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COMPARISON OF SOME COMMERCIAL DISPERSION MODELS FOR HEAVY GAS RELEASES

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Abstract: The commercial operational dispersion models ARGOS and SLAB have been used to calculate downwind concentrations of chlorine and ammonia in urban and rural environments. The models are in fair agreement. The results from the urban dispersion have been compared with LES. While the operational models gave fairly similar results to LES for the sizes of the hazard areas, there were much lower peak concentrations of both chlorine and ammonia close to the release site. One of the releases of chlorine from the Jack Rabbit I field trials was also modelled. The results from ARGOS and SLAB agree with the sensor measurements when the source is modelled as an evaporating pool with duration between 60 sec and 180 sec.

Key words: *Dense gas dispersion models, ARGOS, SLAB, Urban environments, Jack Rabbit I field trials.*

INTRODUCTION

Toxic industrial chemicals are produced, transported and stored in relatively large quantities. Many of the most toxic chemicals, like chlorine and sulphur dioxide, are heavier than air. Ammonia is lighter than air, but since it is most often stored and transported as pressurised, liquefied gas, a release of liquid ammonia will result in a dense cloud close to the release site. Dispersion of a heavy gas is a complex process and challenging to model, especially in urban areas. Some experiments to study the dispersion of dense gases are the field trials Jack Rabbit I and II, conducted at Dugway Proving Ground, Utah, USA in 2010 and 2015-2016 (Hanna *et al*., 2012)(Hanna *et al*., 2016), and the wind tunnel experiments carried out at the University of Surrey, UK during the EDA project MODITIC (Endregard *et al.*, 2016).

This paper describes modelling of the dispersion of chlorine and ammonia with the commercial atmospheric dispersion models ARGOS and SLAB. These models give results quickly, but do not produce highly resolved hazard areas. Some of the simulations have been validated against detailed Large Eddy Simulations or against the Jack Rabbit field experiments.

ARGOS

ARGOS is a software tool, sold by PDC-ARGOS (Denmark), for crisis analysis involving CBRN agents[1]. The dispersion is calculated with the sub-model Rimpuff, which is a local scale puff model taking into account local wind variations and turbulence levels. ARGOS includes a source model for estimating the release rates from containers and pipes as well as evaporation of spills on the ground, and includes a model for dispersion of heavy gasses (HeavyPuff). Obstacles can be taken into account through the sub-model Urban Dispersion Model (URD). These submodules in ARGOS are developed by the Technical University of Denmark (DTU), Department of Wind Energy.

SLAB

SLAB is an atmospheric dispersion model for denser-than-air releases (Ermak, 1990). The gas cloud can be treated as a steady plume, puff or a combination of the two depending of the source characteristics. SLAB handles several release scenarios including ground level and elevated jets, liquid pool evaporation

[1] http://www.pdc-argos.com/

and instantaneous volume sources. SLAB itself is a freeware, but in the present study, the SLAB View Windows graphical user interface from Lakes Environmental Software was used.

LARGE EDDY SIMULATIONS (LES) MODELLING

Computational Fluid Dynamics is a numerical solution of the equations governing the motions and interactions of fluids. Due to the turbulent nature of flows, an analytical solution of these equations is in general not possible. With CFD, the equations are solved iteratively in space and time, and there are several models within CFD with varying degrees of accuracy and computational requirements to choose from. LES is one of these models. The computational requirements for CFD are large compared to operational models. A simulation for gas dispersion with LES can take days to weeks to complete.

COMPARISON OF OPERATIONAL AND CFD MODELLING IN AN URBAN AREA

Earlier studies have shown relatively small differences between ARGOS, SLAB and also the Hazard Prediction and Assessment Capability (HPAC) package from U.S. Defence Threat Reduction Agency (DTRA) for dispersion in rural areas (Tørnes *et al*., 2010). It was therefore of interest to compare the operational models ARGOS and SLAB for dispersion in an urban area. The results are also compared with results from LES of the same scenarios (Wingstedt *et al*., 2012).

