Dispersion model predictions of the Jack Rabbit II chlorine experiments using Drift and Phast

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In 2015 and 2016, two sets of large-scale chlorine release experiments are being performed at the Dugway Proving Ground in Utah, USA. These experiments, known as the Jack Rabbit II trials, are being carried out to improve our understanding of the potential consequences of a tanker truck or railcar release of chlorine. The work is part of a four-year programme involving 5–20 short-tons (4536–18,144 kg) releases of chlorine and dispersion measurements up to a distance of 11 km from the source. The work follows on from the smaller-scale Jack Rabbit I experiments conducted in 2010.

The Health and Safety Executive (HSE) has participated in the Jack Rabbit II Modelling Working Group by providing dispersion model predictions for a 10 short-tons (9072 kg) chlorine release using two different integral models: Drift and Phast. The developers of these models worked with HSE to provide input and feedback on the predictions. The purpose of the simulations was to provide predictions of the likely chlorine concentrations in the dispersing cloud in advance of the 2015 experiments, to help select the locations for concentration sensors.

This paper briefly describes the background to the Jack Rabbit II experiments and provides an overview of the proposed experimental setup. The modelling methodologies used for simulating blowdown of the chlorine vessel are discussed and results are presented from three different models: Stream, Phast and Hysys. Predictions of chlorine concentrations in the dispersing cloud are then presented from both Drift and Phast, and sensitivity tests are performed to assess the impact of liquid rainout and the weather conditions. Based on these results, suggestions are made for the appropriate choice of sensors at the measurement arrays located at distances from 100 m to 11 km downwind from the release point.

Keywords: chlorine, flashing, impinging jet, dense gas dispersion, Jack Rabbit field experiments, consequence modelling

Background and objectives

In 2015 and 2016, two sets of large-scale chlorine release experiments are being performed at the Dugway Proving Ground in Utah, USA. These experiments, known as the Jack Rabbit II trials, are being carried out to improve our understanding of the potential consequences of a tanker truck or railcar release of chlorine. The work is part of a four-year programme led by the U.S. Department of Homeland Security to conduct experiments with releases of 5–20 short-tons (4536–18,144 kg) of chlorine. The work follows on from the smaller-scale Jack Rabbit I experiments conducted in 2010 [Hanna et al., 2012].

The Health and Safety Executive (HSE) has participated in the Jack Rabbit II Modelling Working Group (MWG) by providing dispersion model predictions for a 10 short-tons (9072 kg) chlorine release using two different integral models: Drift and Phast. The developers of the consequence modelling tools worked with HSE to provide input and feedback on the predictions. GT Science & Software contributed towards the work on Drift and DNV GL Software contributed towards the work on Phast.

The purpose of the simulations was to provide predictions of the likely chlorine concentrations in the dispersing cloud in advance of the experiments, in order to help select the most appropriate locations for chlorine concentration sensors. A particular concern was to ensure that the sensors were not exposed to concentrations above their upper (saturation) threshold level, which would prevent them recording any useful data. The upper threshold concentrations for the sensors were 100,000 ppmv (Jaz sensors), 10,000 ppmv (Canary sensors), 2000 ppmv (MiniRAE sensors) and 50 ppmv (ToxiRAE sensors). The modelling methodology was based on the premise of predicting reasonably conservative (upper) estimates of the concentrations and to perform sensitivity tests to examine the possible range in model predictions.

Overview of the Jack Rabbit II field experiment setup

The experiment considered by the MWG consisted of a release of pressure-liquefied chlorine from a storage tank located within an array of large obstacles that were used to represent a mock urban environment. The chlorine was released directly downwards from a six inch (152 mm) diameter hole in the bottom of a storage tank. The bottom of the tank was 1 m above a circular concrete pad that was 25 m in diameter, which was surrounded by a gravelled area with dimensions 183 m long by 122 m wide. The surface level of the gravelled area was approximately 60 cm above the surrounding flat desert surface (the playa). The centreline of the array of Conex shipping containers (the mock urban grid) was aligned towards the prevailing wind direction and the tank was located within the grid, approximately 30 m from the upwind edge. The mock urban grid was approximately 122 m long by 122 m wide. Figure 1 illustrates the proposed geometric layout of the experiment.

The mean obstacle height of the mock urban grid was 2.68 m and the lambda parameter which is used in many empirical urban boundary layer formulas [Britter and Hanna, 2003], was calculated to be 0.18. Accordingly, the surface roughness length (z_0) for the mock urban grid was 0.4 m. For the flat natural playa, z_0 was estimated to be 0.001 m.

Modelling teams participating in the MWG were given a set of target conditions to simulate for the 2015 experiments that consisted of a tank temperature of 20 °C (i.e. a chlorine saturation pressure of approximately 5.8 barg), a wind speed of 2 m/s at a reference height of 10 m and an ambient humidity of 40%. Variations were possible from these conditions and an upper bound of 6 m/s was placed on the wind speed. The experiments were due to take place at 7:00 a.m. Mountain Daylight Time and therefore it was assumed that the atmospheric boundary layer would be stable. The proposed downwind locations of the sensors outside the mock urban grid were along radial arcs at 200 m , 500 m , 1 km , 2 km, 5 km, and 11 km from the tank.

