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Storvirvelsimulering (LES) av spridning i stadsmiljö

Sammanfattning (högst 200 ord)
I ljuset av ett ökat hot för avsiktliga eller oavsiktliga utsläpp av skadliga ämnen som industrikemikalier, radioaktiva utsläpp, giftgas eller biologiska ämnen, finns ett behov av detaljerade spridningsberäkningar. Applicerandet av spridningsmodeller på en urban miljö ställer stora krav på modellen. För en konsistent simulering krävs en detaljerad geometri för staden samt en konsistent behandling av sådana nyckelprocesser som deposition och skiktning. Rent beräkningstekniskt krävs också ett högkvalitativt beräkningsnät. I detta arbete har en första simulering av spridning i stadsmiljö genomförts med så kallad storvirvelsimulering (LES). Simuleringen har genomförts för Gamla Stan i Stockholm som är väl lämpad för modellutveckling då dess läge, omgivet av vatten, borgar för möjligheten att använda enkla randvilkor. Flera utsäpp har simulerats. Totalt har åtta utsläpp simulerats, av fyra olika ämnen, på fem platser. Detta ger sammantaget en god bild av spridningen i staden, i den aktuella simuleringen.

Nyckelord
LES, atmosfärisk, urban turbulens

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Large Eddy Simulation of Urban Dispersion

Abstract (not more than 200 words)
In view of a increased threat of accidental or deliberate release of hazardous substances like industrial chemicals, radioactive releases, poisonous gas or biological agents, detailed dispersion simulations are needed. Application of dispersion modeling to an urban environment is a major simulation challenge. For a consistent simulation a detailed geometry of the city and a consistent treatment of such key processes as deposition and stratification are needed. From a technical point of view, a high quality computational grid is also needed. In this work a first urban dispersion simulation have been performed using Large Eddy Simulation (LES). The simulation has been done for Gamla Stan in Stockholm which is well suited for model development since its location, surrounded by water, guarantees the possibility of using simple boundary conditions. Several releases have been simulated. In total eight releases have been simulated, consisting of four different substances, released on five different locations. Together, this gives a good picture of the dispersion within the city, in the simulation in question.

Keywords
LES, atmospheric, urban, dispersion

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Abbreviations

AHS	Acute Harmful Substance
CFD	Computational Fluid Dynamics
LES	Large Eddy Simulation
MILES	Monotone Integrated LES - A particular way of calculating sub-grid scale turbulent effects on the large scale flow
RANS	Reynolds-Averaged Navier-Stokes
TIC	Toxic Industrial Chemical
V_d	Deposition velocity

1 Introduction

Environmental issues have for a long time motivated the study of atmospheric dispersion, [2]. For air pollution from traffic, factories, house warming etcetera on local scale weather statistics is often used, while for dispersion on a regional scale real weather becomes important. Because of this connection to the weather and atmospheric models, atmospheric dispersion models usually have a resolution similar to that of weather forecast models, see e.g. [6]. The classic atmospheric dispersion model, connected to a weather forecast model is essential in describing the dispersion of contaminants over larger areas. However, in view of the presence of harmful substances in the modern society, and the increased threat of terrorist activity, the issue of deliberate or accidental release of Acute Harmful Substances (from here AHS) within densely populated areas need to be addressed. AHS may consist of Toxic Industrial Chemicals (TIC) or chemical and biological warfare agents.

The successful modeling of a release of a harmful substance in a city poses several challenges. For the purpose of describing differences of AHS concentrations within a city, a very detailed geometrical description of the city is needed. This detail also means that a very high resolution must be used, in order to resolve each individual building. Also, the unsteady, possibly buoyant, flow must be simulated together with the diffusion of the dispersed agent. The latter requirement is motivated by the complex, turbulent flow that can be anticipated in an urban environment.

A successful urban dispersion simulation must adequately simulate the vortex shedding and recirculation from and around buildings. It must take into account the stratification of the atmosphere and the absorption of incoming solar radiation by different surfaces. It must also include a faithful description of deposition and resuspension of gases, and settling of contaminant particles. Such a successful simulation of urban transport and dispersion of an AHS can be used for determining optimal placement of sensors within a city, for training of first-responders, for development of tactics in case of an emergency, for development of fast and easy-to-use means for estimation of hazard areas (templates), for determining the potential effect on civilian population or military personnel and also to e.g. determine visibility in a combat zone.

Here, a first effort at modeling AHS dispersion in an urban environment is presented. The simulation presented here includes many limitations and simplifications. However, even from this rudimentary simulation, we may learn much of what we could expect to happen in the real world. The simulation is also the first step toward a better ability to simulate urban contaminant dispersion.

2 Theory

The numerical simulation of fluid flow is generally referred to as computational fluid dynamics, or CFD, see e.g. [12]. Fluid flow can be described by the Navier-Stokes equations. The Navier-Stokes equations consist of complex, non-linear, coupled, partial differential equations, for which no analytical solution is known. Many simplifications to the Navier-Stokes equations have been made over the years to create solvable subsets of the full solutions. For flow in or around complex geometries, where turbulence effects are important and need to be addressed, the full Navier-Stokes equations are usually used and solved numerically. The two main approaches to CFD today is LES (Large Eddy Simulation, see e.g. [5] and [9]) and RANS (Reynolds-Averaged Navier-Stokes). RANS is by far the most used in engineering applications today, mainly because it is affordable in terms of computational power. However, RANS computes, as it's name implies, averages of the computed fields. In this way all effects of turbulence is modeled. LES on the other hand is presently growing in interest. Mainly perhaps, because computer power have reached a level where practically interesting problems can be simulated using LES, see e.g. [1]. It involves the time dependent simulation of the flow state resolving all turbulence on the scales of the geometry. Turbulence on scales smaller than that resolved are considered only relevant to the larger scale flow through their dissipating effect on energy. This small scale turbulence is therefore modeled. The difference between LES and RANS then, is that from LES we can retrieve the actual large scale turbulence, while RANS only can model the average effects of turbulence. For simulation in complex geometries LES is often preferred. In particular this is the case when simulating dispersion since LES can simulate the actual movement of AHS with the flow field. For highly toxic substances concentration fluctuations may be very important when calculating the toxic effect since a high concentration during a short time generally gives a higher toxic load than a low concentration during a long time, see e.g. [13]. This kind of effect can not be treated in a RANS simulation.

