FFI-rapport 2015/01474

Simulations of the release and dispersion of chlorine and comparison with the Jack Rabbit field trials

Thomas Vik, John Aa Tørnes and Bjørn Anders P. Reif

FFI Forsvarets forskningsinstitutt

Simulations of the release and dispersion of chlorine and comparison with the Jack Rabbit field trials

Thomas Vik, John Aa Tørnes and Bjørn Anders P. Reif

Norwegian Defence Research Establishment (FFI)

7 October 2015

FFI-rapport 2015/01474

1256

P: ISBN 978-82-464-2578-8
E: ISBN 978-82-464-2579-5

Keywords

Klor

Flerfasestrømning

Utslipp

Testing

Approved by

Monica Endregard	Project Manager
Janet Martha Blatny	Director

English summary

The release and dispersion of toxic industrial chemicals as a result of accidents, terrorism or sabotage, represents a possible hazard. Such chemicals are often transported and stored as condensed liquids in pressurized tanks. There is a significant gap of knowledge and a lack of reliable models for calculating the release and dispersion of dense gases, like for example chlorine, and thus on calculating the resulting hazard areas. This knowledge gap is assumed to be relatedto a poor understanding of the source term, especially for massive releases. In order to address this issue, a series of experiments in which two tons of chlorine and ammonia respectively were released from a pressurized tank, were conducted at Dugway Proving Ground, Utah, USA, during spring 2010. FFI assisted in the planning of the experimental setup by conducting numerical simulations of the release of chlorine. In addition, FFI participated in these experiments, as the only non-American institute, and has access to all the experimental data.

This report describes simulations of one of the releases with an advanced Large Eddy Simulation model developed by Cascade Inc., and with the faster hazard prediction tool ARGOS and the dense gas dispersion model SLAB. The results from these are compared with the experimental results. The goal is to gain insight about massive releases of pressurized toxic industrial chemicals and the effectiveness of the fast hazard prediction tools to predict the dispersion and consequences of the release.

Some simplifications and assumptions had to be made in order to use the LES software for simulating the experiment. Even so, near the source, where the dynamics are to a large extent driven by the release jet, good agreement with the experiment is found.

The fast hazard prediction tools cannot resolve the source characterisations of the experiment. A method where the source is specified as anevaporating pool, instead of a two-phase jet from a pressurized tank, was tested. Good agreements with the experiment can be found, however it is quite dependent on the evaporation rate and it is not obvious how to specify this rate a priori.

Sammendrag

Utslipp og spredning av giftige industrikjemikalier som følge av uhell, terror eller sabotasje, representerer en fare. Slike kjemikalier transporteres og oppbevares ofte som væsker i trykksatte tanker. Det er et betydelig kunnskapsgap og mangel på pålitelige modeller for å modellere utslipp og spredning av tunge gasser, som for eksempel klor, og dermed for å beregne fareområdet ved slike hendelser. Det er antatt at forskjellene i stor grad er relatert til mangelfull kildemodellering, spesielt for store utslipp. For å studere kildetermen ved massive utslipp av tunge gasser ble en serie felttester, der to tonn av henholdsvis klor og ammoniakk ble sluppet ut, gjennomført ved Dugway Proving Ground, Utah, i perioden 27. april - 21. mai 2010. FFI deltok i planleggingsfasen av feltforsøkene med to-fase utslippsberegninger av klor for å bidra til å definere forsøksoppsettet.

Denne rapporten beskriver beregninger av utslippene med en avansert Large Eddy Simulation-modell utviklet ved Cascade Inc., USA, og med de raskere farepredikjonsverktøyene ARGOS og SLAB. Hensikten er å erverve økt kunnskap om store utslipp over kort tid av trykk-kondenserte toksiske industrikjemikalier, samt å undersøke de raske farepredikjonsverktøyenes evne til å forutsi spredning av gass og konsekvensene etter et utslipp.

Noen forenklinger og antagelser var nødvendige for å kunne bruke LES-koden til å simulere utslip pet i eksperimentet. Likevel er det god overenstemmelse mellom eksperimentet og simuleringen nær utslippet, der dynamikken til stor grad er styrt av utslippsstrømmen fra tanken.

De raske farepredikjonsverktøyene kan ikke simulere utslippsmekanismen i eksperimentet direkte. En metode der kilden spesifiseres som en dam som fordamper i stedet for en tofasestrøm fra en trykksatt tank ble forsøkt. God overensstemmelse med de eksperimentelle målingene kan oppnås, men resultatene er nokså avhengig av fordampingsraten fra dammen, og det er ikke åpenbart hvordan denne raten bør spesifiseres.

Contents

1 Introduction

The release and dispersion of toxic industrial chemicals as a result of accidents, terrorism or sabotage, represents a possible hazard. Such chemicals are often transported and stored as condensed liquids in pressurised tanks. There is a significant gap of knowledge and a lack of reliable models for calculating the release and dispersion of dense gases, like for example chlorine, and thus on calculating the resulting hazard areas. This knowledge gap is assumed to be related to a poor understanding of the source term, especially for massive releases. In order to address this, the Jack Rabbit field trials were conducted at Dugway Proving Ground, Utah, USA in the spring of 2010. The test program was designed to study source term characteristics for large scale releases of dense gases from pressurised containers, and a total of ten field tests with releases of chlorine and ammonia were conducted.

One of the chlorine releases has been simulated in detailed using a Large Eddy Simulation approach. This report describes the simulation, and the results from the simulation are compared with the experimental results. In addition, the release has been modelled using faster hazard prediction and consequence assessment tools. The results from these are also compared with the experimental results as well as with the LES results.

The Jack Rabbit field trials are briefly described in chapter 2. Chapter 3 describes the various modelling approaches, and the simulations are presented in chapter 4. The results are given in chapter 5 and finally concluding remarks are given in chapter 6.

2 The Jack Rabbit field trials

The Jack Rabbit field trials were conducted at Dugway Proving Ground, Utah, USA, in the period April 27^{th} - May 21^{th} 2010. The test program was managed by the Chemical Security Analysis Center (CSAC) under the Department of Homeland Security (DHS) Science and Technology Directorate. Two pilot tests with the release of one U.S. ton of ammonia and chlorine respectively, and eight tests with the release of two U.S. tons each (four of each chemical) were conducted. Most of the releases were conducted at low ambient wind speeds and stable atmospheric conditions, and the materials were released downward into a dug out depression with a diameter of 50 meters and a depth of two meters. The experimental setup was specified in this way in order to use the two ton releases as simulants for releases of much larger quantities of chlorine, in which the released material lingers at the source location for an extended time. For a description of the test program see [1]. A summary of the experimental measurements is given in [2].

Hanna *et al.* [3] used formulas developed by Briggs *et al.* [4] and the dense gas model SLAB to calculate the downwind chlorine concentrations for two of the chlorine releases, and found satisfactory agreement. The same methodology is used in this work for another case (see chapter 4.2.1 and 5.2). Bauer [5] used one of the chlorine releases to test the atmospheric transport and diffusion model Chemical/Biological Agent Vapor, Liquid, and Solid Tracking (VLSTRACK), which is a

Gaussian dispersion model that includes the density of the plume to account for dense gas effects. VLSTRACK is developed at Naval Surface Warfare Center Dahlgren Division.

Hearn *et al.* [6] studied soils samples at the Jack Rabbit field trials in order to determine the amount of chlorine that can deposit onto soil. They conclude that up to 50 % of a 1814 kg release can deposit within 20 m from the release point for soils with high organic matter and/or water content (not the soil type present at the release site).

The test program is continued as Jack Rabbit II. Several releases are planned in late-summer and autumn of 2015 and 2016. The new tests will focus on chlorine releases exclusively, with releases of 5-20 tons of chlorine in each test.

3 Mathematical modelling

3.1 Large Eddy Simulation and Lagrangian Spray Particles

The compressible solver "vida" developed at CASCADE, INC., [7], has been used for these simulations. Here the mass and momentum equations (Navier-Stokes equation) are solved under the low Mach number approximation, where the thermodynamical parameters are assumed to be decoupled from variations in pressure. In addition a Lagrangian spray particle model (LSP) is used for liquid droplets. The droplets break up and evaporate, and there is a two-way coupling between the gas phase (vida) and liquid phase (lsp) for interphase mass and momentum transport and one-way coupling for the temperature.

The gas phase equations are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \overline{u}_j}{\partial x_j} = S_c \tag{3.1}$$

$$\frac{\partial \rho \overline{u}_i}{\partial t} + \frac{\partial \rho \overline{u}_i \overline{u}_j}{\partial x_j} + \frac{\partial p}{\partial x_i} = \frac{\partial}{\partial x_j}\left[(\mu + \mu_t)\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \overline{u}_k}{\partial x_k}\right)\right] + S_m \tag{3.2}$$

where the bars denotes filtered variables, μ_t is the turbulent viscosity which is modelled by the dynamic Smagorinsky model, and S_c and S_m are source terms for mass and momentum respectively. The density is a dependent on the mass fractions of chlorine vapour and air:

$$\rho = \frac{1}{\overline{Y}/\rho_{vap} + \left(1 - \overline{Y}\right)/\rho_{air}} \tag{3.3}$$

where $\overline{Y}$ is the mass fraction of chlorine vapour.

