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JACK RABBIT II 2015 CHLORINE RELEASE EXPERIMENTS: SIMULATIONS OF THE TRIALS USING DRIFT AND PHAST

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Abstract: Simulations of the Jack Rabbit II 2015 chlorine experiments are presented using two different integral dispersion models: Drift 3.7.2 and Phast 7.11. Comparisons are made to the experimental data in terms of both the peak concentration and toxic load (TL). A global sensitivity analysis is also presented to help assess the impact of uncertainties in the Drift model inputs. The results show that the models produce reasonably good agreement with the Jack Rabbit II data if they account for rainout of liquid chlorine from the two-phase jet and evaporation of the resulting chlorine pool. Peak concentrations and TL are significantly over-predicted if rainout effects are ignored. The sensitivity analysis shows that dry deposition could have a dominating effect on the predicted concentrations of these experiments if a high deposition velocity of 5 cm s^{-1} is assumed.

Key words: *Jack Rabbit experiments, chlorine, dense gas dispersion, toxic load, sensitivity analysis*

INTRODUCTION

In 2015, the first phase of the Jack Rabbit II experiments was carried out at the U.S. Army Dugway Proving Ground in Utah, USA. The experiments consisted of five trials involving large-scale releases of pressure-liquefied chlorine. The work was part of a four-year programme led by the U.S. Department of Homeland Security (DHS) and U.S. Defense Threat Reduction Agency (DTRA), and followed on from the smaller-scale Jack Rabbit I experiments conducted in 2010 (Hanna et al., 2012). Prior to the Jack Rabbit II experiments starting, various modelling teams were invited to participate in a Modelers Working Group (MWG) to help scope out the experiments, validate models and share findings. The UK's Health and Safety Executive (HSE) contributed to the MWG by providing dispersion model predictions for a nominal 9 tonne release of chlorine prior to the 2015 experiments (McKenna et al., 2016). The two integral models used by HSE to model the dispersion of the chlorine cloud were Drift (Tickle and Carlisle, 2008) and Phast (Witlox and Holt, 1999; Witlox and Harper, 2013). The developers of the dispersion modelling software worked with HSE to provide input and feedback on the predictions. Drift is developed by ESR Technology and is used by HSE to model dispersion of toxic and flammable gases for land-use planning public safety advice. Phast is developed by DNV GL Software and is a comprehensive hazard analysis package that contains various sub-models, including vessel discharge, pool evaporation and atmospheric dispersion.

EXPERIMENTS

Phase 1 of the Jack Rabbit II experiments was carried out from late August to early September 2015 and consisted of five trials. Table 1 provides a summary of the experimental release conditions. During these trials, chlorine was released vertically downwards through a 6 inch (0.152 m) diameter hole at the bottom of a pressure vessel, from a height of 1 m above a 25 m diameter concrete pad. The release mechanism involved a blanking plate that was fitted to the end of a short flange using explosive bolts. The discharge was initiated by blowing the bolts. Conex shipping containers were located around the release point to simulate a mock urban array of buildings, and chlorine concentration sensors were placed along radial arcs at distances of 0.2 km, 0.5 km, 1 km, 2 km, 5 km, and 11 km from the vessel. Portable Weather

Instrumentation Data Systems (PWIDS) were deployed over the test site to record weather information, which included wind speed, wind direction, temperature, humidity and pressure.

Table 1. Experimental release conditions for the Jack Rabbit II 2015 trials

Trial	Mass of Chlorine (kg)	Initial Tank Pressure (kPa)	Wind Direction[a] (degrees)	Wind Speed[b] ($m\ s^{-1}$)	Atmospheric Temperature (K)	Relative Humidity (%)	Atmospheric Pressure (kPa)	Pasquill Stability Class
1	4509	738	-18	2.0	290.9	39.2	87	F *
2	8151	693	-7	4.2	295.9	33.6	88	C
3	4512	658	+4	3.9	295.7	30.3	87	D
4	6970	602	+18	2.3	295.7	26.9	87	D
5	8303	674	+17	2.7	295.4	26.5	87	D

[a]Wind direction relative to the centreline of the urban grid, which was aligned 165 degrees to North.
[b]Wind speed measurements were taken at a reference height of 2 m.
*No value given by Dugway, so this was estimated by HSE using a flowchart from Wetmore and Ayres (2000).