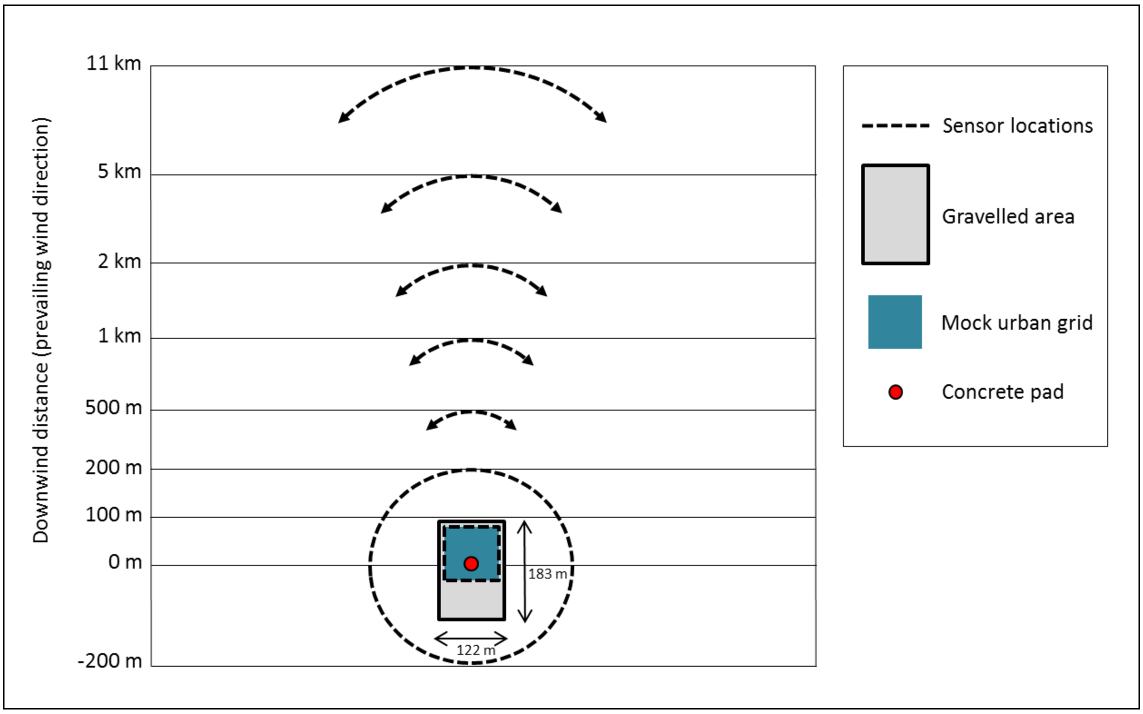

Figure 1. Geometric layout of the experiment (not to scale)

Consequence modelling tools and scenarios predicted

The two main software programs used by HSE for modelling dispersion of the chlorine cloud were the integral models Drift 3.7.2 and Phast 7.11.

Drift was developed by ESR Technology and is used by HSE to model dense gas dispersion. To simulate the proposed Jack Rabbit II experiment Drift was used in conjunction with two other models; the first is Stream A.7 which is an outflow model developed by HSE, the second is Gasp 4.2.12 which is a pool source model also developed by ESR Technology.

Phast was developed by DNV GL Software and is a comprehensive hazard analysis package that contains various sub-models, including ones for vessel discharge, pool evaporation and atmospheric dispersion.

In addition to using Drift and Phast, some simulations of the vessel discharge were also performed by HSE using the process simulation software package Hysys 8.6, which was developed by AspenTech. This work was carried out as an additional check.

One of the significant uncertainties in modelling the 2015 Jack Rabbit II experiments was the fraction of liquid chlorine that would rainout from the two-phase jet as it impinged on the concrete pad and dispersed along the ground. In order to predict reasonably conservative estimates, a baseline configuration was used which assumed no rainout and ‘F2’ weather conditions; F2 weather represents stable atmospheric turbulence (Pasquill stability class ‘F’) and a wind speed of 2 m/s. Two sensitivity cases were also carried out. The first assumed full rainout (i.e. all of the liquid striking the ground was assumed to rainout and form a pool); the second was similar to the baseline configuration (it assumed no rainout) but it used ‘D6’ instead of F2 weather conditions to represent neutral atmospheric stability (Pasquill stability class ‘D’) and a higher wind speed of 6 m/s (the upper bound in which the experiments would take place). Figure 2 illustrates the three scenarios that were modelled, where the red boxes highlight the variations in the sensitivity tests to the Baseline Case.

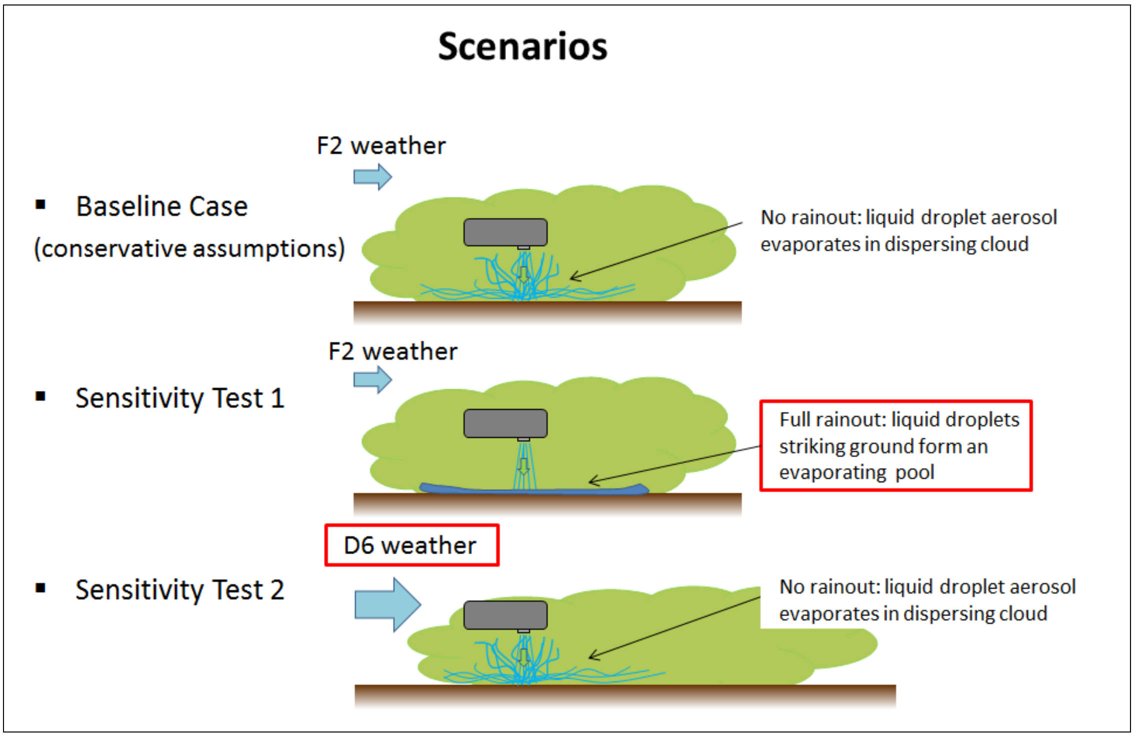

Figure 2. Illustration of Baseline Case and the sensitivity tests

Discharge predictions

The cylindrical chlorine vessel was fitted on its underside with a short flange which had an inside diameter of six inches (152 mm). A blanking plate was fitted to the end of the flange using explosive bolts and the discharge was initiated by blowing the bolts. An uncertainty in modelling the discharge concerned the nature of the flow through the orifice, i.e. whether chlorine would be discharged as liquid or as a flashing two-phase flow of liquid and gas. The mass release rate would be significantly lower for the two-phase flow case, due to choking at the exit. A review [Britter et al., 2011] suggested that for short orifices less than 10 cm in length, the flow would remain as a metastable liquid. This means that the orifice length is considered to be too small for the flow to establish thermodynamic equilibrium, and the chlorine is therefore assumed to remain liquid at the orifice. Therefore, baseline simulations were performed assuming metastable liquid flow. This was consistent with the aim to produce conservative (upper) estimates of the gas concentrations. Sensitivity tests were performed assuming flashing two-phase flow for comparison purposes.

