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Dispersion simulation for CBRNE accident coordination training

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Summary

FFI has developed a virtual training system that can be used to train incident leaders and responders in the mitigation of accidents involving hazardous substances. The virtual training system was successfully used during a course for training incident leaders held by the Norwegian Civil Defence, in which the scenario involved leakage of ammonia gas from a tanker truck after a collision. High-fidelity data of the dispersion of the gas was simulated using Computational Fluid Dynamics and fed into the training system.

In this note, we describe the numerical simulations of the gas dispersion, and the processing of the data necessary to incorporate the dispersion data into the training system. Some insights into the resulting hazard areas at different meteorological conditions and type of hazardous material are also given.



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1 Introduction

The project "Strengthening CBRNE safety and security – Coordination and Standardization", is a collaboration between Poland and Norway, funded under the Norwegian Financial Mechanisms Programme, Programme Home Affairs, area 23 "Prevention of natural disasters and readiness for such disasters". Work Package 3 "Innovative training platforms" aims at establishing innovative e-learning training platforms for CBRNE¹ threats.

FFI has developed the CBRNE Accident Coordination Training (CBRNE-ACT) system to demonstrate the possibility of using virtual training platforms for incident management and response training. CBRNE-ACT uses a computer generated forces application, VR-Forces, as the environment for exercises. FFI has developed plug-ins for VR-Forces to include and visualise the dispersion of toxic gas, and to simulate the effect of the toxic gas on exposed humans.

The Civil Defence regularly hosts exercises where incident leaders for the Fire and Rescue Services, Health and the Police, as well as the Civil Defence, are trained in managing different hazard scenarios. One of the courses, "Interaction at a contaminated damage site CBRN/E", focuses on incidents involving hazardous substances, and was held in September 2023. We used the CBRNE-ACT for virtual training of the incident leaders as one element of this course.

The scenario was a traffic accident involving a tanker truck, which resulted in the release and dispersion of the toxic gas ammonia. High fidelity numerical simulations of the release and dispersion of the ammonia gas and the resulting hazard areas were conducted and incorporated into CBRNE-ACT. Several ammonia simulations were conducted, but only one was used for the exercise. The different simulations conducted was used to indicate differences in the dispersion pattern that can be expected due to different wind speeds and terrain effects. As a reference case, chlorine gas was included to illustrate the consequences of an accident involving a more toxic substance. Apart from the material parameters, the chlorine scenario was equal to the ammonia scenario for the training exercise. The additional ammonia simulations and the chlorine simulation were prepared for an "after action review" and not a part of the exercise itself. The numerical simulations of gas dispersion, the use of the data in CBRNE-ACT, as well as some results and differences between the different meteorological conditions for the ammonia simulations and between the ammonia and chlorine simulations, are described in this report.

Chapter 2 provides background to the scenario, including observations from experimental field trials and accidents. The numerical simulations are presented in chapter 3 and results are given in chapter 4. Finally, concluding remarks are given in chapter 5. The CBRNE-ACT in general, the training exercise and lessons learned from the exercise are described in [1, 2].

¹C: Chemical, B: Biological, R: Radiological, N: Nuclear, E: Explosive

2 Background

2.1 Accident scenario

In the scenario, two trucks collide in the Fetveien/Storgata crossroads at Kjeller outside of Lillestrøm. One of the trucks is a tanker truck, which carries a trailer with a pressurised tank containing about 20 tonnes ammonia. The collision results in a hole in the upper part of the tank, above the liquid surface, from which ammonia gas leaks out into the atmosphere. The Fire and Rescue Service will try to stop the release by covering the hole and tank with tarpaulin. This happens after 20 minutes in the scenario. For more details about the scenario, see [1, 2].