Chlorine vapour has a density of 3.71 kg/m^3 at the boiling point (Tb = −34.1 °C) and atmospheric pressure, that is 2.5 relative to air. Because of this density difference, a massive release of chlorine will greatly influence the micro-meteorology near the release site, resulting in a velocity field which is relatively independent of the ambient wind field. A stable stratified boundary layer is formed in which mixing in the vertical direction is reduced. Therefore the toxic cloud can linger fairly long around the release site.

Ammonia vapour has a density of 0.86 kg/m^3 at the boiling point (Tb = −33.5 °C) and atmospheric pressure, that is 0.6 relative to air. Liquid ammonia released into the atmosphere will evaporate, and heat for the evaporation process is taken from the ambient air, resulting in a cold mixture of ammonia vapour and air that can be denser than the surrounding air. After the evaporation process is finished, new air is introduced to the mixture, the temperature will rise, and eventually the gas will become lighter than air.

During the simulations, two tonnes of respectively chlorine and ammonia were released during one minute with a release rate of 33.3 kg/s. The source was positioned close to the ground and the release directed upward. An ambient wind field with a speed of 3 m/s from west measured at 10 m height was chosen. The ambient temperature was set to 15 °C.

Results for Chlorine

Table 1 gives the maximum travel distances and the time to reach this distance for the AEGL levels (AEGL, 2017) for ARGOS (with URD or HeavyPuff) and SLAB. The combined HeavyPuff+Rimpuff in ARGOS and the SLAB runs give longer maximum travel distances than ARGOS URD+Rimpuff. This is because the heavy gas cloud in ARGOS HeavyPuff and in SLAB is transported closer to the ground in the first phase after the release, and because retention by the buildings in the urban area is not included in the HeavyPuff + Rimpuff run. In both of the ARGOS cases, Rimpuff takes over from URD or HeavyPuff after a certain time. The chlorine plume in HeavyPuff travels very quickly because all the data from HeavyPuff is exported to Rimpuff during the first time step of the simulation even if the actual HeavyPuff dispersion takes several minutes. The chlorine results from ARGOS and SLAB are fairly similar; the maximum distances agree within a factor 1.5 between URD+Rimpuff and HeavyPuff+Rimpuff in ARGOS, and within a factor two between SLAB and ARGOS (HeavyPuff+Rimpuff).

The ARGOS results were compared against LES in (Vik, 2013). The hazard areas for AEGL-3 were fairly similar, while the areas for AEGL-1 and -2 were larger in the ARGOS simulation than in LES. A striking difference, however, between these modelling efforts are that the peak concentrations are larger by a factor of 20-30 in the LES compared to ARGOS (see Table 3 below).

Table 1. Releases of chlorine in central Oslo using 3 m/s wind at 10 m height. The maximum downwind travel distances and times to reach these distances are shown for the three AEGL-limits (10 min exposure times).

Model used	Maximum downwind travel distance (Time to reach maximum distance)		
	AEGL-3	**AEGL-2**	**AEGL-1**
ARGOS (URD+Rimpuff)	0.79 km (10 min)	3.5 km (24 min)	7.0 km (35 min)
ARGOS (HeavyPuff+Rimpuff)	1.2 km (4 min)	3.8 km (12 min)	7.4 km (23 min)
SLAB (measured at 2 m height)	1.7 km (8.5 min)	7.3 km (26 min)	16 km (50 min)

Results for Ammonia

The maximum cloud travel distances and times before the ammonia AEGL concentration limits (AEGL, 2017) are reached, calculated with ARGOS (using URD or HeavyPuff) and SLAB, are given in Table 2. Also in this case, ARGOS (URD+Rimpuff) gives a shorter time to reach the maximum extent for the concentration limits compared to ARGOS (HeavyPuff+Rimpuff) and SLAB (due to the reason explained above for the chlorine case). The downwind travel distances are in fair agreement between the models; the distances to the AEGL limits are within a factor of two.