Several different models were used to simulate the vessel blowdown. Three Phast simulations were performed in total: two of which used its discharge model configured to simulate a metastable liquid flow, with no flashing in the orifice—the first used its compressible liquid model and the second assumed the fluid was incompressible and calculated the discharge velocity from Bernoulli’s equation. In both these cases, the discharge coefficient was set to 0.6. The third Phast simulation assumed flashing two-phase flow through the orifice with a calculated discharge coefficient of 0.96. In all three cases, the expansion of the jet from vena-contracta conditions to atmospheric pressure (final conditions prior to air entrainment) was modelled using Phast’s ‘conservation of momentum’ sub-model.

Two simulations were performed using Stream: one assuming metastable liquid flow and the other assuming flashing two-phase flow. In both cases, the discharge coefficient was set to 0.61. Hysys was also used to model a metastable liquid discharge using the Peng-Robinson equation of state with a discharge coefficient of 0.6. For both Stream and Hysys, the discharge was treated as constant, whereas a time-varying discharge rate was modelled with Phast. The predicted mass release rates from all of the discharge models are compared in Figure 3.

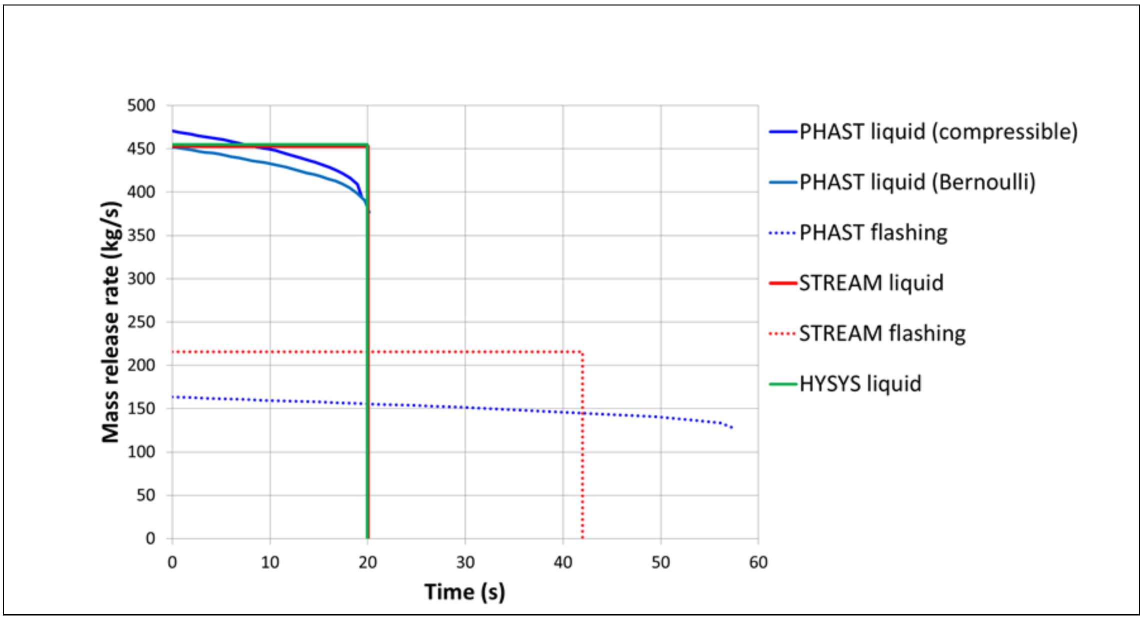

Figure 3. Discharge results for the cases studied

As expected, Figure 3 shows that the metastable liquid release models predicted higher mass release rates than the flashing liquid models. The metastable liquid models all produced similar initial release rates of 450–470 kg/s and release durations of approximately 20 s for the vessel to fully discharge. The Phast release rates using the compressible fluid model were marginally higher than the incompressible (Bernoulli) model. If flashing was assumed to take place within the orifice, the flow was choked and Phast predicted the initial release rate to be 160 kg/s and for the release rate to decrease gradually over time with a total release duration of 57 s. In comparison, the initial release rate using the two-phase model in Stream was 210 kg/s and the vessel took 42 s to fully discharge.

For the subsequent dispersion simulations, the liquid release model from Stream was used to provide source conditions for Drift and the metastable compressible liquid option was used for Phast.

Impinging jet source model

For the Drift dispersion model, the source conditions for the impinging jet were calculated from a separate Drift simulation of a downward-directed two-phase jet. The vaporisation of droplets within the jet was modelled assuming homogeneous equilibrium (i.e. the liquid and vapour shared the same velocity and temperature). Liquid chlorine was assumed to form an ideal solution with condensed water vapour. The conditions predicted at the ground (jet diameter, liquid fraction etc.) were extracted from this simulation and used to provide input conditions for the subsequent atmospheric dispersion simulation with Drift, using its low momentum area source model. The area source model used the diameter of the jet at its impact point on the ground as the initial source size but it allowed for additional gravitational spreading and dilution over the source. For the Baseline Case dispersion simulations and for Sensitivity Test 2 (Figure 2), it was assumed that all of the liquid remained in the dispersing cloud, with no liquid deposition on the ground. For Sensitivity Test 1, Drift predicted that 75% of the mass of chlorine impinged on the ground as a liquid and rained out to form a pool.

To model the impinging jet in Phast, the standard downward-impinging release option was not used, since it is considered to be oversimplified. Instead the chlorine release from the vessel was modelled as a jet with a release angle of -90° relative to horizontal. Two different methods were applied for droplet modelling:

- For the Phast Baseline Case and Sensitivity Test 2 simulations the ‘no rainout, equilibrium’ option was used. This means that rainout is not allowed, separate droplet modelling is not carried out, and a homogeneous equilibrium thermodynamics model is applied for mixing the moist air with the chlorine, where the liquid temperature is presumed to be equal to the vapour temperature.

- For the Phast Sensitivity Test 1 simulation rainout is allowed, and separate droplet modelling is carried out. Here the ‘DNV droplet JIP’ method was used to calculate the initial droplet size [Witlox and Harper, 2013] and the droplet thermodynamics were modelled using the non-equilibrium model, which allowed the droplets to have a different temperature from the surrounding vapour. The non-equilibrium droplet thermodynamics model tends to produce a larger amount of rainout than the alternative equilibrium model. Phast predicted approximately 80% of the chlorine released to rainout and to form a pool.

