FFI-rapport 2015/01986

Preliminary numerical simulation of the dispersion of chlorine vapour in a mock urban environment for the Jack Rabbit II field trials

Thomas Vik, Emma Wingstedt and Bjørn Anders Pettersson Reif

FFI Forsvarets forskningsinstitutt

FFI-rapport 2015/01986

Preliminary numerical simulation of the dispersion of chlorine vapour in a mock urban environment for the Jack Rabbit II field trials

Thomas Vik, Emma Wingstedt and Bjørn Anders Pettersson Reif

Norwegian Defence Research Establishment (FFI)

2 February 2016

FFI-rapport 2015/01986

1392

P: ISBN 978-82-464-2660-0
E: ISBN 978-82-464-2661-7

Keywords

Klor

Utslipp

Spredning

Approved by

Hanne Breivik	Research Manager
Janet Martha Blatny	Director

English summary

The release and dispersion of toxic industrial chemicals as a result of accidents, terrorism, or sabotage represent a possible hazard for life and health. Such chemicals are often transported and stored as condensed liquids in pressurised tanks. Accurate modelling capabilities for the release and dispersion of hazardous chemicals are important for emergency preparedness planning, training and exercises. There is, however, a significant knowledge gap and a lack of reliable models. This knowledge gap is partially assumed to be related to a poor understanding of the source modelling, especially for massive releases.

In order to address this issue, a series of experiments, Jack Rabbit II, is conducted at Dugway Proving Ground, Utah, USA. The first leg of this series was conducted from August 24 to September 3 2015, in which five releases of five to nine tons of chlorine were conducted. The experimental series is planned to continue in 2016.

FFI participated with advanced computational simulations of the release and dispersion of chlorine prior to the experiment in order to assist with the planning of the experimental setup, more specifically to determine the placement of the detectors. This report describes the simulation and gives some preliminary comparisons with the experimental observations. Good qualitative agreement is found between the simulation and the experiments. Initially the vapour is transported symmetrically about the source, and transport of vapour far upwind is seen both in the simulation and the experiments.

By contributing to the modelling work group FFI gets access to all the experimental data from these unique experiments, and will utilise this to gain insight about massive releases of pressurized toxic industrial chemicals, and to improve the modelling capabilities for these events. By validating the simulation methodology against experimental results, the same methodology can be used with confidence for other scenarios for which no experimental results exist. These can in turn be used to test and validate faster, operational hazard prediction tools, and furthermore to describe the source terms for these tools. Therefore this work improves the capability of predicting the dispersion and the resulting consequences after a release of hazardous chemicals, for the Defence as well as for the civil society.

Sammendrag

Utslipp og spredning av giftige industrikjemikalier som følge av uhell, terror eller sabotasje representerer en fare for liv og helse. Slike kjemikalier transporteres og oppbevares ofte som væsker i trykksatte tanker. En pålitelig modelleringskapabilitet for beregning av utslipp og spredning av kjemiske trusselstoffer er viktig med tanke på beredskapsplanlegging, trening og øvelser. Det er imidlertid et betydelig kunnskapsgap og mangel på pålitelige modeller. Det er antatt at forskjellene blant annet skyldes mangelfull kildemodellering, spesielt for store utslipp.

Feltforsøkprogrammet Jack Rabbit II er under utføring ved Dugway Proving Ground, Utah, og skal studere store utslipp av klor. Første del av Jack Rabbit II fant sted i perioden 24. august – 3. september 2015, der totalt fem utslipp med fem til ni tonn klor ble gjennomført. Forsøksserien er planlagt å fortsette sensommeren 2016.

FFI deltok i planleggingsfasen av feltforsøkene med avanserte numeriske beregninger, spesielt med tanke på plassering av sensorer. Denne rapporten beskriver disse beregningene og gir også noen foreløpige sammenligninger med observasjoner av utslippene. Det er god kvalitativ overensstemmelse mellom eksperimentene og simuleringen. Gassen blir spredt symmetrisk rundt utslippspunktet og transportert langt oppvind både i eksperimentene og simuleringen.

Ved å delta i modelleringsgruppen for Jack Rabbit II, får FFI tilgang til alle dataene fra disse unike eksperimentene, og kan bruke disse til å øke kunnskapen om store utslipp over kort tid av trykk-kondenserte giftige industrikjemikalier, og til å forbedre modelleringskapasitetene for slike hendelser. Ved å validere simuleringsmetodologien med eksperimentelle data, kan vi bruke metodologien til å simulere andre scenarioer der det ikke finnes eksperimentelle data. Dette kan videre brukes for å teste og validere raskere, operasjonelle faresprediksjonsverktøy, samt for å gi gode kildebeskrivelser for disse. Arbeidet er derfor med på å styrke kapabiliteten til å forutsi forløp og konsekvenser fra hendelser med utslipp av kjemiske trusselstoffer, både for Forsvaret og for samfunnet for øvrig.

Contents

1 Introduction

Jack Rabbit is a field trials program that aims to study large scale releases of industrial gases. The first leg of this program was conducted at Dugway Proving Ground, Utah, USA during the spring of 2010. In that experimental series, one and two tons[1] of chlorine and ammonia were released in a total of ten trials. For a description of the experimental setup and measurements see [1] and [2]. FFI participated with Computational Fluid Dynamics (CFD) calculations in order to assist with the experimental setup [3], and conducted more elaborate simulations for comparisons with the experimental data, as well as simulations with a faster hazard prediction tools and a dense gas models[4].

The Jack Rabbit program is continued under the name Jack Rabbit II. For the Jack Rabbit II test program only experiments with release of chlorine are conducted. For the first leg of the Jack Rabbit II field trials, a mock urban pad is constructed. A total of five trials with release of five to nine tons of chlorine were conducted in the period from August 24 to September 3 2015. The second leg of Jack Rabbit II is planned to be executed late summer/early autumn 2016, where releases of up to twenty tons of chlorine is planned, but this will not include the urban layout.

This report describes simulations of the dispersion of chlorine vapour through the container built-up environment. This is a preliminary study, which aims to indicate the concentration levels and the temporal evolution of the cloud that can be expected in the field trials, and is a response to a "request for information" that was distributed to the Jack Rabbit II modelling working group[2]. It was conducted to assist with determining the locations of the concentration detectors inside the urban layout.

Chapter 2 gives a brief description of the experimental and computational setup, the results from the simulation is given in chapter 3, and finally conclusions from the simulation and preliminary comparisons with the experiments are given in chapter 4.

2 Mathematical modelling

2.1 Experimental setup

For the 2015 experiments, a mock urban pad was created [5]. The urban pad was about 400 x 400 $\text{ft}^2 \approx 120$ x 120 m^2, and was built up of containers of about two meters height. A circular concrete pad with radius 12.5 meter was placed under the release tank in order to contain the released liquid. The release valve was positioned one meter above the pad pointing down.

---

[1] American tons; 1 U.S. ton $\approx$ 907 kg

[2] The Jack Rabbit II modelling working group consists of participants from, among many other, the Defence Threat Reduction Agency (DTRA), Defence Science and Technology Laboratory (Dstl) and FFI. The group contributes to the test program with various modelling efforts using a variety of models. FFI contributes with advanced computational fluid dynamics simulations.

Specifications for two different layouts were distributed prior to the experiment; these were identical with the exception of a seven meter tall obstacle upwind of the release tank in layout 2 that was not included in layout 1. Layout 1 was used for the experiment. The actual layout was not quite as regular as the specifications sent out in advance; not all containers had the prescribed dimensions, and not all container rows were precisely aligned. Updated specifications will be delivered at a later time.

