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Summary

CT-Analyst® is an operational dispersion prediction tool for urban environments, capable of producing very fast hazard predictions for releases of hazardous substances. A version of CT-Analyst has been developed for Oslo and is being used operationally. CT-Analyst is developed for gases with a density equal to that of air (neutral gases). Some hazardous substances, however, have densities larger than that of air (dense gases). Dense gases will have a somewhat different dispersion pattern than neutral gases. They tend to disperse closer to the ground and are to a lesser degree transported vertically, resulting in a flat plume that spreads out wide laterally, and can also be transported counter to the ambient wind direction. Far from the source, the dense gas will be diluted by infiltration of air and at some point behave like a neutral gas.

We propose a simple method for taking dense gas effects into account with CT-Analyst: to increase the spatial dimensions of the source in CT-Analyst. The idea is that the increased spatial extent of the source will, to some degree, account for the lateral and upwind transport of the dense cloud.

In order to determine the factor by which the default source size should be scaled to account for the dense gas effects, we have conducted a series of numerical simulations of instant releases of some commonly occurring dense gases, using high-fidelity large eddy simulations. We have then investigated the ratios of the size of the resulting plumes to the size of the instantaneous source, and used this to provide a rule-of-thumb: Increasing the source size of about a factor 5–6 could account for the effect the density of the gas has on the dispersion.

In addition, we have conducted full-scale urban simulations of a neutral and a dense gas, using the same large eddy simulations methodology as for the instant release simulations, as well as CT-Analyst predictions with default and extended source sizes. The results indicate that increasing the source will to some degree indeed account for the large spatial extension of the plume after the release. However, the area covered by the dense plume is larger than indicated by the instantaneous simulations. The urban simulations indicate that an increase of the source by a factor of 5–10 might be more appropriate. The reason for this discrepancy could be influence by the buildings or the terrain in the full-scale simulation. Another reason could be the fact that the full-scale simulations have a continuous source for a duration of 15 minutes, instead of an instantaneous release.

Sammendrag

CT-Analyst® er et operasjonelt verktøy for spredningsprediksjon i urbane miljøer. Det gir meget raske prediksjoner av fareområder etter utslipp av farlige stoffer, og en versjon av CT-Analyst er utviklet for Oslo og blir brukt operasjonelt. CT-Analyst er i utgangspunktet utviklet for å gi prediksjoner for spredning av nøytrale gasser, det vil si gasser med samme tetthet som luft. En del kjemikalier har imidlertid en tetthet som er høyere enn tettheten til luft (tunge gasser) og disse gassene kan ha et spredningsmønster som skiller seg fra nøytrale gasser. Tunge gasser transporteres oppover i mindre grad enn nøytrale gasser og holder seg i større grad langs bakken der den kan spres nokså uavhengig av den generelle vindretningen. En tung gass vil dermed typisk gi en gassky som er mindre utstrakt i vertikal retning og mer utstrakt i horisontal retning enn en nøytral gassky. Etter hvert som gassen transporteres vekk, vil den tynnes ut med luft og oppføre seg mer som en nøytral gass.

Vi forslår en enkel metode for å ta hensyn til tunggasseffekter i CT-Analyst: å øke den romlige utstrekningen av kilden i horisontal retning. Tanken er at den økte utstrekningen i horisontalplanet gjør rede for den økte spredningen sidelengs og oppvinds ved tunggassutslipp, spesielt i urbane områder.

Vi har gjennomført en serie numeriske simuleringer av utslipp av noen alminnelige tunge gasser, ved hjelp av såkalte LES-simuleringer ("large eddy simulations"), med formål å bestemme hvor mye den romlige utstrekningen bør økes for å ta hensyn til tunggasseffekter. Forholdet mellom størrelsen av den resulterende gasskyen og størrelsen på kilden er brukt til å gi en tommelfingerregel om at tunggasseffektene til en viss grad kan inkluderes ved å øke kildestørrelsen med en faktor 5–6.

Dernest har vi gjennomført numeriske simuleringer av utslipp og spredning av en nøytral og en tung gass i et urbant område med den samme LES-metodologien. Vi har også gjennomført CT-Analyst-beregninger med kilde med standardstørrelse og med forstørret kilde. Resultatene herfra indikerer at å øke kildestørrelsen i CT-Analyst kan bidra til å ta hensyn til tunggasseffektene i nærområdet. Arealet som dekkes av den tunge gassen i disse tilfellene er imidlertid større enn det som ble indikert med øyeblikksutslippene. Resultatene fra fullskalasimuleringene indikerer at en økning av kildestørrelsen med en faktor på omlag 5–10 kan være passende. Årsaken til forskjellen kan dels være at bygningene og terrenget i fullskalasimuleringene har en innflytelse på spredningsmønsteret. En annen årsak kan være at fullskalasimuleringene er gjort med et kontinuerlig utslipp over 15 minutter i stedet for et øyeblikksutslipp.

Contents

1 Introduction

The release and atmospheric dispersion of toxic substances, either due to accidents or intentional acts, constitute a threat to public health as well as the environment. The ability to predict the affected areas is important for crisis management, both for preparing and conducting consequence assessment and mitigation efforts, as well as in the aftermath of the crisis. Very accurate numerical simulations of the dispersion can be conducted for city planning, resource allocation and so on. Such simulations can also be employed after an incident, for example in the investigation of the chain of events, and to guide the efforts to restore the affected area. Computational Fluid Dynamics (CFD) are commonly employed for such studies. CFD simulations are, however, time-consuming, and during an emergency faster hazard prediction tools are required to calculate affected areas, identify areas which should be evacuated, plan evacuation routes, and so on. Several fast dispersion models exist, differing in both the time required to conduct the calculations and the accuracy of the dispersion predictions.

CT-Analyst® (Contaminant Transport Analyst), developed by Naval Research Laboratory, U.S, is a software tool for instantaneous and accurate prediction of urban dispersion of hazardous materials in urban environments [1, 2, 3]. A version of CT-Analyst for Oslo was developed in FFI-project 1394, [4, 5] and is currently in operational use. A version for the Haakonsvern area outside of Bergen is being developed in FFI-project 1575.

CT-Analyst calculates the dispersion of gases with assumed densities similar to that of the surrounding air, referred to as neutral gases. These are passively transported with the ambient wind field. Some chemical contaminants, however, have densities which differs from that of air. These gases are in reality not transported passively by the ambient wind, but may in fact affect the ambient wind field. The toxic industrial chemicals chlorine and sulphur dioxide are examples of gases which are denser than air. These gases have negative buoyancy and will tend to be transported closer to the ground than neutral gases. Furthermore, the density difference can cause the gas to be dispersed relatively independent of the ambient wind direction, especially in urban environments. The resulting plume from a release of a dense gas can therefore be much wider spanwise than a neutral gas, as well as extend substantially upwind [6, 7, 8].

The dense-gas effects will be most profound in the area near the source, since air entrainment will eventually dilute the gas concentration to the degree where it will behave like a neutral gas. The large horizontal extent of the negatively buoyant plume, may however affect the gas concentration also at longer distances. We propose that a very simple method for considering dense gas dispersion in CT-Analyst can be to simply increase the spatial extent of the source in CT-Analyst.

To estimate the size of the dense cloud after a dense gas release, the release and dispersion of some commonly occurring dense gases have been simulated using Large Eddy Simulations (LES). The radius of the dense gas cloud (source) before the gas is transported away by the ambient wind field have been calculated and used to give a rule-of-thumb for the source size of a dense gas release. In addition, full scale simulations of the transport of dense and neutral gases in an urban environment are conducted with LES, and compared with hazard area predictions with CT-Analyst with default and extended source size values.

The simulations for calculating the source sizes and the resulting negatively buoyant plume sizes are presented in chapter 2, while chapter 3 presents the urban dispersion simulations, including the comparisons of the full scale LES with CT-Analyst. Both chapters include descriptions of the numerical procedures. Finally, concluding remarks are given in chapter 4.