Four simulations with the release and dispersion of ammonia were conducted, although only one was used in the exercise. The different simulations were used to illustrate differences in the dispersion pattern and the resulting hazard areas, due to different meteorological conditions and different terrain effects. A simulation with the more toxic substance chlorine was also conducted as an illustration of possible effects following a more hazardous toxic release. The comparisons between the four ammonia simulations and the chlorine simulation were prepared for an "after action review" and not for the actual exercise.

2.2 Material parameters

Ammonia is a toxic industrial chemical which is in much use worldwide. It is used among other in agriculture (as a source of nitrogen), fertiliser industry, water treatment and as a refrigerant. Liquid ammonia is lighter than water and ammonia gas is lighter than air. At a pressure of one atmosphere and temperature zero degrees Celsius, the relative density of ammonia gas to air is 0.6 [3].

Chlorine is also a common toxic industrial chemical. It is used among other for water purification. The transportation of chlorine is more restricted compared to ammonia, due to it's higher toxicity. At a pressure of one atmosphere and temperature zero degrees Celsius, chlorine gas has a relative density to air of 2.5.

As a measure of the toxicity of ammonia and chlorine, we use the Acute Exposure Guideline Levels (AEGLs), which are threshold levels for various effects of exposed personnel². The threshold depends on the exposure time. For this scenario, we use the concentration thresholds for ten minute exposure times, which are given in table 2.1 [4, 5].

²The three AEGLs are defined:

[•] AEGL-1 is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic non-sensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.

[•] AEGL-2 is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

[•] AEGL-3 is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

Substance	AEGL-1	AEGL-2	AEGL-3
Ammonio	30 ppm	220 ppm	2700 ppm
Ammonia	21 mg/m^3	154 mg/m ³	1888 mg/m ³
Chloring	0.5 ppm	2.8 ppm	50 ppm
Chiornie	1.5 mg/m^3	8.1 mg/m ³	145 mg/m ³

Table 2.1 The AEGLs for ten minute exposure of ammonia and chlorine gas.

2.3 Observations from experiments and accidents with releases from railcars

Over the years, there has been conducted quite a few field trials of the release and dispersion of toxic industrial chemicals. One fairly recent experimental campaign is the Jack Rabbit field trials. In USA, there were three well documented accidents involving the release of chlorine from railcars in the 2000s. These experiments and accidents are briefly described here.

2.3.1 Experimentally measured release rates

The Jack Rabbit II field trials, executed at Dugway Proving Ground, Utah, USA, in 2015 and 2016, studied large releases of chlorine into the environment. One of the trials studied the release from a pressurised tank containing nine short tons of chlorine through a hole directed upward. Gas ventilation was observed for the first 1–2 seconds, followed by a two-phase release for about half a minute, and then a gas release until about 100 seconds after start of the release. After that, the release rate was negligible. About 70% of the liquid was still contained in the tank. The observed release rates was estimated by Hanna et al. [6] and are listed in table 2.2.

Time after start of the release (s)	Period (s)	Rate (kg/s)
5	5	139.4
10	5	66.8
15	5	48.8
20	5	37.8
25	5	30.1
30	5	24.3
40	10	18.1
50	10	12.4
60	10	8.64
80	20	5.24
100	20	2.71

Table 2.2Observed release rater for Jack Rabbit II trial 8.

It should be noted that there are some important differences between ammonia and chlorine gas which could affect the release rates. Ammonia has a higher vapour pressure and thus require higher storage pressure than chlorine. The higher pressure will give a higher speed of the jet. On the other hand, ammonia is less dense than chlorine, which will lower the mass release rate, and thus counteract the effect of the higher speed. The Jack Rabbit field trials in 2010 studied releases of both ammonia and chlorine. In these trials, the initial storage pressure was typically about three

to four atmospheres for chlorine and about seven to eight atmospheres for ammonia. Two short tonnes were released in each trial, and the duration of the releases were roughly about one minute for each trial [7]. In these trials, as well as for most of the Jack Rabbit II trials, the release was directed straight down toward the ground from the bottom of the tank, and these trials are therefore not so relevant for describing the release of gas horizontally from the upper part of a tank.

