. On the other hand, both models present good agreement with the second measurement at 2555 s. The performance of LES model for the area of sensor 27 is very good for the first measurement, as shown in Figure 1(b), while the RANS model presents a small overestimation. For the second measurement, the RANS performance is better than LES model. In Figure 1(c), it is seen that the performance for both models are similar for the first measurement, while for the second measurement both models overpredict the concentration value, but LES overprediction is relatively smaller than RANS. It should be noted that the numerical results of LES model for sensors no. 26 and no. 27, in general, follow satisfactory the trajectory of the AGREE measurements. Figure 1(d) presents the numerical predictions for LES and RANS models, together with the two available measurements from AGREE data set for sensor no. 64. It is noticed that the LES model' s performance is very good for both measurements, while RANS model achieves good agreement only for the first measurement at 1583 s, as shown in Figure 1(d).

The observed differences between the numerical results and measurements are also due to the variation of incident wind direction and speed which based on the position of the AGREE sensors. The different performance between LES and RANS can be explained by the fact that in the former only the small, isotropic turbulent scales are modelled and not the entire spectrum as it is the case in the latter (Argyropoulos and Markatos, 2015).

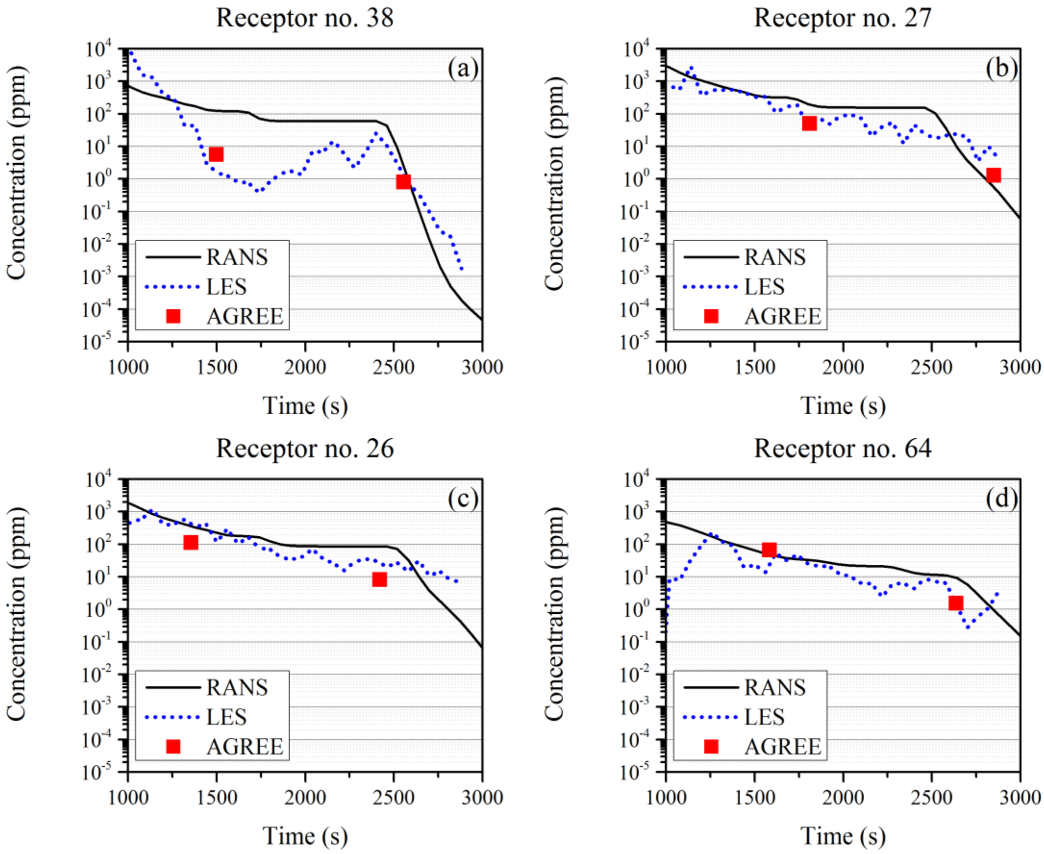

Figure 1: Concentration values vs. time for different receptors and models.

CONCLUSIONS

This work investigates the dispersion of a toxic gas during a real industrial accident at the building exterior from where the source release took place, but inside the complex industrial facility. According to our initial results, LES approach is more accurate than RANS approach. However, RANS is less computationally demanding than LES. Generally, both models can be considered to perform satisfactory taking into account the complexity of the flow and the meteorological uncertainties. The harmonisation of the selected models with the appropriate meteorological data, emission rate and temporal variability of the wind is of high importance in order to reduce the uncertainty of our computations.

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