The transport of vapour is calculated by:

$$\frac{\partial \rho \overline{Y}}{\partial t} + \frac{\partial \rho \overline{u}_j \overline{Y}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\rho D_Y + \frac{\mu_t}{Sc_t}\right)\frac{\partial \overline{Z}}{\partial x_j}\right] + S_z \tag{3.4}$$

where D_Y is the molecular diffusion coefficient, Sc_t is the turbulent Schmidt number, and and S_z is a source term for vapour mixture fraction.

A scalar equation is solved for the temperature:

$$\frac{\partial \rho \overline{T}}{\partial t} + \frac{\partial \rho \overline{u}_j \overline{T}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\rho D_T + \frac{\mu_t}{Sc_t}\right)\frac{\partial \overline{T}}{\partial x_j}\right] + S_T \tag{3.5}$$

where D_T is the thermal diffusion coefficient and S_T a source term.

The vida solver is coupled to a Lagrangian spray particle model. The methodology for calculating the particle transport and evaporation is taken from [8]. The equations governing the particle transport are:

$$\frac{d\mathbf{x_p}}{dt} = \mathbf{u_p} \tag{3.6}$$

$$\frac{d\mathbf{u_p}}{dt} = D_p\left(\mathbf{u} - \mathbf{u_p}\right) \tag{3.7}$$

where $\mathbf{x_p}$ is the particle position, $\mathbf{u_p}$ the particle velocity, $\mathbf{u}$ the gas velocity and D_p the drag coefficient modelled as:

$$D_p = \frac{f_1}{\tau_p} \tag{3.8}$$

where $\tau_p = \rho_p d_p^2/18\mu_g$ is the particle time constant for Stokes flow, d_p is the particle diameter, ρ_p the particle density, and μ_g the gas viscosity. The factor f_1 is a correction to Stokes drag for droplet motion and evaporation and is a function of the particle Reynold's number:

$$Re_p = \frac{\rho_g d_p \mid \mathbf{u} - \mathbf{u_p} \mid}{\mu_g} \tag{3.9}$$

The evaporation is calculated from the equilibrium Langmuir-Knudsen formula as:

$$\frac{dm_p}{dt} = -\frac{Sh}{Sc_G}\left(\frac{m_d}{\tau_d}\right)\ln\left(1 + B_{M,eq}\right) \tag{3.10}$$

where the widely used Ranz-Marshall correlation is used for the Shearwood number:

$$Sh = 2 + 0.552 Re_p^{1/2} Sc_G^{1/3} \tag{3.11}$$

and the Spalding transfer number for the mass is:

$$B_{M,eq} = \frac{Y_{s,eq} - Y_G}{1 - Y_{s,eq}} \tag{3.12}$$

where the subscript s means at the droplet surface and G denotes in the carrier gas.

The temperature of the droplets are calculated as:

$$\frac{dT_p}{dt} = \frac{GNu}{3Pr_G}\left(\frac{\theta}{\tau_p}\right)\left(T - T_p\right) + \left(\frac{L_V}{C_L}\right)\frac{\dot{m}_p}{m_d} \tag{3.13}$$

where $\dot{m}_p = dm_p/dt$ is negative for evaporation, and

$$G = \frac{\beta}{e^{\beta} - 1} \tag{3.14}$$

where the non-dimensional evaporation parameter β is:

$$\beta = -\left(\frac{3Pr_G\tau_d}{2}\right)\frac{\dot{m}_p}{m_p} \tag{3.15}$$

$Pr_G = \mu_G C_{p,G}/\lambda_G$ is the gas phase Prandtl number given by the gas phase viscosity (μ_G), heat capacity at constant pressure ($C_{p,G}$) and thermal conductivity (λ_G). Nu is the Nusselt number, which is given by the Ranz-Marshall correlation:

$$Nu = 2 + 0.552Re_p^{1/2}Pr_G^{1/3} \tag{3.16}$$

$\theta = C_{p,G}/C_L$ is the ratio of of gas heat capacity to liquid heat capacity, T_G is the gas temperature, and L_V the latent heat of vaporisation.

Droplets break up when the cross flow Weber number exceeds six. The Weber number is given by:

$$We = \frac{\rho_G(u-u_p)^2 r_p}{\sigma} \tag{3.17}$$

where r_p is the droplet radius and σ is the surface tension.

The evaporated mass is given as a source for the gas phase (equation 3.1 and 3.4), and the change of particle momentum is given as source for the gas momentum equation (equation 3.2).

The effect on the air temperature due to evaporation is neglected in this simulation, the source term in equation 3.5 is zero. In reality heat is taken from the surrounding air for evaporation of the droplets and consequently the temperature of air would decrease. This would then create a denser air-chlorine vapour mixture than that calculated as described above. However, in the temperatures measured in the depression during the experiments were not particularly low (down to -10°C [2]). In this case, for a vapour mass fraction of 50% chlorine vapour, the difference in density as calculated above compared to the real case is below 10%.

3.2 ARGOS

The Accident Reporting and Guiding Operational System (ARGOS) [9] is a decision support system for enhancing crisis management for incidents involving CBRN releases developed by Beredskapsstyrelsen (Danish Emergency Management Agency, DEMA), Risø National Laboratory and PDC-ARGOS in Denmark. Originally developed for supporting decisions for nuclear emergencies, a chemical module has later been included.

For the Jack Rabbit chlorine gas release simulations, the HeavyPuff module in ARGOS was used. This is a box model that was developed by the Technical University of Denmark (DTU, Risø) some years ago, but has never been developed further from the original prototype level [10]. It is designed to simulate the behaviour of a heavy gas plume near (up to 500 m) from the source.

In HeavyPuff, the dense gas cloud from an instantaneous release is approximated by a cylinder with a given radius and height. In the classic box model all properties (concentration, density, absolute temperature, enthalpy difference, et cetera) are assumed to be uniformly distributed

within this volume. The radius grows with a front velocity and the centre of mass moves with the advection velocity. The vertical mixing of the gas cloud is modelled by an entrainment velocity through the top cloud interface, and the enhanced mixing at the front is modelled by the front entrainment velocity [10].

After the near source region of the dense gas, further dispersion of the gas is simulated by the Rimpuff model [9], which is a Gaussian puff model in which the gas cloud is simulated as a series of puffs with maximum concentrations in the centre and Gaussian concentration profiles.

3.3 SLAB

The SLAB model [11] is an atmospheric dispersion model for denser-than-air releases, developed in 1990 by Donald L. Ermak of the Lawrence Livermore National Laboratory, Livermore, CA, with support from the U.S. Department of Energy (DOE), USAF Engineering and Services Center, and the American Petroleum Institute. The SLAB model treats denser-than-air releases by solving one-dimensional spatially averaged equations of momentum, conservation of mass, species, and energy, and the equation of state (ideal gas). The gas cloud can be treated as a steady plume, puff or a combination of the two depending in the source characteristics. SLAB handles several release scenarios including ground level and elevated jets, liquid pool evaporation, and instantaneous volume sources. SLAB is one of the most widely used dense gas models and it is also recognised as the easiest-to-use dense gas model in the public domain.

SLAB itself is a freeware and in the present investigation the SLAB View Windows graphical user interface from Lakes Environmental Software was used.

4 Numerical approach

One of the chlorine release trials, test number 5, is used in this case. For this test, two U.S. tons of chlorine was released. The ambient wind speed was about 1.5 m/s for this case, and the air temperature at the time of the release was 3.5°C. For more details concerning this test and the weather conditions see [2].

4.1 Large Eddy Simulation

4.1.1 Computational mesh

The computational domain includes the tank and the depression as specified according to the experimental setup, see [1] and [2]. The total computational domain consists of a box with a length of 400 meter, a width of 200 meter, and a height of 100 meter. The velocity inlet plane is positioned 100 meter upwind of the tank. Figure 4.1 shows a close-up of the tank and the depression.

