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A Numerical Study of Effects of an Industrial Hazardous Release On People Egress

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The release and dispersion of toxic materials from industrial equipment may pose severe concerns and have tragic consequences. The assessment of such scenarios relies on broad literature, approaches, and modelling tools that support estimating the impact area. However, hazard assessments do not generally embed the egress modelling and the impact of a toxic release on people evacuating. The present work couples a gas dispersion model with evacuation dynamics to estimate the near-field impact on people approaching a safe place. It is applied to a hypothetical case study concerning a release of dense chlorine, in which the effect of adopting different assumptions is discussed.

1. Introduction

To meet challenges, chemical plants need to provide safer plant operations. Simulation practices can provide quantitative measures to assess accidental scenarios that may impact men, goods, and the environment (Hossam et al., 2003; Vianello et al., 2014). These include loss of containment from tanks and reactors, ignited scenarios evolving in fires or explosions, and toxic dispersion. Every possible risk has to be investigated carefully, and hazard potentials must be reduced as much as reasonably possible. This can be accomplished by adopting low-risk process solutions, chemicals, devices, and operative strategies (Oberhoff Konig safety management in a chemical plant). Holistically, these approaches should tend to an acceptable safety standard based on robust risk analysis approaches and contribute to preventing accidents and preparing for emergency response (Mocellin and Maschio, 2016).

Risk scenarios can be approached according to different methods, i.e. deterministic, probabilistic, qualitative, and quantitative. The classification is based on the type of output data expected for the safety assessment.

One crucial step is related to the quantification of consequences of identified Top Events and scenarios. More in detail, the determination of chemical and physical properties concerning leak and dispersion and further possible harm and damage by fire, explosions and toxicity have to be known (Pasman, 2015).

These approaches allow for estimating concentration maps that can be used to assess the impact on people through exposure models, including dose-response and Probit (Gwynne et al., 1999). In fact, the evaluation of the impact of toxic gases and fires and explosions on humans represents the final step of risk assessment. However, despite the availability of various methodologies and tools for risk assessment, approaches to egress dynamics are typically available for indoor contexts, and related investigations rely on the analysis of specific parameters and concepts. This is to say that existing concepts do not fully embed human behaviour during emergency contexts, especially in industrial settings. Moreover, risk assessment in complex geometries that links dense gas spreading to human exposure is still not systematically addressed in the literature (Epstein et al., 2011). People activities and the exposure to a dose of toxic material or heat effects related to fires is of crucial interest for evacuation purposes and to assess the impact of hazardous scenarios on a human target evacuating. However, although evacuation models are available, an integrated approach to risk assessment in open domains interested in toxic gas dispersion or fires with evacuating people is still not fully investigated in the literature. Moreover, the impact of different models for gas dispersion on the estimated absorbed dose by evacuating people need to be assessed.

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The primary purpose of this work is to discuss a strategy that embeds gas dispersion modelling and egress dynamics applied to an industrial context. The impact of the toxic dispersion is addressed in terms of absorbed dose from evacuees in the trajectories to the safe place. Different approaches to gas dispersion are compared with respect to the impact on the final results of absorbed dose. The case study deals with a release of dense chlorine from a storage tank.

2. Methodology

This section illustrates the methodology adopted for gas dispersion and modelling individuals' behaviour around the threatening area (Figure 1).

The methodology starts with analysing the context in terms of processed or stored hazardous materials and layout. Then, credible accident scenarios are identified and formulated according to the typical quantitative risk assessment tree. In general, at the basis of atmospheric dispersion, a loss of containment from a process unit occurs due to failures, external actions, or terrorist attacks. The loss of containment involves a release whose features are determined by process or storage conditions and by the type and geometry of the source. A liquid evaporating pool or a solid sublimating system (Mocellin et al., 2018) may be formed if peculiar materials are interested under specific conditions.

Once the release scenario is defined, the gas dispersion is addressed for threat zones and extension, according to atmospheric conditions and the geometry of the surrounding area. Predicting gas dispersion and concentrations can be approached with different modelling approaches with increasing complexity and detail. In fact, different categories exist, including Gaussian models, Lagrangian and particle models, analytical models, and the more complex computational fluid dynamics (CFD) models. The selection of a specific modelling approach deals with different factors, including the scale of the problem and the required detail.