The LES simulations presented here have been performed with a finite volume formulation (see [4]) on a grid including the islands Stadsholmen, where the Stockholm old town is situated, Helgeandsholmen, Strömsborg and Riddarholmen. Sub-grid scale turbulence have been modeled using the MILES approach, see [3]. The inflow boundary supplied a log-linear velocity profile with a 'free-atmosphere' wind of 3 ms^{-1} (equivalent to a 10 meter wind of about 2 ms^{-1}). The outflow uses transmissive boundary conditions for the flow to be able to pass through, while the lateral and upper boundaries use a symmetry plane boundary condition. Lower boundary conditions depend on the surfaces: ground and water surfaces as well as roofs are considered no-slip surfaces while walls are considered free-slip surfaces. The reason for this unphysical treatment of wall friction is that the resolution in many streets and alleys is too poor for an adequate viscous formulation. Using only three cells across an alley, both the outer cells would be heavily retarded by the proximity to the walls and exaggerate the retarding effect on the dispersion. It should be noted though, that the present no-slip formulation means that the flow through the alleys may instead be too easy and thus somewhat high.

No atmospheric stratification is assumed for the present simulation. The atmosphere within the domain is instead considered isentropic. This may be a severe simplification in non-neutral situations (see e.g. [11] for a introduction to the static stability in the atmospheric boundary layer), as will be shown in section 3. It was however a necessary simplification for the present simulation. Work is in progress on including the effects of stratification into the simulations, see e.g. [14].

Dispersed gases are neutrally buoyant, i.e. gases have the same density as the air, and deposit on the ground, water, walls and roofs. Deposition is modeled using a deposition velocity formulation, see e.g. Zhang and Brook [8]. The deposition velocities vary between the substances being dispersed. The deposition velocity is also different between dry and wet surfaces. Finally, all chemical species are considered inert. No chemistry is included in the simulation. Transport is calculated according to

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot grad(c) - \nabla(\nu \nabla \cdot c) = 0, \tag{2.1}$$

where c is the species concentration, t is the time, $\mathbf{v}$ is the velocity field and ν is the kinematic viscosity.

2.1 Computational grid

Part of the computational grid used in the simulation is presented in Figure 1. The grid is a structured, hexahedral grid, consisting of 1’622’897 cells. The domain is 1750 x 830 x 1000 m^3. Hexahedral grids are often used for CFD calculations. One reason for this is their good ability of resolving boundary layers. However, in the present case, the structured hexahedral grid also shows a weakness. Figure 1 shows that the complex geometry means that it is impossible for the structured grid to have a uniform resolution. To achieve a sufficient resolution on the lee side of a spreading object, like the house of parliament, a unnecessary high resolution is required on the windward side.

3 Results

The simulation was started from an initial state at rest with the prescribed boundary value on the inflow boundary. After 548 simulated seconds, the simulation was restarted including releases

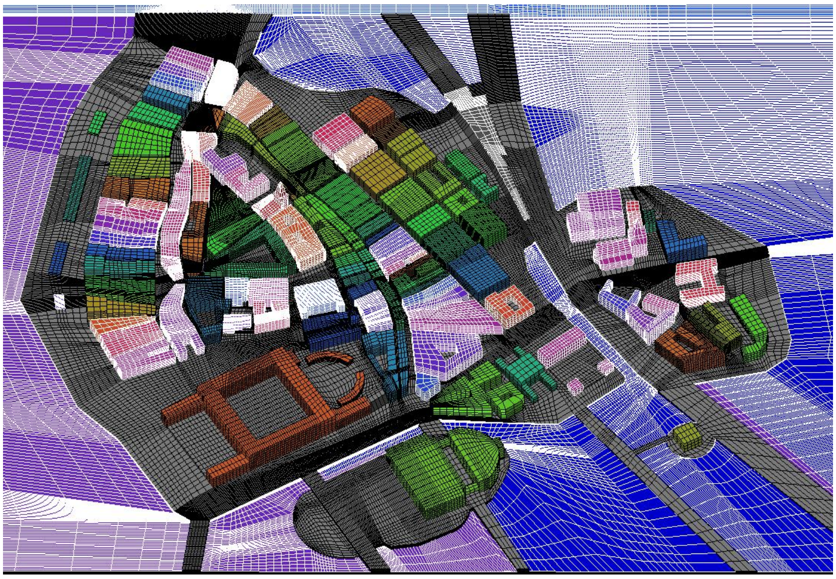

Figure 1: The domain and the grid used for the simulation. A structured hexahedral grid has been used. Notice how 'parallel' lines are spread or contracted in fan like patterns by semi-circular buildings. NB, although praxis in this report is that north is up, in this particular figure north is down. The House of Parliament is the single green building on the small island in the bottom of the figure.

and depositions. The simulation was successfully carried out for a total simulated time after initialization of 29 minutes.

Although this simulation with its many deficiencies can not be taken as a simulation of a true outcome, the results bear witness of many interesting features of the flow, and of dispersion. These features in them self are sufficient motivation for the present work, but also hint at what could be done.

The results will be presented in two subsections, subsection 3.1 describing the simulated flow and subsection 3.2 describing the the simulated dispersion and conclusions following from studying those results.

From the study of the dispersion of releases several conclusions can be drawn. The most obvious is that it is possible to see how the respective releases would affect the local environment. However, conclusions can also be drawn on a more general level regarding dispersion in an urban environment. Sections 3.3-3.5 presents some of the features that have been found in studying the simulated dispersion.