A mesh with about 25 million tetrahedra cells was created. The cells nearest the ground have a

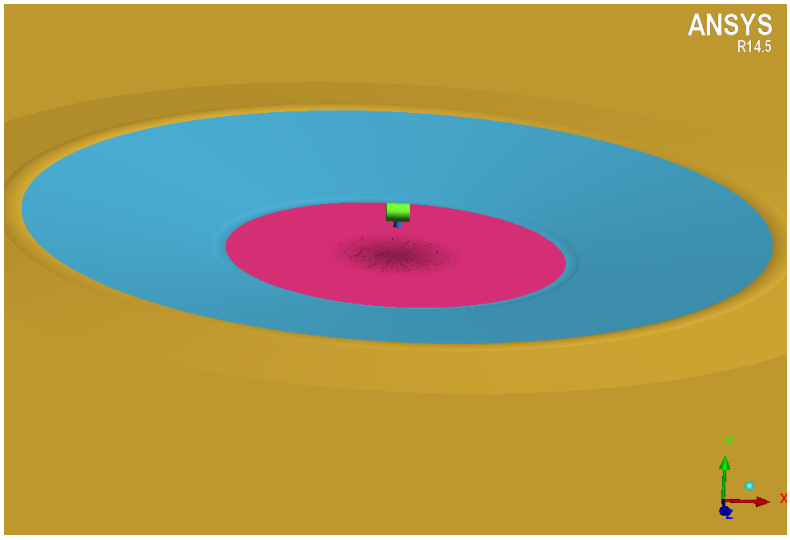


Figure 4.1 *The geometrical model of the tank (green) and the depression, which has a flat area with a diameter of about 24 meters (red) and a 2 meter high hill toward the rim (blue). The total diameter of the depression is 50 meters.*

resolution of 20 cm, while the cells grow larger in the vertical direction. The finest resolution is in the region between the tank and the bottom of the depression with cell lengths of about 2.5 cm.

4.1.2 Boundary conditions

In the experiments, the released material was transported through a 30 cm long pipe before entering the environment where subsequent flashing[1] of the liquid occurred (some flashing of the liquid also occurred within the pipe). To simulate this would require a separate simulation, as a combination of the resolution required to resolve the processes in the pipe and the subsequent flashing with the large scale simulation of the dispersion of liquid would result in a very time consuming simulation. Instead it was planned to start the simulation after the adiabatic expansion of the jet. From thermodynamics, about 12% of the liquid is expected to flash immediately, and before air entrainment the jet would then have a diameter of about 0.5 meter.

However, the current code for coupling the variable density solver with Lagrangian spray particles cannot account for such large fractions of liquid because is does not include the volumetric displacement of the gas by the droplets. It is valid only for a dilute regime. Therefore a jet consisting of 10% liquid droplets and 90% vapour was used in the simulation. The area of the jet was increased to a radius of 0.665 meter.

The vapour is released from a circular area with the dimension specified above. The jet velocity was chosen to give the release time observed in the experiment (about one minute). The droplets are released from a number of rings co-located with this area, and the droplets are given radii in

[1] Flashing means immediate evaporation of liquid due to the pressure difference between storage pressure and the ambient pressure.

Height above ground (m)	Wind speed (m/s)
2	1.44
4	1.63
8	1.87
16	1.90
32	1.96

Table 4.1 Wind speed at different heights measured during trial 5.

the range $[1 \cdot 10^{-6}, 1 \cdot 10^{-4}]$ meter according to the Rosin-Rammler distribution.

The droplets evaporate according to the evaporation model in equation 3.10, however the Spalding transfer number in equation 3.12, $B_{M,eq}$, gets unrealistic values when the mass fraction at the droplet surface and in the carrier gas are both near one. Therefore when the gas mass fraction in the carrier gas is near one, evaporation of the droplets are suppressed.

A velocity profile based on the measured mean velocity components (shown in table 4.1) and the six components of the Reynold's stress tensor at heights of 2, 4, 8, 16 and 32 meters above ground level was given at the inlet plane. A synthetic turbulence model with a integral length scale of one meter and a bulk wind speed of 1.44 m/s was included to create a turbulent boundary layer.

4.2 Operational models

The chlorine release described above is quite unusual with a vertical release from a tank into a depression in the ground, making the source term definition quite complex. It might, therefore, be better to simulate the release as a continuous evaporating pool on the ground. This has been done by Hanna *et al.* using two of the other Jack Rabbit trials (trial 2 and 6) as examples [3] (they have not simulated the release from trial 5). The same methodology is used for trial 5 in this work.

In the simulations, the chlorine assumed to fill the depression. The surface roughness for grassland (0.05 m) [3], an air temperature of 3.5 °C (276.7 K), a ground temperature of 3.2 °C, and the measured wind speed at a meteorological mast 50 meters south of the source location (table 4.1) [2] were used in the calculations.

4.2.1 SLAB

4.2.1.1 Instantaneous or short duration evaporating pool release

The chlorine concentration was calculated by SLAB using two different options. First, the release was defined as an instantaneous or short duration evaporating pool release from a tank source. In this case SLAB calculates the initial liquid mass fraction ($m_{f,liq}$) from the thermodynamical formula:

$$m_{f,liq} = 1 - C_{liq} \cdot (T_s - T_{BP})/L \tag{4.1}$$

where C_{liq} is the liquid heat capacity, T_s the material storage temperature, T_{BP} the material boiling point and L the heat of vaporisation at the boiling point. Using this formula, a liquid mass fraction of 0.878 is calculated. The release is then calculated from a combination of two sources: an instantaneous volume source (mass fraction 0.122), which could be either pure vapour or a mixture of vapour and liquid droplets, and a short-duration ground level area source (mass fraction 0.878). The source area was taken as the area of the 50 m diameter depression (1960 m^2) and the total mass released was 1826 kg. The temperature of the source material was set to the boiling temperature of chlorine, 239.1 K.

4.2.1.2 As an evaporation pool

In addition, the chlorine concentration from an evaporating pool from the same source area as used above (1960 m^2), but without any instantaneous vapour or liquid droplet fraction, was calculated. Also for this case, the temperature of the source material was set to 239.1 K.

The source duration had to be estimated from the videos recorded during the field trials or calculated. In the release, quite a lot of the released material is transported out of the depression during the release. However once the release is finished, the gas fills out the depression and remains in the depression for at least five minutes (which is the duration of the available videos) and is very slowly transported out. Briggs *et al.* developed a model for dense gas removal from a valley by cross-winds [4], also used in [3]. Even though this is a model for the removal of dense gas trapped in a valley, it has been used to set the evaporation rate from a pool filling out the depression in the current simulation. The model gives a source duration of 900 seconds for a wind speed of 1.44 m/s (although this might be too high wind speed for this model, the velocity closer to the evaporating surface would be more appropriate; this would give an even longer evaporation time). It was therefore decided to use four different pool durations: 60, 120, 180 and 900 seconds. The release rate (source rate) was adjusted accordingly (30.4 kg/s, 15.2 kg/s, 10.1 kg/s and 2.0 kg/s) in order to obtain the total source mass (1826 kg).

4.2.2 ARGOS

The chlorine concentration was calculated by ARGOS as a release from a pool with diameter 50 meter in the same way as described for SLAB in chapter 4.2.1.2 (no initial vapour fraction). The chlorine was released with two different release rates: 30.4 kg/s over 60 seconds and 15.2 kg/s over 120 seconds. The surface under the pool and the surrounding environment were set to dry sand.

Height (meter)	Maximum concentration (mg/m^3)
0.5	$1.4{\cdot}10^5$
1.0	$2.0{\cdot}10^4$
1.5	$9.9{\cdot}10^3$
2.0	$9.9{\cdot}10^3$

Table 5.1 Maximum chlorine vapour concentration 25 meters downwind at different heights.

5 Results

5.1 Dispersion

5.1.1 LES

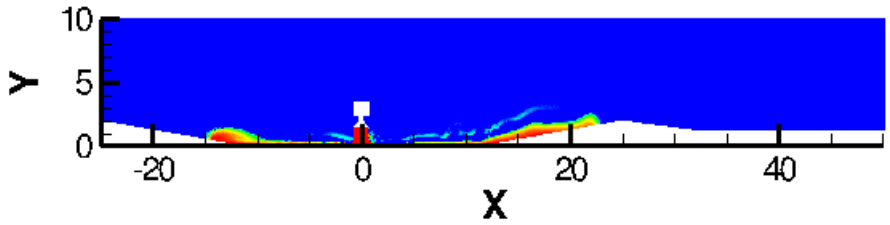
Figure 5.1 shows the concentration of chlorine vapour in a vertical plane through the source location at various time steps. Figure 5.2 shows the simulated three dimensional vapour cloud at two time steps.

During the release, at first the gas is transported symmetrically outwards in all directions close to the ground. The transport along the ground is opposed by the incoming ambient velocity field upwind, gravitational forces at the rise toward the rim of the depression, and by frictional forces, and the gas soon falls back into the depression. Initially a lot of mixing in the vertical direction occurs. Toward the end of the release however, the vertical mixing diminish, and after the release has finished, the gas remains quite still in the depression for a long time, and is slowly transported out of the depression. This is very similar to what was observed in the experiments.