In the present work, we approached the gas dispersion through two approaches: a simplified Gaussian model for dense gas dispersion and a detailed CFD approach carried out with the code Fire Dynamic Simulator (FDS). FDS is a Large Eddy Simulation (LES) code that solves, for low-Mach numbers, the Navier-Stokes equations coupled to balance on chemical species and energy. In this way, we wanted to demonstrate how the selection of a specific approach, characterized by different degrees of detail and computational burden, may affect the absorbed dose results and impact human targets egressing from the scenario.

The gas dispersion concentration was coupled with the evacuation model. In this regard, we simulated the evacuation trajectories of each egressing agent, and we calculated the dose absorbed by evacuees during the movement related to the attempt to evacuate the area of the scenario. The dose of a toxic gas absorbed by an individual *i* is calculated according to Figure 1. It is based on the Haber approach, where C_i is the concentration of the gas, t_e is the duration of the exposure, and n depends on the specific toxic gas considered.

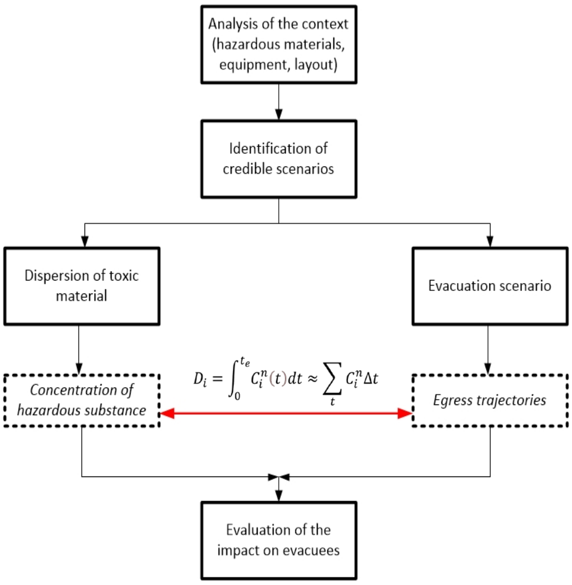


Figure 1: Methodology for assessing the impact of gas dispersion on evacuees.

3. Case study

The case study refers to an industrial installation that processes various hazardous substances to synthesise fine chemicals developed on a 20000 m^2 surface. It consists of three production departments, pilot plants, dedicated wastewater and gas treatment parks, R&D facilities, and buildings allocated to offices and workshops. The industrial park is also equipped with a tank farm that covers about 2000 m^2 where both liquid and gaseous hazardous materials are stored in atmospheric and pressurized equipment, for total quantities of more than 40 t. Hazardous materials include solvent hydrocarbon-derived compounds, pressurized gases including chlorine and hydrogen, and other various substances (technical gases, intermediates). According to CLP labelling (EC Regulation No 1272/2008), most are classified as H2, H3, and H4 with related physical, health, and environmental hazards. In addition, some hazardous materials are toxic and stored as compressed gas, i.e. chlorine.In the investigated context, different credible scenarios were formulated according to a coupled Hazard Investigation (HAZID) and Hazard and Operability Analysis (HAZOP). Focusing on the tank area, these include:

- Release of pressurized chlorine from a hole in a storage tank
- Release of flammable hazardous materials forming a pool fire.

In the present work, we discuss the case of a pressurized release of chlorine from a storage tank located in the tank farm of the industrial installation (Figure 2).

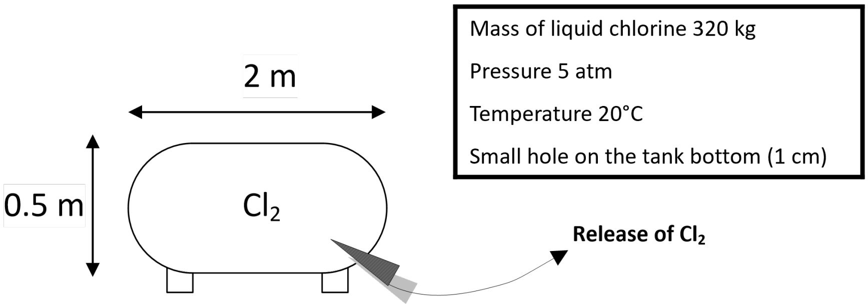


Figure 2: Source term for chlorine toxic dispersion.