Evaporating pool source model

For Sensitivity Test 1, where all of the liquid striking the ground was assumed to rainout, two different models were used to predict the rate of pool spread and evaporation:

- The first model was Gasp, which was used to provide source conditions for the Drift dispersion model. Gasp calculates the heat transfer rate from the concrete substrate assuming perfect thermal contact, and its heat transfer model accounts for cooling of the substrate. The predicted time-varying vaporisation rate from Gasp was combined with the 25% of vapour from the two-phase jet to provide the source conditions for the Drift dispersion model.
- Secondly, the Phast dispersion simulations for Sensitivity Test 1 used the default pool evaporation model. In this case where rainout is modelled, Phast accounts for the addition of chlorine vapour from the pool back into the dispersing cloud.

In both cases, with Gasp and Phast, the pools were allowed to spread unrestricted across the ground. The concrete test pad in the experiments was fitted with a small lip at its edge to try to limit any spill-over onto the surrounding gravelled area. However, the presence of the lip was not modelled. The lip was installed in the experiments following previous experience in the Jack Rabbit I trials, where it was found that if chlorine liquid seeped into the porous desert surface it could take a long time to evaporate (which led to logistical problems in setting up repeated experiments). Because the lip at the edge of the pad was not modelled, Gasp and Phast would tend to over-estimate the pool vaporisation rate when the pool reaches its maximal extent.

Figure 4 shows the pool model results for Gasp and Phast for Sensitivity Test 1. The pool was predicted to spread beyond the edge of the 12.5 m radius concrete test pad using both models. Gasp predicted the pool to reach a maximum radius of 23 m whilst Phast predicted a maximum radius of 16 m. Phast reaches its maximum radius at the time when the pool thickness reaches its minimum value; afterwards the pool breaks up into ‘blobs’ resulting in a reduction of the ‘effective’ pool area and the associated ‘effective’ pool radius. Thus the Phast ‘pool radius’ shown in Figure 3 is the ‘effective’ pool radius and not the visible actual pool radius. To account for unevenness of the ground Gasp can use puddle depth, in which case there is a similar interpretation to Phast. However, the Gasp modelling work undertaken here includes no such minimum pool depth. The Gasp and Phast rainout results are conservative in the sense that they assume that all of the liquid striking the ground rains out, whereas in reality some of the liquid will disperse as an aerosol.

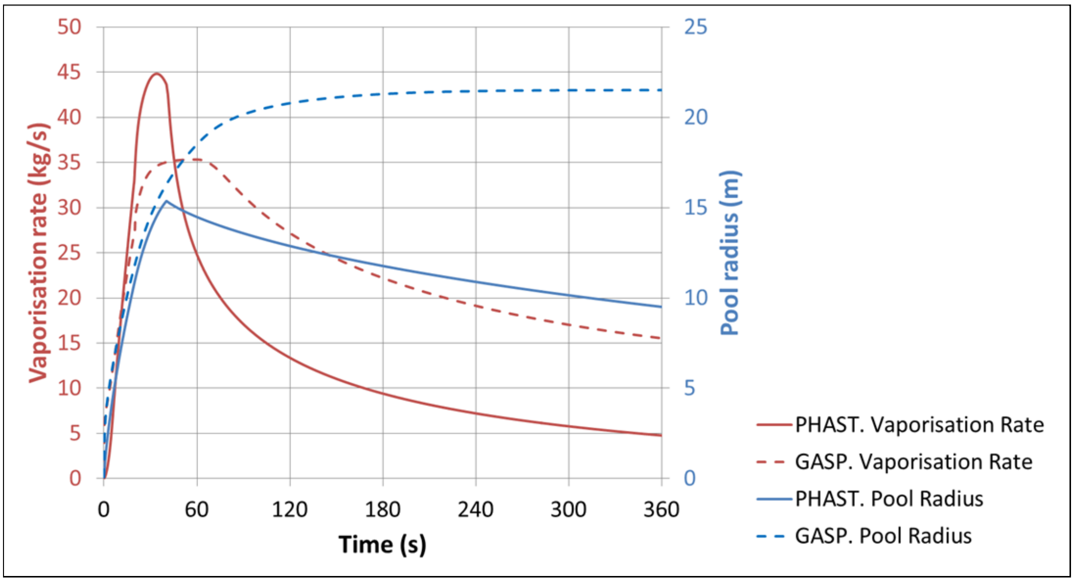

Figure 4. Pool vaporisation results

One of the effects of pool formation on the dispersion predictions was that the duration of the chlorine vapour source was extended considerably. Figure 3 shows that the vessel discharge was predicted to terminate within 20 s (assuming metastable liquid flow through the orifice), whereas the pools were predicted to remain evaporating for more than 360 s. A comparison of Figures 3 and 4 also shows that the mass flow rate of vapour produced by the pool models reached a maximum of around 10% of the total mass flow rate (45 kg/s of vapour from the pool as compared to a discharge rate from the vessel of 450 kg/s, using Phast).

Dispersion modelling

Methodology

In the experiments, the mock urban grid spanned a distance of approximately 100 m downstream from the release point (Figure 1). Within this area the surface roughness length, $z_{0,}$ was assumed to be 0.4 m. Further downstream, z_0 was taken as 0.001 m to represent the flat natural playa. Drift and Phast do not allow for a change in surface roughness at different distances within a single dispersion simulation. For this reason, two simulations were performed for each scenario: a ‘near-field' scenario that used a uniform z_0 of 0.4 m, and a 'far-field' scenario that used a uniform roughness of 0.001 m. At 100 m downwind, the centreline concentrations of the 0.001 m z_0 simulations were often higher than those produced using a z_0 of 0.4 m. Where there was a significant discontinuity, the results were blended together by matching the centreline concentrations at 100 m as shown in Figure 5. This method was proposed during the modelling work by Graham Tickle.