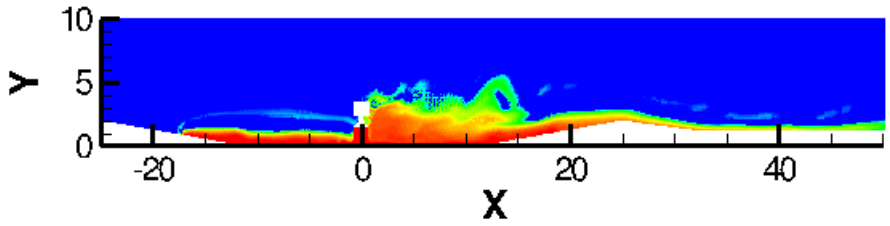
Figure 5.3 shows the predicted vapour concentrations 25 and 50 meters downwind the release point as function of time. This is five seconds averages of the maximum concentrations. However, the concentration drops rapidly with height in the simulation. Table 5.1 gives the predicted maximum concentration at height of 0.5, 1, 1.5 and 2 meters above ground 25 meters downwind. The maximum concentration shown in figure 5.3 is taken fairly close to the ground.

Figure 5.4 shows the concentration profiles measured with the Jaz UV-Viz sensors during the experiment. The concentration peaks corresponds fairly well with the maximum concentration measured in the experiment, see also figure 5.6. However, the measured time concentration profiles decrease much quicker than the simulated time concentration profiles. It should be noted that the maximum concentration is not necessarily found directly downwind; kinematic blocking of the gas upwind and the gravitational forces blocking the dispersion at the edges may induce build up of vapour at these locations.

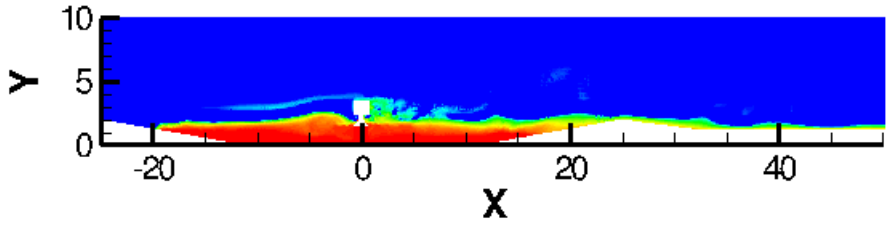
Figure 5.5 shows the predicted amount of vapour inside the depression as function of time. If this curve is extrapolated, it would take a long time before all the gas is transported out of the depression (about one hour). This is a much longer time than what was observed in the experiments. Both the transport of vapour out of the depression and the vertical mixing of the



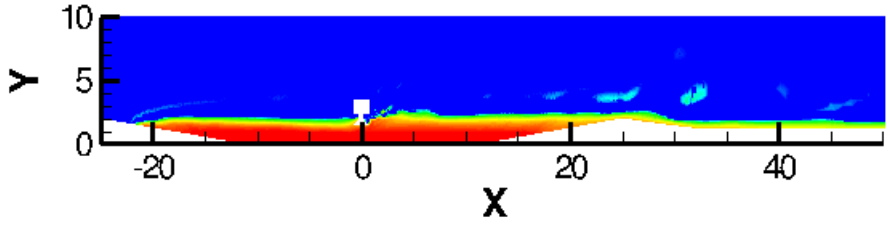
(a) 10 s



(b) 30 s

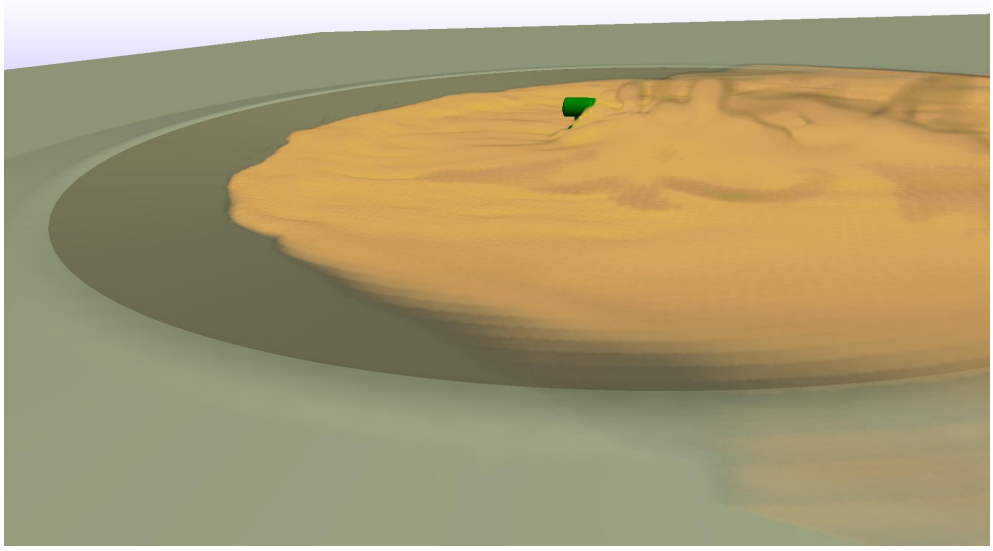


(c) 50 s

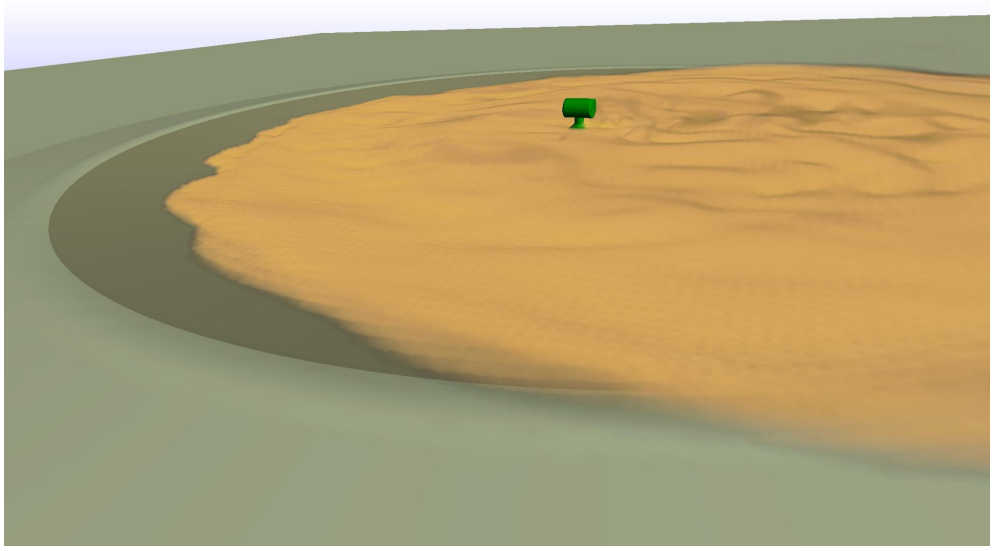


(d) 90 s

Figure 5.1 *The chlorine vapour concentration in a vertical plane through the source at various time steps after the start of the release. The release starts at $t = 0$ s and ends at $t = 60$ s. The mean wind direction is in the positive x-direction.*

