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Mathematical modelling and computer simulation of toxic gas building infiltration

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ABSTRACT

A toxic gas release, e.g. H_2S, from pipeline accidents or sour wells, although improbable, may lead to serious consequences for the health of people and the environment. Such incidents might also jeopardize occupants of nearby indoor environments via infiltration of toxic contaminants. Despite that risk, there is still a lack of data and of comparative studies concerning the appropriate models and mitigation methods.

The purpose of this work is, therefore, the improved modelling of toxic gas building infiltration, by a combination of tools and approaches. Using a realistic release scenario, the present comprehensive analysis demonstrates the need to consider the detailed building characteristics and meteorology. Significant deviations are observed between simple and advanced building ingress models. Furthermore, the consequences assessment leads to contradicting conclusions depending on the employed dose-response approaches. The proposed methodology could serve as a guide for the improvement of relevant risk-assessment tools and of future studies.

1. Introduction

Although the majority of incidents involving toxic gas release in oil and gas industry affects outdoor environments, industrial accidents such as those of Poza Rica of Mexico (24-Nov-1950, 25 died) (McCabe and Clayton, 1952), Denver city of Texas (02-Feb-1975, 9 died) (Layton et al., 1983), Lodgepole in Alberta of Canada (17-Oct-1982, 3 died) (Leahey and Schroeder, 1986) and the relatively recent in the town of Gaoqiao, Kai Xian of China (23-Dec-2003, 243 died) (Jianwen et al., 2014), support the fact that the nearby buildings and indoor environments are also at risk with possible serious consequences for the occupants. Non-process areas such as administration buildings and warehouses are often the least protected, despite being in the vicinity of potential sources. Outdoor contaminants can penetrate indoors through the ventilation system, and any kind of openings. The process of air infiltration between building and outdoor environment is known as ingress. Building ingress depends on wind pressures, ventilation system, wind turbulence and buoyancy, as well as on the leakage characteristics of the building envelope. Other driving factors which affect the infiltration rates and indoor concentration levels are the building height and the effect of sheltering from the surrounding buildings. The latter factor can reduce the speed of the exposed wind on the building exterior, while the building height has significant effect in building ventilation, due to the buoyancy forces and wind speed to which a building is exposed (Hall and Spanton, 2012). The aforementioned factors can lead to uncertainties when trying to quantify them. Therefore, it is necessary to select a suitable method for the investigation of toxic gas building ingress.

Sour natural gas (>7 ppmv H_2S) is commonly found in many explorations, in particular to deep and high-pressure deposits (e.g. North America, Central Asia) and occupies nearly 40% of the global gas reserves (Total, 2007). Moreover, the H_2S level for most of the natural gas wells increases along with the "age" of the reserve. Hydrogen sulphide is flammable, corrosive, with a characteristic rotten egg smell, heavier (denser) than air (specific gravity of ~1.19 at 15 °C) and extremely poisonous (fatal) even at low concentrations (e.g. 76 ppmv for a 10 min

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exposure) (http://naturalgas.org/naturalgas/processing-ng/). The characteristic rotten egg odour can be detected at concentrations less than 0.01 ppmv, while a loss of odour detection capability occurs at 150 ppmv or after a prolonged exposure above 20 ppmv. A dosage of more than 1000 ppmv could have acute fatal effects for the population (Leahey and Schroeder, 1986). Natural gas is mainly transported by long pipelines which pose a potential risk for the nearby communities in case of a leak or rupture. Only in Alberta, Canada, there are 18,000 km of operating sour gas pipelines and more than 6000 sour gas wells. Although, the probability of a pipeline leak or rupture is very low (making it an unlikely event), it is still possible, and then the eminent consequences, of the toxic release, can be severe and thus this risk should not be ignored.

In the unlikely event of a sour gas release combined with fire, the transport of hydrogen sulphide along with other combustion products (e.g. sulphur oxides) by a wind-blown plume can distribute poisonous materials over a large area and may lead to serious consequences for the health of people and environment (Argyropoulos et al., 2013, 2010; Assael and Kakosimos, 2010; Markatos et al., 2009). More details in relation to the health impact of H_2S exposure on oil and gas workers and surrounding population may be found in the works of Hessel et al. (1997) and Lambert et al. (2006).

In order to model the indoor exposure, there are three types of indoor air quality models: statistical regression (Valero et al., 2009), micro-environmental (Duan, 1982) and Computational Fluid Dynamics (CFD) models (Béghein et al., 2005; Choi and Edwards, 2012). The first category uses empirical techniques in order to relate, via simple analytical expressions, the indoor environment exposure to parameters such as contaminant concentration, source strength and building characteristic. Micro-environmental class of models is further classified into the measurement-based (Kornartit et al., 2010; Ozkaynak et al., 2007), mass-balance (Dimitroulopoulou et al., 2006; Gerharz et al., 2009), multi-zone (Srebric et al., 2008; Wang and Chen, 2007; Wang et al., 2010) and sub-zonal models (Megri and Haghighat, 2007; Stewart and Ren, 2006). These models assume that the pollutant concentration is well mixed within the micro-environments and their results can be used relatively easily to compare with exposure data. However, it is known that the "well mixed" assumption does not always hold true (Wang and Chen, 2008). To surpass this difficulty, advanced CFD techniques are used for modelling the indoor air flow using Large Eddy Simulation (LES) techniques (Choi and Edwards, 2008; Emmerich and McGrattan, 1998) or less computational demanding approaches such as Reynolds-Averaged Navier-Stokes (RANS) (Chen et al., 2006; Karadimou and Markatos, 2016) and Unsteady Reynolds-Averaged Navier-Stokes (URANS) (Cehlin et al., 2014). Comparison of the models can be found in the work of Deevy et al. (2008) the review papers by Milner et al. (2011) and Wang and Zhai (2016).