Table 2. Releases of ammonia in central Oslo using 3 m/s wind at 10 m height. The maximum downwind travel distances and times to reach these distances are shown for the three AEGL-limits (10 min exposure times).

Model used	Maximum downwind travel distance (Time to reach maximum distance)		
	AEGL-3	**AEGL-2**	**AEGL-1**
ARGOS (URD+rimpuff)	0.14 km (4 min)	0.8 km (7 min)	2.1 km (14 min)
ARGOS (HeavyPuff+Rimpuff)	0.15 km (2 min)	1.2 km (4 min)	2.3 km (7 min)
SLAB (measured at 2 m height)	0.29 km (2.5 min)	1.4 km (7.0 min)	4.2 km (17 min)

The ARGOS simulations in this case were also compared with LES in (Vik, 2013). In the LES, concentrations above the AEGL-3 limit remains near the source location during the entire simulation time, while for ARGOS/URD the concentration of ammonia drops below the AEGL-3-level less than one minute after the end of the release. The extension of the ammonia cloud from ARGOS/URD in the upwind direction for the AEGL-1 and -2 levels are a factor three larger than with LES. For the other directions the extensions of the clouds are fairly similar. Also in this case, the peak concentrations are much larger in LES than in ARGOS (see Table 3).

Table 3 shows the peak concentration one and two minutes after the end of the release in the ARGOS and SLAB simulations and in the LES. LES produce much higher peak values than the operational tools. By comparing the peak values for chlorine and ammonia in the ARGOS/URD simulation, it is evident that ARGOS/URD treats these chemicals identically; since dense gas effects are not included in ARGOS/URD, and the source terms for the two scenarios are equal. SLAB has peak concentrations roughly a factor 3-4 larger than ARGOS, but still an order of magnitude lower than LES.

Table 3. Concentration peaks for LES, ARGOS/URD and SLAB one and two minutes after the end of the releases.

	Time after end of the release	**Maximum concentration (mg/m^3)**		
		LES	**ARGOS/URD**	**SLAB**
Chlorine	1 minute	$6.0 \cdot 10^4$	$1.9 \cdot 10^3$	$6.2 \cdot 10^3$
	2 minutes	$1.5 \cdot 10^4$	$5.6 \cdot 10^2$	$2.0 \cdot 10^3$
Ammonia	1 minute	$1.6 \cdot 10^5$	$1.9 \cdot 10^3$	$7.0 \cdot 10^3$
	2 minutes	$7.5 \cdot 10^4$	$5.6 \cdot 10^2$	$1.4 \cdot 10^3$

RESULTS FROM THE JACK RABBIT FIELD TRIALS, 2010

The Jack Rabbit field trials were conducted at Dugway Proving Ground, Utah, USA, in the period April 27th to May 21th 2010. Ammonia or chlorine was released downward into a depression with a diameter of

50 meters and a depth of two meters. For a description of the test program see (Storwold, 2010). In this paper, test number 5 with the release of two U.S. tons of chlorine has been used. The ambient wind speed was about 1.5 m/s and the air temperature was 3.5 °C at the time of the release. The depression was intended to hold up the released material for some time after the release. Therefore, in addition to a short duration vapour source, a source where vapour was released from a pool with the same dimension as the depression was used for the simulations. Various pool durations up to 900 seconds (15 minutes) were tested. The latter duration correspond roughly to the time calculated with the method described in (Briggs *et al.*, 1990) for dense gas removal from a valley by crosswinds, and also roughly with the observed time for all the vapour to be transported away in the experiment (although the transportation rate is higher early after the release and then decreases with time).