3.1 Simulated flow

The computations reveal a very complex flow field containing many interesting flow structures such as large vortices behind buildings like the royal palace and the parliament buildings. These results are for the instantaneous velocity field. Back flow is found both behind and in front of buildings with walls perpendicular to the prevailing, westerly wind. One example of this is the royal palace in Figure 2. There the wind 2m above the ground is plotted as velocity vectors colored by the magnitude of the flow velocity, where red represent 1.5 m/s and blue 0 m/s. The undisturbed wind, approximately 2ms^{-1} at 10m above sea level, comes from left moving in positive x direction while the wind mostly goes in the opposite direction in both the outer and inner courtyard of the royal palace, again at 2m above the ground. Another example is a place called Köpmansbrinken in the eastern part of the old town, see Figure 3. Here the approaching wind coming through the street Köpmangatan have the expected direction but the down hill slope here generates a recirculation zone, giving wind in the opposite direction in the other streets approaching this location. A Karman Vortex Street can be found around the top of the German church (Tyska kyrkan) at the central part of the Old Town. The plots in Figure 4 contain images of the absolute value of the velocity at 50m above the sea level, i.e. approximately 20m above the roofs of the houses in the surrounding area. The resolution is not sufficient to get a complete vortex street but there are significant traces of it in the wake. In Figure 4 it can also be seen that there are no vortex street behind the top of the church close to the Royal Palace (Storkyrkan). This is probably due to the coarse grid resolution in this area.

The area behind the parliament contains a large vortex structure, see Figure 5. This area

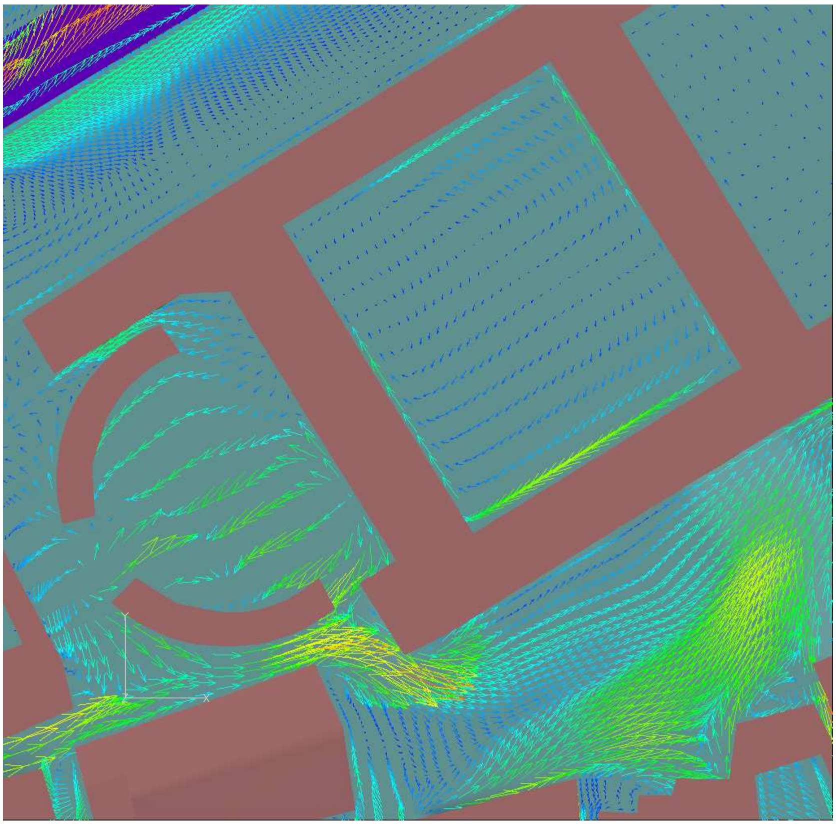

Figure 2: Wind velocity vector 2 m above ground around the royal palace. North is up.

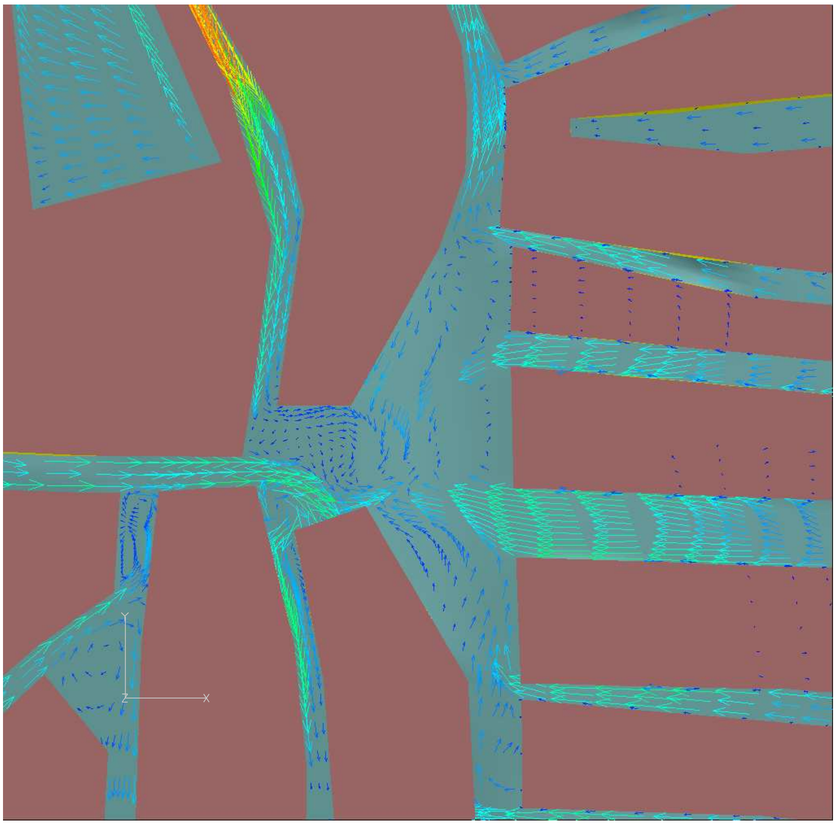

Figure 3: Wind velocity vector 2 m above ground at Köpmansbrinken in the eastern part of the Helgeandsholmen

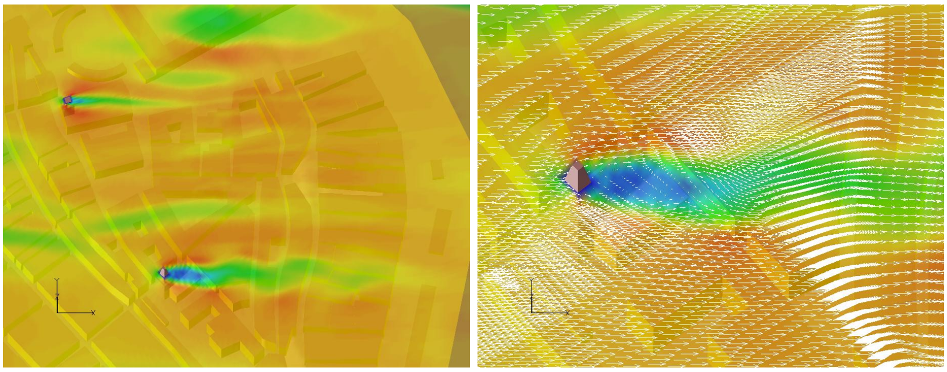

Figure 4: Absolute value of the wind velocity and velocity vectors at 50 m above sea level at the German Church.

