18th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
9-12 October 2017, Bologna, Italy

MULTI-SCALE MODELLING POLLUTANT DISPERSION AND EXPOSURE AGAINST AN ACCIDENTAL TOXIC RELEASE IN AN ADMINISTRATION BUILDING USING LARGE EDDY SIMULATION AND EVACUATION MODELS

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Abstract: Administration or non-process buildings, which are located in industrial facilities often have a large number of occupants. In the unlike event of a toxic gas release, large amounts of pollutants can penetrate into the building shell through openings and cracks and could lead to serious consequences for the health of people and the environment. Lethal dosages can be reached indoors because of the gas ingress and its entrapment. A multi-scale modelling methodology is presented for a H_2S release affecting an administration building. The proposed methodology extends ordinary numerical modelling approaches one step further by using evacuation models for better understanding, protecting and mitigating the vulnerability of the building occupants during their evacuation to safer places.

Key words: *Multi-zone, infiltration, LES, CFD, evacuation modelling.*

INTRODUCTION

Industrial accidents involving toxic gas release (e.g. H_2S) from a pipeline leak or oil wells are associated with high risk for nearby administration buildings and indoor environments due to the dispersion and penetration of contaminated outdoor air. The pressure difference between the outdoor and building environment allows the unintentional or accidental flow of outside air into the buildings through openings, cracks and the ventilation system. This phenomenon of air infiltration in buildings is also known as ingress. Building ingress depends on many factors, such as wind pressures, leakage characteristics of building envelope, ventilation system and turbulence, among others (Kukadia and Hall, 2004; Hall and Spanton, 2012). All these factors can introduce significant uncertainties when trying to quantify them (Ashraf et al., 2016; Argyropoulos et al, 2017). Therefore, it is important to choose the appropriate tool in order to investigate the indoor air quality (Argyropoulos et al., 2016). Building ingress can be calculated by using simple statistical regression and mass balance approaches to more complex multi-zone and computational fluid dynamics (CFD) models (Milner et al., 2011). Both approaches have advantages and disadvantages (Wang et al., 2010), however, a combination of multi-zone and CFD models for studying the building infiltration is a good selection for large buildings, compromising accuracy and computational demands (Srebric et al., 2008; Argyropoulos et al., 2017).

As mentioned above, building ingress is responsible for the penetration of contaminated outdoor air inside the building, however, it is also important to calculate the concentration levels of the toxic gas (e.g. H_2S) inside the building due to the indoor dispersion from the gas infiltration. Although there are many proposed methodologies that assess the impact of toxic gas concentration on humans (Parker and Coffey, 2011; Ashraf et al., 2016), the majority of them assume the person to be a "stationary observer". As a result, the acute dose is estimated using the assumption that the occupant's position is at a particular place during the release event. Nevertheless, these approaches do not consider that the person might be moving to a safer area (Lovreglio et al., 2016). Thus, the risk assessment should consider the individual's position with respect to time while estimating their health impact. Using the predicted concentrations as an input parameter, the impact of the infiltrated toxic gas on the indoor population is usually assessed by using correlations that can estimate percentage fatalities. However, standard risk assessment methodologies do not take into account the human behaviour and the movement of people during an emergency situation.

Evacuation modelling can be mainly categorised into the cases which are considered only human movement and those that combine human movement and human behaviour (Gwynne et al. 1999). In addition, evacuation research also ignores (in most cases) the dynamics of fire and smoke spreading which altering the moving behaviour of the occupants (Zheng et al. 2017). Recently, Lovreglio et al. (2016) proposed a quazi-dynamic approach for risk assessment using a combination of gas dispersion modelling (CFD approach) and evacuation modelling. Two evacuation scenarios with (people move to escape) and without people movement (static) were presented and discussed, respectively.

In the present study, we propose a multi-scale modelling methodology for a H_2S release affecting an administration building in a natural gas facility based on the combination of the following models for outdoor dispersion (SLAB (Ermak, 1990) and QUIC (Nelson and Brown, 2013)), building infiltration (CONTAM (Wang et al., 2010)), indoor dispersion (FDS (McGrattan et al., 2013)) and evacuation (Pathfinder (Thunderhead Engineering, 2015)). This work investigates the dispersion of the pollutant in an administration building and at the same time examines a number of evacuation scenarios for the safe evacuation of the building occupants.