EXPERIMENTAL MEASUREMENTS COMPARED AGAINST MODEL PREDICTIONS

After the 2015 experiments were conducted, Drift 3.7.2 and Phast 7.11 were again used by HSE to model dispersion of the chlorine released, but this time the simulations were refined to take account of the release conditions and weather data recorded for each trial. The modelling methodology was described by McKenna et al. (2016, 2017). Since Drift and Phast do not allow for variations of surface roughness within a single simulation, two simulations were performed for each trial using different roughnesses for the urban array and the downwind desert playa. The predicted concentrations were later blended together at the edge of the urban array. A 'baseline' case, which sets the anticipated upper bound to concentration predictions, was modelled assuming metastable liquid outflow and no rainout of liquid from the chlorine jet. However, video footage from the trials showed that pools of liquid chlorine formed on the concrete pad. Sensitivity tests were therefore performed in which all of the liquid hitting the pad rained out and formed an evaporating pool. The choice of full liquid rainout was to provide a bounding case and, in reality, it is likely that a fraction of the liquid remained in the dispersing cloud as an aerosol. Figure 1 compares the model predictions to the concentration data for the five trials. Uncertainties in the experimental data are identified using coloured symbols. Both models gave best agreement with the data when rainout was taken into account.

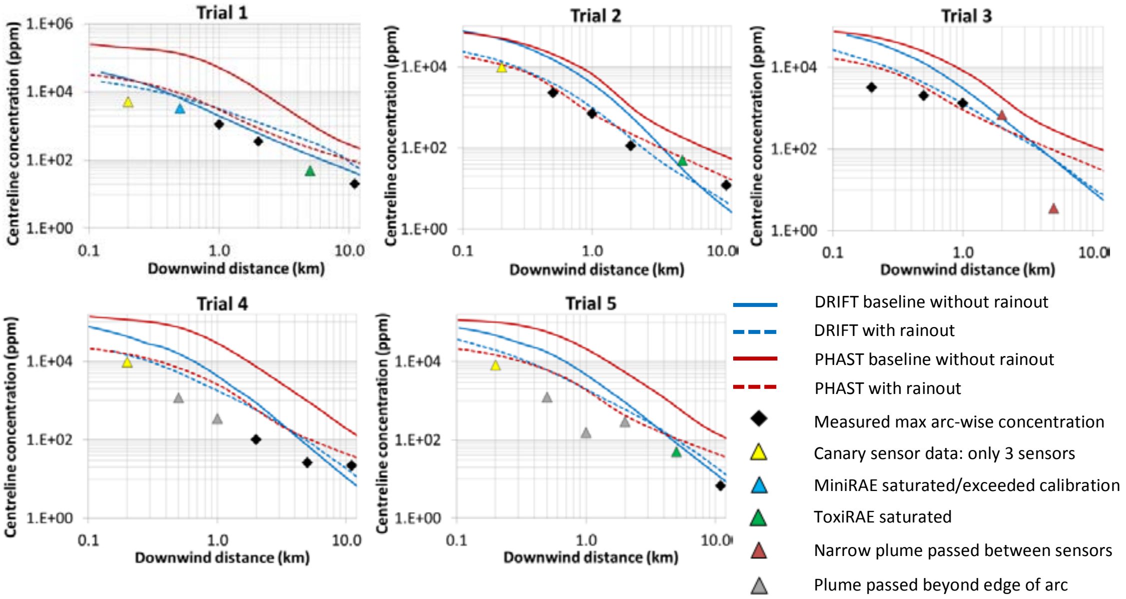

Figure 1. Comparison of Drift and Phast predictions against concentration data for the Jack Rabbit II 2015 trials

In future work, a new version of Phast (version 8.0) may be used that should result in lower predicted concentrations in the far-field, due to its inclusion of along-wind diffusion effects. These along-wind diffusion effects are already taken into account by Drift 3.7.2.

Maximum concentrations, like those shown in Figure 1, provide a standard means of assessing dispersion model performance. However, for risk assessment purposes, the toxic load (TL) is instead more useful to assess the harm to people from exposure to a toxic chemical. The TL is calculated by integrating the time-varying chlorine concentration raised to the power *n* over the duration of the cloud passage time. Figure 2 compares the Drift predictions of TL for the five trials against the experimental data for TL, which was kindly provided to HSE by the U.S. Institute for Defense Analyses (IDA) using the HSE *n* value of 2. Two threshold levels of TL are shown in these plots: the ‘Specified Level of Toxicity’ (SLOT) which equates to approximately 1% fatalities in the general population, as well as injuries to others, and severe distress to practically everyone; and the ‘Significant Likelihood of Death’ (SLOD) which equates to 50% fatalities in an exposed general population. The SLOT and SLOD values for various chemicals are available on HSE’s website (HSE, 2015). IDA provided the TL data from concentrations that were smoothed using either a 0.1 min or 1.0 min running average. Results were also produced from Drift simulations using a lateral meander averaging time of 0.1 min and 1.0 min. However, the choice of either 0.1 min or 1.0 min averaging time was found to have no significant effect on the results.