2.2 Computational geometry and mesh

For the simulation, a computational geometry of layout 2 was created, figure 2.1. The concrete pad beneath the tank is disregarded in the simulation.

In total the computational domain has dimensions 250 meters (streamwise) $\times$ 200 meters (spanwise) $\times$ 100 meters (vertical). An unstructured mesh of approximately 40 million tetrahedral cells was created, the mesh sizes inside the mock urban area was 10-30 cm.

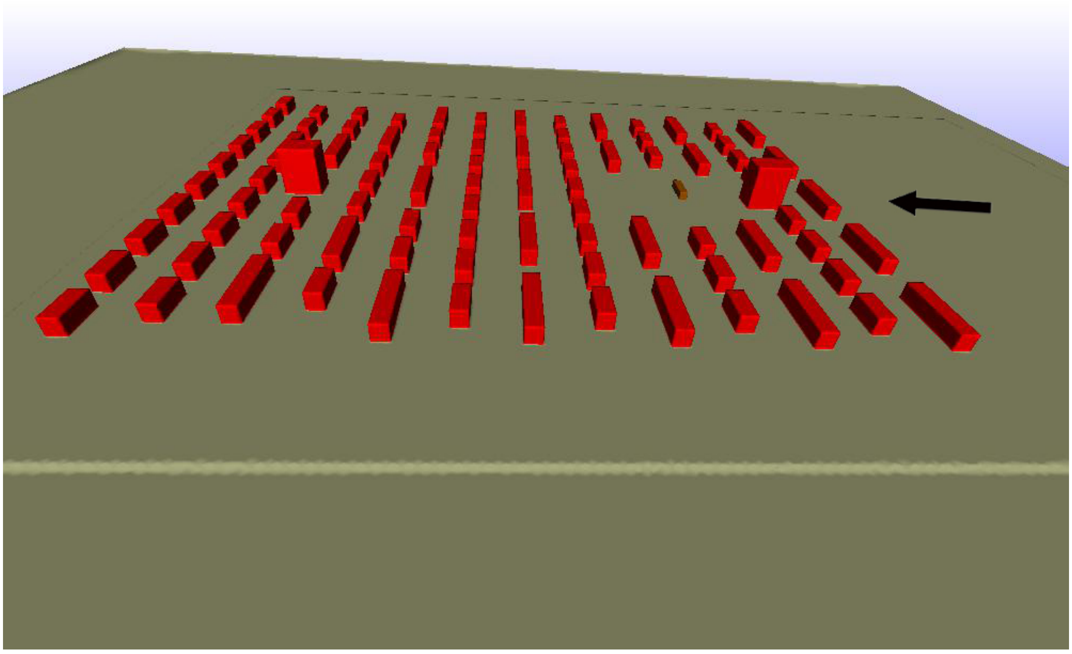
2.3 Simulation

The variable density Large Eddy Simulation (LES) code "Vida" developed by Cascade Technologies Inc. [6] is used. The liquid chlorine is disregarded; only the transport of chlorine vapour is included, and the density of the chlorine-air mixture is calculated with the ideal gas law.

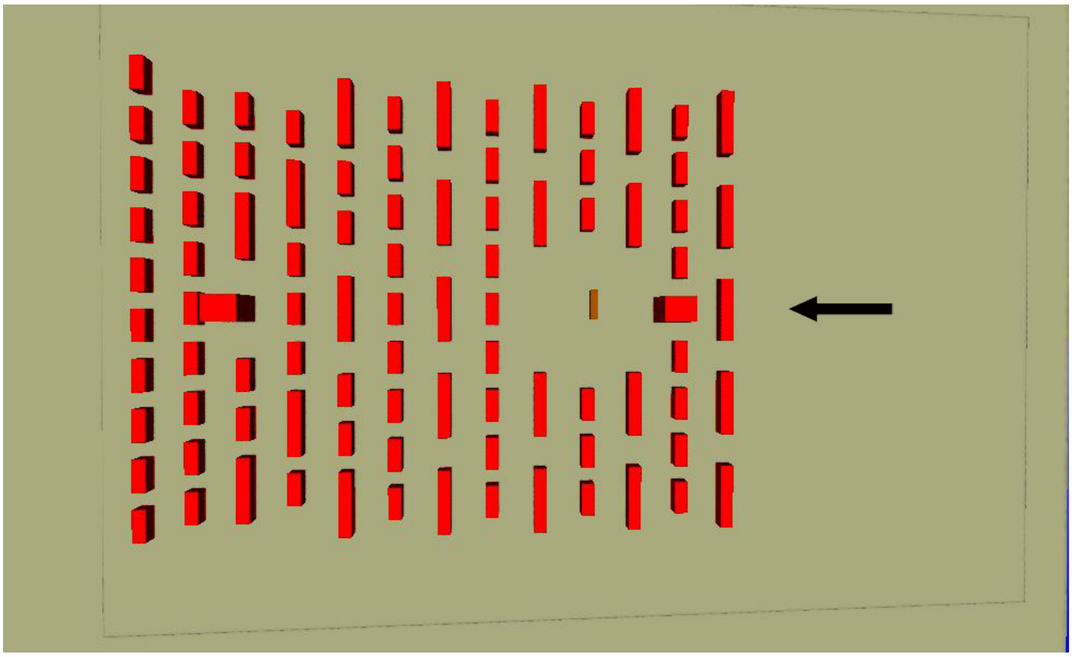
A source description for a ten ton release from a downward-pointing large hole one meter above the concrete pad was calculated with a tank blowdown model developed by Richard Babarsky[3] and distributed to the Jack Rabbit II modelling working group [5]. A two-phase jet was predicted for the first 20 seconds after opening the valve, then a single-phase vapour jet was predicted to continue for some time (with much lower release rate). For this simulation, only chlorine gas is considered, and only the first 20 seconds of release is included. The whole bottom plane of the tank with an area of 7.74 m^2 was used as inlet plane for the jet. A jet velocity of 15 m/s was chosen; this is approximately the mean jet velocity for the first 20 seconds from the specified source. This results in a release of about 8600 kg vapour in the simulation (about the same amount as the tank blowdown model predicts as two-phase flow for the same time slot).

The ambient wind field was specified according to the measurements for test 05RC in the Jack Rabbit field trials (see [4]). The three mean wind field components and the fluctuations were given at the inlet plane. Furthermore a synthetic turbulence model was used. The wind field was simulated for about one flow-through time before the chlorine vapour was released. Chlorine vapour was released for twenty seconds, and the simulation was continued for five more minutes.

[3] Richard J. Babarsky, National Ground Intelligence Center, Charlottesville, VA, USA



(a) Side view



(b) Top view

Figure 2.1 The geometry for the simulation seen from the side and top respectively. The tank is coloured brown while the containers are coloured red. The arrow points in the mean wind direction.