THE MULTI-SCALE MODELLING APPROACH

We consider the realistic release of natural gas from a feed pipeline, of around 0.77% (w/w) H_2S in methane, due to full bore rupture. Leak duration of 60 min and a mass source rate equal to 11,500 kg/s are also considered. The release of H_2S is directed to the non-process building, while the temperature and pressure of pipeline are assumed to be maintained at 27^{o}C and 83 bars, respectively. The H_2S is a well-studied toxic agent with adverse health effects even at sub-ppm concentrations. The area surrounding the facility is flat, and the prevailing wind velocity is set to 5 ms^{-1} while the atmospheric stability is neutral. The outdoor atmospheric dispersion of the hazardous agent was modelled using the U.S. Environmental Protection Agency's (USEPA) SLAB model for the case of a horizontal jet source release. The output from SLAB is used by CONTAM (building ingress model) via ambient contaminant (CTM) file along with suitable meteorological data acting on the building exterior. CONTAM is a widely used multi-zone model capable of handling infiltration, indoor air quality and airflow path calculations, among others. CONTAM generates a path location data (PLD) file which can be adopted by QUIC in order to select the exact points of the airflow paths (Argyropoulos et al, 2017). QUIC is equipped with a diagnostic tool (QUIC-URB) and a CFD algorithm (QUIC-CFD) with a simple zero-equation model (Argyropoulos and Markatos, 2015), both capable of predicting the 3-D flow field around complex buildings either using empirical algorithms or CFD techniques, respectively.

By coupling the SLAB, QUIC and CONTAM models, we derive the appropriate inputs for the Fire Dynamic Simulator (FDS). It is a CFD code developed by National Institute of Standards and Technology (NIST). The code employs a Large Eddy Simulation (LES) approach (McGrattan et al., 2013; Argyropoulos and Markatos, 2015) for fire-driven flows. In the present study, the FDS code has been modified for gas ingress and implemented in the graphical user interface PyroSim. Next, we import to Pathfinder the appropriate output data from FDS to extract the walking space and exposure levels of the occupants, according to the predicted H_2S concentration levels in the building. Pathfinder (Thunderhead Engineering, 2015) is characterised as an emergency egress simulator. It comprises an integrated user interface and animated 3D results. It models the occupant's evacuation using an Agent based modelling approach and can simulate a large number of evacuees (>5000 agents) (Lovreglio et al., 2016). As a result, we are able to consider a number of evacuation scenarios in order to examine the occupants' movement, closest exit path and evacuation estimate time.

RESULTS

Every window and doors of the building exterior are considered to be closed and a leakage area of 1.73 cm^{2}m^{-1} per window and 187.5 cm^2 per door are assumed (Persily and Grot, 1986). The building is constituted by 102 rooms on the first floor and 94 rooms on the ground floor. Figure 1 presents the idealised building geometry for the ground floor as incorporated in FDS together with the calculated mass fraction of H_2S (kg/kg) during the indoor dispersion for 20 min approximately after the building ingress of H_2S. The turbulence modelling in FDS is achieved by using a LES approach. Since the multi-zone models (CONTAM) are not appropriate for large rooms/areas due to the low accuracy, the use of FDS is considered necessary. Multi-zone models (e.g. CONTAM) assume a spatially uniform concentration at the building exterior and a “well mixed” zone at the building interior. However, when the flow is non-uniform the “well-mixed” assumption is not valid. On the other hand, FDS calculations are characterised by high time and computational demands compared to the multi-zone models.