2 Source term spatial size

A series of numerical simulations of instantaneous releases from volumetric sources of the three dense gases chlorine (Cl_2), sulphur dioxide (SO_2) and carbon dioxide (CO_2) as well as neutral gas (air) have been conducted. Cl_2, SO_2 and CO_2 have a density of 2.5, 2.3 and 1.6 times that of air respectively. The aim is to estimate the size of the dense plume at the source location, before the gas is transported downwind with the ambient wind field. In order to make an estimate of the size of the dense gas plume, first an analytic estimate of the mass fraction that can be expected to give a dense gas effect is given.

2.1 Mass fraction threshold for the onset of dense gas effects

The Richardson number is a measure of the relative importance of buoyancy and shear forcing. The gradient Richardson number is defined by

$$Ri_g = \frac{N^2}{S^2}. \tag{2.1}$$

N is the Brunt-Väisälä frequency given by

$$N = \sqrt{-g\frac{1}{\rho_0}\frac{\partial \rho}{\partial z}} \tag{2.2}$$

and $S = \sqrt{2S_{ij}S_{ij}}$ is the norm of the strain tensor

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{2.3}$$

where u_i is the instantaneous velocity and x_i the spatial coordinates. It is assumed that when the gradient Richardson number exceeds an critical value, the flow field is locally stable. The critical value varies between 0.2 and 1, typically a value of 0.25 is used [9].

If we assume that the vertical gradient of the streamwise wind velocity dominates the velocity gradient:

$$\frac{\partial u_i}{\partial x_j} \approx \frac{\partial u}{\partial z}, \tag{2.4}$$

the shear stress tensor can be approximated as

$$S_{ij} \approx \frac{1}{2}\left(\frac{\partial u}{\partial z}\right) \approx \frac{1}{2}\left(\frac{U_\infty - U_0}{\delta}\right) = \frac{1}{2}\left(\frac{U_\infty}{\delta}\right) \tag{2.5}$$

and

$$S \approx \sqrt{\frac{1}{2}}\frac{U_\infty}{\delta}, \tag{2.6}$$

where U_∞ is the ambient speed at the mixing layer height δ and $U_0 = 0$ is the wind speed at the ground. The density gradient is approximated as

$$\frac{\partial \rho}{\partial z} \approx \frac{\rho_0 - \rho}{\delta} = -\frac{\rho - \rho_0}{\delta}, \tag{2.7}$$

Wind speed (m/s)	Mixing height (m)	Mass fraction threshold		
		Cl_2	SO_2	CO_2
2	2	0.04	0.04	0.06
	5	0.02	0.02	0.03
	10	0.01	0.01	0.01
4	2	0.15	0.17	0.24
	5	0.07	0.07	0.10
	10	0.03	0.04	0.05
8	2	0.49	0.52	0.75
	5	0.23	0.25	0.36
	10	0.13	0.14	0.19

Table 2.1 Mass fraction limits for dense gas effects.

where we assume that the density at the mixing layer height equals the density of air, and the density at ground is the density of the dense gas mixture. This gives the following expression for the Brunt–Väisälä frequency:

$$N \approx \sqrt{\frac{g}{\rho_0}\frac{\rho - \rho_0}{\partial}} = \sqrt{\frac{g'}{\delta}}. \tag{2.8}$$

The gradient Richardson number can then be expressed as

$$Ri_g \approx \frac{2g'\delta}{U_\infty^2}. \tag{2.9}$$

Equation 2.9 is used to estimate the mass fractions above which dense gas effects are assumed to be important. The threshold value of $Ri > 0.25$ for stable stratification is used as the criteria for the onset of dense gas effects. Table 2.1 lists the calculated mass fraction thresholds for the dense gases Cl_2, SO_s and CO_2, for mixing heights 2, 5 and 10 m, and wind speeds of 2, 4 and 8 m/s. For a mixing height of 10 meters, a mass fraction of about 0.01–0.1 should give dense-gas effects for the chlorine release, while for the less dense carbon dioxide, a mass fraction of about 0.01-0.2 should give dense gas effects.

2.2 Numerical procedure

The low-Mach number, variable density solver vida, from Cascade Technologies, is used in this study. This is an unstructured, finite-volume based LES solver with a low-dissipation numerical scheme. A second order central difference scheme for the momentum and a first order upwind scheme for the scalar field is employed.

Dense gas effects are accounted for by a reduced gravity term:

$$g' = g\frac{\rho'}{\rho_0} = g\frac{\rho - \rho_0}{\rho_0}, \tag{2.10}$$

where ρ is the local density, ρ_0 the ambient density (the density of air) and g the gravitational acceleration. The local density of the gas-air mixture is calculated by

$$\rho = \frac{1}{m_f/\rho_g + \left(1 - m_f\right)/\rho_0}, \tag{2.11}$$

Substance	ρ/ρ_{air}	Amount (kg)	Radius (r)	Wind speed (m/s)
Cl_2	2.5	500	3.24	2
Cl_2	2.5	2,000	6.45	0, 2, 4, 8
Cl_2	2.5	20,000	20.47	0, 2, 4, 8
SO_2	2.3	2,000	6.65	0, 2, 4, 8
SO_2	2.3	20,000	21.44	0, 2, 4, 8
CO_2	1.6	2,000	7.83	0, 2, 4, 8
CO_2	1.6	20,000	25.23	0, 2, 4, 8
Air	1	2,000	10	2, 4, 8
Air	1	20,000	32.2	2, 4, 8

Table 2.2 The simulation matrix for the source term simulations.

where ρ_g is the density of the gas and m_f the mass fraction of the dense gas. See for instance [6] for a more detailed description of vida.

2.2.1 Computational geometry and mesh

The computational domain for this study is a box with spatial dimensions 1,000 meter in the streamwise direction, 600 meters in the spanwise direction and 1,000 meters in the vertical direction. A number of roughness elements with heights six meters and horizontal dimensions 6–10 meters are placed between the inlet plane and the source location in order to generate a turbulent boundary layer. Except for these roughness elements, the surfaces are flat. The computational mesh has a cell size of about 1 m within 20 meters from the source and about 2 m within 80 meters.

2.2.2 Simulation setup

A set of simulations of instantaneous releases of 500, 2,000 and 20,000 kg gas are conducted from a cylinder with a height of five meters. The radius of the cylinder is calculated from the volume of the gas in each simulation, keeping the height of the cylinder constant. This is a idealistic release mechanism, but is similar to the method used for the source description in CT-Analyst. The wind velocity is varied between $U = 2, 4$ and 8 m/s. A plug flow with the given wind velocity is used as input, and a boundary layer is developed from the roughness elements. In addition, some simulations with zero wind were also conducted. The simulations were conducted for five minutes after the start of the release, except for the two-tonne air release, which was conducted for 1 minutes and 40 seconds. Table 2.2 lists the simulations.

2.3 Results

The horizontal plane is divided into 20 sectors of 18 degrees each, and each sector is further divided into radial segments of 5 meters, see figure 2.1. Within each radial segment, the mean mass fraction is calculated. For each sector, the radius of the plume to the threshold values are calculated, and an effective radius, R, is finally calculated as the average radius over the 20 sectors. Four threshold values are chosen: $m_f = 0.03, 0.1, 0.2$ and 0.5. Unless otherwise stated, the results are given for a threshold value of $m_f = 0.1$, based on the estimate for the critical Richardson number in table 2.1.