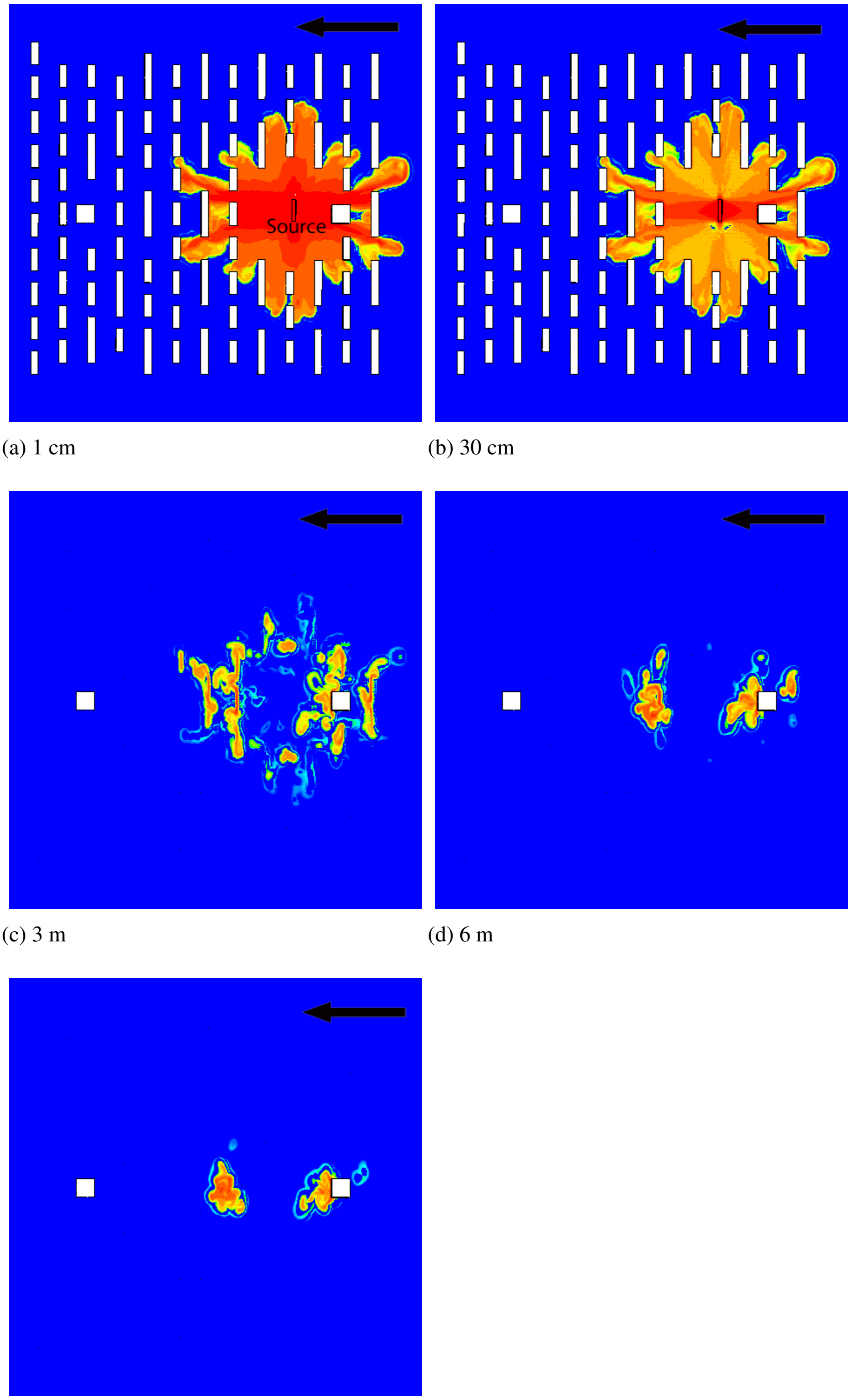
3 Results

Figure 3.1 shows the concentration in various horizontal planes through the mock urban pad five seconds after the start of the release. Figures 3.2 , 3.3, and 3.4 show the corresponding concentrations at the end of the release (20 seconds after the start), and 24 and 44 seconds after the end of the release. Figure 3.5 shows the concentration in a vertical plane in the streamwise direction at the same four instances.

Figures 3.6, 3.7, 3.8, and 3.9 show three-dimensional pictures of the vapour cloud seen from up-wind of the release at the same four instances as in figures 3.1 through 3.4, while figures 3.10, 3.11, 3.12, and 3.13 show three-dimensional pictures of the vapour cloud seen from the side. It should be noted that the vapour cloud extends further than what is shown in the pictures in the downwind direction for the last two time steps.

During the release, the vapour is transported above the 2 meter containers. The vapour is lifted quite high at the first buildings downwind and by the 7 meter obstacle in front. When the release is stopped, the vapour falls down to ground level. The vapour is also transported efficiently towards the mean ambient wind direction. The vapour cloud is fairly symmetrical, not unlike observations from the Jack Rabbit field trials in 2010.

Near the ground, high concentration levels of about 100 000 parts per million by volume (ppmv) is expected. Even at 7.6 meters above ground, such concentration levels are predicted during the release, but the concentration drops to 10 000 ppmv after the release stops at height 3 meters and above (at ground level high concentrations prevail). Immediately below the release location there is only chlorine vapour (all air is pushed away), and at the sides of the obstacle and the first row of containers downwind toward the release location, very high levels of chlorine vapour can be expected.