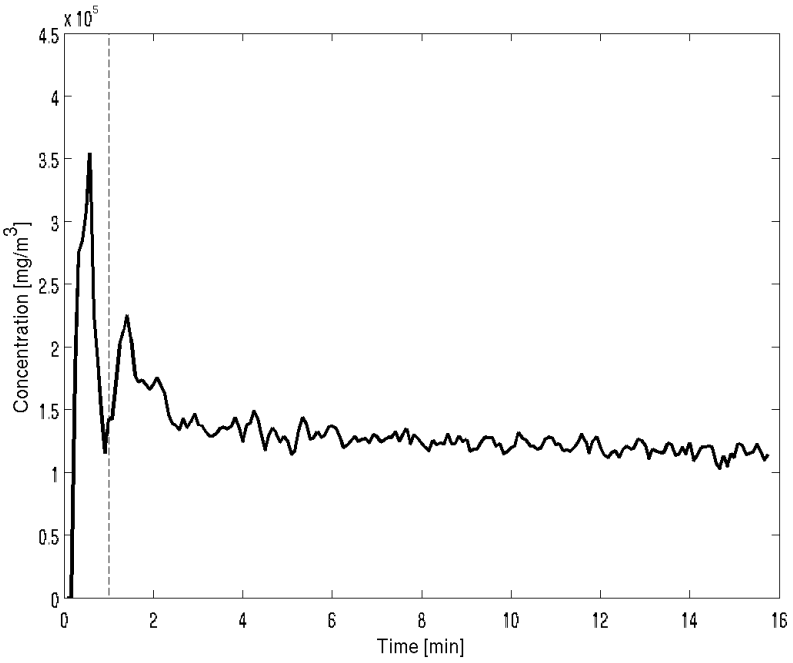


(a) 30 s

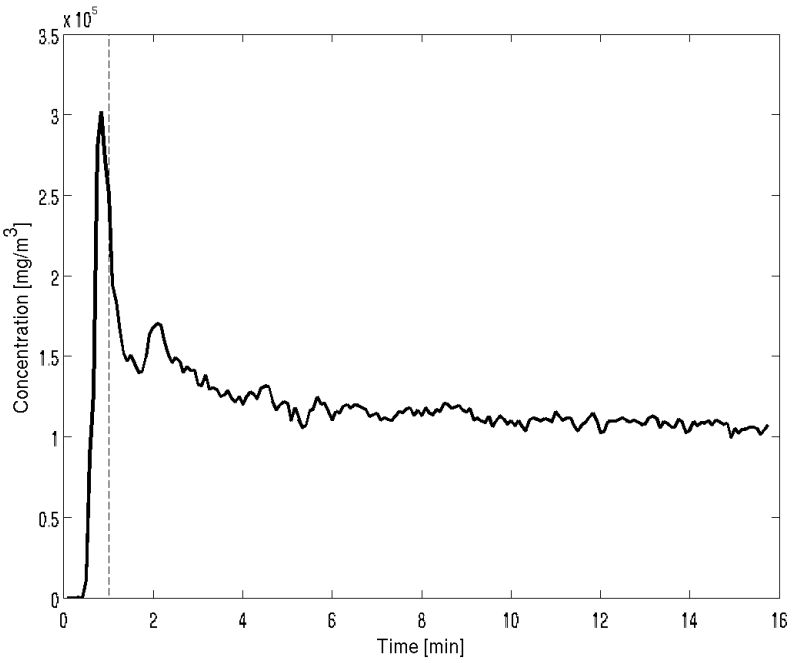


(b) 60 s

Figure 5.2 The simulated vapour cloud at various time steps after the start of the release. The release starts at $t = 0$ s and ends at $t = 60$ s.

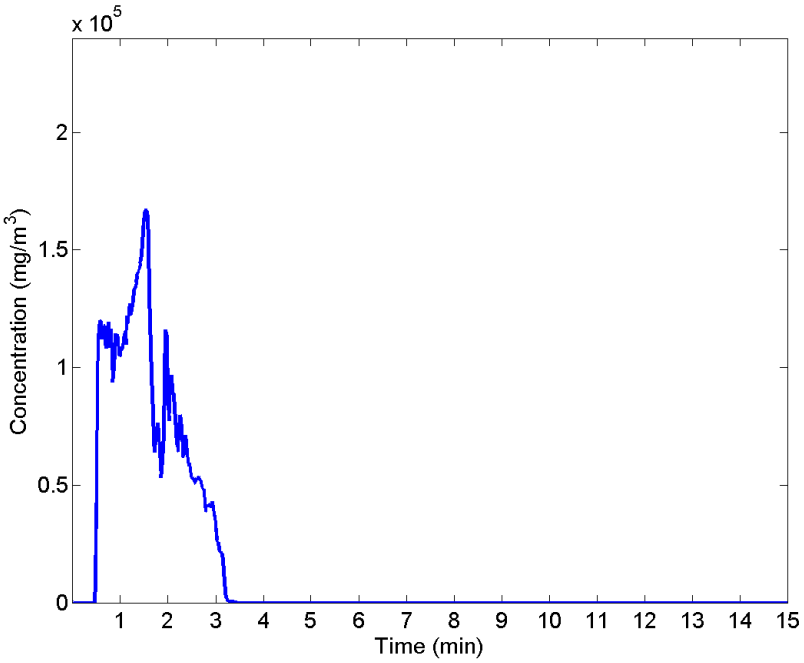


(a) 25 meter

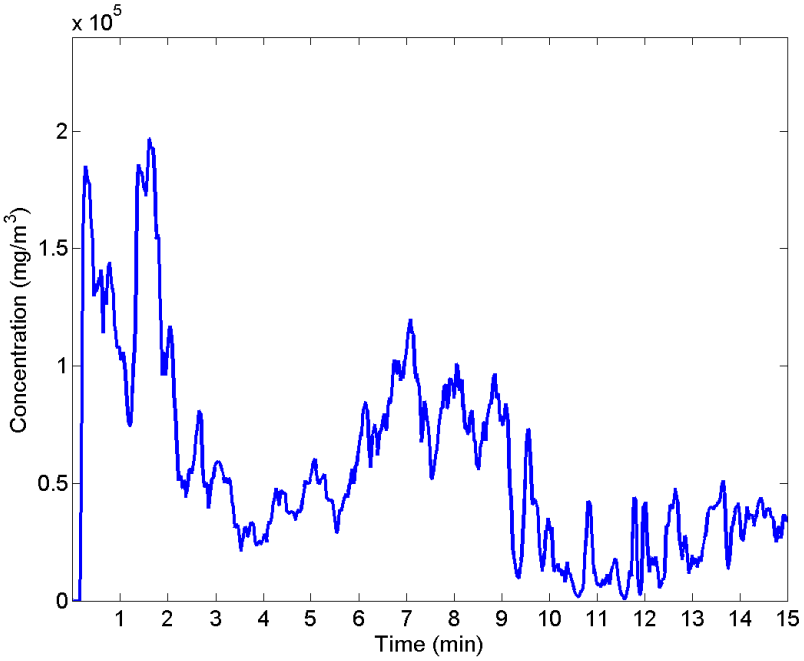


(b) 50 meter

Figure 5.3 The predicted concentration 25 and 50 meters downwind the release point. The stapled line denotes the end of the release.



(a) 25 meter



(b) 50 meter

Figure 5.4 The chlorine vapour concentration 25 and 50 meters downwind the release point measured with the Jaz UV-Viz sensors. The sensor at 25 meters is almost directly downwind of the source (within 20°), while the sensor at 50 meters is almost 90° off.

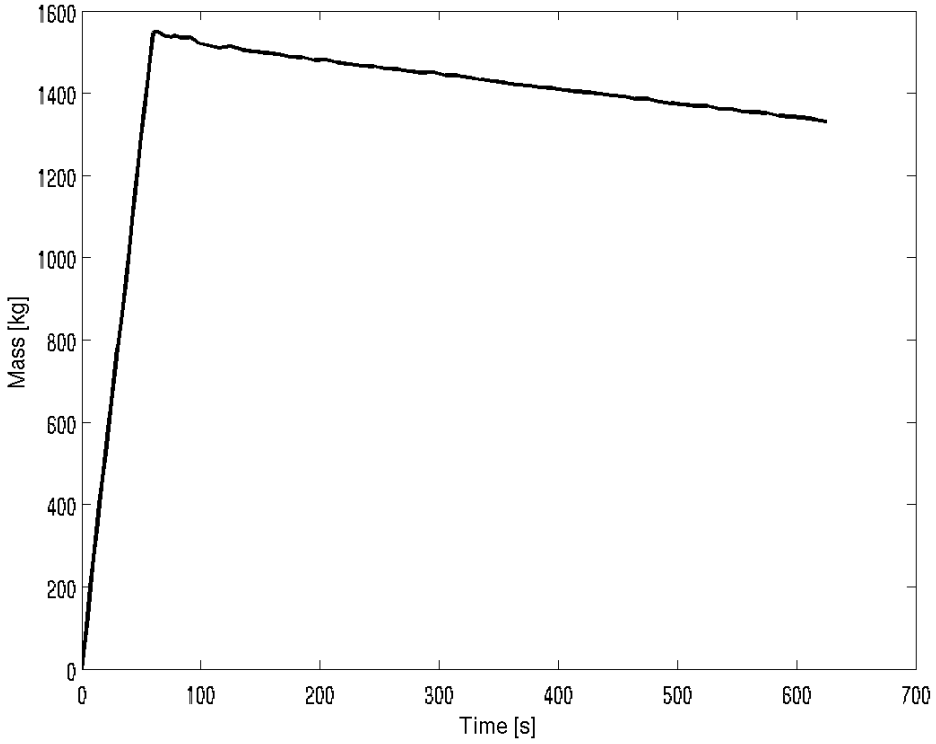


Figure 5.5 The predicted chlorine capour mass contained in the depression as function of time.

vapour downwind the depression is underestimated. As long as the release occurs, the motion of the dense gas jet induces all the motion near the source location, and the simulation shows good agreement with the experiment (even though the characteristics of the jet is different from the experimental jet). After the release has finished however, some discrepancies becomes apparent. The reason for this is most likely that the atmospheric boundary layer near the ground is too poorly resolved in the simulation.

5.2 Operational models

In figure 5.6 a plot of the centreline chlorine concentration at different distances from the source is shown. In addition, the maximum obtained readings from field measurements at three distances (25 , 50 and 100 meters) and the maximum concentration levels with LES at two distances (25, and 50 meters) from the source are also shown.

When evaporation from a pool is selected in SLAB, the maximum airborne concentration is achieved at about 22 m from the source for all three source durations. This corresponds with the edge of the 50 m diameter depression. The chlorine cloud gets more and more diluted as it travels further away from the source.