Figure 2.2 shows the temporal evolution of the radii of the plume for the two and twenty tonnes

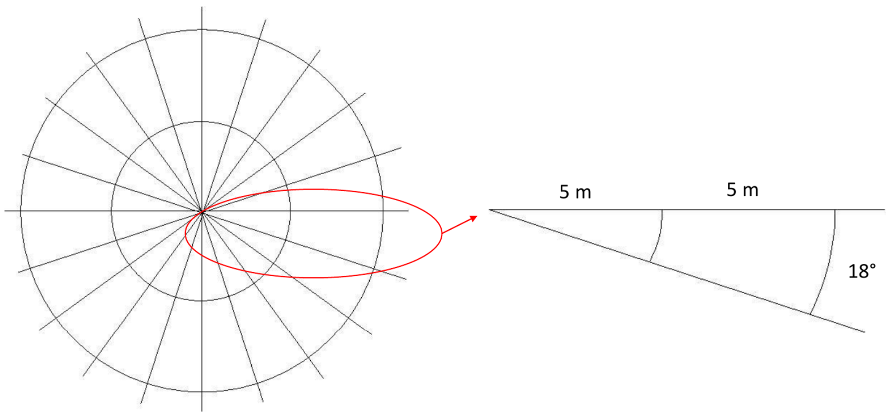


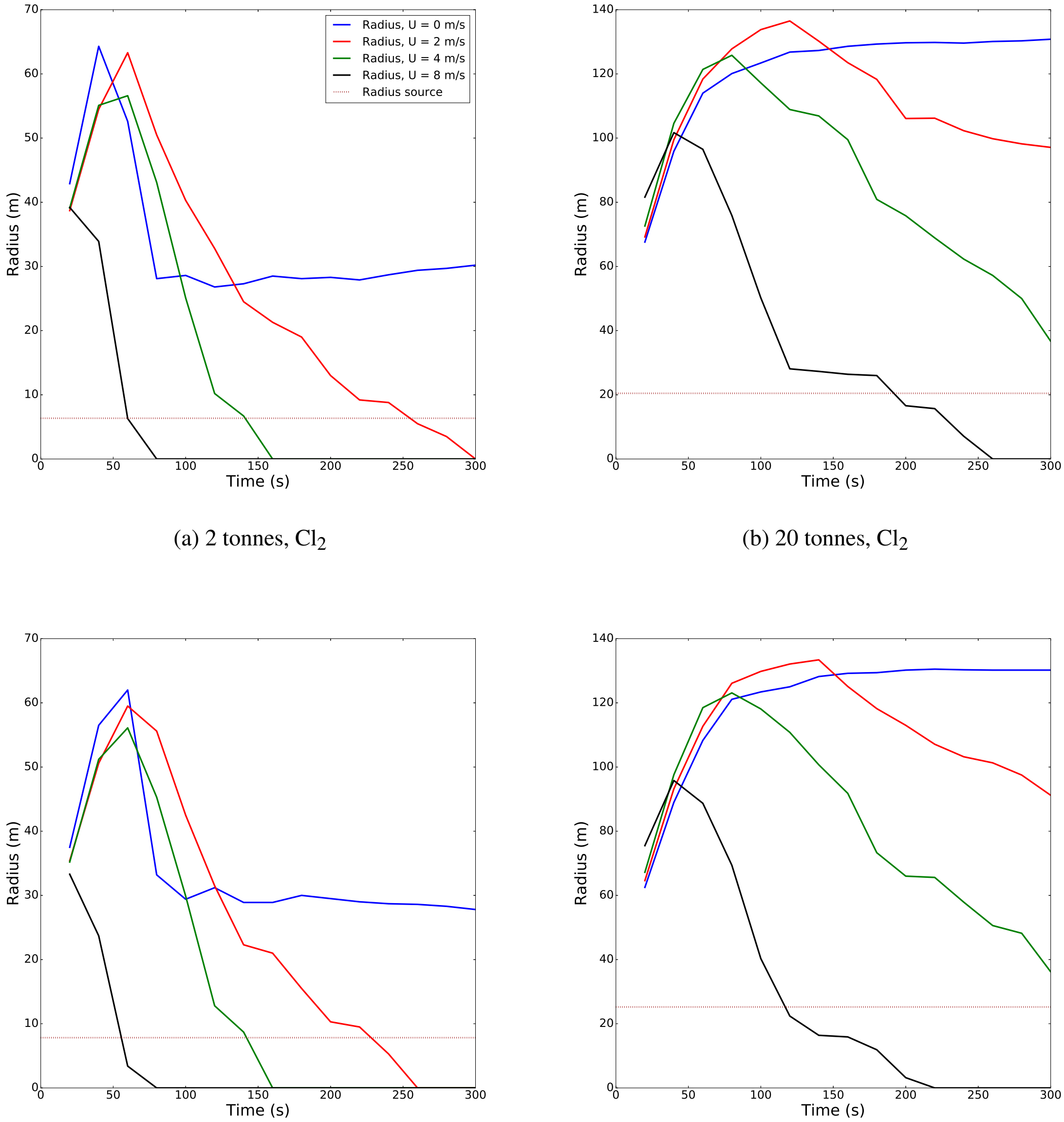
Figure 2.1 Sketch of how the horizontal plane is divided into 20 segments of 18 degrees each and each segment is divided into radial segments of five meters.

chlorine and carbon dioxide releases. There is a steep rise in the radius for the first minute or so for the two tonnes release and the first two–three minutes for the 20 tonnes releases. For the simulations with no wind, the radius stabilises when the momentum from the release subsides. For the simulations with wind, the radii decrease faster with increasing wind. Note that for the 20 tonnes releases, the effective radius is still larger than the source radius at 300 seconds.

Figure 2.3 shows the radii for mass fraction above 0.03, 0.1, 0.2 and 0.5 for the 500 kg, 2,000 kg and 20,000 kg chlorine releases at a wind speed of 2 m/s. Even for the 500 kg release, the radius of the plume to mass fraction of 0.1 is about six times the source radius. Only the 20 tonnes releases have mass fractions above 0.5, and in this case only for about a minute.

Figure 2.4 shows birds-eye views of the chlorine cloud 40 seconds after the start of the release at wind speed of 2 m/s for the 500 kg, 2 tonnes and 20 tonnes releases, as well as for the 20 tonnes release at 8 m/s wind speed. Data from height of 0 – 20 meters are averaged and projected on a horizontal plane. For a wind speed of 2 m/s, the initial dispersion pattern is very symmetric, while for a wind speed of 8 meters, the plume is more prolonged in the downwind direction.

Table 2.3 lists the average effective radii and the average normalised effective radii R/R_0, where R_0 is the radius of the source, for the dense clouds. These are average values for the time the effective radii are larger than the source radius. The averaging time is given in the table. It is interesting to note that the three dense gases have fairly similar effective radii. All the cases have a ratio of the effective radius to the source radius of 4–6, except for the 20,000 kg releases at wind speeds of 4 and 8, which have ratios of about 3. The time the dense gas lingers at the source area differs with the wind speeds, at larger wind speeds the gas is transported away faster. For the 20,000 kg dense gas releases with wind speeds of 2 and 4 m/s, the gas is still present after five minutes (the end of the simulation).