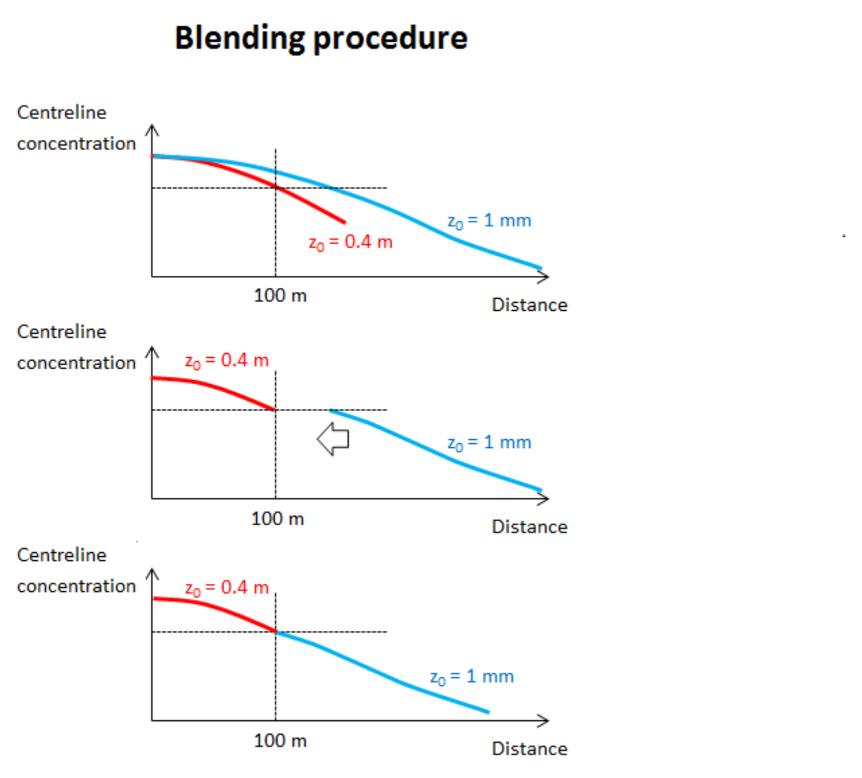

Figure 5. Illustration of the blending procedure used to combine dispersion model predictions obtained using two different (uniform) roughness lengths of 0.4 m and 0.001 m.

The effect of the short release duration was represented using Drift's finite-duration model. This accounts for mixing and spreading at the front and back edges of the cloud, i.e. diffusion and gravity-spreading effects in the along-wind direction. One of the acknowledged limitations of the model is that it uses a Froude number that has been tuned for continuous dense gas releases. It may therefore over-predict concentrations in the far-field for short releases, where the behaviour is closer to an instantaneous 'puff'. A short averaging time of 5 s was used, since the focus of the study was to assess whether concentration sensors could momentarily be exposed to high concentrations.

The release was modelled in Phast using the time-varying leak option in the Unified Dispersion Model (UDM) [Witlox and Holt, 1999]. This model splits the source strength into a number of time steps (release segments) with uniform source strength. For each release segment, a corresponding dispersion calculation is carried out. For each of the release segments the UDM calculations are similar to a finite-duration cloud; however, no quasi-instantaneous transition occurs and, therefore, the effects of along-wind diffusion and along-wind gravity-spreading are not taken into account. It is also possible that neighbouring cloud time fragments overlap at a given time. One of the consequences of this approach is that maximum concentrations may be over-predicted in the far-field, due to the lack of along-wind diffusion. The default short averaging time of 18.75 s was used. Furthermore in the near-field there may be inaccuracies in the Phast concentration predictions due to (a) absence of added air entrainment due to jet impingement on the ground, (b) a possible inaccurate value of the concrete heat conductivity and therefore inaccurate pool evaporation rate, and (c) the presence of obstacles (containers) which may cause trapping of the cloud.

Results

The predicted centreline gas concentrations from Drift and Phast for the Baseline Case are shown in Figure 6. For both Drift and Phast, there is virtually no discontinuity between the predicted concentrations 100 m downwind from the release point using either a uniform surface roughness of 0.4 m or 0.001 m, and therefore no blending was required to join the two results together at 100 m. The Phast centreline concentrations are consistently higher than those produced by Drift. At 1000 m the difference is around a factor of 20 (89,200 ppmv for Phast versus 4200 ppmv for Drift at a distance of 1 km). The 100,000 ppmv upper concentration limit for the Jaz sensors is predicted to extend as far as 250 m or 1000 m from the release point (depending upon whether one uses Drift or Phast, respectively). The 50 ppmv upper concentration limit for the ToxiRAE sensors is reached at 10.5 km downwind for Drift and 33.9 km for Phast. The higher concentrations produced using Phast are likely to result from the model ignoring the effects of diffusion and gravity-spreading in the along-wind direction. The jagged nature of the Phast result is due to the processing of raw data where cloud time fragments overlap. The peak concentrations produced by Phast are the values of primary interest here.

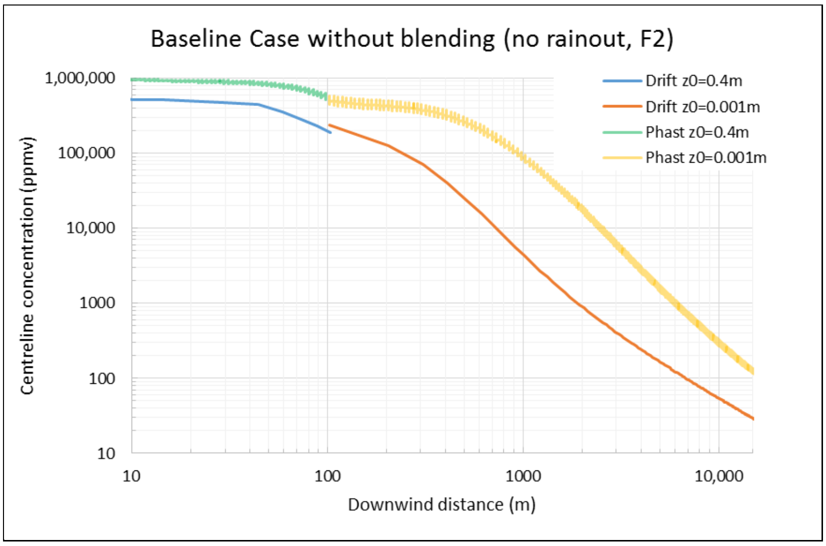

Figure 6. Predicted centreline concentrations for the Baseline Case without blending

Figure 7 shows the results from the same simulations as Figure 6, but with the results from the simulations using 0.4 m and 0.001 m roughness lengths extending from the source into the far-field, rather than cutting and joining them at 100 m. The results show that it is only in the far-field (beyond 100 m) where the simulations with different z_0 values begin to separate from each other, with the 0.001 m results becoming higher than those using z_0 = 0.4 m, due to the greater mixing and dilution in the higher roughness case.