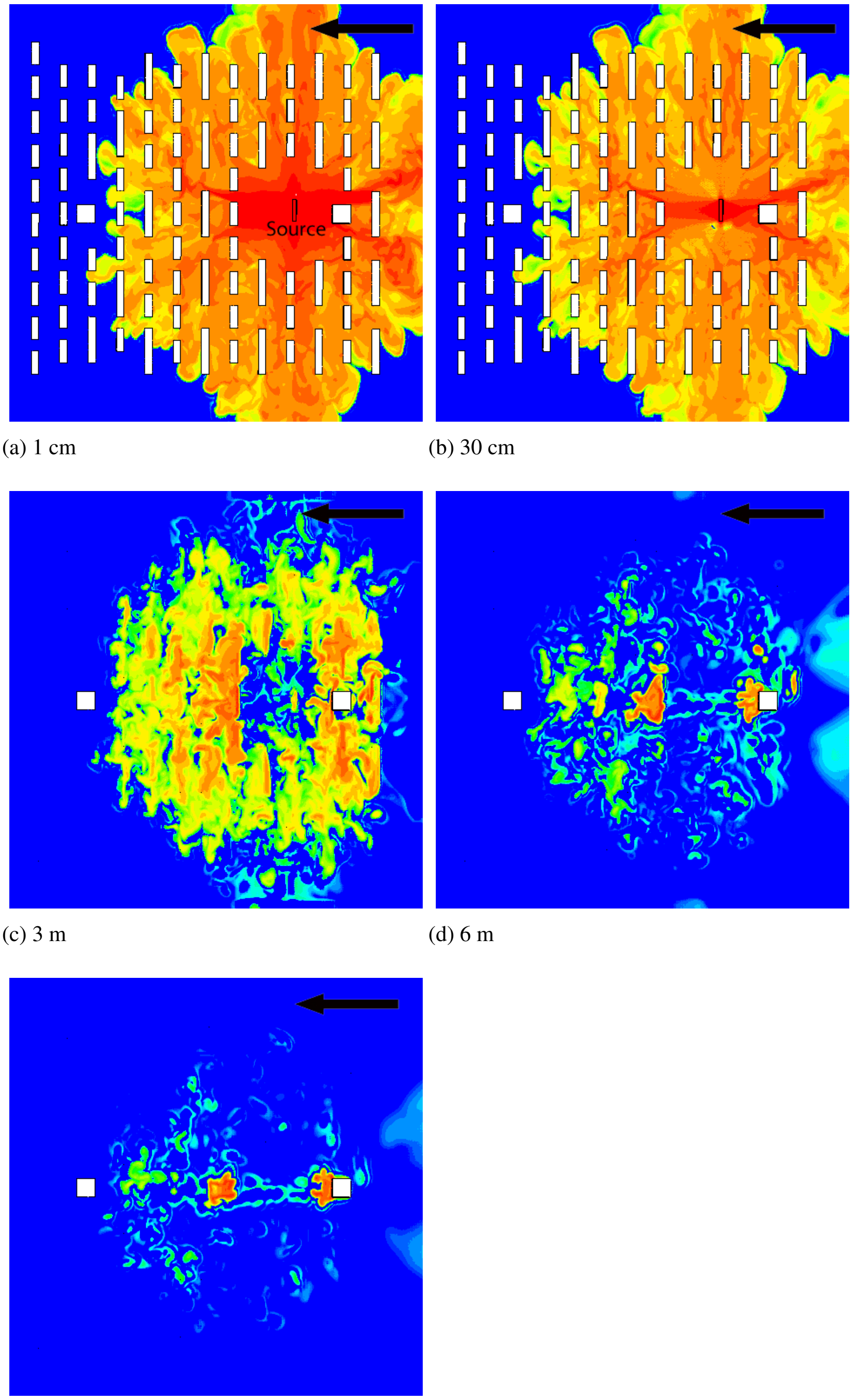


(a) 1 cm (b) 30 cm

(c) 3 m (d) 6 m

(e) 7.6 m

Figure 3.1 *The concentration of chlorine vapour at heights of 1 cm, 30 cm, 3 m, 6 m, and 7.6 m five seconds after start of the release. The arrow points in the mean wind direction. The source is indicated in figure (a). The colours denotes concentration in parts per million by volume (ppmv), dark blue denotes < 10, light blue ~ 100, green $\sim 10\,000$, yellow $\sim 100\,000$ and red $\sim 1000\,000$.*

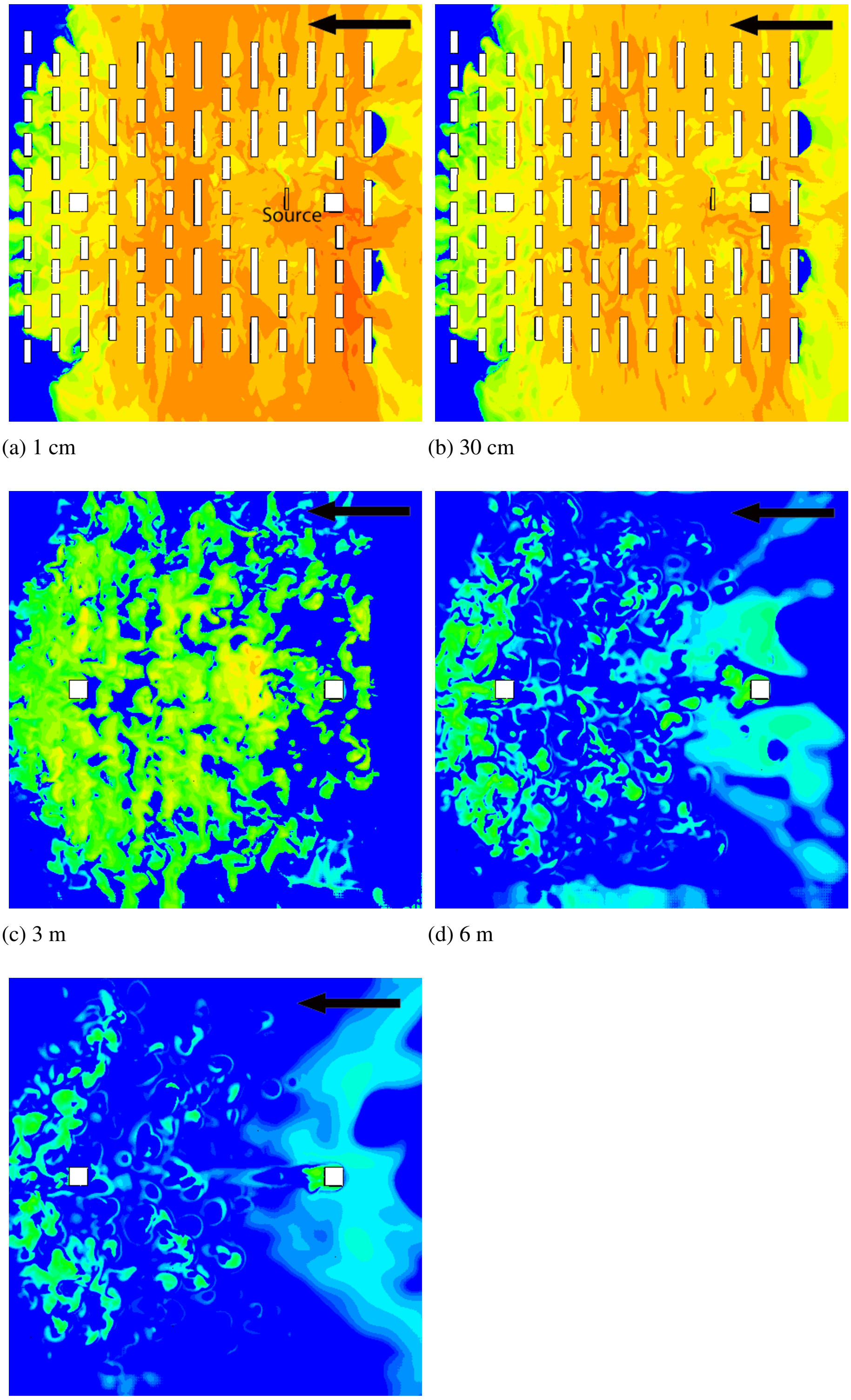


(a) 1 cm (b) 30 cm

(c) 3 m (d) 6 m

(e) 7.6 m

Figure 3.2 The concentration of chlorine vapour at heights of 1 cm, 30 cm, 3 m, 6 m, and 7.6 m 20 seconds after the start of the release. The arrow points in the mean wind direction. The source is indicated in figure (a). The colour legend is the same as for figure 3.1.