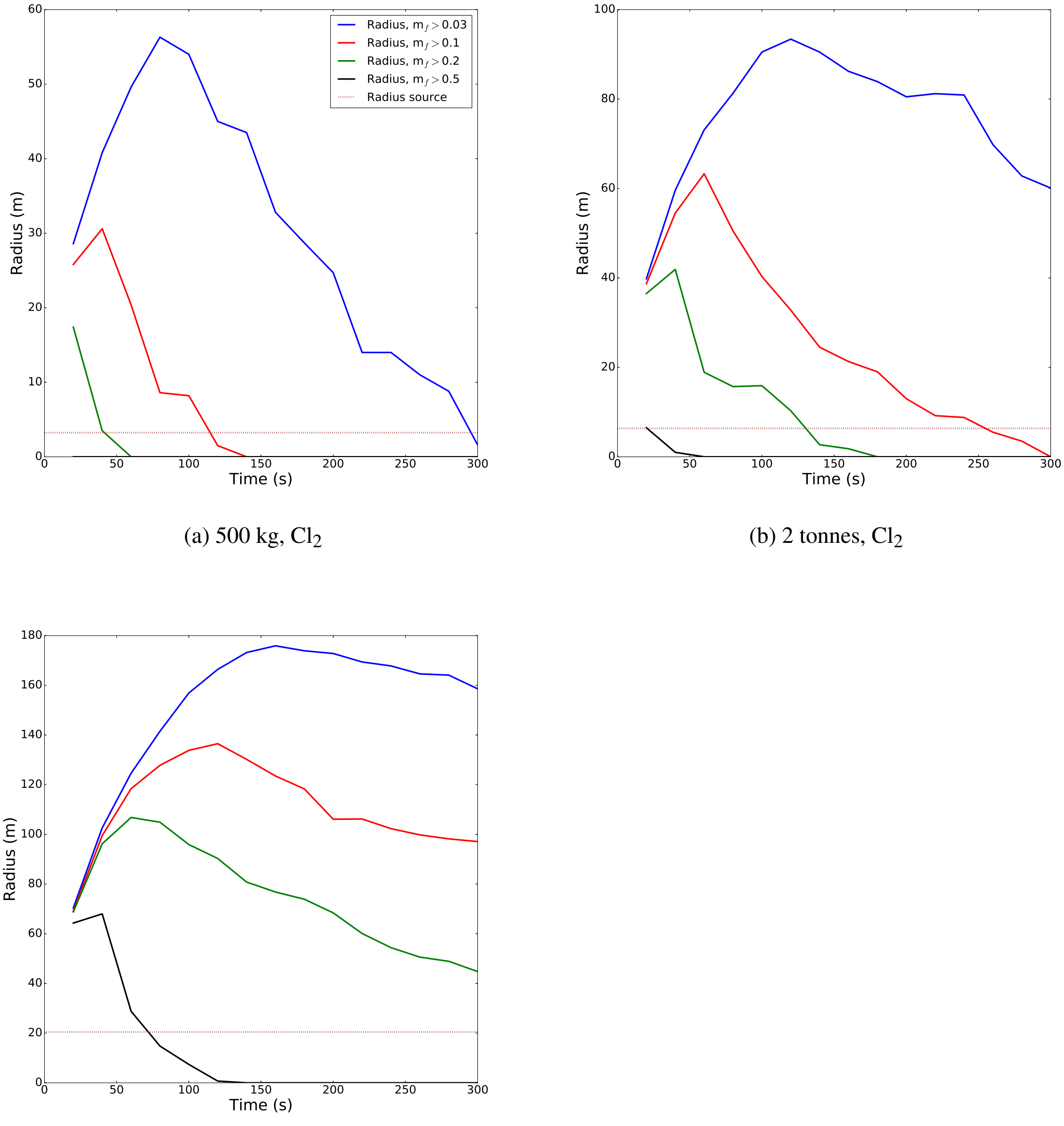
(a) 2 tonnes, Cl_2

(b) 20 tonnes, Cl_2

(c) 2 tonnes, CO_2

(d) 20 tonnes, CO_2

Figure 2.2 The radius of the cloud as function of time for the 2 and 20 tonnes chlorine and carbon dioxide releases at threshold $m_f = 0.1$. *The gas is released at time zero.*

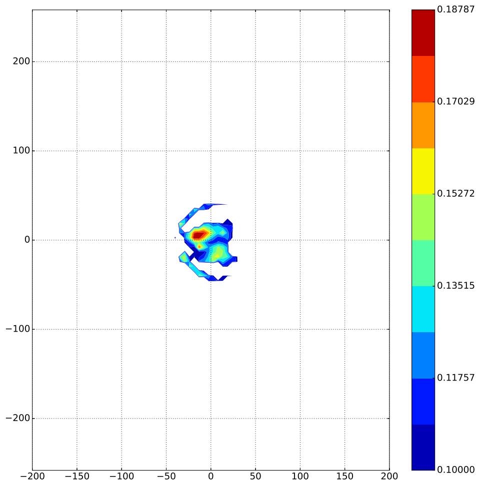


(a) 500 kg, Cl_2

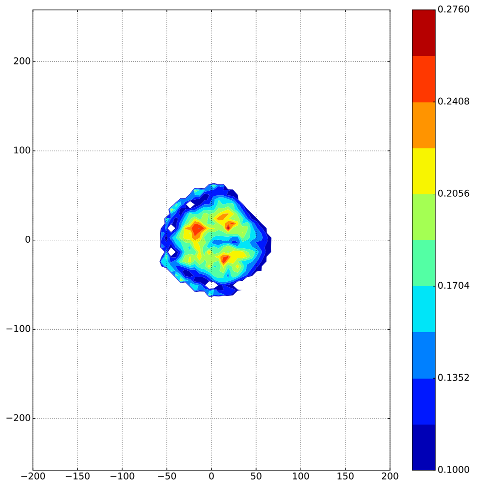
(b) 2 tonnes, Cl_2

(c) 20 tonnes, Cl_2

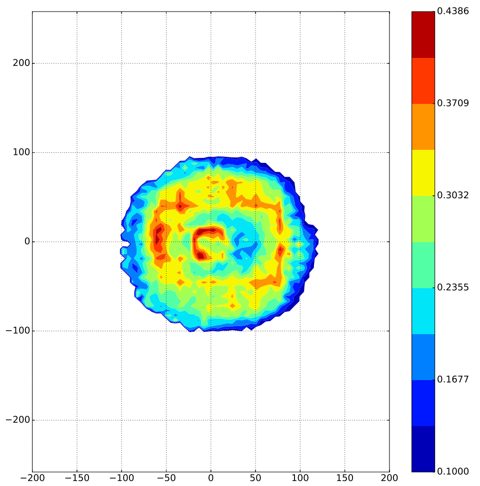
Figure 2.3 The radius of the cloud above $m_f = 0.03, 0.1, 0.2$ *and* 0.5 *as function of time for the 500 kg, 2 and 20 tonnes chlorine releases at a wind speed of 2 m/s. The release is at time zero.*



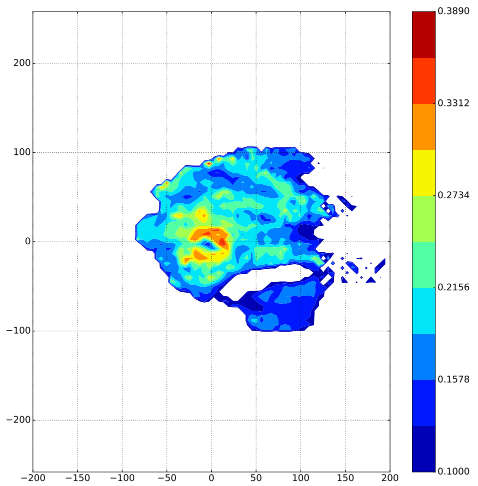
(a) 500 kg, U = 2 m/s



(b) 2 tonnes, U = 2 m/s



(c) 20 tonnes, U = 2 m/s



(d) 20 tonnes, U = 8 m/s

Figure 2.4 Birdseye view of the chlorine clouds for $m_f > 0.1$ *40 seconds after the release. The release location is in origo (0,0). Note that the maximum concentration and the colour levels are different for the four plots.*

500 kg release

Substance	Wind speed (m/s)	Effective radius (m)	R/R_0	Time (s)
Cl_2	2	19	6	100

2,000 kg release

Substance	Wind speed (m/s)	Effective radius (m)	R/R_0	Time (s)
Cl_2	0	33	5	>300
	2	31	5	240
	4	34	5	140
	8	37	6	40
SO_2	0	33	5	> 300
	2	32	5	220
	4	38	6	120
	8	35	5	40
CO_2	0	34	4	> 300
	2	32	4	220
	4	34	4	140
	8	29	4	40
Air	2	14	1	60
	4	11	1	40
	8	16	2	20

20,000 kg release

Substance	Wind speed (m/s)	Effective radius (m)	R/R_0	Time (s)
Cl_2	0	121	6	> 300
	2	111	5	> 300
	4	86	4	> 300
	8	57	3	180
SO_2	0	123	6	> 300
	2	111	5	> 300
	4	85	4	> 300
	8	56	3	180
CO_2	0	120	5	> 300
	2	110	4	> 300
	4	82	3	> 300
	8	74	3	100
Air	2	38	1	140
	4	42	1	40
	8	37	1	40

Table 2.3 Average radius for the dense cloud for the instantaneous release simulations.

Trial	Amount (kg)	Wind speed (m/s)	Observed upwind transport
1	4,500	1.9	At least tens of meters upwind of containers
2	8,100	4.3	Fills grid, but very little upwind
3	4,500	4.0	As for trial 2
4	7,000	2.3	As for trial 1
5	8,300	2.8	100 meter

Table 2.4 Estimates of upwind transport for JRII

2.4 Discussion

The Jack Rabbit II experiment series studied the release and dispersion of chlorine vapour following the release of 4.5–18 tonnes of chlorine [10, 11]. Five of the releases were conducted within a mock urban grid built up of shipping containers extending about 30 meters upwind, 80 meters downwind and 40 meters in the spanwise directions. Table 2.4 lists estimates of the upwind transport for four of the releases in the mock urban grid. In a report from the Utah Valley University [8], it is stated that in trial 5, where 8300 kg chlorine was released in the mock urban grid and the ambient wind speed was about 3 m/s, retrograde creep to more than 100 meters upwind was observed visually. For the remaining trials, which where conducted without an urban grid, no visible gas was transported more than 35 meters upwind [8].