Chlorine is stored in the form of pressurized gas (b.p. -33°C at 1 atm) and, during the release, undergoes a liquid-vapour transformation. According to initial conditions, we estimated an initial vaporized fraction of 0.17. The main features of the release are reported in Table 1. The release was modelled with the approach proposed in (CCPS, 2010). As a conservative approach, it is assumed that all unflashed liquid is entrained into the gas jet as an aerosol. The estimated cloud density ranges from 1.3 to 23 kg m^{-3}; the lowest values were recorded in correspondence to cold chlorine released from the tank at the initial stages.

Therefore, the gas dispersion involves heavy gas and requires appropriate treatment, especially when working with a substance like chlorine, toxic at concentrations as low as ppm. The accuracy of estimations depend on the specific modelling approach adopted, and this directly impacts the calculated dose inhaled by evacuees (Figure 1).

For the sake of comparison, in the present work, we dealt with the estimation of toxic gas concentrations with two distinct approaches:

a- Dense gas dispersion model, according to Britter and McQuaid (Britter and McQuaid, 1988),
b- Computation Fluid Dynamics with Fire Dynamic Simulator (FDS).

Both are able to predict the atmospheric dispersion of vapours that behave as negatively buoyant and include the relevant effect of weather conditions that is known to affect the extent of dispersion. Despite related assumptions, the first approach can provide good insight into physical processes essential for the transport and dispersion of chlorine. It is suitable for conservative estimations, but it is less effective in dealing with complex geometries, such as industrial installations (CCPS, 2010). Instead, the second approach provides very detailed insight and can accommodate any complex geometry, including the effect of local obstacles on mixing and dispersion. A Computational fluid dynamic approach (CFD), in a trade-off between detail and computational burden, may be beneficial in dealing with the spread of very toxic materials like chlorine.

Starting from the source term calculation of Table 1 and Figure 2, we calculated the peak concentrations of chlorine at the ground on the downwind coordinate (Figure 3).

According to the results, the chlorine concentration exceeds the AEGL-3 (10 min) within the release source's 15-20 m downwind. Values over the AEGL-2 (10 min) threshold is observed up to 60-70 m from the accident. Therefore, considering the industrial installation's layout, this simplified approach (a) suggests that outdoor chlorine concentration may be persistently over the AEGL-2 or AEGL-3 limit (10 min) for a certain period, i.e.

life-threatening health effects or death on the general population can occur. However, related risk of intoxication or death is a matter of toxic adsorbed dose, namely the amount of chlorine that gets into the body of any evacuee by inhalation. This is often calculated by multiplying the gas concentration and exposure time (Figure 1), alternatively by adopting the Fractional Effective Dose (FED) concept. According to Figure 1, this accounts for people behaviour during the emergency that goes with the toxic release scenario and related trajectories, i.e. the position over time of threatened targets by the toxic gas.On this basis, we reproduced the release and dispersion of chlorine in the exact geometry of the industrial installation with the CFD approach. We used the Fire Dynamic Simulation (FDS) on a computational domain shaped on the complex geometry of the tank farm under atmospheric conditions of Table 1. We preserved the parameters of the source and boundary conditions of the study to ensure a common basis for comparison. The computational domain of the numerical simulation was allocated with different grids according to the distance from the release source. Consequently, we adopted 20 cm cubic cells on the total number of about 2000000, progressively increasing to 40 cm near the boundaries of the computational domain. The domain is extended for 50x70x50 m, and results are non-sensitive to further grid refinement.