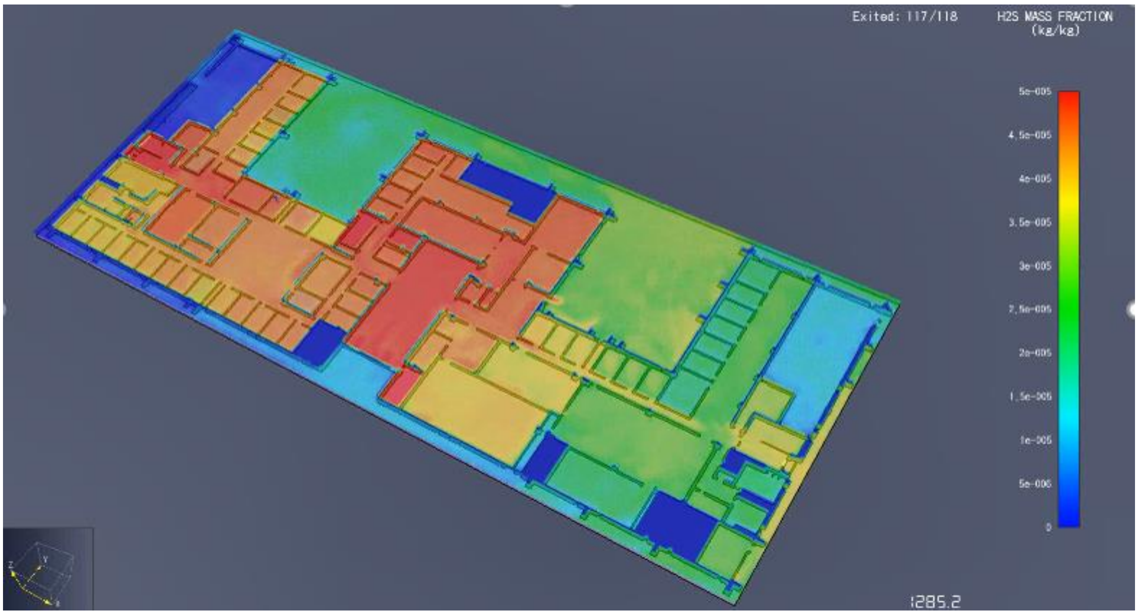

Figure 1: LES modelling of indoor dispersion of H_2S in the administration building.

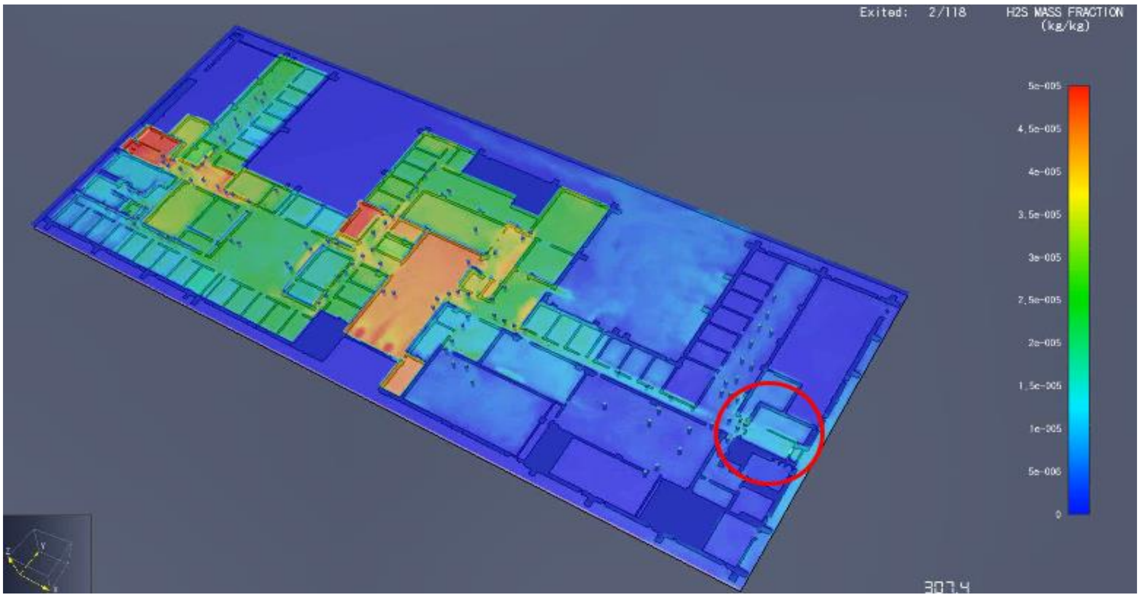

Figure 2: Occupants’ evacuation modelling using pathfinder software.