2.3.2 Accidents

In USA, there were three well documented accidents involving releases of chlorine from railcars in the 2000s [8]. Here follows a brief description.

- **Festus, Missouri, August 14, 2002.** An accident occurred while chlorine was off-loaded from a railcar. A hose with dimensions of about one inch got a hole about two-three metres from the tank at a height of about three metres. The release sustained for about three hours with an estimated average release rate of 2.02 kg/s. A total of 48,000 lb = 22,000 kg was released.
- Macdona, Texas, June 28, 2014. A collision between two trains resulted in a chlorine release that lasted for seven hours. The release was terminated by forcing wooden plugs into the hole, which had a size of about 2 inches and was located in the lower part of the tank. Most of the chlorine leaked out during the first three minutes, after that a minor gas release continued for seven hours. A total amount of about 120,000 lb = 54,000 kg was released.
- **Graniteville, South Carolina, January 6, 2005.** A moving train collided with a standing train. A "fist-sized" hole on the side of the tank was reported. There was a large gas release for about one minute, followed by a lower gas release for several hours. A total amount of about 183,000 lb = 83,000 kg was released.

The organisation *Fertilizers Europe* have analysed 38 European ammonia rail transport accidents, and found that in none of these cases did the loss of containment of ammonia lead to injuries or casualties [9]. It should, however, be noted that the risks may be higher in scenarios involving road transport, as trucks may move through, or closer to, areas with a higher density of people possibly increasing the probability of exposure.

2.4 About transportation tanks

Some general data about tanks mounted on trucks in the USA is found in the Handbook of compressed gases, Compressed Gas Ass., Inc.[10]. Tanker track tanks have design pressures of 265 psig (1830 kPa, about 18 atm). Before 1960, truck tanks typically had a capacity of 26 short tons (24000 kg). After 1960, they typically have a capacity of 80 short tons (73000 kg). The maximum filling degree by weight is about 56%, which corresponds to a filling degree by volume of 82%.

3 Numerical dispersion simulation

In this chapter, we describe the numerical simulation of the gas dispersion. First, we estimate the release rate of gas from the tank, and then we describe the numerical method for simulating the transport of gas in air. Lastly, we describe how this data is converted and distributed into CBRNE-ACT.

3.1 Source term

The TNO Yellow Book [11] provides the following general expression for calculating the release of gas from a pressurised tank:

$$q = C_d A \Psi \sqrt{\rho_0 P_0 \gamma \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}},$$
(3.1)

where C_d is the so-called discharge-coefficient, A the area of the hole, ρ_0 the initial gas density, P the pressure, $\gamma = C_p/C_v$ is the ratio of the heat capacity at constant pressure and volume, and

$$\Psi^{2} = \begin{cases} 1 & \text{if } \frac{P_{0}}{P_{a}} \ge \left(\frac{\gamma+1}{2}\right)^{\frac{\gamma}{\gamma-1}} \\ \frac{2}{\gamma-1} \left(\frac{\gamma+1}{2}\right)^{\frac{\gamma+1}{\gamma-1}} \left(\frac{P_{a}}{P_{0}}\right)^{\frac{2}{\gamma}} \left(1 - \frac{P_{a}}{P_{0}}\right)^{\frac{\gamma-1}{\gamma}} & \text{otherwise.} \end{cases}$$

Index "0" denotes the conditions in the tank and "a" atmospheric conditions.