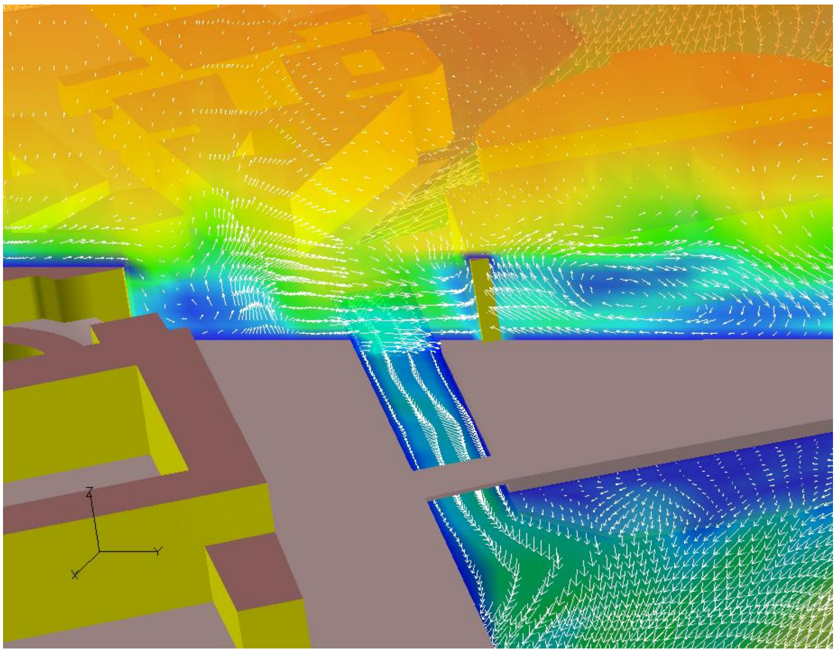

Figure 5: Velocity contours and vectors at a plane 2 m above sea level and a vertical plane with constant x coordinate right behind the parliament. View from north-east.

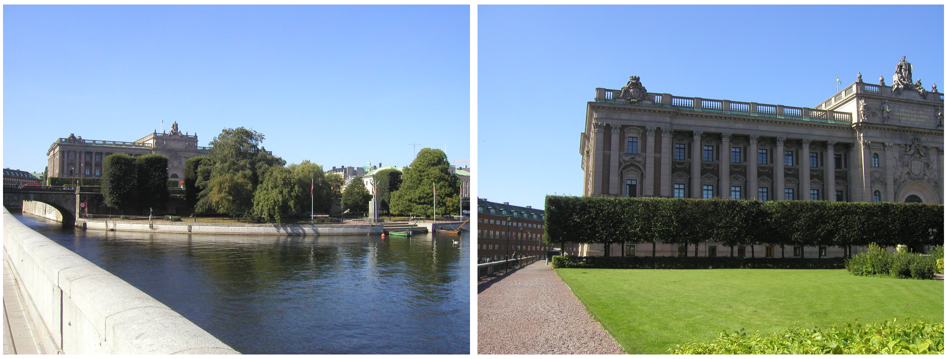

Figure 6: Photos of the area behind the parliament. View from north-east.

is partially covered by trees in the real world, see Figure 6. These trees will probably reduce the velocities and the rotation of the vortices here. This is an effect that is not captured since there is presently no treatment of the damping effect of trees included in the simulations. A tree reduces the wind velocity but it does not stop it totally and the reduction is dependent on how many branches and leaves the tree has in different parts of it. The old town contains many houses and around each of them there can be found interesting flow fields. However, because of their abundance, only a few examples are presented here.

3.2 Dispersed substances

To study the effect of dispersion on a release of some AHS, a total of 8 releases were considered. The releases were computed at the same time but are not affecting each other. The releases are grouped based on their type and whether they represent a accidental or deliberate release. Then, one release represents the accidental release of an industrial chemical. Five releases represent the deliberate release of a nerve gas. These releases are partitioned between two substances (Sarin and VX), two release locations, and one release that does not deposit. Finally, two releases are made of a biological substance (Anthrax). The respective release locations are given in figure 7. Details on the releases are given in subsections 3.2.1-3.2.4. For the releases of SO_2, Sarin and VX a toxic model based on the toxic load concept is use. The basic idea in the model is described in [13]. Values on the model parameters are taken from [7]. For Anthrax a dose response relation described in [10] is used.

3.2.1 Industrial chemical (SO_2, field 1)

The first release is hypothesized to be a ruptured tanker on the track at Centralbron, just next to the mouth of the railway tunnel. The tank is filled with 45 tons of liquid SO_2 that vaporizes as

Figure 7: Locations of the different releases, cf subsections 3.2.1-3.2.4.

the pressure drops and creates a jet of gas flowing out of the tank through a hole with a diameter of 5 cm. This yields an area source on the highway just next to the mouth of the railway tunnel. The source is considered an area source, 6m x 22m at a distance of 40m from the tank (which positions it right on the highway). The release is continuous in time for 23 minutes, after which it is switched off. The resulting dosage resulting from this release (under the assumption that people do not move during the full 29 minutes) is presented in Figure 8. The colors indicate a dose giving light injuries (yellow) and severe injuries (orange). Lethal injuries (red) are not present, the simulated concentrations never reached sufficiently high levels for sufficient time during the simulation. It should be noted here that because the when the simulation was terminated, there was still SO_2 gas present in the domain. Therefore it is possible that the dose might increase somewhat if the simulation was continued.