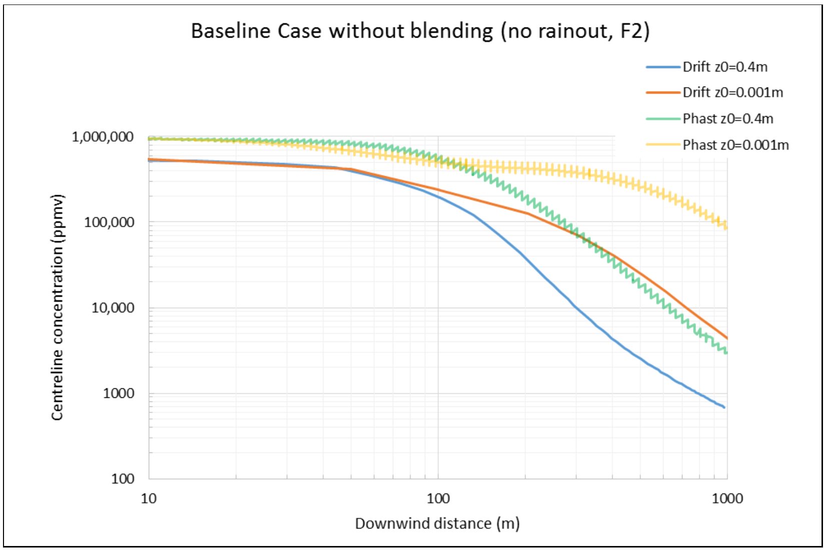

Figure 7. Predicted centreline concentrations for the Baseline Case, with the results using two different roughness lengths shown uncut, extending from the source to a distance of 1 km downwind

Figure 8 shows the results of Sensitivity Test 1 (which assumed rainout and pool formation) without blending. There is a clear discontinuity in the predicted centreline concentrations at 100 m using both Drift and Phast, with higher concentrations using z_0 = 0.001 m than 0.4 m. The Drift Baseline Case is included for comparison purposes.

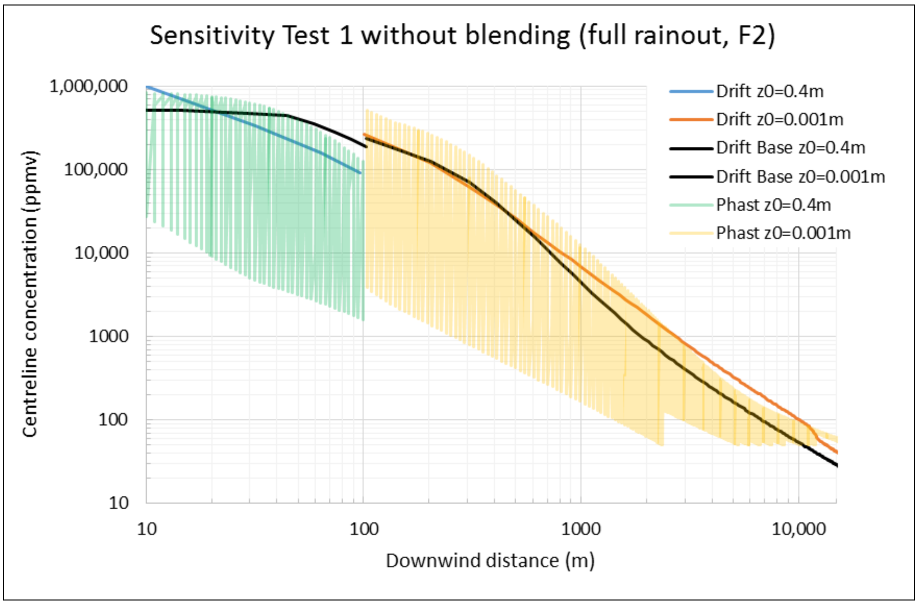

Figure 8. Predicted centreline concentrations for Sensitivity Test 1 without blending

Figure 9 shows the same results for Sensitivity Test 1 after blending has been applied. Above the pool source (up to a distance of around 20 m for Drift and 40 m for Phast) the concentrations are predicted to be higher for Sensitivity Test 1 than for the Drift Baseline Case. Further downwind the concentrations become lower than those of the Drift Baseline Case, before they rise up again above the Drift Baseline Case at around 600 m downwind for Phast and 900 m downwind for Drift. The lower concentrations in the near-field are probably due to the fact that the liquid chlorine in the impinging jet rains out to form a pool, whereas in the Baseline Case the liquid remains suspended in the dispersing cloud as an aerosol, where it evaporates and maintains high vapour concentrations. Further downwind, the higher concentrations with Sensitivity Test 1 are probably due to the longer duration of the vapour source from the pool. Overall, the Drift and Phast results are in closer agreement with each other for Sensitivity Test 1 than for the Baseline Case.

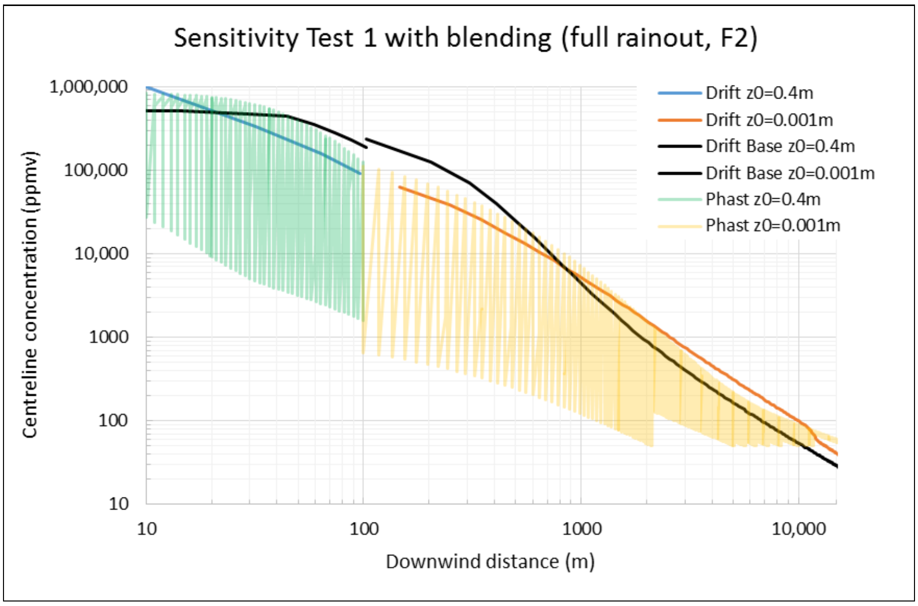

Figure 9. Predicted centreline concentrations for Sensitivity Test 1 with blending

Figure 10 shows the results for Sensitivity Test 2 (D6 weather conditions) without blending. Again, the Drift Baseline Case is included for comparison purposes. A similar discontinuity to Sensitivity Test 1 is observed at 100 m and the results are re-plotted in Figure 11 after blending.