The Yellow Book also describes a method for calculating releases from the top of a tank. This method starts with calculation of the gas release given above and proceeds with a calculation of the "bubble rise" velocity in the liquid. A criteria for determining whether the content is released as pure vapour or as a two-phase flow (bubbly or churn type two-phase flow) is given. If vapour outflow is predicted, the release rate is calculated with equation 3.1. If two-phase outflow is predicted, the quality, Φ (the mass fraction of vapour), of the jet is calculated with the implicit function

$$\frac{\Phi q}{F_1 u_b \rho_v A_L} = \frac{1}{1 - CF_2 \left(\rho_v / \rho_l\right) \left(1 - \Phi\right) / \Phi},\tag{3.2}$$

where F_1 , F_2 and C are flow dependent parameters, u_b is the bubble rise velocity, A_L the normal liquid surface area, ρ_v and ρ_l the vapour and liquid densities. The release rate is then calculated by

$$q = C_d A \sqrt{2 (P_0 - P_a) \rho_f},$$
(3.3)

where ρ_f is the average fluid density. These two latter equations must be solved iteratively.

We assume a storage temperature of 15°C and an initial tank pressure of 7.4 bar. At this point, the ammonia liquid and vapour densities are $\rho_l = 681.7 \text{ kg/m}^3$ and $\rho_v = 5.7 \text{ kg/m}^3$, respectively. The ratio of specific heats and the discharge-coefficient is set at $\gamma = 1.4$ and $C_d = 0.62$ m (which is recommended for sharp orifices). We assume a liquid surface area of 20 m², which corresponds to a ten metre long and two metre wide tank. The type of flow and calculated release rates from holes with areas of A = 1, 5 and 10 cm at these conditions, as well as with the vapour density at atmospheric pressure and temperatures of 15°C ($\rho_{vap} = 0.71$) and the boiling point ($\rho_{vap} = 0.86 \text{ kg/m}^3$), are given in table 3.1.

Padius (cm)	Gas density (kg/m ³)	Rate liquid (kg/s)		Rate gas (kg/s)
Kaulus (CIII)		Rate	Gas fraction	
	0.71	-	-	0.10
1	0.86	-	-	0.11
	5.7	-	-	0.27
	0.71	33.2	0.02	2.39
5	0.86	33.2	0.02	2.63
	5.7	33.5	0.16	6.8
	0.71	333.3	0.002	9.6
10	0.86	333.5	0.003	10.5
	5.7	335.0	0.02	27.1

Table 3.1 Release rates.

If we have an initial two-phase release, then some of the liquid will instantly evaporate and be dispersed immediately as gas, while a fraction of the liquid will likely form a pool on the ground which will evaporate for some time. The evaporating pool thus constitutes a secondary source, and could be included in the simulation by calculating the amount that forms the pool and the evaporation rate. If a two-phase release with rate 33.5 kg/s endures for one minute, about 1400 kg of liquid will form a pool on the ground. Using methodology from the TNO Yellow Book [11], the evaporation rate from the pool is estimated to be about 0.5 kg/s for the first minute. At ten minutes, the rate has decreased to below 0.1 kg/s. The vapour source from the evaporating pool is thus quite small compared to the gas release from the tank (at least initially), and is disregarded in the simulation.

Based on these calculations, the observations from the chlorine accidents and the field trials described in section 2.3, the following estimate for the gas release rate in the scenario is used in the simulation:

- 6.8 kg/s for the first four minutes,
- 2.0 kg/s for the next 16 or 26 minutes³.

The speed of this jet right after exiting the tank is on the order of 100 m/s. We, however, choose to start the dispersion simulation after the adiabatic expansion of the jet, when the jet speed is much reduced. The gas in the simulation is released from an area of 1 m^2 with a speed of 5.5 m/s from the first part of the release and a speed of 1.63 m/s for the subsequent release.

The chlorine simulation is conducted with the same amount released. Since the density of chlorine gas is higher, the speed of the jet is lower for the chlorine simulation than the ammonia simulation: 2.2 m/s for the first four minutes and 1.66 m/s for the next 16 or 26 minutes.

³As previously stated, the Fire and Rescue Service will cover the hole with tarpaulin and thus end the release after twenty minutes. We have however also calculated the release for a further ten minutes to visualise the effect of ending the release after twenty minutes.