The simulation shows that the release is not sufficient to cause widespread severe injuries, or even deaths. The area of light injuries on the other hand covers a major part of the island, a sign of the strong dispersive effects for this case. It should be noted that the low dosages are closely connected to the release location and the prevailing 'weather', i.e. stratification and wind. This feature will be further discussed in section 3.3.

Figure 8: Resulting dosage for release of SO_2 from ruptured tank. The release location is marked with a white cross. North is up.

3.2.2 Sarin (field 2 and 3)

The first of the supposed deliberate releases is that of the nerve gas Sarin. It is assumed that a small bomb filled with 10 kg of Sarin is exploded and that 90% of the substance is vapourized while 10% of the substance is found in liquid phase on the ground. The surface coverage is distributed over an area of 10m x 50m, while the initial cloud of gas is 10m x 10m x 10m with its center at 6m above the ground. The ground contamination evaporates for five minutes with a speed of 0.00333 times the concentration of the substance on the ground (in kg/m^2). Sarin deposits on dry surfaces with $V_d = 0.007ms^{-1}$ and on wet surfaces with $V_d = 0.02ms^{-1}$.

The release is done at two distinct locations, one on Västerlånggatan and one outside the House of Nobility. The resulting dosages for the two releases can be seen in Figure 9. In that figure yellow indicates light injuries, orange indicates severe injuries and red indicates lethal injuries. Due to code errors the evaporation from the ground contamination was not started immediately but first after 980 seconds (approximately 16 minutes) of simulated time. The dosages from the evaporated gas are negligible in comparison to the dosages from the primary release and are not further presented here.

The obvious differences due to release location will be further discussed in section 3.4. The dosages still show that large areas of the town are affected. In the case of a release on Västerlånggatan, the entire street, including the streets upstream of the release has received a lethal dosage. The same is true for the streets south-west of Västerlånggatan. This spread of the

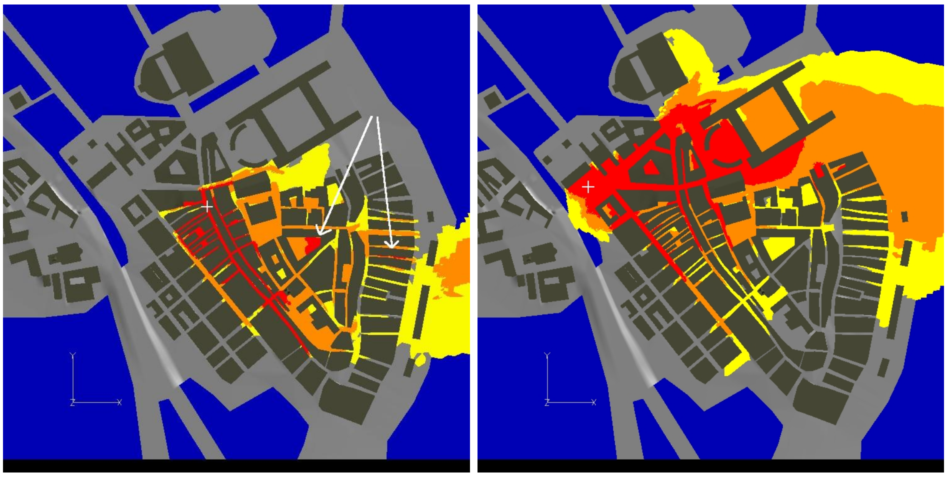

Figure 9: Resulting dosage for release of the nerve gas Sarin at two locations. One on Västerlånggatan and one just outside the House of Nobility. The respective release locations are marked with white crosses. North is up.

AHS up-wind is interesting. It is most probably caused by the the hill-shaped curvature of the island. That means that approaching air passing over the houses on Riddarholmen, approaches the houses close to the release. Part of the flow then passes over the houses while a smaller part goes down and flows back through the alleys. Another interesting feature of this release is the high dosage seen (red) in the yard of a triangular building about two blocks downstream of the release, marked by an arrow. Obviously, the flow at this location has been such that although 'only' severe injuries have affected the area around this house, this particular location is lethal. A similar effect can be seen in an alley even further down-stream (also marked by an arrow).

Similarly, the release just off the House of Nobility has a much less obstructed way down-stream and in consequence the dosage along that path is also lethal. However, due to channeling into the streets large doses are seen also along the streets leading south-east from the release location.

3.2.3 VX (field 4, 5 and 8)

The second of the supposed deliberate releases is of the nerve gas VX. The bomb here is identical to the Sarin bomb. The bomb is filled with 10 kg of VX. In the explosion of the bomb, 40$\%$ of the VX is vapourized while the remaining 60$\%$ forms a ground contamination. The ground contamination is 10m x 50m, with the initial cloud being 10m x 10m x 10m with center at 6m above ground. The surface contamination evaporates with a speed of $2.8 \cdot 10^{-6}$ times the contamination density (g/m^2). This corresponds to a ground temperature of approximately 5^oC.

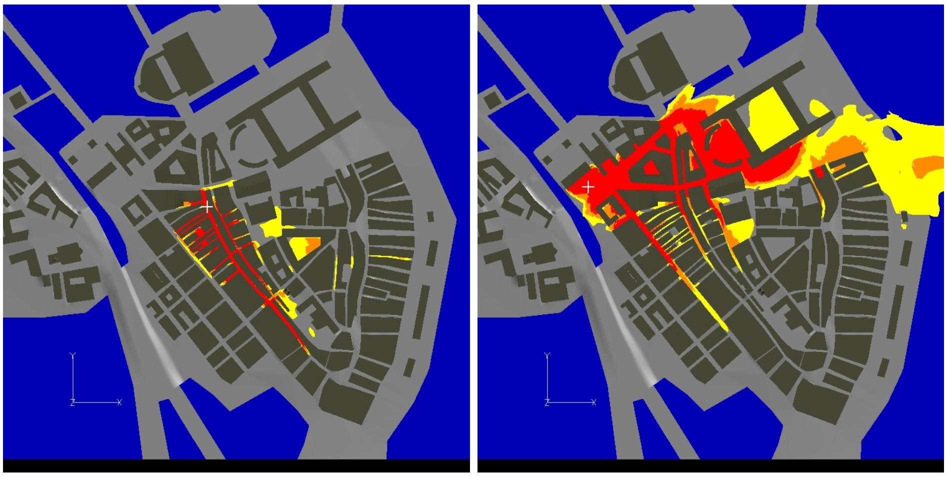

Figure 10: Resulting dosage for release of the nerve gas VX at two locations. One on Västerlånggatan and one just outside the House of Nobility. The respective release locations are marked with white crosses. North is up.