Table 1: Release of chlorine. Source term and environmental parameters

Peak emission rate	1.78 kg/s
Minimum temperature	-33°C
Total release time	160 s
Environmental temperature	25°C
Stability class	B
Realtive humidity	50 %

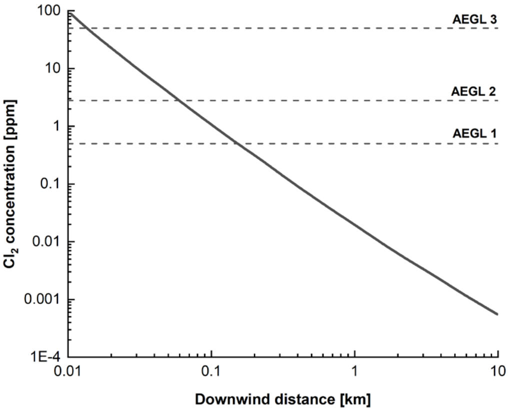
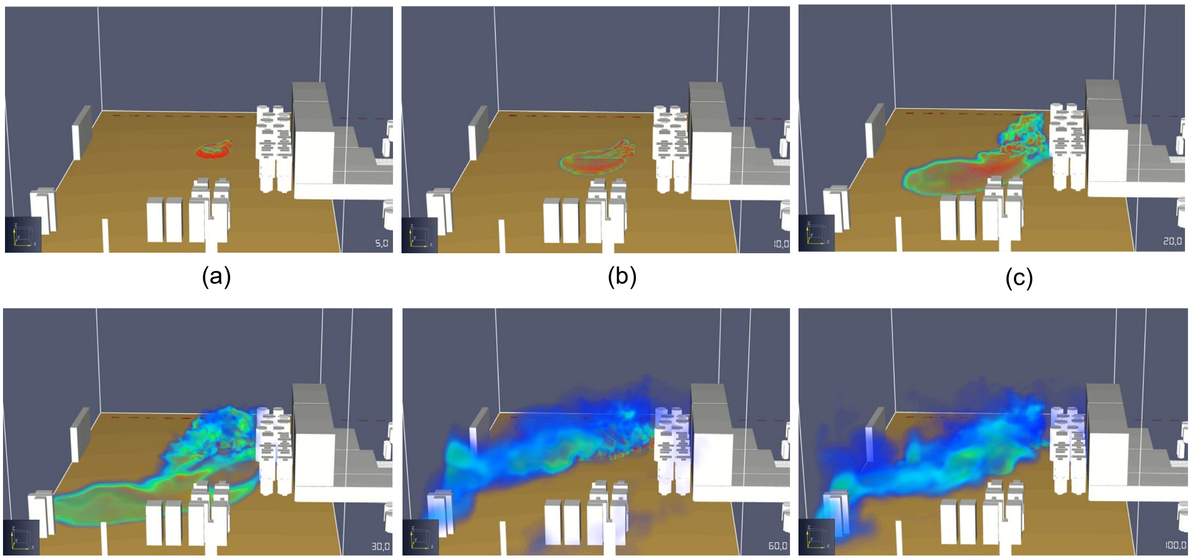


Figure 3: Outdoor toxic concentration of chlorine along the downwind distance according to the modelled source. AEGLs (Acute Exposure Guideline Levels) refer to 10 min exposure, comparable to timing for egress operations.

Figure 4 shows some relevant timeframes of the chlorine dispersion in the industrial installation. The numerical simulation underlines the heavy gas behaviour of chlorine that is enhanced by both low temperature and high density. This approach requires a higher level of sophistication and modelling effort, but different authors suggest it may allow more accurate results, especially in complex geometries (Zhang and Chen, 2010). However, the considered parameters in the numerical approach (e.g. wind direction can impact the predictions modifying the direction of dispersion and resulting toxic chlorine. In the present investigation, we considered constant parameters for local wind.

We built the egress scenario with Pathfinder® that includes relevant behavioural aspects and allows investigating the impact of different human factors and evacuations strategies. According to Figure 1, the approach provides that gas dispersion and human behaviour are modelled independently. Therefore, we neglected eventual deteriorations in human behaviours due to the impact of toxic gases on the speed and capability of decision making of evacuees.

According to indications, we considered a total occupancy resulting in 45 non-vulnerable evacuees representing a relevant part of the farm’s employees. The behavioural pattern was implemented according to the primary components that determine the response of an evacuee dealing with an emergency (Figure 5). We used an average velocity for agents ranging from 1.52 to 1.79 m/s representative of a quick walk and light running, respectively. However, we considered some agents to behave specifically, i.e. a small group initially approached the release source to acquire an awareness of the event.