3.2 Gas dispersion simulations

3.2.1 Computational model and mesh

The computational domain for the three dimensional wind and dispersion simulation covers an area of 2600 metres in the east-west direction, 2400 metres in the north-south direction and 1000 metres in the vertical direction.

Maps of the terrain and the buildings in this area are downloaded from GeoNorge (Kartverket) and used to create a computational model with the methodology described in [12]. A crude model of a tanker truck is created "by hand", and put in the crossroads at Fetveien, Storgata. A map of the domain and the computational model is shown in figure 3.1. It is evident that the terrain is very different toward west and east from the source location. Toward east, there are quite a lot of buildings and a steep hill. Toward west on the other hand, the terrain is mainly flat, open land.

A computational mesh is created with a mesh size of 0.1 metre at the source location and four metres around the buildings, see figure 3.2.

3.2.2 Density effects

We treat ammonia gas as a neutral gas, meaning that the gas density is taken as equal to that of air. In other words, this means that the gas is passively transported by the wind. In reality, ammonia gas is quite complex when it comes to buoyancy. While the gas is lighter than air and can therefore be expected to have positive buoyancy, initially the ammonia-air-gas mixture can be denser than the surrounding air. The dense ammonia-air gas mixture is a result of evaporation of liquid, which consumes heat from the ambient air and gives a cold mixture. Since we assume release of pure vapour in the scenario, we can disregard the initial dense gas effect. Disregarding the positive buoyancy is conservative in the sense that we will then over-estimate rather than under-estimate the concentration of gas at ground level.

For the chlorine simulation the density is included. Chlorine gas is about 2.5 times denser than air, and this affects the concentration at ground level significantly.

3.2.3 Numerical simulations

The numerical simulations are conducted by Computational Fluid Dynamics (CFD). This is a method for numerically solving the Navier-Stokes equations, which are equations for the conservation of mass and momentum. There are different CFD models available for modelling the turbulence. In this work, large eddy simulation (LES) is used, where the fluid flow is divided into a resolved domain (where the equations are explicitly solved) and an unresolved (subgrid) domain which is modelled. The dispersion of the gas in air is modelled by scalar transport.

A detailed description of LES can be found in textbooks, see for instance [13]. For a description of the LES methodology for urban dispersion, see [14, 15].

Five simulations have been conducted. Four simulations with the release of ammonia and one simulation with the release of chlorine. The ammonia simulations are conducted for two wind directions with two wind speeds each. The conducted simulations are listed in table 3.2. Simulation '3A' was used in the exercise.

For each of the simulations, a neutral boundary layer is imposed and a turbulent boundary layer develops due to the roughness elements (buildings) in the domain. The wind flow is first simulated for 2000 seconds, ensuring that more than one flow through of the domain is completed, before the



(a) A map of the incident area. The accident location (release site) is shown with the black star.



(b) The computational model. The buildings can be seen as the dark areas and the release location is indicated with the black star. The dark grey area to the right of the release location indicates a hill.

Figure 3.1 A map of the incident area and the computational model.



(a) The computational mesh at the accident location.



(b) The computational mesh close to the source.

Figure 3.2 The terrain, buildings and tank with surface mesh.

Index	Substance	Wind speed (m/s)	Wind direction
1A	Ammonia	1.5	270° (West)
2A	Ammonia	1.5	90° (East)
3A	Ammonia	3	270° (West)
4A	Ammonia	3	90° (East)
1C	Chlorine	3	270° (West)

Table 3.2The numerical simulations. Simulation 3A was used for CBRN ACT. The wind
speed is at ten metres height. The wind direction is the direction from which the
wind blows.

gas is released. Figure 3.3 shows the vertical velocity profiles before the releases are started, at the location of the accident. The wind directions are from west and from east, and the wind speeds are about 1.5 m/s and 3 m/s at 10 metres height. The time step for the simulations is 0.02 seconds.