The effective radii from the simulations for the instantaneous releases are about 30 meters for the two tonnes releases and 80–100 meter for the 20 tonnes releases at wind speeds comparable to the listed Jack Rabbit II field trials. Although the amounts released in the simulations differs from the field trials, the upwind extend of the plumes are roughly of the same size.

The effective radius divided by the radius of the source are fairly similar for the different instantaneous release simulations. The results indicate a rule of thumb that the source radius should be increased by a factor of five from the default radius used in CT-Analyst for dense-gas releases.

3 Full-scale simulations

The overall aim of the work presented in this report is to investigate whether increasing the spatial size of a dense gas source in CT-Analyst can account (to some degree) for the effects of the density on the hazard areas. Full-scale LES of the dispersion of the dense gas chlorine and a neutral gas (air) in a part of Oslo are conducted. The results from these simulations are compared with CT-Analyst predictions with the default source size and extended source sizes.

3.1 Numerical procedure

These simulations employ the same LES methodology as described in section 2.2 and [6].

3.1.1 Geometrical domain and mesh

A geometrical model of a part of Oslo is created using the method described in [4], see figure 3.1. The spatial extent of the domain is about 5 km in the streamwise direction (north–south) and 2 km in the spanwise direction (east–west), extending from the harbour on the south and beyond Ullevaal stadium to the north. The royal palace is seen in the lower part of the figure, and the source area is located in a park just north of the palace.

The source for the gas is a 300 m^2 area on the ground in a park area. A computational box with horizontal dimensions given by the geometrical domain above and vertical dimension up to 1,000 meter is created. The mesh resolution is about 0.25 m around the source location, then increased up to 1–2 meter resolution about 100 meters from the source area. The maximum cell size in the domain is 64 meters.

3.1.2 Agent specifications

Chlorine is chosen as the dense gas. This is a widely used industrial chemical with a boiling point of -34°C, and is therefore a gas at normal atmospheric conditions. It is normally stored and transported as a liquefied, pressurised gas. Chlorine has a density of 3.71 kg/m^3 at the boiling point and 3.04 kg/m^3 at atmospheric pressure, that is about 2.5 times that of air.

The Acute Exposure Guideline Levels (AEGLs) are thresholds above which various consequences are expected to occur[1] [12]. AEGLs are defined for various exposure times. CT-Analyst use the 1 hour Acute Exposure Guideline Levels (AEGLs) shown in table 3.1 for estimating health effects.

[1] The three AEGLs are defined as:

- 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 asymptotic 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 adverse health effects or death.

Figure 3.1 The geometrical domain for the full-scale urban simulations. The source location is indicated just north of the royal palace. The average wind direction from the south is indicated with the arrow.

Threshold	**Concentration**	
	mg/m^3	**ppm$_v$**
AEGL-1	1.5	0.5
AEGL-2	5.8	2.0
AEGL-3	58	20.0

Table 3.1 Acute exposure guideline levels (AEGLs) for one hour exposure to chlorine [12] expressed in mg/m^3 and parts-per-million of volume.

3.1.3 Setup

An area of 300 m^2 on the ground is specified as the gas source. A continuous release with release rate 10 kg/s is specified for both the dense and neutral gas releases. The resulting release velocities are 0.011 m/s for the chlorine gas release and 0.027 m/s for the neutral gas release, much lower than the ambient air velocity. The momentum effects from these releases should therefore be small. However, in order to ensure numerical stability, the velocity fields of the release is set up at first, and the mass fraction of the gas is increased from 0 to 1 during 10 seconds.

The inlet velocity field is based in Stull (2015) for neutral conditions. The vertical wind profile at the inlet plane is

$$
\begin{aligned}
V(z) &= \begin{cases} U_\infty \cdot \left(\dfrac{z}{H_z}\right)^\alpha, & z \leq H \\ U_\infty, & z > H \end{cases}, \\
U(z) &= 0, \\
W(z) &= 0,
\end{aligned}
$$

where $H = 500$ m is the atmospheric boundary layer height, z the height above ground, $U_\infty = 3$ m/s the free stream wind speed and $\alpha = 0.25$ a model parameter. The wind direction is from south to north, as indicated in figure 3.1. The fluctuations below the atmospheric boundary layer height are

$$
\begin{aligned}
\sigma_{uu} &= (1.6u_* (1 - 0.5 (z/H))))^2, \\
\sigma_{vv} &= \left(2.5u_* e^{-1.5z/H}\right)^2, \\
\sigma_{ww} &= (1.25u_* (1 - 0.5 (z/H)))^2, \\
\sigma_{uv} &= 0, \\
\sigma_{uw} &= 0, \\
\sigma_{vw} &= 0.
\end{aligned}
$$

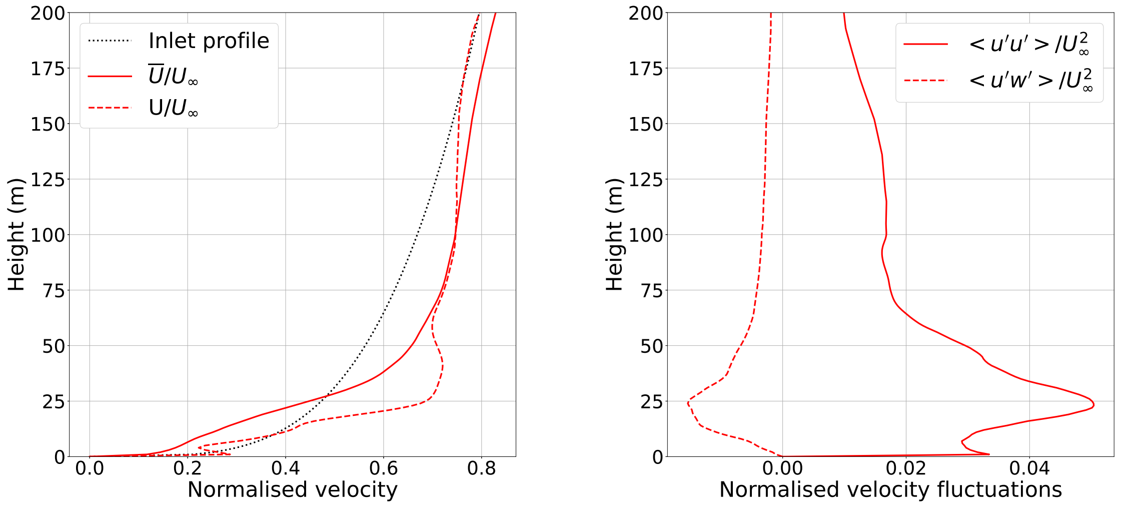
First, the velocity field was simulated for a total simulation time of about 4500 seconds (75 minutes), that is more than enough time to ensure one flow-through of the entire domain.

Then a dense-gas and a neutral-gas dispersion simulation were conducted. The dense-gas simulation used chlorine gas at atmospheric pressure and a temperature of 15°C, at which point the chlorine gas density is $\rho_{Cl_2} = 3.04$ kg/m^3. The neutral-gas simulation used air ($\rho_{air} = 1.225$ kg/m^3). A time step of 0.02 seconds was used during the releases. The releases were simulated for 15 minutes.

3.1.4 CT-Analyst

CT-Analyst is an operational dispersion tool providing instantaneous predictions of the dispersion of hazardous materials in urban environments. It utilises wind fields for urban environments, which are precomputed using high-fidelity Large Eddy Simulations and stored in a database. CT-Analyst uses these databases to give an instantaneous prediction of the hazard areas following a release of a toxic agent. Detailed descriptions of CT-Analyst can be found in [1, 2, 3, 4, 5]

CT-Analyst of continuous releases with rate 10 kg/s from a source with a horizontal radius of ten meter (default source size) and extended radii of 50, 100 and 150 meters have been conducted. A wind velocity of 3 m/s from the south was specified.