(a) (b) (c)

(d) (e) (f)

Figure 4: View of the computational domain and spatial spread of chlorine as simulated by the Computational Fluid Dynamic approach. (a) 5 s; (b) 10 s; (c) 20 s; (d) 30 s; (e) 60 s; (f) 100 s. Spreading areas in red are characterized by about 500 ppm of chlorine values.

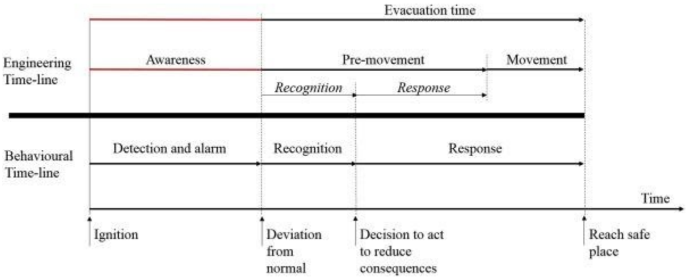


Figure 5: Behavioural and engineering components before and during egress.

According to the results, the simplified approach (Figure 3) suggests an effect on people egressing. In fact, we calculated the maximum inhaled dose of chlorine as high as $18\text{-}20 \cdot 10^3$ $ppm^2 \cdot min$. Within the evacuee's population, this is suffered by a group representing less than 5 % of the total population (2 people) that persist in the hazardous area for some minutes. A large part of the evacuees (60-75 %) inhales a dose of chlorine in the range from 500 to 3500 $ppm^2 \cdot min$. It should be noted that this modelling approach for gas dispersion can manage neither local fluctuations of concentrations nor stratification effects, i.e. the concentration map is uniform within the target area, which means conceptually that evacuees experience a constant maximum chlorine concentration of about 70-90 ppm. A related effect is strictly sensitive to the exposure time. According to this, no mortality is expected, but part of the population is exposed to dangerous concentrations for a short exposure (threshold limit of 40-60 ppm). The Probit function for non-lethal injuries suggests that evacuees experiencing such concentrations have more than 90% of the probability of non-lethal injuries.

A more detailed approach to toxic dispersion, i.e. based on CFD, may support more rigorous estimations.

In this regard, it should be noted that the chlorine discharge lasts about 4.5 min. Instead, the evacuation to a safe place (emergency meeting places, indoor areas) requires 40 s to 2 min depending on the position of the evacuee and actions taken according to simulated results. Our CFD simulation concluded that the expected concentration is constantly over the AEGL-3 (10 min) within 20 m from the source of release and at 1.5 m from the ground. This is partially in line with the conclusions of the simplified approach, but we simulated concentration peaks as high as 500 ppm in specific areas (Figure 4). In this regard, it should be noted that concentrations higher than 100 ppm can incapacitate men in a few seconds, while 1000 ppm is a threshold for lethality (Chauhan et al., 2008). Matching the CFD gas dispersion modelling with the egress scenario of the case study, we calculated a maximum value of absorbed dose higher than the simplified approach of about $60 \cdot 10^3$ $ppm^2 \cdot min$. Therefore the simplified approach tends to underestimate in the near-field. In addition, we observed that evacuees that initially found themselves in an area within 15 m from the release source would have a probability of mortality of 90-95 % according to the Probit equation based on cumulative inhaled dose. On the contrary, this scenario was discarded by the simplified approach. All evacuees, independently on their initial outdoor location, suffered consequences with an average probability of 60 % of injuring.

4. Conclusions

Including behavioural modelling in quantitative risk assessment can improve our estimations in dealing with the impact of highly toxic materials on evacuees during risk scenarios. Critical is an advanced treatment of local gas dispersion, especially for heavy gases and specific materials active at ppm like chlorine. Our case study showed how a simplified approach to gas dispersion shaped on evacuation trajectories underestimates the effects of inhaled dose and impact on people. Instead, a computational fluid dynamics treatment resulted in more accurate considerations that have re-evaluated the absorbed dose and probability of mortality. In the specific case, the simplified strategy resulted only in injuries for part of the population. Instead, detailed CFD modelling coupled to egress simulation suggested non-negligible mortality and different near-field impact zones driven by stratification and obstacles in complex geometries.

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