VX deposits on dry surfaces with $V_d = 0.01ms^{-1}$ and on wet surfaces with $V_d = 0.02ms^{-1}$.

The releases are collocated with the two Sarin releases. The resulting dosage of the VX releases can be seen in Figure 10. Like for Sarin a code error meant that the agent did not start to evaporate until after 980 seconds. Also for VX the dosages for this secondary release are negligible compared to the primary release. For this reason the secondary release is not further presented here. Also like Sarin, in Figure 10 yellow indicates dosage representative of light injuries, orange indicates severe injuries and red indicates lethal injuries. Direct contamination of human skin or clothes have also not been considered here.

Similar results like those drawn from the Sarin releases in subsection 3.2.2 can be drawn from the VX releases. Since these releases were made at the same places and at the same times, the differences in dosages relate mainly to the toxicity of the substances and what part of the release that is initially gaseous (as opposed to forming a ground contamination).

3.2.4 Anthrax (field 6 and 7)

Anthrax spores were chosen for a biological agent to be released. Two locations were chosen; one on top of the roof of a house across the street from the House of Nobility (field 6), and one in the passageway between the parliament and the old national treasury (field 7). The biological releases are continuous all through the simulation, with 10^9 spores being released every second. The releases are in one single grid cell. The deposition is given by $V_d = 0.002ms^{-1}$. The resulting dosages for the biological releases can be seen in Figure 11. In that figure yellow

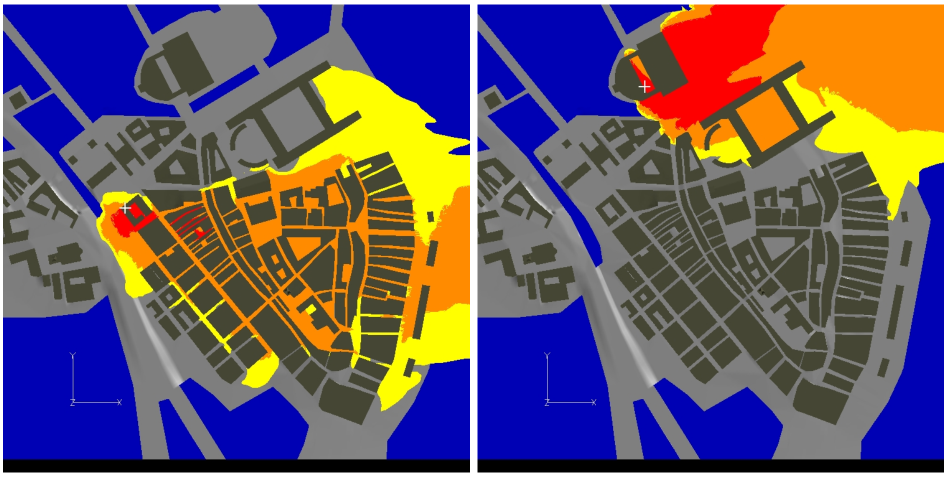

Figure 11: Resulting dosage for release of anthrax spores at two locations. One near the wall in the passageway between the parliament and the old national treasury, the other on the roof of a building near the House of Nobility. The respective release locations are marked with white crosses. North is up.

indicates that 5 $\%$ of the population has been infected by the spores, orange indicates that 15 $\%$ has been infected and red indicates that 50 $\%$ has been infected by the Anthrax spores.

A distinct difference can be seen in the size of the area of high level of infection (red). It is apparent that the source on the top of the roof (field 6) spreads much of the spores over the city while only a lesser amount of spores reaches the ground level and can infect people there. In the release in front of the House of Nobility (field 6) an area of large dosage can be seen just in the lee of the release. This area of high dosage is probably caused by the same kind of flow that causes the back flow of gas from Västerlånggatan, i.e. the increasing altitude of the ground. Since the settling velocity is ignored in the calculation the results should mainly be valid for a released aerosol with small aerosol particles. A diameter $d = 2\mu m$ yields a total settling distance (the distance in the vertical that the particle falls relative to the surrounding air, due to gravity) less than $1m$. If $d = 20\mu m$ the corresponding value would be approximately $18m$ which of course would alter the results by giving shorter distances for the particles to disperse over.

3.3 Point source versus line source

The releases have been placed at several locations in order to find interesting features in the dispersive patterns. One such interesting feature appears in the dispersion of field 1. Referring back to Figure 8 the release location can be seen marked by a white cross. However, due to the