In Figure 1, the predicted centreline chlorine concentration at different distances from the source using ARGOS and SLAB is shown. The maximum readings from field measurements at three distances (25 , 50 and 100 meters) and the maximum predicted concentrations from a LES of the release at two distances (25 and 50 meters) from the source are also shown (Vik, 2015). When evaporation from a pool is selected in SLAB, the maximum airborne concentration is achieved at the edge of the 50 m diameter depression for all three source durations. The chlorine cloud is diluted as it travels further away from the source.

Figure 1 shows that SLAB predicts a higher initial chlorine concentration with the instantaneous or short duration pool simulation compared to evaporation from a pool. This is because a part of the release (12.8 %) during the first method was calculated as either pure vapour or a mixture of vapour and airborne liquid droplets, which, since SLAB does not take topography into account, is quickly transported downwind. In our view it is more realistic to represent the chlorine contained in the depression as a liquid pool only (no initial vapour or airborne droplet phase). The four SLAB calculations with evaporating pool gave different air concentrations close to the source, but approximately the same concentration of chlorine farther downwind, except for the longest pool duration (900 seconds).

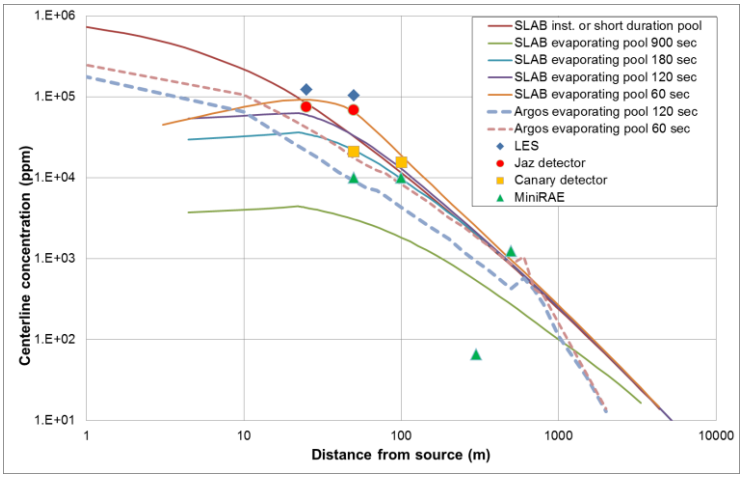

Figure 1. Comparison of chlorine centreline concentrations calculated by SLAB and ARGOS using different modelling options (see text for details). Maximum concentrations from field measurements using Jaz UV-VIS, Canary UV and MiniRAE photoionization sensors, and from LES are also shown in the figure. Not all the sensors are placed at the centreline downwind from the release site. Note that MiniRAE readings both at 50 m and 100 m are above the maximum range (> 10 000 ppm).

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

There are too few concentration measurements from vapour detectors in the area to conclude which method that best predicts the concentration. The available measurements fits relatively well with all the performed simulations, except for the SLAB simulation with 900 seconds pool duration (Figure 1). Since the transport rate out of the depression is largest in the start and then drops off, it seems reasonable that a pool duration less than 900 s is appropriate for this source characterisation.

CONCLUSIONS

No single existing operational dispersion model can be used in all possible scenarios. It is, however, important to have a good understanding of the tools in order to use them correctly and get meaningful results and to quickly be able to select the most suitable tool when a real incident occurs. The aim of this work is not to provide recommendations on which model performs best, but rather to demonstrate the similarities and differences of the models.

The comparison of the models that were carried out shows that the dispersion of heavy gases in urban areas are complex and not handled good enough using operational models and that there is a need for better source term modelling. The examples in this report show that ARGOS and SLAB produce similar results for the release of chlorine and ammonia in both rural and urban areas within the limitations of the models described above. An important difference between the operational models and LES, is that LES gave much higher peak concentrations close to the release site compared to ARGOS/URD. This can have a huge impact when calculating the toxic effects. ARGOS and SLAB simulations are also compared with the Jack Rabbit chlorine field trials; good agreement with the experimental measurements is found when the release is modelled as an evaporating pool.

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