(a) 1 cm

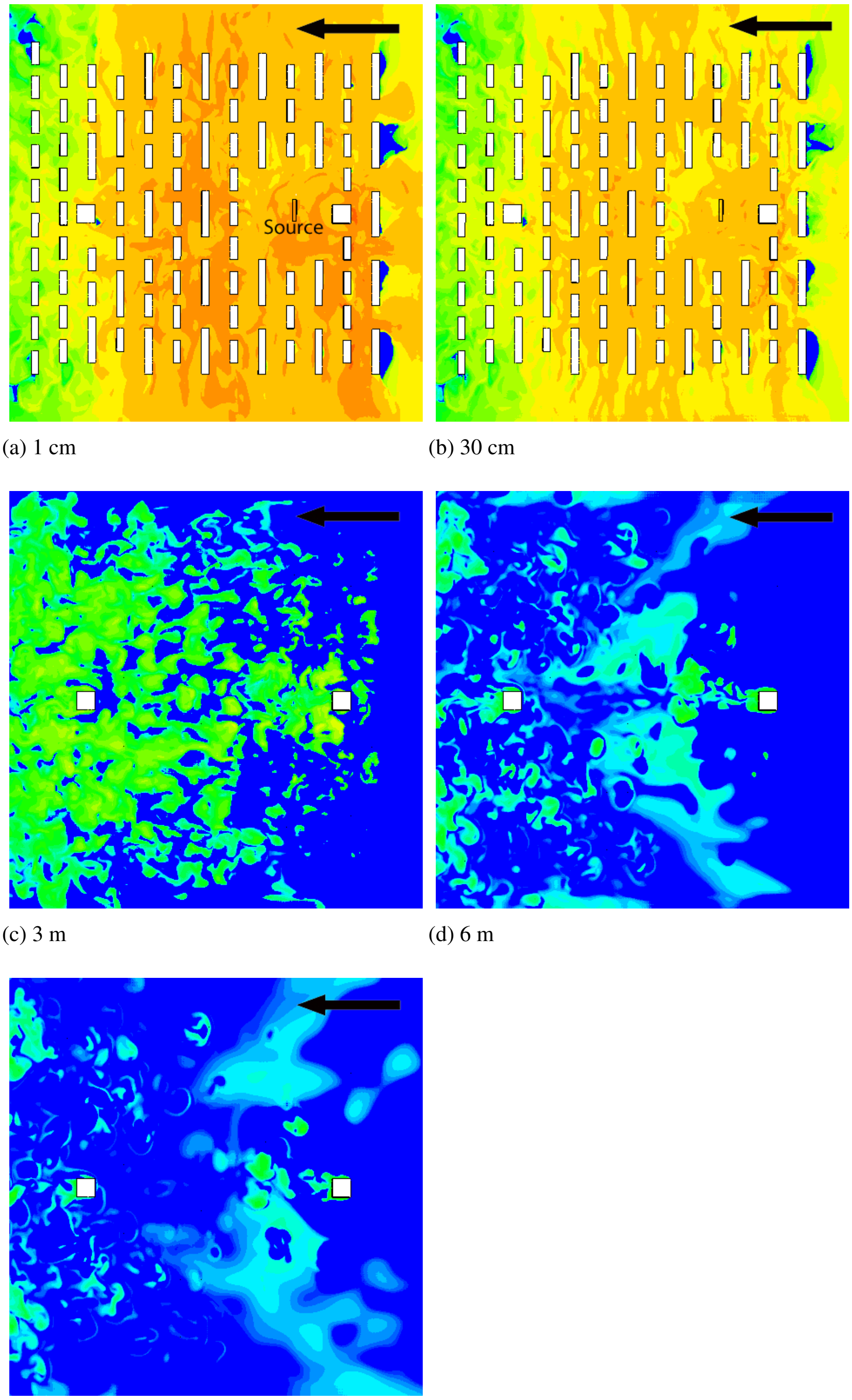
(b) 30 cm

(c) 3 m

(d) 6 m

(e) 7.6 m

Figure 3.3 The concentration of chlorine vapour at heights of 1 cm, 30 cm, 3 m, 6 m, and 7.6 m 24 seconds after the end of the release. The arrow points in the mean wind direction. The source is indicated in figure (a). The colour legend is the same as for figure 3.1.



(a) 1 cm

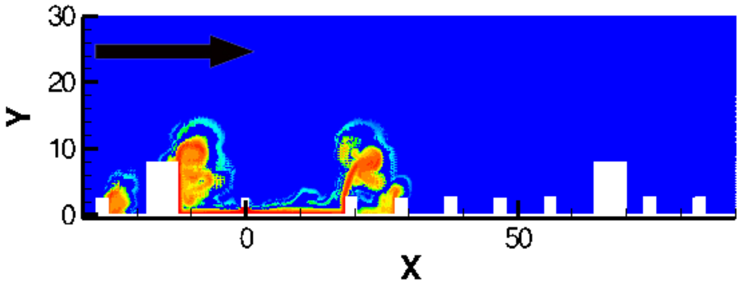
(b) 30 cm

(c) 3 m

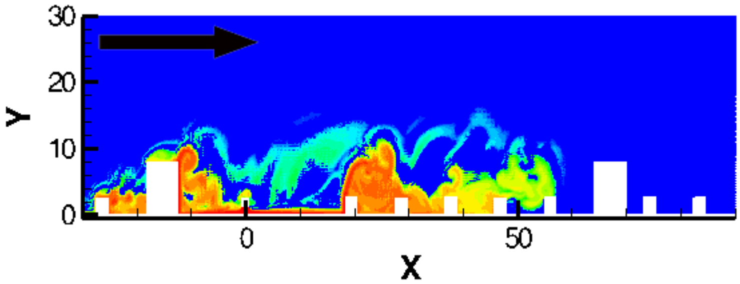
(d) 6 m

(e) 7.6 m

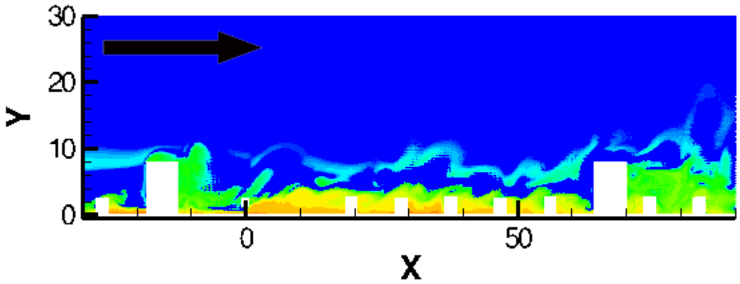
Figure 3.4 The concentration of chlorine vapour at heights of 1 cm, 30 cm, 3 m, 6 m, and 7.6 m 44 seconds after the end of the release. The arrow points in the mean wind direction. The source is indicated in figure (a). The colour legend is the same as for figure 3.1.



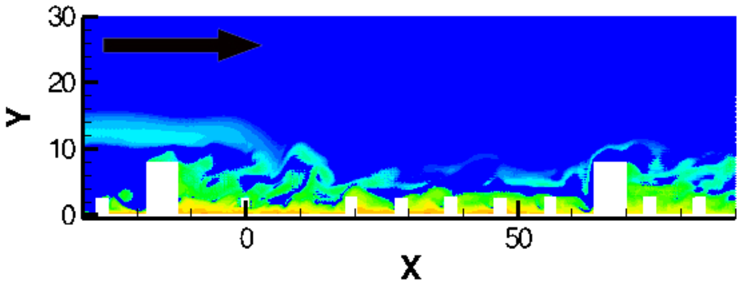
(a) 5 seconds after the start



(b) The end of the release



(c) 24 seconds after the end of the release



(d) 44 seconds after the end of the release

Figure 3.5 The concentration of chlorine vapour in a vertical plane through the source. The arrow points in the mean wind direction. The source is located at x = 0. The colour legend is the same as for figure 3.1.

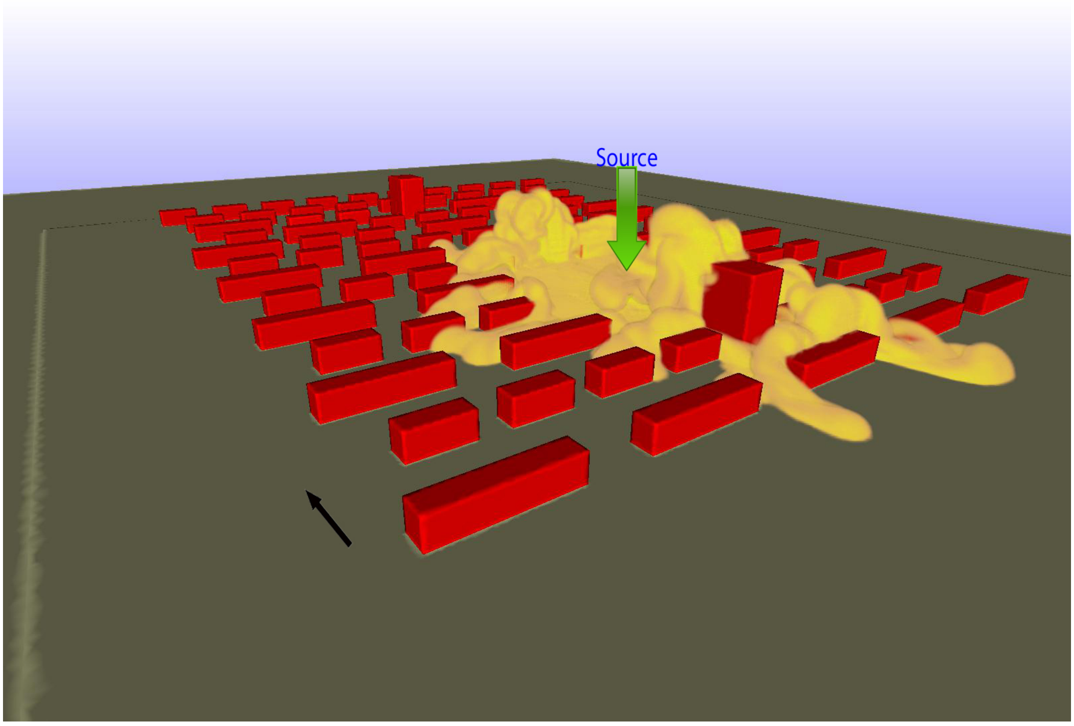


Figure 3.6 *Upwind front view of the three-dimensional cloud 5 seconds after the start of the release. The black arrow points in the mean wind direction. The green arrow indicates the source location.*