Figure 5.6 shows that SLAB predicts a higher initial chlorine concentration with the instantaneous or short duration pool simulation compared to evaporation from a pool. This is because a part of

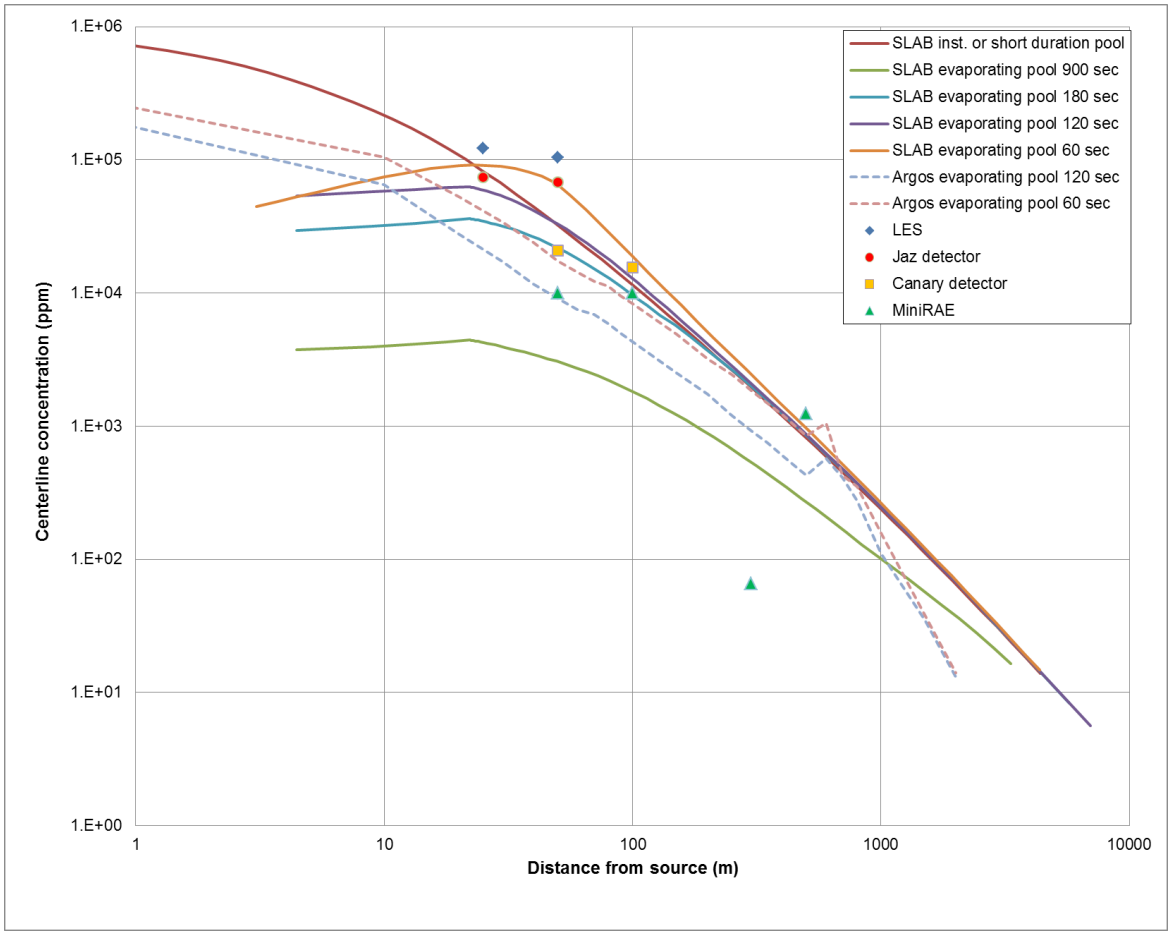


Figure 5.6 Comparison of chlorine centreline concentrations calculated by SLAB and ARGOS using different modelling options (see text for details). Maximum concentrations from field measurements using Jaz UV-VIS, Canary UV and MiniRAE photoionization sensors, and from LES are also shown in the figure. Not all the sensors are placed at the centreline downwind from the release site. Note that MiniRAE readings both at 50 m and 100 m are above the maximum range (> 10 000 ppm).

the release (12.8 %) during the first method was calculated as either pure vapour or a mixture of vapour and airborne liquid droplets, which, since SLAB does not take topography into account, is quickly transported downwind. In our view it is more realistic to represent the chlorine contained in the depression as a liquid pool only (no initial vapour or airborne droplet phase). The four SLAB calculations with evaporating pool only gave different air concentrations close to the source, but approximately the same concentration of chlorine farther downwind, i.e. more than about 300 meter downwind from the source, except for the longest pool duration (900 seconds).

Heavy gas calculations using ARGOS was carried out using the pool only method described for SLAB above. The calculated chlorine concentration outside the depression (more than 25 m) is higher with SLAB (up to about a factor four) compared to the concentration calculated by ARGOS using the same pool duration. The difference between SLAB and ARGOS gets smaller when the cloud moves towards 500 m from the source.

At 500 m distance, Gaussian puff calculation takes over form the box model. The discontinuity in the ARGOS results is due to the change of dispersion models at this distance. The calculated concentration drops quicker with distance after this transition. This is reasonable as the chlorine cloud does not behave like a dense cloud anymore and therefore dilutes more quickly in the surrounding air

There are too few concentration measurements from vapour detectors in the area to be able to draw any conclusions on which method that best predicts the concentration. The measurements fits relatively well with all the performed simulations, except for the SLAB simulation with 900 seconds pool duration. This indicates that the duration calculated with the model by Briggs *et al* is too long for this modelling procedure, even though this corresponds better with the observations from the experiment.

The plume widths at 50 m and 500 m from the source centre are shown in table 5.2. The difference between the plume widths for AEGL-1, AEGL-2 and AEGL-3 levels are very small, and therefore the plume widths for only one concentration limit are shown. The initial plume width (at 50 meter) is larger for the instantaneous or short duration evaporating pool release with SLAB and smaller with ARGOS compared to the release from a pool using SLAB. At 50 meter distance, the plume width is larger from 120 second pool duration compared to shorter and longer pool durations. At 500 meter from the source centre, all four SLAB calculations gave almost the same plume width, except from the longest pool duration, whereas ARGOS gave a wider plume.

With LES, the width of the plume to the AEGL concentration levels 50 meters downwind of the release is about 50 meters at the end of the release, and grows to about 150 meters after the release stops.

The dimensions of the gas cloud was estimated by cameras. It is not clear to the authors at what concentration level the gas was detected. From these cameras a cloud with of about 300 meters is estimated three minutes after start of the release. The center of the plume is by that time about 160 meters from the release location. It should however be noted that because the wind direction shifts,

Model	Pool duration (sec)	Distance from source centre	
		50 m	500 m
SLAB-inst		260	500
SLAB-pool	60	180	470
SLAB-pool	120	240	500
SLAB-pool	180	190	480
SLAB-pool	900	110	300
ARGOS-pool	60	120	600
ARGOS-pool	120	110	600

Table 5.2 Maximum plume width (m) at 50 m and 500 m from source centre. SLAB-inst is calculated as an instantaneous or short duration evaporating pool release while SLAB-pool and ARGOS-pool is calculated as an evaporating pool with different pool duration times.

the plume has travelled a longer distance than that at this point. The width then decrease with time to 200 - 250 meters.

5.3 The wind field

Figure 5.7 shows velocity profile given as input to the simulation together with the profile from the simulation at a vertical line 50 meters downwind the inlet plane (and 25 meters upwind the nearest rim of the depression). The velocity profile from the simulation is an average of 600 time steps before the release is started. The measured velocity profile is fairly well reproduced.

Figure 5.8 shows the streamwise velocity before and during the release. The mean velocity plots show time averages over 470 seconds before the release, and for the duration of the release (60 seconds) for the release. It is evident that the dense gas release reduce the velocity near the release, while the fluctuations are increased.