In a real event, the first responders will likely try to stop the release by covering the release with a tarpaulin. In the script for the exercise, this is done 20 minutes after start of the release. For the ammonia simulations, we have calculated the ammonia release for 20 and 30 minutes in order to visualise the effect of ending the release after 20 minutes. The chlorine release is only simulated for a 30 minute release. All the simulations are conducted for 30 minutes after start of the release.

3.3 Dispersion data in CBRNE-ACT

The 3D LES data is calculated on an unstructured grid. The results are stored at planes two metres above the ground as csv-files. The data is then post-processed and resampled onto a regular grid with grid size of 5 metre in the horizontal directions. Within each grid cell (in the regular grid), the concentration is taken to be the maximum concentration from the data points (in the numerical simulation) that falls within the grid cell.

The data are distributed to VR-Forces (and CBRNE-ACT) through a plug-in (which is coded by FFI). To ensure a smooth running of the CBRN-ACT scenario and to avoid time lags during the exercise, the data is compressed in two ways: 1) the dispersion data is sampled (and updated to CBRNE-ACT) with a temporal resolution of 30 seconds, and 2) the concentration data is smoothed by an averaging filter before distribution. A more detailed representation of the gas plume can be obtained by increasing the number of time samples and/or by skipping the smoothing filter.

The simulated data are used in the two following ways in CBRNE-ACT: it is included visually to show the dispersion of the gas, and the time integral of the concentration is used to estimate the effects on exposed people. For the visualisation, the gas is shown as plumes to the AEGLs for ten minute exposure (table 2.1). For the effect estimation, ten concentration levels ranging from: $m_f = 30$ to 3500 ppm is used⁴. At each point in the simulation, the concentration (within these levels) are logged. When the integrated value exceeds the AEGL exposure limits for 10 minute exposure, the affected simulated entities experience health effects.

⁴We have only conducted effect modelling for the ammonia simulation that was used for the training exercise.



Figure 3.3 The wind profile in the lowest 100 metres above ground for the four ammonia simulations. Height of 10 metres is indicated with the dashed lines.

4 Results

4.1 The gas plume from LES, converted data and in CBRNE-ACT

Figure 4.1 shows the instantaneous plume for gas concentration above AEGL-1 at four and ten minutes after start of the release, as well as the corresponding plumes converted onto the regular grid. Figure 4.2 shows the plume at 1, 2, 3, 4, 5 and 10 minutes in VR-Forces.

4.2 The effect of terrain and wind speed

Figure 4.3 shows the time average plume corresponding to the AEGL thresholds four, ten and twenty minutes after start of the release for the ammonia simulations 3A and 4A, with wind speed 3 m/s at ten metres height from west and east, respectively. With wind from the west, the buildings and the hill will tend to increase the dispersion in the lateral direction, giving a wide plume laterally. Also with wind from the east, there are a few buildings downwind which affects the dispersion, transporting the plume to the north. The overall plume, however, is more narrow with wind from the east, as the terrain after the small group of buildings is open and flat.

Figure 4.4 shows the average concentration after twenty minutes for the four ammonia simulations. The areas of the AEGL-levels are larger for the lowest wind speed for both directions, which is reasonable as the mixing of the gas is higher for higher wind speeds. The simulation with wind 3 m/s from east gives a shorter average plume to the AEGL-1 threshold than the simulation with wind 1.5 m/s. The reason is probably that the gas is transported more quickly away, and more efficiently mixed with the ambient air, with the higher wind speed. For the lower wind speed, however, the gas lingers for a longer period with concentration above AEGL-1.



(a) Instantaneous plume, 4 minutes

(b) Instantaneous plume, 10 minutes



Figure 4.1 The gas plume at four and ten minutes after start of the release. Figures (a) and (b) show the instantaneous plumes from the numerical simulation at a plane two metres above ground (visualised with the software paraview). Figures (c) and (d) show the plume converted into the regular grid. Green indicates concentration above the AEGL-1 threshold, yellow above AEGL-2, and red indicates concentrations above AEGL-3.