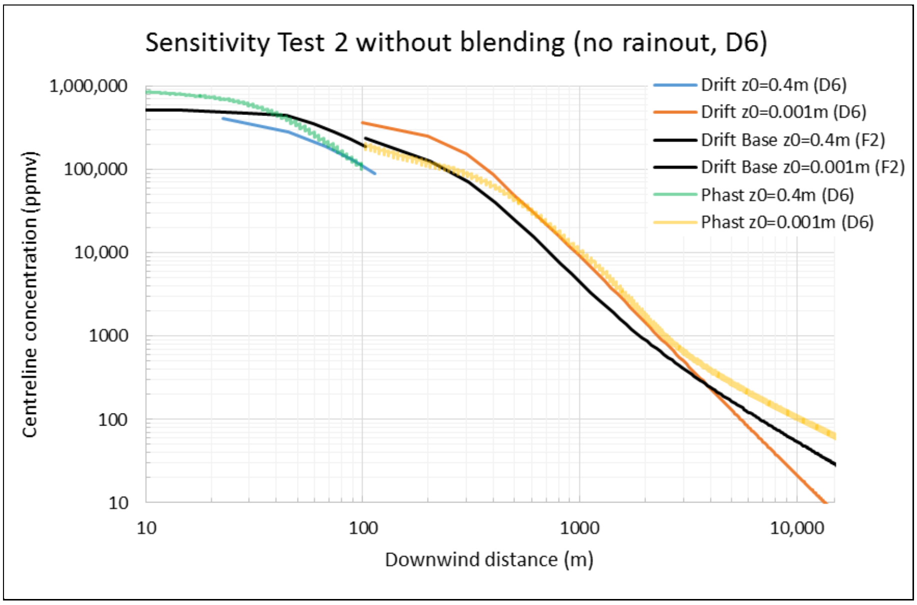

Figure 10. Predicted centreline concentrations for Sensitivity Test 2 without blending

Figure 11 shows that the change in weather conditions from F2 to D6 causes a factor of two decrease in the Drift centreline concentrations in a region spanning from 40 m to 400 m downstream from the source. Further downstream, between 700 m and 4000 m, the two weather conditions give comparable results. Beyond 4000 m, the concentrations are higher with F2 than for D6. Analysis of the results showed that steady conditions were quickly established in D6 weather conditions, whereas for F2 the release terminated before steady conditions could become established—in which case the F2 dispersion run is effectively treated as an instantaneous release (but with a Froude number tuned for continuous releases).

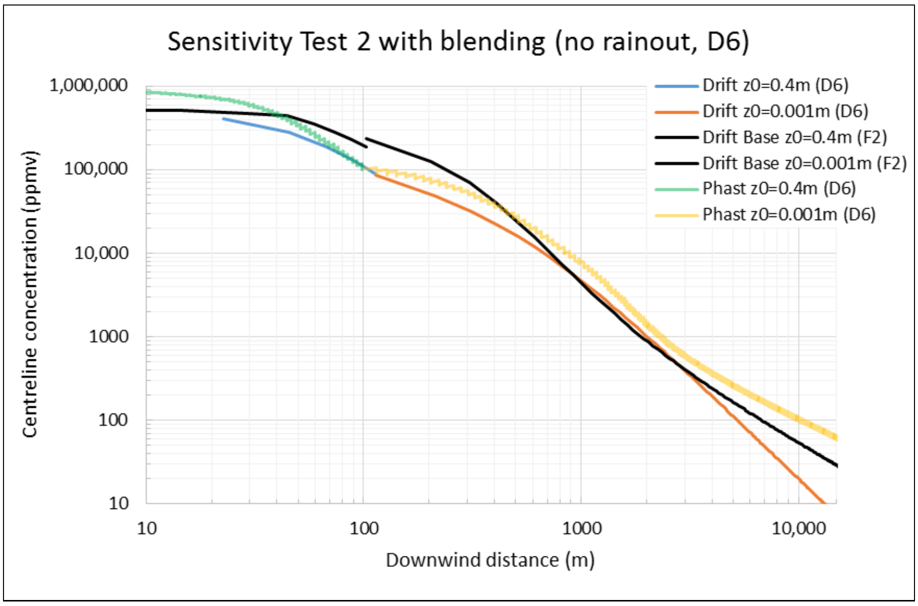

Figure 11. Predicted centreline concentrations for Sensitivity Test 2 with blending

Comparing the Phast results to those from Drift for Sensitivity Test 2, the two models produce similar results (within a factor of two) until a distance of around 4 km is reached. Further downwind from 4 km, Drift predicts a steady reduction in concentration whilst Phast predicts a more gradual decrease. As for the Baseline Case, the higher far-field concentrations predicted by Phast are likely to result from the model ignoring along-wind diffusion effects.

It is commonly assumed that concentrations in dispersing plumes are higher in stable, low wind speed conditions, but for short duration dense gas releases this is not always the case [Hanna and Chang, 2014].

Figure 12 shows a summary of all the dispersion model predictions at the seven sensor locations that range in distance from 100 m to 11 km from the source. Upper threshold concentrations for the four different sensors are shown as horizontal dashed lines. The Jaz sensors have the highest upper concentration limit of 100,000 ppmv and the dispersion model predictions suggest that these sensors should be placed close to the source, up to a distance of 1000 m downwind. The Drift and Phast Baseline Case results suggest that these sensors may become saturated at distances of up to 200 m (for Drift) or 500 m (for Phast). However, the maximum centreline concentrations for the Baseline Case results are notably higher than for the other sensitivity tests results, and they make the strong assumption that no liquid pool will be formed, which means that the models will tend to over-predict concentrations in the near-field.