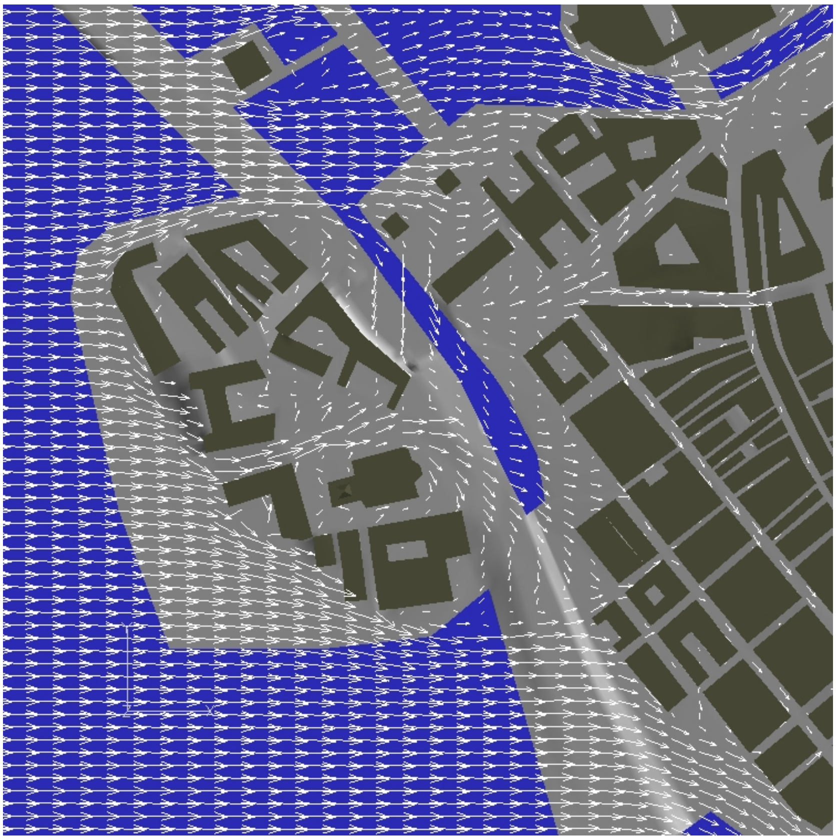

Figure 12: Wind vectors 10m above ground at Riddarholmen. The vortex in the center of the figure is a persistent feature of the simulation and has vital implications for the first AHS release (see 3.2.1).

westerly wind (coming from left in the figure) being blocked by Riddarholmen a considerable portion of air sweeps around the northern corner of Riddarholmen and proceeds south-east along the highway. An example of this for one single instant in time (timestep 50, $t = 250s$) can be seen in Figure 12 where the wind at 10m above ground is plotted as vectors. The vortex that can be seen turning clock-wise around the north-eastern corner of Riddarholmen and on to the highway is in fact a very persistent feature and this vortex has two important implications. The persistence of the vortex means that air is continuously pumped southward (down in the figure) over the highway. This in turn means that although there is really a point source, the dosage (see Figure 8) seem to originate from a line source. Also, the flow from the vortex onto the houses on Riddarholmen transports much of the AHS this way that there is in fact a considerable dosage on locations upwind of the release location.

This vortex structure and the flow south-east over the highway is important for many of the

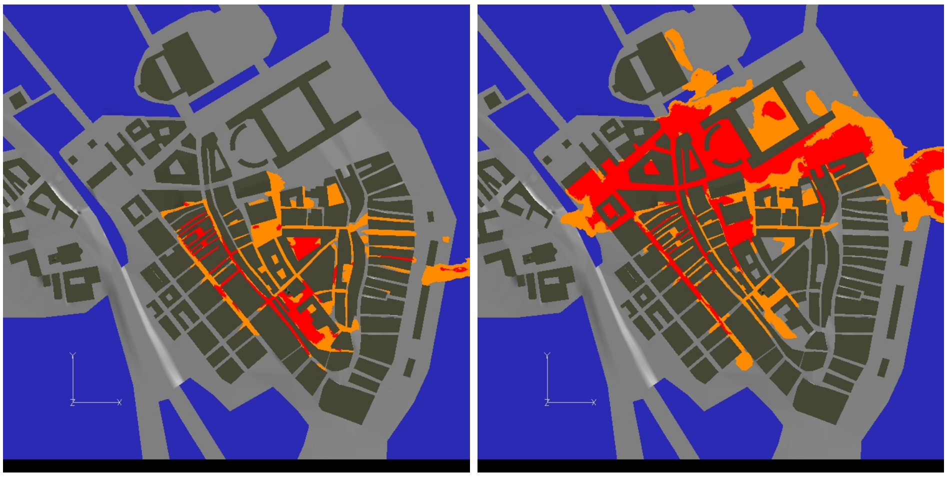

Figure 13: Concentration 3 m above ground level for VX at two release locations.

releases. Referring back to subsections 3.2.1-3.2.4, all releases but the one at the parliament have been affected by the flow along the highway. The influence have been either like bringing gas upwind (like subsection 3.2.1 and the releases on Västerlånggatan) or by bringing substance down (like the biological release off the House of Nobility). It is also most likely that this vortex structure and the associated effects on releases would differ greatly even for a modest change in inflow direction or speed.

3.4 Dependence on release location

The dependence on release location is illustrated by Figure 13 and Figure 14, already briefly mentioned in subsections 3.2.2 and 3.2.3. Figure 13 shows instantaneous concentrations (timestep 100, $t = 500s$) at three meters above ground level. The figure shows clearly the difference in how efficiently the AHS is transported through the city.

Figure 14 shows streamlines originating at the two release locations for four different timesteps in the simulation. The streamlines show that consistently, the airflow passing by the release on Västerlånggatan continues along Västerlånggatan. Any flow leaving Västerlånggatan does so by going vertically over the roofs of the houses. Once the air have risen over the houses, it is caught by the mean stream going over the city and is quickly swept away downstream of the island, thus removing the harmful substances from the city (for the moment we ignore parts of the actual city that are not included in the computational domain).

Conversely, the air passing the release point off the House of Nobility, does not show such a consistent flow pattern. Rather, that flow is characterized by a lot of turbulence. At one instant