(a) 1 minute

(b) 2 minutes



(c) 3 minutes

(d) 4 minutes



(e) 5 minutes

(f) 10 minutes

Figure 4.2 The gas plume in VR-Forces and different instances. Yellow indicates concentration above AEGL-1, orange indicates AEGL-2 and red indicates AEGL-3.



(a) Wind from west, 4 minutes



(c) Wind from west, 10 minutes



(b) Wind from east, 4 minutes



(d) Wind from east, 10 minutes



Figure 4.3 The time average plume at four, ten and twenty minutes after start of the release with wind from west and east respectively. Green indicates concentration above the AEGL-1 threshold, yellow above AEGL-2, and red indicates concentration above AEGL-3.



(a) Wind 1.5 m/s from west



(b) Wind 1.5 m/s from east



(c) Wind 3 m/s from west

(d) Wind 3 m/s from east

Figure 4.4 The average concentration after twenty minutes release for the four ammonia simulations. Green indicates concentration above the AEGL-1 threshold, yellow above AEGL-2, and red indicates concentration above AEGL-3.

4.3 The effect of stopping the release

The Fire and Rescue Service will try to terminate the release by covering the hole with a tarpaulin. In the scenario, the hole is covered after 20 minutes. At this point the pressure in the tank has decreased substantially, probably to about the atmospheric pressure level of the surroundings. In the simulations, we assume that covering the hole terminates the release completely.

Figure 4.5 shows the instantaneous concentration 25 minutes after start of the release for the ammonia simulations with wind from west for both the full half hours release simulation and the simulation where the release is terminated after 20 minutes. At the highest wind speed, the gas is quickly transported away and only small amounts linger five minutes after the release is stopped. At lower wind speed on the other hand, a substantial amount remains at the accident site even five minutes after the release is stopped.

4.4 Comparison with a more toxic chemical.

Figure 4.6 shows the instantaneous plumes to the AEGLs for chlorine and ammonia gas at four, ten and twenty minutes after start of the release. The wind speed is 3 m/s at ten metres height from west.

The AEGL-thresholds for chlorine are about 20 times less than for ammonia. This naturally has a great impact on the hazard areas. The high density of chlorine will also affect the hazard areas, as this causes the gas to be transported closer to the ground and thus cover a larger area. The dense gas is also transported some distance against the incoming wind direction, as can be seen in the figures.



(a) Wind speed 3 m/s, continuous release



(b) Wind speed 3 m/s, release stopped after 20 minutes



(c) Wind speed 1.5 m/s, continuous release



(d) Wind speed 1.5 m/s, release stopped after 20 minutes

Figure 4.5 The instantaneous plume after 25 minutes release with continuous release for 30 minutes and with released stopped after 20 minutes. Green indicates concentration above the AEGL-1 threshold, yellow above AEGL-2, and red indicates concentration above AEGL-3.



(a) 4 minutes, chlorine

(b) 4 minutes, ammonia





Figure 4.6 The instantaneous plume four, ten and twenty minutes after start of the release for the chlorine and ammonia gas simulation with wind speed of 3 m/s from west. Green indicates concentration above the AEGL-1 threshold, yellow above AEGL-2, and red indicates concentration above AEGL-3.

5 Concluding remarks

Numerical simulations of the release and dispersion of ammonia and chlorine gas have been conducted with Large Eddy Simulations. The performed computations were four simulations of ammonia dispersion with different meteorological conditions and terrain effects, and one simulation of chlorine dispersion. One of the ammonia simulations was included in the virtual training platform CBRNE-ACT and successfully used in a course conducted at the Civil Defence, where incident leaders from the Fire and Rescue Service, Police and Health, as well as the Civil Defence were trained in managing a scenario involving the release of ammonia gas. The additional ammonia simulations and the chlorine simulation were prepared for an "after action review" to highlight the effects of buildings, wind speed and toxicity.