(a) Streamwise velocity profile (b) Fluctuating velocity profile

Figure 3.2 Mean and instantaneous streamwise velocity profile and the inlet velocity profile (a) and streamwise Reynolds stress and shear stress (b).

3.2 Results

3.2.1 Wind field

Figure 3.2a shows the vertical profile of the mean ($\overline{U}$) and instantaneous (U) streamwise velocity at the source location. The specified inlet profile is also shown. The streamwise Reynolds stress, $\overline{u'u'}/U_\infty^2$, and the shear stress, $\overline{u'w'}/u_\infty^2$, are shown in 3.2b. Here u' and w' is the fluctuating velocity component in the streamwise and vertical directions respectively. There is a difference between the mean streamwise velocity and the inlet profile. Some difference, however, is expected due to the urban geometry that will affect the velocity profile.

Figure 3.3 shows the turbulence kinetic energy

$$k = 1/2\left(\overline{u'u'} + \overline{v'v'} + \overline{w'w'}\right),$$

where u', v' and $'w$ are the fluctuating velocities in the streamwise, spanwise and vertical directions respectively before the gas is released, in a plane four meters above the ground. The turbulence levels are about the same as in the urban dispersion simulations presented in [5], which are used for the Oslo version of CT-Analyst. CT-Analyst used the turbulence kinetic energy values to calculate the "spreading angle" used in its dispersion predictions.

3.2.2 Dispersion

For comparison with CT-Analyst dispersion data, data from the LES was taken in a plane 4 meters above the ground. The comparison of LES with CT-Analyst uses two different sample sets: resampled grid and sector segments. For the former method, the horizontal plane is gridded to a

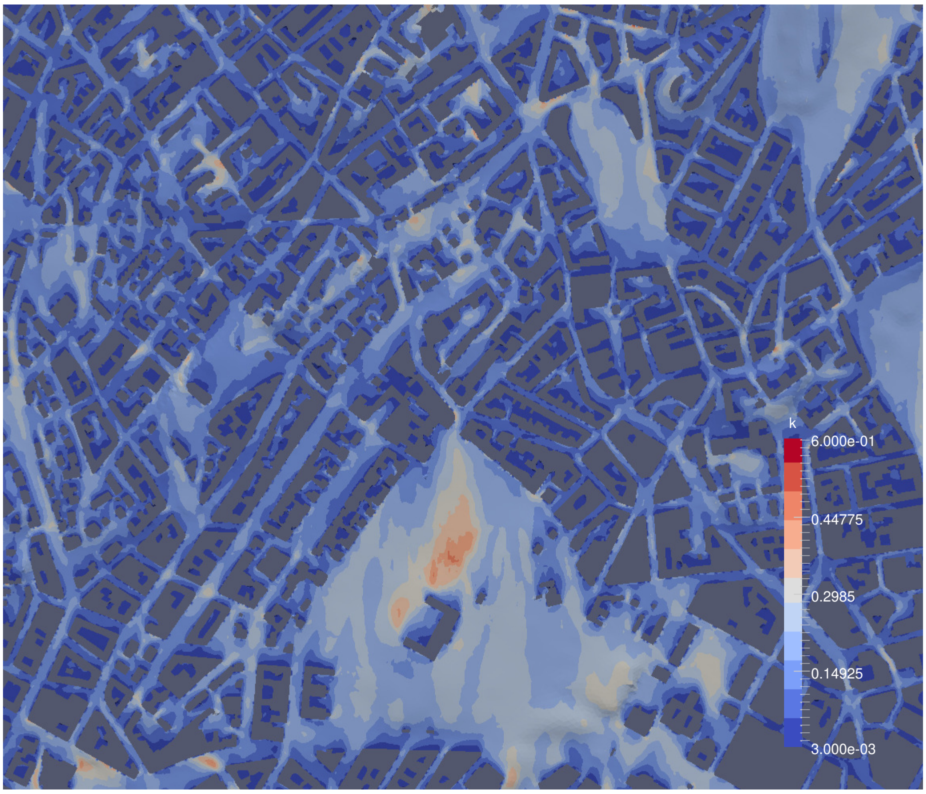


Figure 3.3 Turbulence kinetic energy in a plane 4 meters above ground. Dark blue denotes energy less than 0.003 m^2/s^2, the highest value in the region shown is about 0.5 m^2/s^2, displayed in red.

mesh with grid size 50 meter. Both the CT-Analyst and the LES results are resampled onto this mesh. All of the contour plots in the following are shown for this resample mesh. The latter method is to divide the horizontal plane into 24 sectors of 15° each: (0°, 15°), (15°, 30°) and so on, with 0° being true north (which coincides with the mean streamwise wind direction)[2]. For each sector, the maximum range of the gas to given threshold values for the LES and CT-Analyst are found. For both methods, the concentration results given are for the maximum concentration achieved at a given point in space.

The baseline for the comparison is the neutral gas simulation, as CT-Analyst is developed for the dispersion of passive (neutral gases). Figure 3.4 shows the concentration field contours of the plume to the 60-minute AEGL-thresholds as well as ten concentration levels[3] for the neutral gas simulation in the resample grid of 50 meter grid size. The CT-Analyst and the neutral gas LES are in good agreement, especially for the AEGL contours. For concentration higher than AEGL-3, CT-Analyst yields shorter hazard distances than LES.

Figure 3.5 shows the concentration contours for the AEGL threshold values for the dense and neutral LES at the end of the releases (15 minutes after start of the releases). It is evident that the dense-gas plume is much wider than the neutral-gas plume, whereas the downwind distances to the AEGL thresholds are much longer for the neutral gas than the dense gas.

[2]This division into sectors is slightly different than the division used in chapter 2

[3]The ten concentration levels are: $C = 1, 2, 5, 10, 20, 50, 100, 500, 1000, 5000$ mg/m^3.

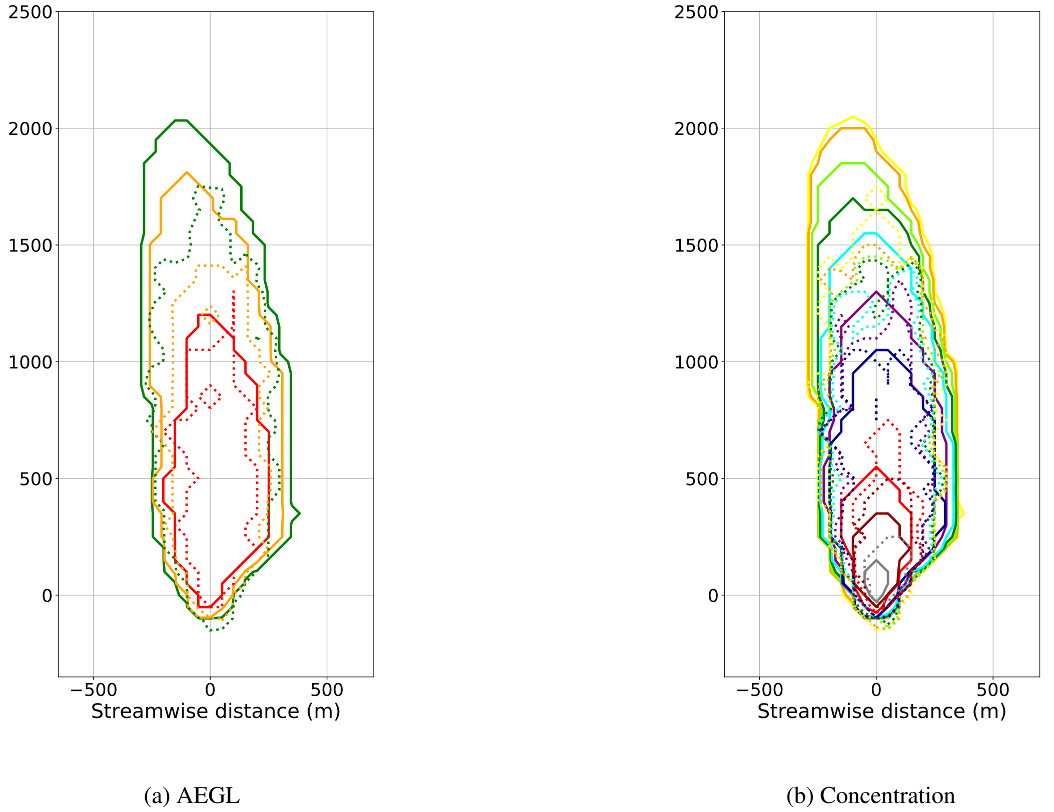


Figure 3.4 *(a) The plumes to the AEGL-1 (green), AEGL-2 (yellow) and AEGL-3 (red) thresholds for CT-Analyst (full lines) and LES neutral gas (stapled lines) after 15 minutes release of neutral gas. (b) Corresponding figure to ten concentration levels:* $C = 1, 2, 5, 10, 20, 50, 100, 500, 1000, 5000$ *mg/m*^{3}.