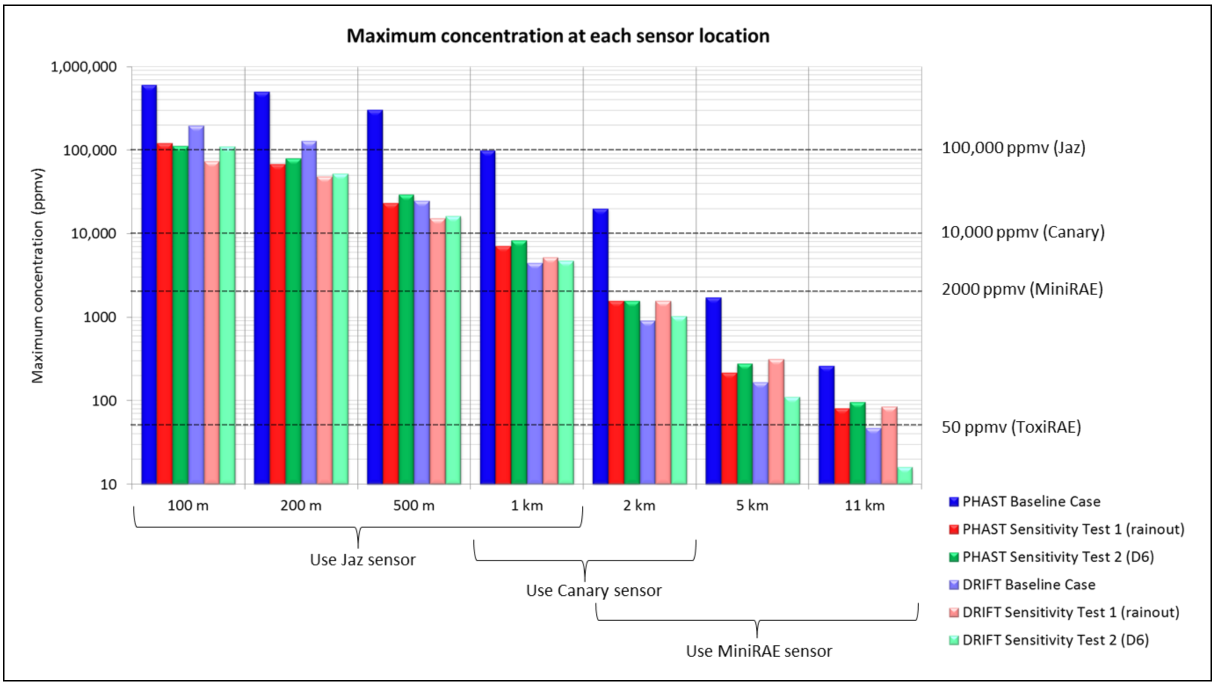

Figure 12. Predicted maximum centreline concentrations at each sensor location

The Canary sensors have an upper concentration threshold of 10,000 ppmv and the results suggest that they should therefore be located at a distance of 1–2 km downwind from the source. The MiniRAE sensors have a lower saturation limit of 2000 ppmv and should therefore be located at 2–11 km. The ToxiRAE sensors have an upper concentration threshold of 50 ppmv and the results indicate that they could reach saturation levels at a distance of 11 km. The only result that is significantly below the 50 ppmv threshold concentration is from Drift for Sensitivity Test 2 (D6 weather conditions). The Baseline Case result from Drift is 47 ppmv at 11 km, which is only marginally less than the 50 ppmv limit.

Conclusions

Dispersion model predictions have been presented using Drift and Phast for a 10 short-tons (9072 kg) release of pressure-liquefied chlorine through a six inch (152 mm) hole in the underside of a vessel, at a height of 1 m above the ground. The predictions were produced by HSE in support of the MWG to help select the location of the concentration sensors in the experiments. In order to provide reasonably conservative (upper) estimates of the concentration, a baseline configuration was modelled which assumed that the chlorine was discharged from the vessel in a metastable liquid state. The two-phase jet impinging on the ground was assumed not to produce a pool but instead the liquid was assumed to remain in the dispersing cloud as an evaporating aerosol of droplets. Atmospheric conditions were assumed to be low wind speed and stable (F2). Sensitivity tests were then performed to examine the effect of flashing in the orifice on the discharge rate predictions. A further two sensitivity tests were carried out which assumed that all of the liquid impinging upon the ground rained out to form a pool (Sensitivity Test 1) or that the wind speed was higher and the atmospheric stability neutral (Sensitivity Test 2—D6 weather conditions).

Phast predicted centreline concentrations that were generally higher than Drift (up to 20 times higher for the Baseline Case). This was probably due to the current model for time-varying releases in Phast not accounting for the effects of diffusion or gravity-spreading in the along-wind direction, which are accounted for by Drift. A planned future release of Phast will address this issue.

The dispersion results for the two sensitivity tests generally gave lower centreline concentrations than the Baseline Case. An exception was the Drift results for Sensitivity Test 1, where concentrations were higher in the far-field. This appeared to be due to the longer duration of the vapour source from the evaporating pool.

The conclusion from the dispersion results in terms of the placement of concentration sensors was that the Jaz sensors should be placed in the near-field up to 1 km from the release point. The Canary sensors should be placed 1–2 km downwind of the release and the MiniRAE sensors 2–11 km downwind of the release. The ToxiRAE sensors could be placed at the 11 km arc but, according to the dispersion model results, their upper concentration threshold of 50 ppmv may be exceeded.

These results were produced prior to the 2015 Jack Rabbit II experiments, to help select the appropriate location of concentration sensors. Once the experimental data becomes available in 2016, the simulations will be revisited and a model validation exercise will be undertaken. In the summer of 2016, the second set of Jack Rabbit II experiments are planned to take place which will involve horizontal jet releases of chlorine across open, unobstructed flat terrain, without the presence of the mock urban array. HSE plans to perform further dispersion model predictions in preparation for those tests, to help position the concentration sensors, and to conduct a second validation exercise afterwards, when the data is made available.

Disclaimer

The final configuration of the Jack Rabbit II experiments may be slightly different from the conditions summarised in this paper. The conditions modelled here were solely used to help inform the location of concentration sensors and were based on nominal ‘target’ conditions for the experiments.

DNV GL Software provided HSE with guidance on the appropriate methodology to use with Phast, but the Phast simulations presented in this paper were performed by HSE and have not been independently checked by DNV GL Software. As part of separate work by DNV GL Software (not reported as part of the current paper), additional results were submitted to the MWG by DNV GL Software using new, improved discharge and dispersion models that will be included in a future release of Phast.

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References

Britter, R., Weil, J., Leung, J. and Hanna, S., 2011, Toxic industrial chemical (TIC) source emission modeling for pressurized liquefied gases, Atmospheric Environment, 45, p1–25.

Britter, R. E. and Hanna, S.R., 2003, Flow and dispersion in urban area, Annu. Rev. Fluid Mech., 35, p469–96.

Hanna, S., Britter, R., Argenta, E. and Chang, J., 2012, The Jack Rabbit chlorine release experiments: Implications of dense gas removal from a depression and downwind concentrations, Journal of Hazardous Materials, 213–214, p406–412.

Hanna, S. and Chang, J., 2014, Puff or plume? American Meteorological Society (AMS) Annual Meeting, Paper 4.3, Atlanta, Georgia, USA, 4 February 2014.

Witlox, H.W.M. and Harper, M., 2013, Two-phase jet releases, droplet dispersion and rainout, I. Overview and model validation, Journal of Loss Prevention in the Process Industries, 3, 453–461.

Witlox, H.W.M. and Holt, A., 1999, A unified model for jet, heavy and passive dispersion including droplet rainout and re-evaporation, Det Norske Veritas, London, UK, CCPS 1999 UDM paper.