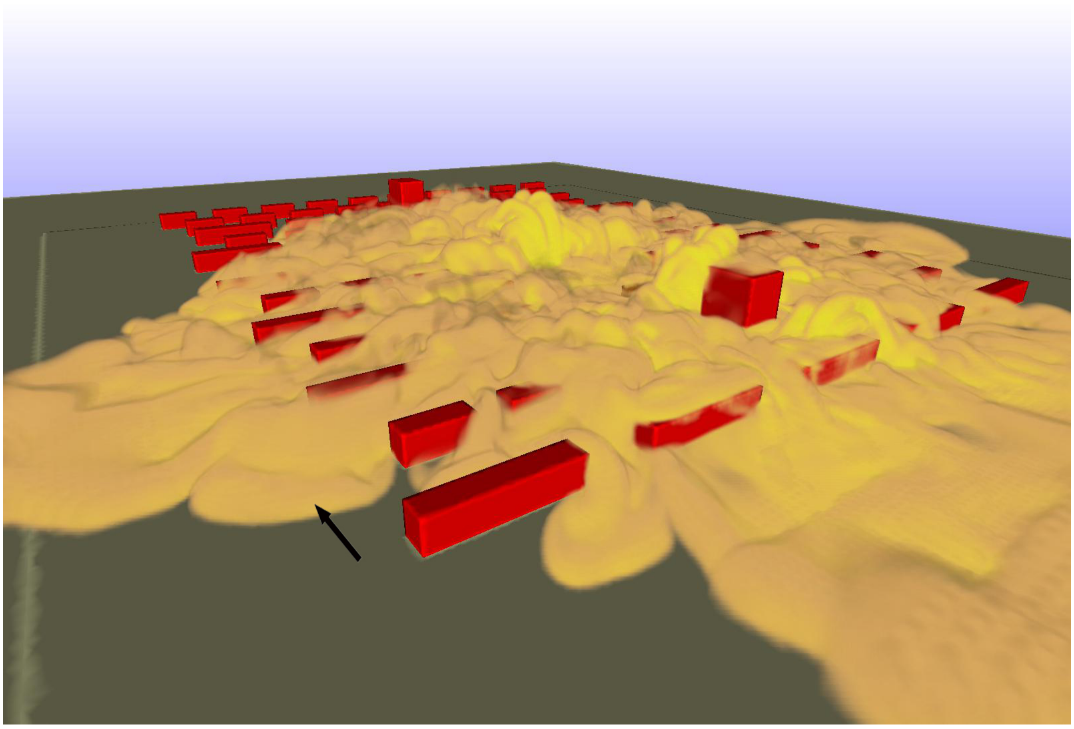


Figure 3.7 *Upwind front view of the three-dimensional cloud at the end of the release. The arrow points in the mean wind direction.*

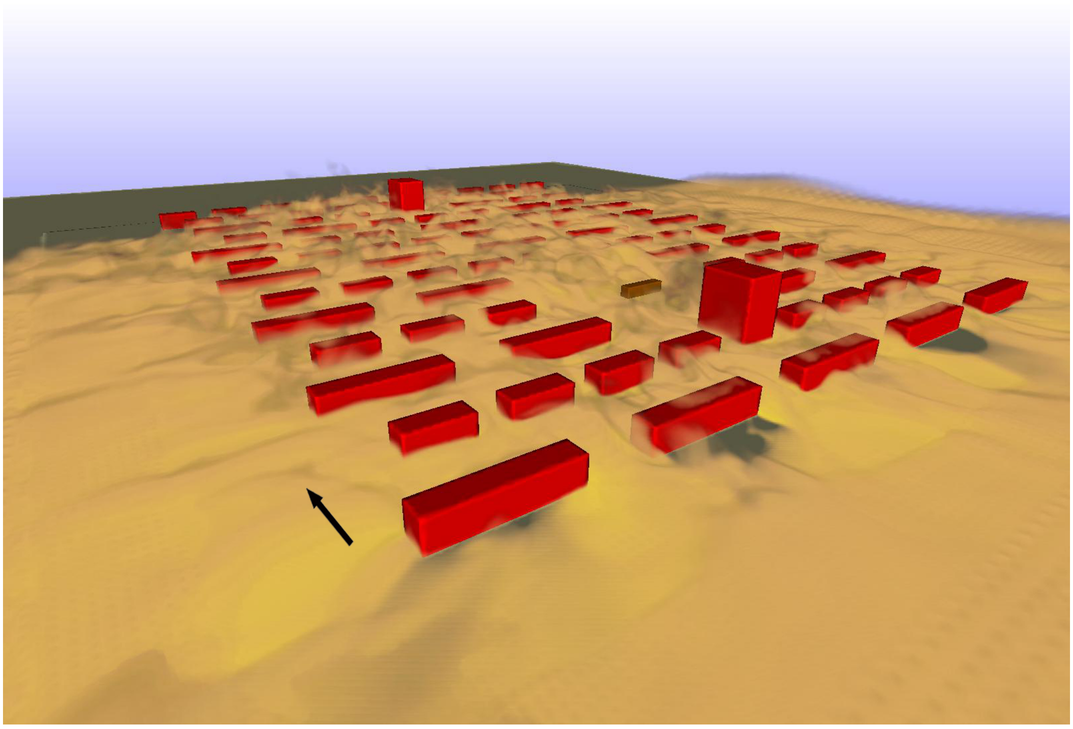


Figure 3.8 Upwind front view of the three-dimensional cloud 24 seconds after the end of the release. The arrow points in the mean wind direction.