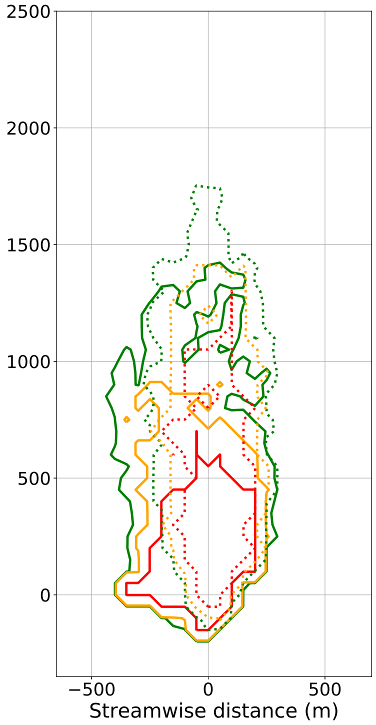


Figure 3.5 The plume to the AEGL-1 (green), AEGL-2 (yellow) and AEGL-3 (red) values for the dense gas (full lines) and neutral gas (stapled lines) LES. The results are shown in a resampled grid with mesh size 50 meters 15 minutes after start of the release.

Figure 3.6 shows the maximum mass fraction projected on a horizontal and a vertical plane 15 minutes after the start of the release for the dense and neutral gas simulations. There are quite large differences between the dense and neutral gas releases. Most strikingly is perhaps the lateral dispersion of the dense gas. The dense-gas is also transported further upwind than the neutral-gas. We see that the neutral-gas is much more efficiently mixed in the vertical direction than the dense gas. The source is located at $(x, y) = (0, 0)$, but it is an area source which extends about 20 meters in each direction.

Figure 3.7 shows AEGL contour plots for CT-Analyst and LES for the dense-gas release. The CT-Analyst results are predictions with the default source radius of 10 meters and extended radii of 50, 100 and 150 meters. The transport of the dense gas to the south-west in the LES can be captured by increasing the source size in CT-Analyst by about an order of magnitude. Increasing the source size gives a larger plume size in the spanwise direction also far downwind from the release site. The downwind distances to the AEGL thresholds are, however, not greatly affected. An extended source of 150 meters (a factor of 15 increase) reduces the downwind distance to the AEGL thresholds somewhat, but CT-Analyst still give much larger downwind hazard distances than LES.

A dense-gas release can affect the ambient wind field such that the magnitude of the wind field generally decreases, and thereby affect the temporal evolution of the dispersion process. The dense-gas can therefore remain at the source site for a long period, and relatively slowly be mixed with and transported by the ambient air stream. This may explain the shorter downwind distances to the AEGL levels in the dense-gas LES compared with the neutral-gas LES. CT-Analyst assumes a neutral-gas plume and therefore cannot take this effect into account. This may explain the fact that the contours to the AEGLs downwind are relatively unaffected by increasing the spatial source size.

3.2.3 Statistical analysis

In order to evaluate the performance of increasing the source term in CT-Analyst, the following two metrics are calculated: the fractional bias (FB) and the modified normalised mean bias (MNMB). These are commonly used for evaluating dispersion models with experimental data, see for instance [13]. For observations X_O and predictions X_P, FB and $MNMB$ are defined as

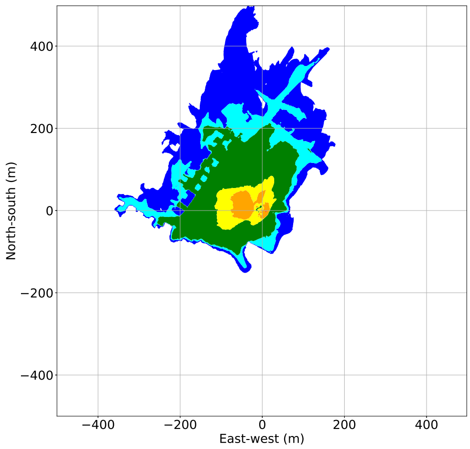
$$\mathrm{FB} = \frac{\overline{\mathrm{X}}_\mathrm{O} - \overline{\mathrm{X}}_\mathrm{P}}{0.5\left(\overline{\mathrm{X}}_\mathrm{O} + \overline{\mathrm{X}}_\mathrm{P}\right)}, \tag{3.1}$$

$$\mathrm{MNMB} = \frac{2}{\mathrm{N}} \sum_{\mathrm{i}=1}^{\mathrm{N}} \left(\frac{\mathrm{X}_\mathrm{O} - \mathrm{X}_\mathrm{P}}{\mathrm{X}_\mathrm{O} + \mathrm{X}_\mathrm{P}}\right). \tag{3.2}$$

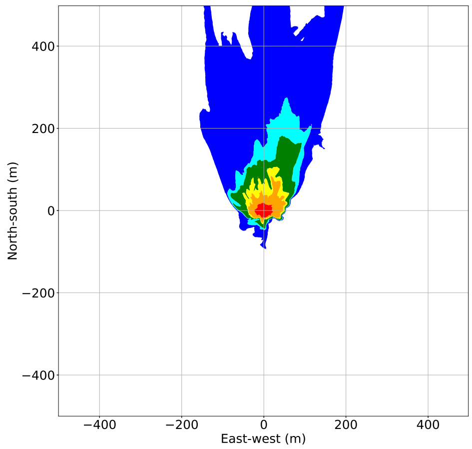
The bars $(\overline{X})$ indicates averaging over N values in the dataset. FB and MNMB ranges between -2 and 2. A value of 0 indicates perfect match between the observations and the predictions, positive values indicate underprediction and negative values indicate overprediction.

FB and MNMB are calculated for the maximum distances to the AEGL-1, -2 and -3 threshold values in the sector segments presented in section 3.2.2. LES is taken as the observations and CT-Analyst is taken as the predictions. FBs for each AEGL individually, as well as the entire dataset (all AEGLs), and MNMB are given in table 3.2.

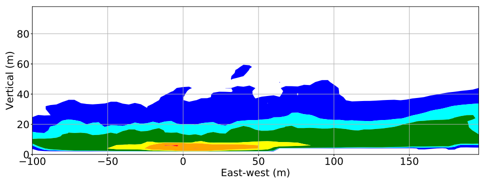
As an operational hazard prediction tool, CT-Analyst should overestimate rather than underestimate the hazard area. Therefore a negative value of the metric is better than a positive value. The neutral gas scenario is the reference case, and therefore the metric at default spatial source size for the neutral gas release can be taken as the reference.