Figure 2 exhibits one of the considered evacuation scenarios using Pathfinder software with input data from FDS. We assumed a number of 118 occupants with arbitrary locations in the building, while the onset of occupants’ movement is initiated after a delay of 300s. The selection of 300s (5 min) was considered a reasonable reaction time. Examination of the results revealed important setbacks of the evacuation plan. For example, during the evacuation a large number of people has been blocked close to the right exits (see red circle) owe to its narrow size. At the same time, the left exit lead directly to the

H_2S plume, thus to higher exposures. Eventually, for the studied scenario, both exits maybe proven inadequate for the emergency evacuation..

Figure 3 illustrates the toxic load estimation of H_2S (ppm) during the evacuation procedure. More specifically, in Figure 3a, it is observed that the levels of H_2S exposure for four moving occupants are high for a short period of time, particularly for two of the occupants (>27 ppm). This concentration values can lead to notable discomfort or disability according to Acute Exposure Guideline Levels (AEGLs) (NCR, 2013). On the other hand, in Figure 3b, it is seen that the exposure levels of H_2S are different for the two selected models, CFD (FDS) and multi-zone (CONTAM), considering the same four but static occupants. The CFD results are also above the AEGL2 limit for H_2S (NCR, 2013), while the multizone model underestimates the exposure levels. Such differences between models and approaches raise the need for more experimental studies, in order to validate the obtained numerical results, and for more advanced numerical methods, for the prediction of indoor toxic levels in large rooms/areas.

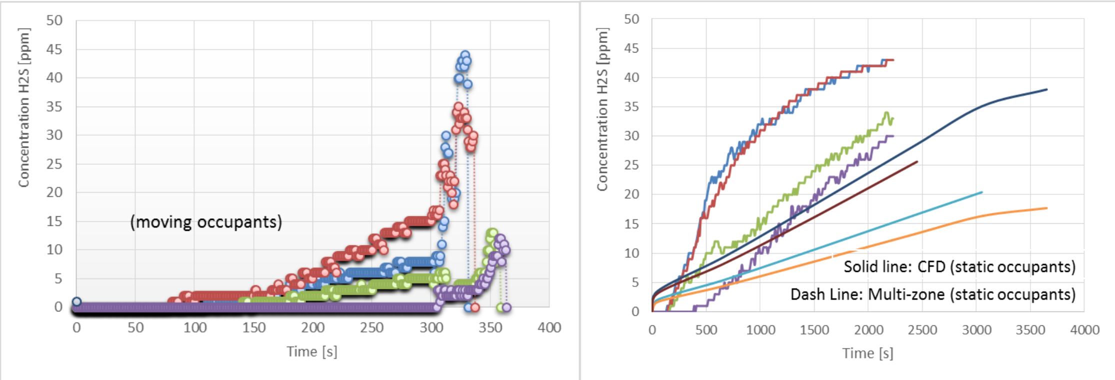

Figure 3. Toxic load estimation of the moving evacuees after a delay of 300 s: a) CFD results for moving occupants and b) CFD vs multi-zone (CONTAM) results for static occupants.

CONCLUSIONS

A multi-scale modelling methodology is presented for the dispersion of toxic gas using a combination of dispersion, ingress and evacuation models. The CFD model was able to model the indoor dispersion of H_2S inside the building by taking into account obstacles and large volume areas. The CFD results obtained were combined with the evacuation model to predict the toxic gas exposure to occupants. Initial toxic load results indicate that the multi-zone model predictions are lower than CFD estimations and since moving occupants mimic real life scenarios, toxic load estimations utilizing CFD model can be considered more accurate compared to multi-zone (CONTAM) model, due to better performance for large rooms/areas. Finally, a qualitative assessment of the occupant's exposure indicated that the standard route of the nearest exit may not always be the optimal approach depending on a number of factors such as meteorology, location of the release and building characteristics. It is concluded that the present methodology is appropriate for the assessment of evacuation scenarios regarding the exposure levels of toxic ingress gas. Plausible results are obtained for such complicated and interacting phenomena and it is hoped that this methodoly to be beneficial for the risk assessment community.

ACKNOWLEDGEMENTS

This publication was made possible by a NPRP award [NPRP 7-674-2-252] from the Qatar National Research Fund (a member of The Qatar Foundation) and the support of the Mary Kay 'O Connor Process Safety Center at Qatar. The statements made herein are solely the responsibility of the authors.

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