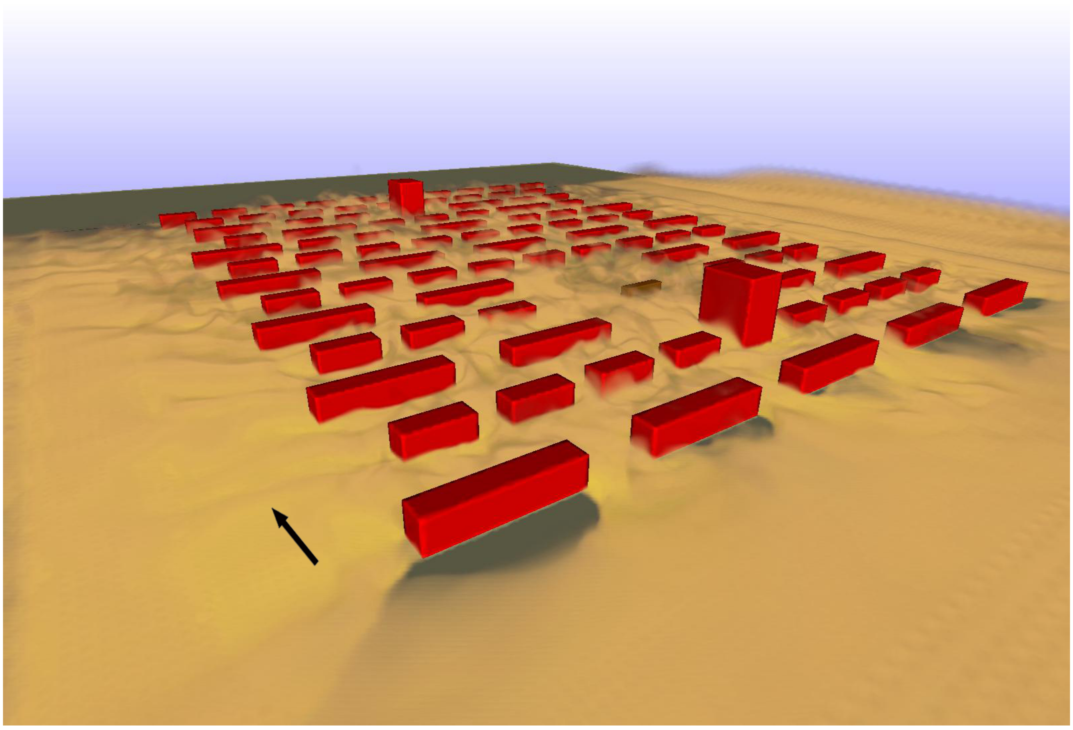


Figure 3.9 Upwind front view of the three-dimensional cloud 44 seconds after the end of the release. The arrow points in the mean wind direction.

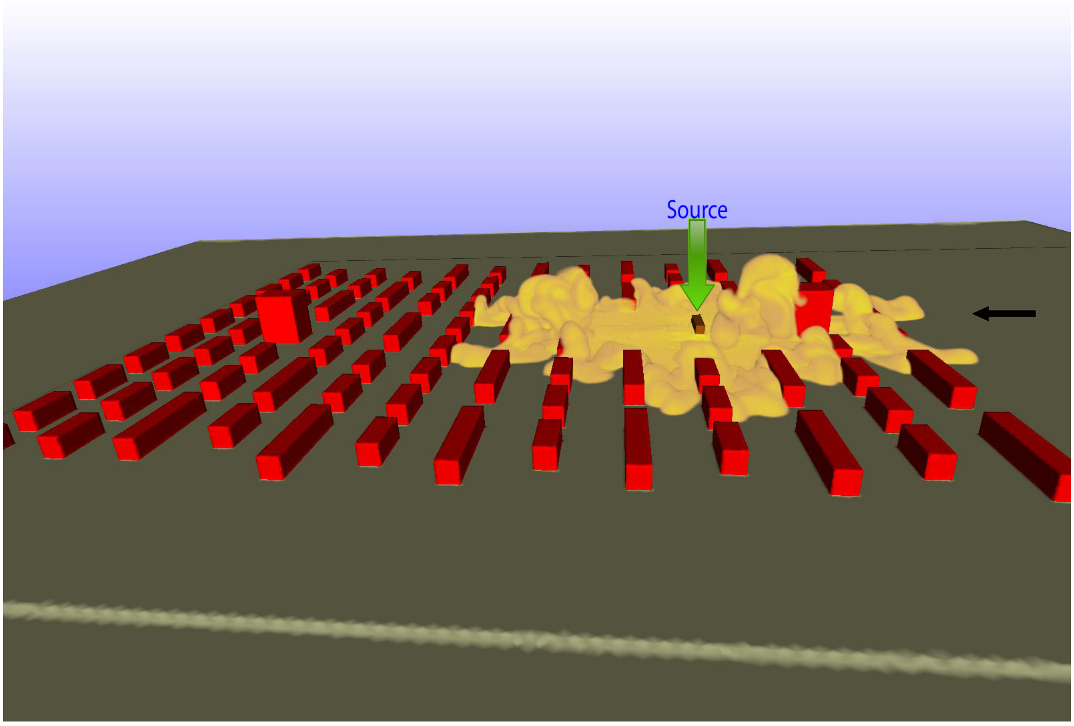


Figure 3.10 *Side view of the three-dimensional cloud five seconds after the start of the release. The black arrow points in the mean wind direction. The green arrow points to the source location.*

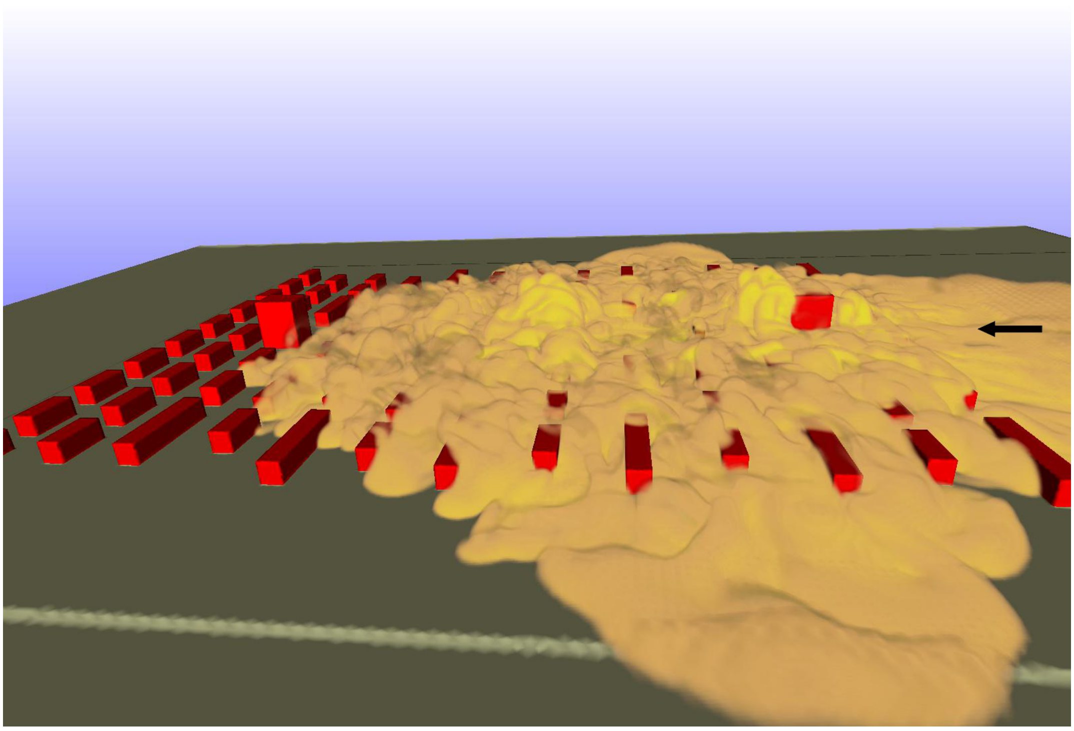


Figure 3.11 *Side view of the three-dimensional cloud at the end of the release. The arrow points in the mean wind direction.*