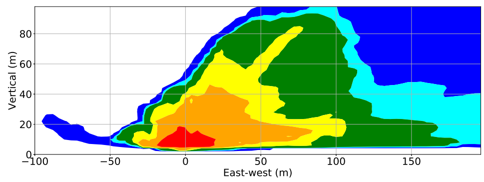
(a) Dense gas, horizontal plane



(b) Neutral gas, horizontal plane

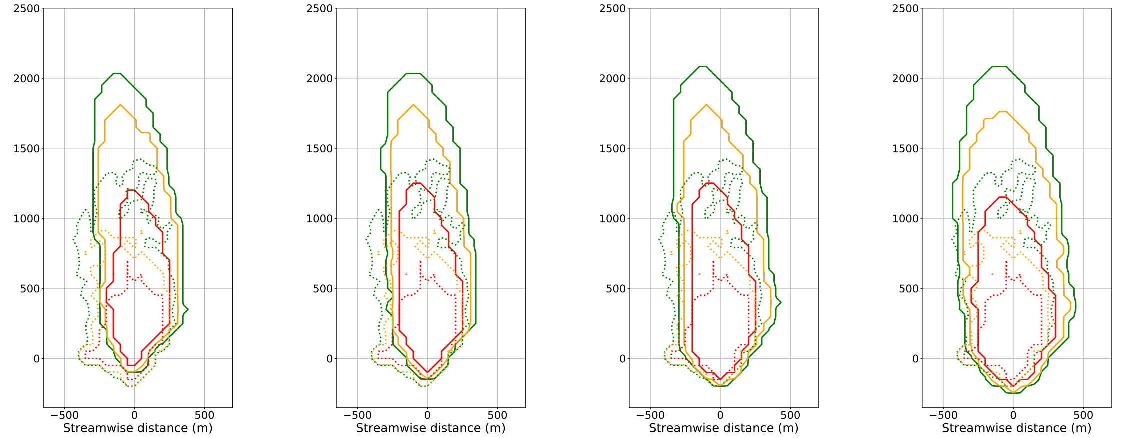


(c) Dense gas, vertical plane



(d) Neutral gas, vertical plane

Figure 3.6 *The maximum mass fractions obtained 15 minutes after start in projected horizontal and vertical planes for the dense and neutral gas releases respectively. The colours denotes mass fractions as follows: red > 0.5, orange > 0.1, yellow > 0.05, green > 0.01, cyan > 0.005 and blue > 0.001.*



(a) Default source radius 10 m

(b) Extended source radius 50 m

(c) Extended source radius 100 m

(d) Extended source radius 150 m

Figure 3.7 Contour plots for CT-Analyst (stapled line) and LES (full lines) to the AEGL-1 (green), AEGL-2 (yellow) and AEGL-3 (red) thresholds after 15 minutes release. Figure (a) shows results from CT-Analyst with default source size while (b), (c) and (d) show CT-Analyst results with extended source sizes of 50, 100 and 150 meters respectively.

	Threshold	**CT-Analyst data**			
		R = 10 m	**R = 50 m**	**R = 100 m**	**R = 150 m**
Dense gas	FB AEGL-1	0.018	-0.076	-0.217	-0.341
	FB AEGL-2	-0.034	-0.124	-0.253	-0.374
	FB AEGL-3	0.029	-0.111	-0.214	-0.325
	FB All AEGLs	0.003	-0.102	-0.228	-0.348
	MNMB	0.313	0.05	-0.193	-0.382
Neutral gas	FB AEGL-1	-0.189	-0.282	-0.419	-0.539
	FB AEGL-2	-0.224	-0.313	-0.438	-0.554
	FB AEGL-3	-0.09	-0.229	-0.331	-0.44
	FB All AEGLs	-0.173	-0.277	-0.401	-0.516
	MNMB	-0.146	-0.42	-0.646	-0.809

Table 3.2 Fractional bias (FB) and modified normalised mean bias (MNMB) calculated from the maximum ranges to AEGL-1, -2 and 3 in 18 sector segments.

For the dense gas scenario, the default CT-Analyst source gives an underprediction of the hazard area. Extended source sizes of 50 meters (five times the default source) and 100 meters (ten times) yield metric values in the same area as the reference case.

4 Concluding remarks

A very simple method for considering the effect of dense-gas dispersion in CT-Analyst is proposed, namely to increase the size of the source from the default source size in CT-Analyst. A dispersion of a dense gas will typically be dominated by the negative buoyancy effects due to the density (as well as the momentum from a jet release). This results in an initial dispersion pattern where the gas is transported in all directions in the horizontal plane including upwind) quite close to the ground. A natural gas will on the other hand be transported dominantly in the down wind direction, and also be more efficiently transported upward. As the dense gas is diluted with ambient air, the buoyancy effects will diminish and the gas will at some point behave like a neutral gas that is transported passively by the ambient wind field. The large horizontal dense plume cloud may, however, affect the resulting long distance dispersion pattern, even at distances where the negative buoyancy effects are negligible. The idea behind the proposed simple method, is that by increasing the spatial source size in CT-Analyst, the increased initial horizontal transport of the gas, and the effect this has on the long-distance transport, can be accounted for. The investigation was conducted in two steps: first by studying the gas dispersion in the first phase after a release, when negative buoyancy effects are important; next by conducting full scale numerical simulations of the release and dispersion of dense and neutral gases in an urban environment, and compare with predictions from CT-Analyst with default and extended source sizes.

In order to study the initial gas dispersion when the negative buoyancy effects are important, the release and dispersion of some dense gases in an open environment were conducted using LES. The purpose of these simulations was to estimate the initial sizes of the dense-gas plumes after a release. The radii for the initial dense plumes are 3–6 times larger than the radius of the sources. The radii are roughly in agreement with the results from field trials of chlorine releases in the Jack Rabbit II experiment series. This would indicate that increasing the spatial dimension of the source by a factor five for a CT-Analyst prediction could be a rule-of-thumb for dense gases.

Next, full scale large-eddy simulations of the dispersion of the dense chlorine gas and a neutral gas in a part of Oslo have been conducted. The dense-gas simulation produce a vertically thinner plume which extends much wider laterally and a longer distance upwind than the neutral gas release. The dense-gas simulation has been compared with CT-Analyst predictions of the gas dispersion with the default source radius of 10 meters as well as with extended radii of 50, 100 and 150 meters. The results of the study indicates that increasing the source radius can to some extent capture the transport upwind and spanwise. Increasing the source size leads to a wider plume in the spanwise directions also far downwind of the release, but the length of the cloud is only affected in a small amount. It should be noted that an initial thin and horizontally extended plume is just one effect from the dense gas. Another effect is that the temporal evolution of the plume can be prolonged as the dense gas tends to remain in the near-source area for a longer period of time than a neutral gas, and this can influence the far field dispersion pattern. This simple model does not take the dense gas effects on the temporal evolution into account, even though the build up urban environment also leads to a similar effect of “trapping” the gas at the source location.

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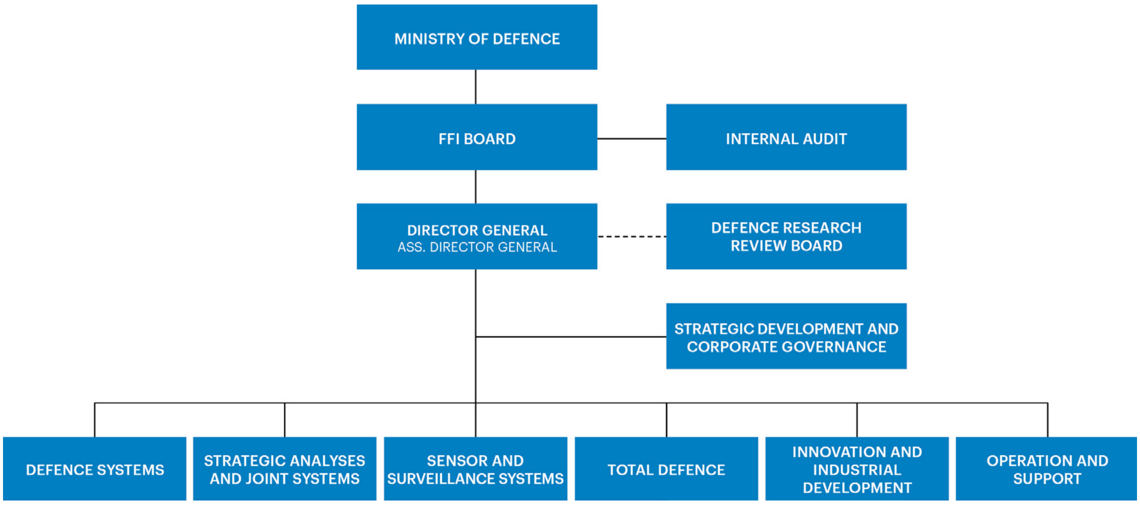

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