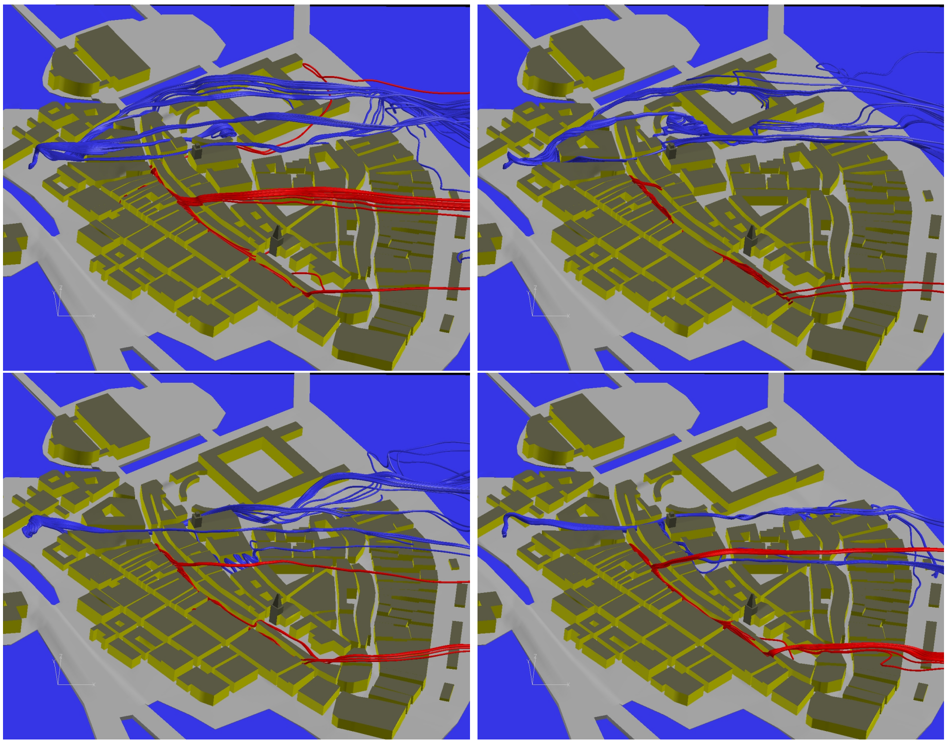

Figure 14: Instantaneous streamlines from the release positions at Västerlånggatan and outside the House of Nobility. The panels show timesteps 1, 50, 100 and 200 respectively, equaling times 5, 250, 500 and 1000 seconds.

the flow passes rather far to the north, and mainly above the houses. At another, the flow passes through the alleys rather far south. Similarly the air passing this release location is going up above one house, then diving to the ground again, and so on. The resulting effect is that the substance release off the House of Nobility is dispersed more efficiently than the release on Västerlånggatan. The toxicity is however so large with these substances that although the dispersion is greater at the release off the House of Nobility, it is not sufficient to make the dosage less than lethal. In fact, looking in detail (not shown in figures), the dosage on Västerlånggatan is much higher than that around the royal palace, for the same releases at these locations. Since the lower dose around the palace is still lethal however, that difference is not important, except for the study of the flow field. However, for a smaller release the differences could be crucial.

3.5 The urban dome

In Figure 13 an isolated area of rather high concentration can be seen on Skeppsbron. The lack of connections between this area and the polluted area upwind is due to vertical motion. In fact, the high-concentration in the air at this location comes from above. In lack of static stability stopping vertical motion a large part of the released substances rise vertically over the houses, attach to the free flow there and is transported over the city. Part of this flow going over the city will re-attach to the ground, bringing polluted air from Västerlånggatan directly to Skeppsbron.

This feature points at the importance of atmospheric static stability. The present simulation is performed with neutral stratification. The real city may however experience deviations from strong stable stability during winters to unstable conditions during hot summer convection. Needless to say, such difference in the stability would yield strong differences in the dispersion patterns and thereby in the dosages affecting inhabitants.

4 Conclusions

In the present work we report on a LES simulation of releases of several different contaminants and their dispersion through the city. The simulation points to several important features of urban contaminant transport and dispersion.

- The urban geometry creates vortex structures that may transport AHS against the direction of mean flow.
- Stratification is likely to be very important when estimating the transport/dispersion of an AHS release.
- The structure of houses near the release location can be very important
  - A point source may appear like a line or area source to locations down stream
  - A dominant direction of streets leads the AHS in that direction.

The simulation presented in this report has several limitations and simplifications. Therefore the conclusions listed above are most likely dependent on a number of prerequisites. Some of the major limitations of the current model will be summarized here.

The model does not treat or take into account:

- time of day / time of year
- deviation of the atmospheric stratification from neutral stratification

- temperature / solar radiation
- chemical composition of the AHS
- different partitions between gaseous form and ground contaminant
- different boundary conditions

The present simulation is not an exhaustive description of an outcome. Rather, it is an example of what can be done.

5 Discussion

In view of the increased threat of deliberate or accidental release of acute harmful substances such as toxic gas, biological agents or radiological material there is a demand for detailed simulations of such releases. The application of such models to an urban environment, where the threat is likely to be largest and where the effect would be the worst, poses a challenge. Successful simulation of such releases require a detailed geometry for the city, a grid resolution sufficient to satisfactorily resolve the city and relevant flow features within that. Hexahedral grids are often used for LES applications. The reason for this is mainly in their ability to resolve boundary layers. The down side of using a structured grid, like the hexahedral grid used here, is that the lines from which the grid is made, may not cross. This has the effect that semi-circular geometries forces the grid to either expand or contract. This in turn gives unnecessary high (or too low) resolution in different parts of the grid. A possible relief for this problem would be to use a tetrahedral grid in which the resolution can be kept more uniform. The down side of that solution may be a lower numerical accuracy. The ability of a tetrahedral grid (which could perhaps also be auto generated) to support an accurate simulation of urban dispersion is yet unknown. This is a question calling for further investigation. The simulation also need to take into account such complex physical features as deposition on various surfaces, stratification, and differences in solar radiation.

The simulation presented here constitutes a first effort at simulating urban dispersion. The simulation has many simplifications and limitations. Perhaps the most severe limitation is that no stratification is included. LES is well known to often be strongly dependent on boundary conditions. In an urban simulation, the boundary conditions form a further challenge. The urban environment presents several very complicated boundary conditions. For example, traffic will produce both turbulence, momentum, heat, and possibly mass (exhausts). Similarly, trees contribute a very complex obstruction to the flow. These boundary conditions are probably important, but they are also very difficult to describe in a consistent way. The present simulation does however show that it is possible to simulate urban flows. When this kind of simulations have been sufficiently validated, and important physical features like stratification and perhaps advanced boundary forcing (e.g. from trees, traffic) have been added, it can be used for a multitude of functions. Among these are

- Time dependent realistic scenarios.
- Training and education of rescue personnel.
- Risk assessment for exposed regions
- Preparations for possible accidents
- Validation and calibration of fast-response models (templates) or similar for use by first-responders on the scene of an accident
- Creation of tactics for urban warfare through simulation of visibility in presence of pyroclastic flows, i.e. battle-dust

With the fast evolution in computer power it is likely that very soon the computer power will not be the main impediment for accurate simulations of urban contaminant transport.

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