Figure 5.9 shows the difference between the mean streamwise velocity before the release and the mean during the release as function of time at four locations, two within the depression and two locations downwind. The mean before the release is time averaged over 470 seconds, while the mean velocity during the release is the mean velocity over the given time since the start of the release. The velocities are shown in heights of one and two meters above ground. The difference is calculated as:

$$U_{diff} = \frac{U(t) - U(t=0)}{U(t=0)} \tag{5.1}$$

Figure 5.10 shows the corresponding velocity difference for the vertical component. At the height of one meter, the streamwise velocities at the two locations within the depression first have a brief rise, then quickly drops, especially at the downwind location. Also at the rim of the depression there is a decrease in velocity at one meter, while the velocity at the location downwind the depression is not so affected by the dense gas. At two meters, the upwind location inside

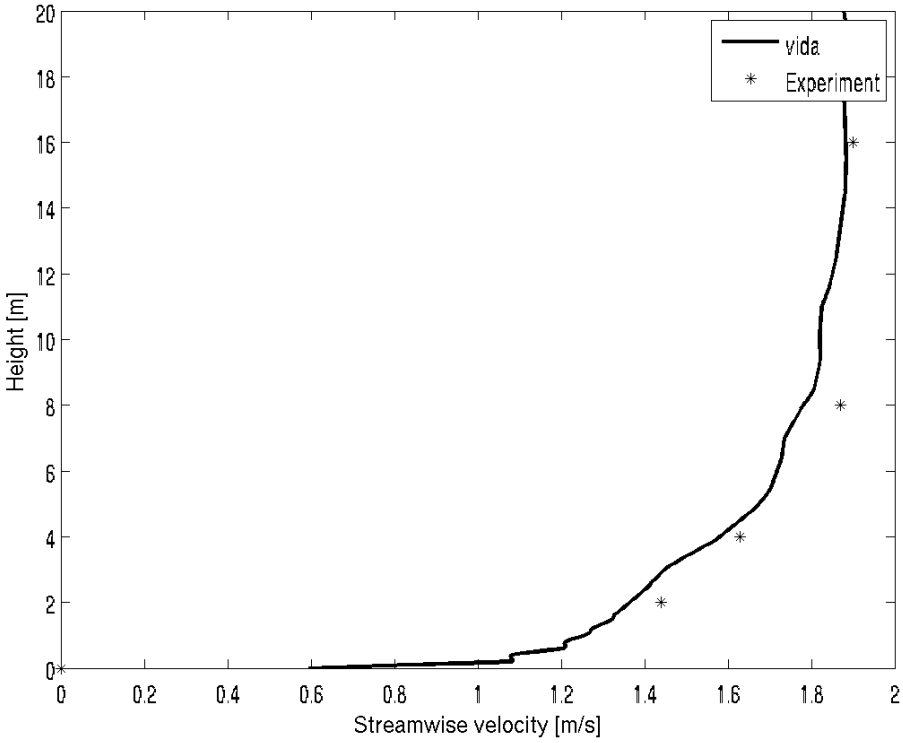
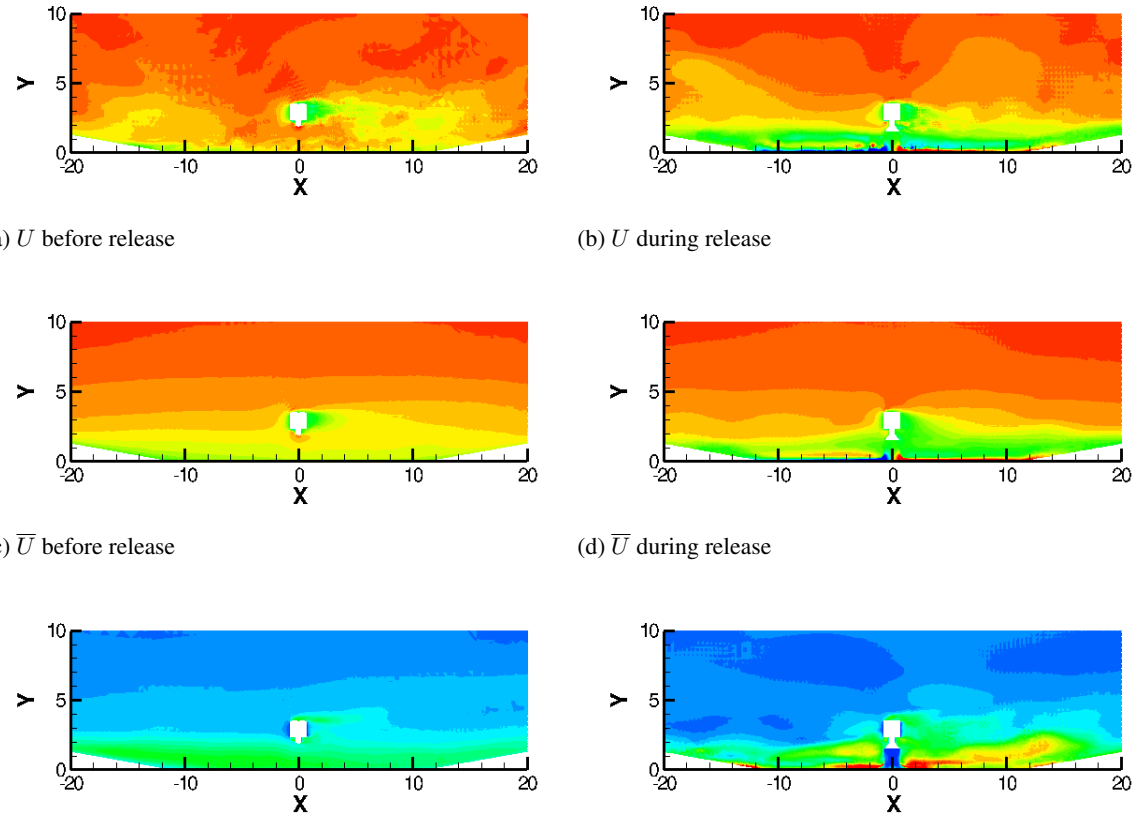


Figure 5.7 The streamwise velocity profiles measured in the experiment (and given as inlet conditions to the LES), and from the simulation 50 meters downwind the inlet plane.



(a) U before release

(b) U during release

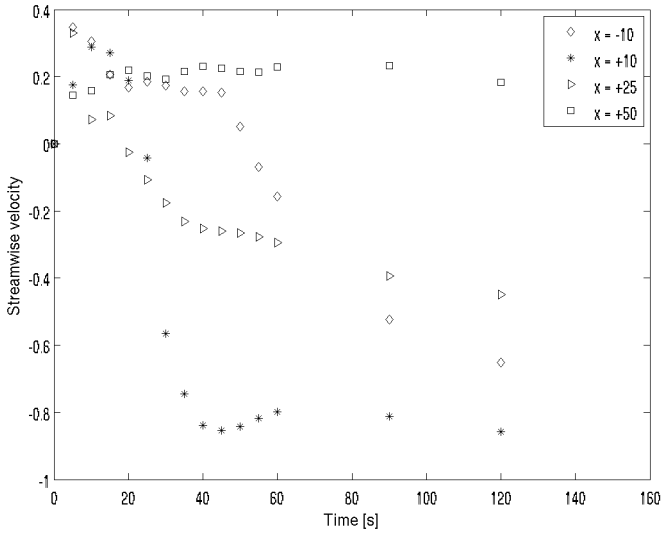
(c) $\overline{U}$ before release

(d) $\overline{U}$ during release

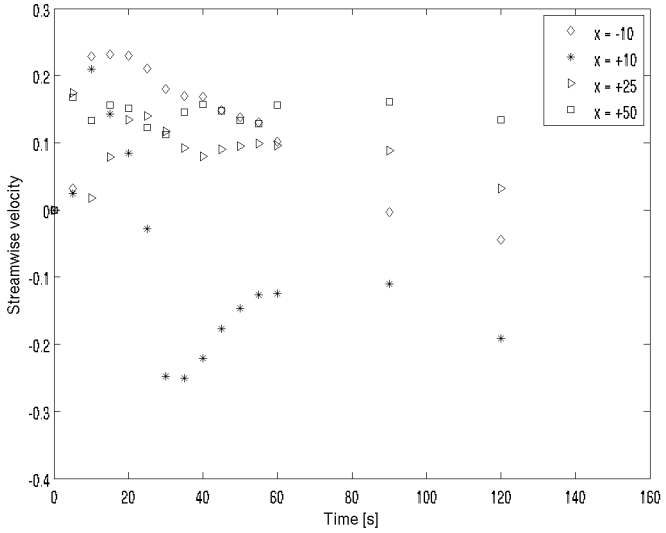
(e) U_{RMS} before release

(f) U_{RMS} during release

Figure 5.8 The instantaneous streamwise velocity (U), the mean streamwise velocity ($\overline{U}$), and the root-mean-square (U_{RMS}) before the release (a, c, e) and during the release (b, d, f). U and $\overline{U}$ are shown i the range < -2 (blue) , 2 (red) $>$ m/s, with green being low velocities, U_{RMS} are shown in the range < 0 (blue) , 1 (red) $>$ m/s.