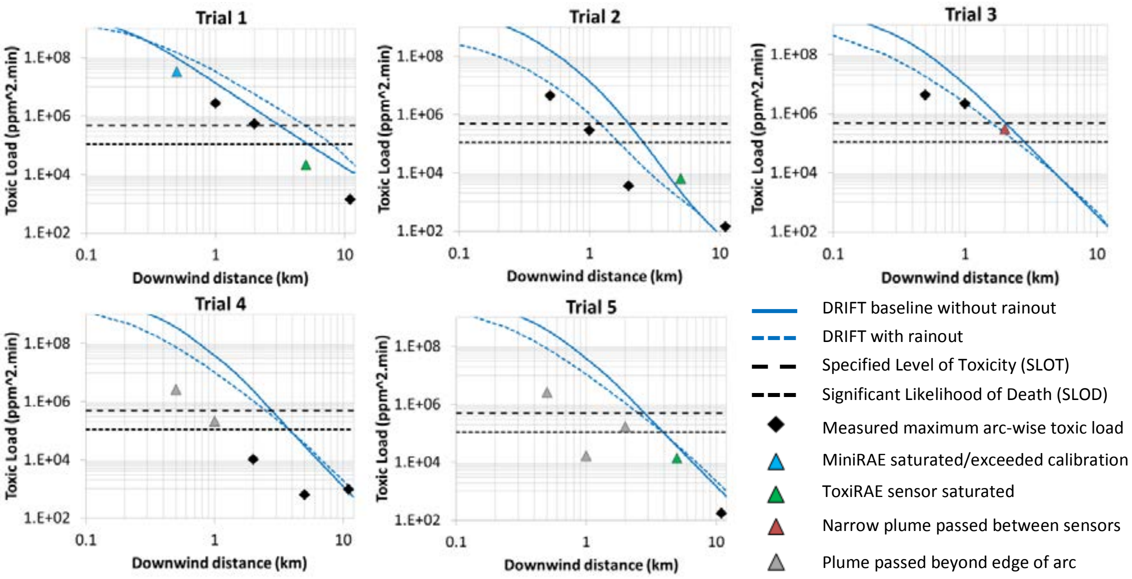

Figure 2. Drift predictions of TL (blue lines) against measurement data (symbols) for the Jack Rabbit II 2015 trials using *n* = 2. Black lines show two different toxic effects thresholds (SLOT and SLOD).

GLOBAL SENSITIVITY ANALYSIS

To help understand the impact of uncertainties in the dispersion model inputs, a global sensitivity analysis was performed on a modified development version of Drift (version 3.7.11) using the Gaussian Emulation Machine (GEM)[1]. This version of Drift includes a deposition model. The input parameters varied in the study are given in Table 2. The minimum and maximum values of the inventory, wind speed, temperature and Monin-Obukhov length were taken as the limits across the five Jack Rabbit II 2015 trials. The rainout fraction was varied from maximum physical limits of 0 to 1, and the discharge model was switched from the metastable liquid to the flashing model. The vapour deposition was varied from zero to a maximum value of 5 cm s^{-1}, which represents the highest value found in the literature from previous studies (Hanna and Chang, 2008).

[1] https://www.tonyohagan.co.uk/academic/GEM/, accessed 24 August 2017.

It should be noted that there is significant uncertainty in the value of the deposition velocity. Deposition experiments are ongoing at Arkansas University and previous work has shown the velocity to be affected by the organic content of the soil and other factors. The model used in Drift assumes the deposition flux to be simply the product of the deposition velocity and concentration and it does not account for saturation effects or other complexities. The value of 5 cm s^{-1} is probably far too high for the Dugway Proving Ground playa; it was chosen purely as an upper bound to assess the significance of deposition effects.

A Sobol' sequence was used to sample the ranges of these 7 inputs and in total 127 Drift simulations were performed. The sensitivity of the model to the inputs was assessed by considering their effect on the variance of two model outputs: the distance to the predicted centreline concentration of either 100 ppm or 10 ppm. The latter value is the Immediately Dangerous to Life and Health (IDLH) concentration for chlorine[2]. Independent analyses were performed on the choice of the discharge model.