Early attempts to investigate the occupants' exposure to air contaminants in industrial buildings were performed by Andreopoulos et al. (1992), Papakonstantinou et al. (2000) and Ren and Stewart (2005). In the latter work, a modified version of COMIS with sub-zones (COwZ) model was used for assessing personal exposure. The numerical results were compared with available experimental and numerical (CFD) data, indicating the importance of the location and orientation of the occupant. Chan et al. (2007) proposed two metrics for quantifying the performance of shelter-in-place (SIP) as protective action for the population during an unintentional toxic release. The two introduced metrics are the casualty reduction factor and safety-factor multiplier, which adopt the nonlinear dose response effect. The proposed methodology uses a combination of models for the pollutant dispersion (Gaussian model), the indoor concentrations (well-mixed box model), and health effects (power-law toxic load model). Several other studies have also been devoted to assess the SIP effective mitigation measure during the release of a hazardous airborne material (Kulmala et al., 2016; Mannan and Kilpatrick, 2000; Sorensen et al., 2004) and to provide analytical expression for the exposure in buildings or shelters (Parker et al., 2014; Parker and Coffey, 2011) and building ventilation strategies for the protection of the occupants (Stewart-Evans, 2014).

Kassomenos et al. (2008) developed a CFD model for assessing the indoor impact to the toxic Vinyl Chloride Monomer (VCM) in a chemical plant. The model was implemented using the commercial computer program PHOENICS, as used earlier by Andreopoulos et al. (1992). Their numerical results showed that the CFD model is capable of assessing the occupational exposure. Zhang and Chen (2010) presented a combined numerical approach for quantifying the risk from an accidental toxic gas (H_2S) release. The method comprises CFD and dose-response models. The former is used for dispersion modelling, while the latter is adopted for estimating the fatality percentage of the exposed personnel. Recently, Ashraf et al. (2016) presented a combined numerical methodology for computing building ingress during a toxic gas release from a natural gas feed pipeline. The study exhibits a consequence analysis based on the predicted indoor H_2S concentration.

The above mentioned studies adopt either sub-zones or CFD models for the occupants' exposure, excluding the work of Ashraf et al. (2016) which utilises a combination of multi-zone and CFD models. However, the main focus of these works is on simple quantifying approaches for risk assessment. In the present study, advantage is taken of the manual coupling of multi-zone and CFD models, while the proposed methodology implements advanced dose-response techniques for quantifying the occupants' exposure. In addition, the proposed methodology is faster than the advanced CFD approaches and as a result it can be used as a tool to assist the preparedness and response for a hazardous material release event, as well as a guide for the improvement of relevant risk assessment tools.

The purpose of the present effort is to improve the modelling of toxic gases building infiltration, thus a specific numerical study for predicting the H_2S ingress in a non-process building of industrial area has been selected. A combination of multi-zone and CFD models, such as CONTAM (Wang et al., 2010), SLAB (Ermak, 1990; Ermak et al., 1982) and Quick Urban & Industrial Complex (QUIC) (Nelson and Brown, 2013), together with available meteorological data are employed for investigating the ingress dynamics. Furthermore, a number of dosage procedures along with various scenarios are examined for proposing adequate mitigation measures, in order to prevent any health impact on the working personnel.

2. The proposed methodology

Consequences analysis of a toxic gas incident involves estimation of the release, atmospheric transport, (potentially) building ingress, and health effects. The present study focuses mainly on last two, therefore to cover the other two use is made of available information for an H_2S release scenario and the well-established atmospheric transport model SLAB by United States Environmental Protection Agency (US EPA) (Ermak, 1990; Ermak et al., 1982). SLAB (see Section 2.1) predicts the outdoor contaminant concentration and provides information on the time taken for the plume to reach the building, for example, the maximum concentration that building is exposed to as well as the duration of the exposure. Then, the predicted values of outdoor concentration are used as input parameter for the building ingress model. For the latter, CONTAM ((Wang et al., 2010); see Section 2.2) was selected, and the impact of the external wind pressures (see Section 2.3), the most critical parameter for building infiltration, was investigated by using the simple American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) correlation (Swami and Chandra, 1998) and a CFD model QUIC (Nelson and Brown, 2013). The former applies to low rise single and isolated cubical buildings, while the latter one resolves the detailed building geometry and predicts numerically the wind field around it. Finally, different mitigation scenarios and the expected health effects were assessed using the Acute Expo-