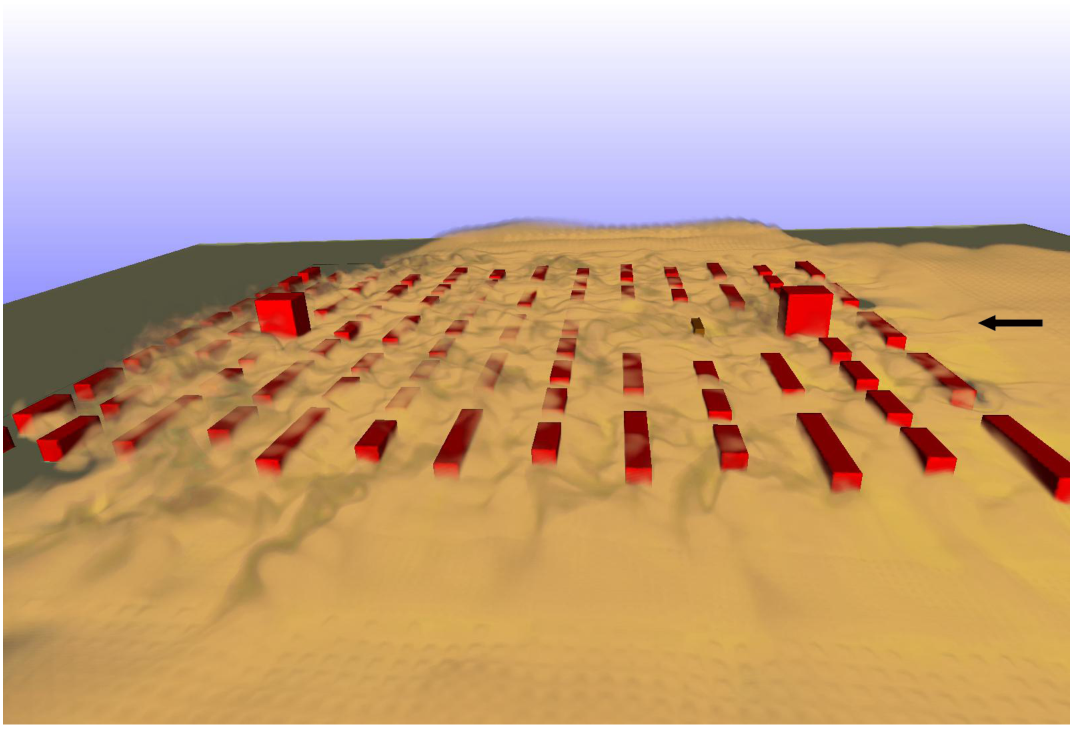


Figure 3.12 *Side view of the three-dimensional cloud 24 seconds after the end of the release. The arrow points in the mean wind direction.*

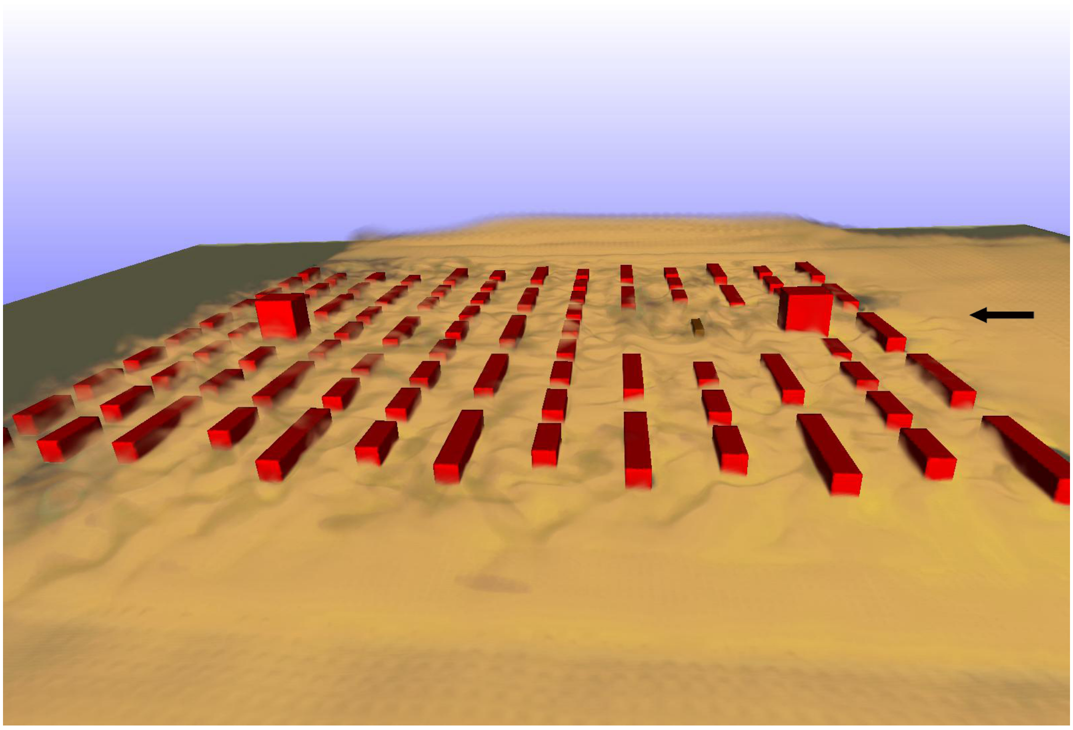


Figure 3.13 *Side view of the three-dimensional cloud 44 seconds after the end of the release. The arrow points in the mean wind direction.*

4 Preliminary conclusions

4.1 Conclusions from the simulation

There are some simplifications in this preliminary simulation:

- Only vapour is released. In reality a two-phase jet will be released, it will take some time for the liquid phase to evaporate.
- Rain-out on the ground and condensation of the vapour are not included.
- Infiltration and absorption in the ground are not included.
- The release rate corresponding to the 10 ton downward pointing release is used and the simulated release time is 20 seconds; for the experiments the maximum amount released was about 9 tons.

Even so, the simulation gives an indication on the concentration levels that can be expected in the field trials. The main findings are:

- High concentration levels, in the order of 100 000 ppmv, can be expected near the ground. In the mock urban pad, the vapour is expected to reach above the containers with concentration levels of the order of 10 000 ppmv.
- The cloud remains symmetrical about the mean wind direction.
- The cloud becomes almost perfectly circular with the source in origo during the release, but drifts downwind as time passes.
- The mixing created by the containers, in particular the highest one, lifts the plume up above eight meters and upwind transport of the cloud is induced; the cloud will be transported far upstream of the source (in the order of 100 meters).
- The cloud will cover the mock urban area entirely less than one minute after the release starts.
- The urban mock up appears to act as surface roughness rather than an urban area; it will thus be challenging to scale up the experimental results to a full scale urban environment.

4.2 Preliminary observations from the experiments

The experiments with the mock urban layout were conducted late August 2015. FFI was present at Dugway Proving Ground for two of the tests. Five tests were executed with a release mass of 5-9 tons. Even with the five ton release, the vapour was transported above the containers very quickly. However after the release was finished, the vapour sunk toward the ground and remained below the level of the container tops (two meters above ground) for quite some time. The gas cloud covered all of the built-up area for a few minutes and it took about 15 minutes for all the vapour to be transported away from the container area. Also, transport of vapour quite far upwind was observed (at least a few tens of meters). The initial observations thus correspond fairly well with the preliminary simulation. It can be concluded that the model is useful for emergency preparedness planning.

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] Thomas Vik and Bjørn Anders Pettersson Reif. Preliminary assessment of the vertical release of liquefied chlorine inside a depression. FFI-rapport 2009/01251, Forsvarets forskningsinstitutt, 2009.

[4] Thomas Vik, John Aa Tørnes, and Bjørn Anders P Reif. Simulations of the release and dispersion of chlorine and comparison with the jack rabbit field trials. FFI-rapport 2015/01474, Forsvarets forskningsinstitutt, 2015.

[5] John Boyd. Email to the Jack Rabbit modelling group dated 4/29/2015.

[6] http://www.cascadetechnologies.com/, 11/09/2015.