Table 2. Minimum and maximum values of the input parameters varied in the global sensitivity analysis

	Chlorine Inventory (kg)	Rainout Fraction	Wind Speed (m s^{-1})	Ambient Temperature (K)	Inverse Monin-Obukhov length (m^{-1})	Vapour Deposition Velocity (cm s^{-1})	Discharge Model
Min.	4000	0	1.5	288	-0.12	0	Metastable liquid
Max.	9000	1	5.0	303	0.08	5.0	Flashing

Results from the variance-based global sensitivity analysis are presented in Figure 3 in the form of a 'Lowry' plot which shows the main and total effects for each input, together with the cumulative main and total effects. The main effect of an input parameter describes its influence on the output due to changing its value alone. The total effect includes any additional influence due to its interactions with other varying input parameters. The plot shows the results for the metastable liquid discharge model for the 100 ppm concentration. Similar trends were produced for the flashing discharge model and for the 10 ppm concentration. The results show that the deposition velocity has the dominant effect, whilst the wind speed, Monin-Obukhov length and rainout fraction have some limited effects and interactions, and the inventory and temperature have practically no effect.

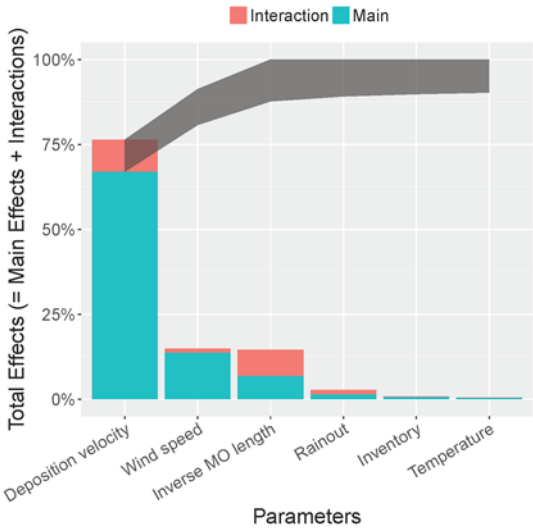

Figure 3. 'Lowry' plot showing main and total effects for the range of inputs given in Table 2 (but only for the metastable liquid discharge model) for the predicted distance to a concentration of 100 ppm

The inventory probably had little effect since the model assumed a downwards release from a 6 inch diameter hole in all cases, which meant that the inventory primarily affected the release duration rather

[2] https://www.cdc.gov/niosh/idlh/7782505.html, accessed 24 August 2017.

than release rate. The dominance of the deposition velocity suggests that great care should be taken in using deposition models in practice where the value of deposition velocity is uncertain. These results from the sensitivity analysis are only preliminary and further work is ongoing, in particular to examine the model behaviour within a narrower range of the deposition velocity.

CONCLUSIONS

Results have been presented from Drift and Phast for peak concentrations and TL in the Jack Rabbit II 2015 trials. The predictions were in reasonably good agreement with the data when the two models accounted for rainout from the two-phase jet, but significantly over-predicted concentrations when rainout was ignored. A global sensitivity analysis on Drift showed that dry deposition could have a dominating effect on the predicted concentrations of these trials if a high deposition velocity of 5 cm s^{-1} was assumed.

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REFERENCES

Hanna, S. and J. Chang, 2008: Gaps in toxic industrial chemical (TIC) model systems, 12th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Cavtat, Croatia, 6–9 October 2008.

Hanna, S., R. Britter, E. Argenta and J. Chang, 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.

HSE, 2015: Assessment of the Dangerous Toxic Load (DTL) for Specified Level of Toxicity (SLOT) and Significant Likelihood of Death (SLOD), from http://www.hse.gov.uk/chemicals/haztox.htm, accessed 24 August 2017.

McKenna, B., M. Mallafrè Garcia, S. Gant, R. Batt, M. Wardman, H. Tucker, G. Tickle, H. Witlox, M. Fernandez, M. Harper and J. Stene, 2016: Dispersion model predictions of the Jack Rabbit II chlorine experiments using Drift and Phast, IChemE Hazards 26 Conference, Edinburgh, UK, 24–26 May 2016.

McKenna, B., M. Mallafrè Garcia, S. Gant, R. Batt, M. Wardman, H. Tucker, G. Tickle, H. Witlox, M. Fernandez, M. Harper and J. Stene, 2017: Jack Rabbit II 2015 trials: preliminary comparison of the experimental results against Drift and Phast dispersion model predictions, IChemE Hazards 27 Conference, Birmingham, UK, 10–12 May 2017.

Tickle, G.A. and J.E. Carlisle, 2008: Extension of the dense gas dispersion model DRIFT to include buoyant lift-off and buoyant rise, Health and Safety Executive (HSE) Research Report RR629, from http://www.hse.gov.uk/research/rrhtm/rr629.htm, accessed 6 December 2016.

Wetmore, A. and S.D. Ayres, 2000: COMBIC, Combined Obscuration Model for Battlefield Induced Contaminants: Volume 1 – Technical Documentation and Users Guide, Army Research Laboratory.

Witlox, H.W.M. and A. Holt, 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.

Witlox, H.W.M. and M. Harper, 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.