A comparison of the four ammonia simulations shows some difference in the instantaneous plumes. The terrain and built up environment influence the dispersion substantially. With wind from the west, the gas is transported toward an area with several buildings and a hill, while wind from the opposite direction transport the plume toward a flat, open area. The resulting plume is wider laterally in the direction of the houses and the hill. Two wind speeds were compared, and larger hazard areas are found at the lower wind speeds.

The effect of ending the release after twenty minutes was investigated. At the highest wind speed simulated (3 m/s at 10 metres height), the ammonia gas is quickly transported away after ending the release. At the low wind speed (1.5 m/s at 10 metres height) however, the gas remains at the source location for some time after the release is ended.

A simulation with the release and dispersion of the more toxic substance chlorine was simulated, to illustrate the effects of using a more dangerous scenario. Due to the higher toxicity of chlorine, the hazard areas are much larger in the chlorine gas scenario than for the ammonia scenario.

References

- Arild Skjeltorp, Cecilie Jackbo Gran, Martin Asprusten, Ole Martin Mevassvik, Thomas Vik, and Anders Helgeland. CBRNE Accident Coordination Training System (CBRNE-ACT) Technical description. Technical Report FFI-rapport 24/01122, Norwegian Defence Research Establishment (FFI), 2024.
- [2] Cecilie Jackbo Gran, Arild Skjeltorp, Martin Asprusten, Ole Martin Mevassvik, Thomas Vik, and Anders Helgeland. Simulation supported CBRNE accident coordination training. Technical Report FFI-rapport 24/01544, Norwegian Defence Research Establishment (FFI), 2024.
- [3] Compressed Gas Association et al. *Handbook of compressed gases*. Springer Science & Business Media, 2012.
- [4] United States Environmental Protection Agency. https://www.epa.gov/aegl/ammonia-results-aegl-program7, retrived November 27, 2023.
- [5] United States Environmental Protection Agency. https://www.epa.gov/aegl/chlorine-resultsaegl-program, retrived November 27, 2023.
- [6] Steven Hanna, Graham Tickle, Thomas Mazzola, and Simon Gant. Dense gas plume rise and touchdown for Jack Rabbit II trial 8 chlorine field experiment. *Atmospheric Environment*, 260:118551, 2021.
- [7] U.S. Department of Homeland Security and Dugway Proving Ground. Record Customer Package, database of Jack Rabbit field trials results.
- [8] Steven Hanna, Seshu Dharmavaram, John Zhang, Ian Sykes, Henk Witlox, Shah Khajehnajafi, and Kay Koslan. Comparison of six widely-used dense gas dispersion models for three recent chlorine railcar accidents. *Process Safety Progress*, 27(3):248–259, 2008.
- [9] Fertilizers Europe. Guidance for transporting ammonia by rail. *Fertilizers Europe: Etterbeek, Belgium*, 2007.
- [10] Compressed Gas Association et al. *Handbook of compressed gases*. Springer Science & Business Media, 2012.
- [11] TNO. Methods for the calculation of physical effects due to releases of hazardous materials (liquids and gases), 2005. Third edition.
- [12] Hannibal E. Fossum and Anders Helgeland. Creating computational meshes from geographical information-system data for urban environments - a general and robust methodology. FFIrapport 2017/16283, Forsvarets forskningsinstitutt, 2017.
- [13] Stephen B Pope. Turbulent flows. *Measurement Science and Technology*, 12(11):2020–2021, 2001.
- [14] Hannibal E. Fossum and Anders Helgeland. Computational fluid dynamics simulations of local wind in large urban areas. FFI-rapport 2020/02365, Forsvarets forskningsinstitutt, 2020.

[15] Emma My Maria Wingstedt, Andreas Nygård Osnes, Espen Åkervik, Daniel Eriksson, and BA Pettersson Reif. Large-eddy simulation of dense gas dispersion over a simplified urban area. *Atmospheric Environment*, 152:605–616, 2017.

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