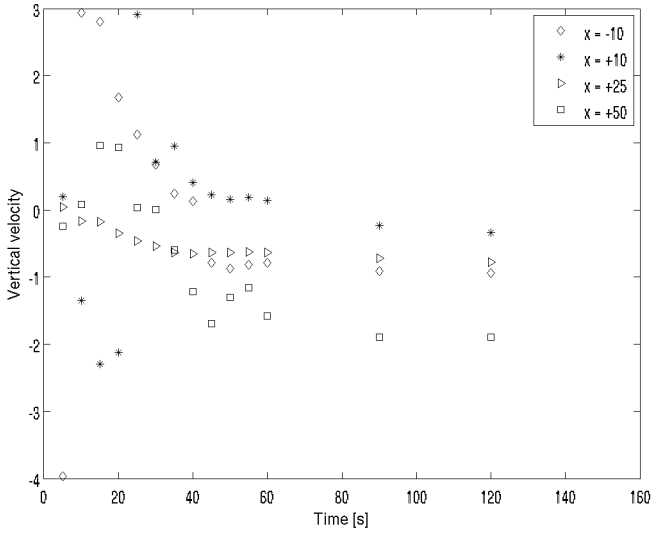


(a) Height = 1 meter

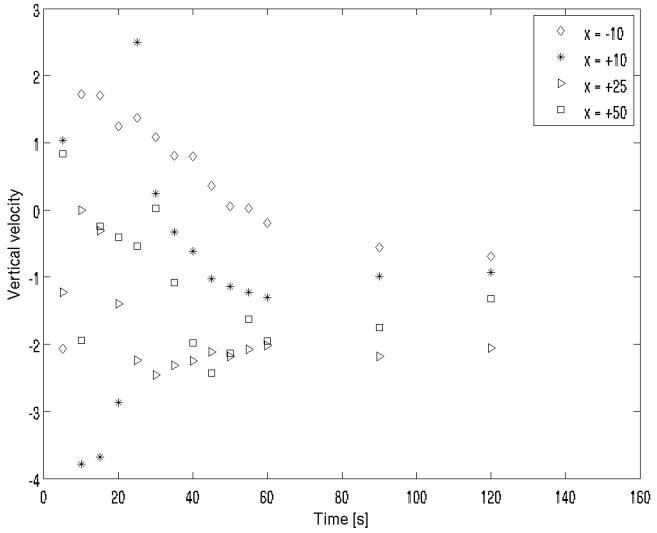


(b) Height = 2 meter

Figure 5.9 The difference of the mean streamwise velocity before and during the release as function of time. The release starts at $t = 0$ and ends at $t = 120$ s. The locations at $x = -10$ and $x = 10$ are within the depression (10 meters upwind and downwind of the tank respectively), while $x = 25$ are at the edge of the depression and $x = 50$ downwind. The velocity at $t = 0$ is the time average up to the point where the release starts, while the other times are time averages for the period since the start of the release.



(a) Height = 1 meter



(b) Height = 2 meter

Figure 5.10 *The difference of the mean vertical velocity before and during the release as function of time. The release starts at $t = 0$ and ends at $t = 120$ s. The locations at $x = -10$ and $x = 10$ are within the depression (10 meters upwind and downwind of the tank respectively), while $x = 25$ are at the edge of the depression and $x = 50$ downwind. The velocity at $t = 0$ is the time average up to the point where the release starts, while the other times are time averages for the period since the start of the release.*

the depression also shows a decrease in the velocities, while the other locations are relatively unaffected, or shows a slight increase in the velocity.

For the vertical velocity component, at first there are a lot of movement within the depression; fairly large vortices will be induced by the release jet. However, these structures diminish after some time, and the vertical velocity is subdued as compared to the situation before the release.

6 Concluding remarks

6.1 Large eddy simulations

The condition of the release jet was not measured very precisely during the experiments, so the quantity of vapour and liquid must be estimated based on analytical models. From pure thermodynamics, about 12% is expected to flash immediately due to the difference between the storage pressure and the ambient pressure. Thus most of the material is expected to be released as liquid. Some of this liquid will be dispersed as airborne droplets (which evaporates over time), some will evaporate immediately and some liquid will form a pool on the ground and subsequently evaporate, creating a secondary vapour source.

In the current CFD modelling approach it is not possible to take into account such a large quantity of liquid compared to vapour. Instead only 10% was released as liquid droplets and the rest released as vapour. There is therefore a discrepancy between the actual release jet and the simulated jet, and this will likely result in some differences in the velocity fields and the corresponding gas dispersion.

Another deficiency with the current LES methodology is the treatment of temperature. The energy equation is not solved explicitly, instead a scalar transport equation for temperature is solved. The gas temperature calculated by this is used for the Lagrangian spray model for calculating the evaporation and the temperature of the droplets, but there is no coupling back to the gas temperature transport equation. This will lead to an overestimation of the gas temperature, and thereby an underestimation of the density.

Even so, within the depression, where the dynamics are to a large extent driven by the momentum of the release jet, there is a fairly good agreement between the experiment and the simulation, indicating that the dynamics are quite well captured.

Outside of the depression there seems to be an underestimation of the mixing of the gas in the simulation when compared to the experiment. One reason for this is probably that the resolution of the computational mesh is too coarse to resolve the atmospheric boundary layer in this region.

6.2 Operational models

An approach described by Hanna *et al.* in which evaporation from a pool with the dimensions of the depression, where the evaporation rate is specified according to a model of dense gas

removal from a valley by cross-wind, has been tested both with SLAB and ARGOS. For both models good agreement with the experimental results can be found, however it is quite dependent on the evaporation rate and it is not obvious how to specify this rate *a priori*. In fact, the rate corresponding to the vapour removal time frame most consistent with the experimental observation (15 minutes) yields the least agreement with the experimental measurements of downwind concentration of vapour.

The dense gas atmospheric dispersion model SLAB predicts a higher initial chlorine concentration using the instantaneous or short duration pool option, compared to evaporation from a pool only. It is believed that the pool only option better represent the release from the depression used in the Jack Rabbit exercise because the gas is trapped inside the depression for a longer time compared to a release in a flat area.

Heavy gas calculations using ARGOS was carried out as a release from a pool only in the same way as described for SLAB. The predicted chlorine concentration outside the depression is lower (about $\frac{1}{4}$) than calculated by SLAB for the same pool duration times. This could partly be explained by the somewhat wider plume predicted by ARGOS compared to SLAB, especially at longer distances from the source.

6.3 Further work

The Jack Rabbit field trials was designed to use a relatively small scale release (two tons) to simulate a much larger release (twenty tons). However, it is observed that the source behaviour is non-linear with increasing release volumes [12]. Therefore the test program continues as Jack Rabbit II, in which experiments with the release of 5-20 tons of chlorine will be conducted. For the field trials in 2015 a mock urban test environment was constructed for the trials, while the experiments in 2016 will be in open terrain. This time there will be measurements of chlorine vapour concentrations up to 11 km downwind the release site, as well as within the mock urban environment. FFI has contributed with numerical simulations in order to assist with the experimental setup and sensor placement. FFI was also present at the 2015 trials, and we will have access to all the experimental data from these field trials.

We are quite confident that the LES methodology used for the Jack Rabbit simulations can capture the dynamics of the releases at least in the near field. Data from Jack Rabbit II as well as numerical simulations will be used to investigate dense gas releases further and in more detail. Jack Rabbit II will also be more appropriate for testing the faster hazard prediction tools, as it is for dispersion over large areas that these models really have their use.

References

[1] Donald P. Storwold JR. Detailed test plan for the jack rabbit test program. Technical report, West Desert Test Center, U.S. Army Dugway Proving Ground, March 2010. ATEC Project No. 2012-DT-DPG-SNIMT-E5835, WDTC Document No. WDTC-TP-10-011.

[2] Thomas Vik. Jack rabbit field trials - systematisering av eksperimentelle resultater. FFI-rapport 2013/02771, Forsvarets forskningsinstitutt, 2013. In norwegian.

[3] Steven Hanna, Rex Britter, Edward Argenta, and Joseph Chang. The jack rabbit chlorine release experiments: Implications of dense gas removal from a depression and downwind concentrations. *Journal of hazardous materials*, 213:406–412, 2012.

[4] Gary A Briggs, Roger S Thompson, and William H Snyder. Dense gas removal from a valley by crosswinds. *Journal of Hazardous Materials*, 24(1):1–38, 1990.

[5] Timothy J Bauer. Comparison of chlorine and ammonia concentration field trial data with calculated results from a gaussian atmospheric transport and dispersion model. *Journal of hazardous materials*, 254:325–335, 2013.

[6] John D Hearn, Richard Weber, Robert Nichols, Michael V Henley, and Shannon Fox. Deposition of cl 2 on soils during outdoor releases. *Journal of hazardous materials*, 252:107–114, 2013.

[7] http://www.cascadetechnologies.com/.

[8] RS Miller, K Harstad, and J Bellan. Evaluation of equilibrium and non-equilibrium evaporation models for many-droplet gas-liquid flow simulations. *International Journal of Multiphase Flow*, 24(6):1025–1055, 1998.

[9] Danish Emergency Management Agency, Risø DTU National Laboratory, Danish Meteorological Institute, and Prolog Development Center AS. Whitepaper, ARGOS CBRN Information System for Emergency Management, March 2011.

[10] Morten Nielsen. Dense gas dispersion in the atmosphere. Technical report, Risø National Laboratory, Roskilde, Denmark, September 1998. Risø-R-1030 (EN).

[11] Donald R Ermak. User's manul for SLAB: an atmospheric dispersion model for denser-than-air releases, June 1990. UCRL-MA-105607.

[12] Shannon Fox. The Jack Rabbit II Program. Presentation at the Jack Rabbit II Stakeholder Kickoff Meeting, American Chemistry Council HQ, Washington D.C., March 27, 2015.