DRIFT Dispersion Model Predictions for the Jack Rabbit II Model Inter-Comparison Exercise

Simon Gant[1]*, Graham Tickle[2], Adrian Kelsey[1] and Harvey Tucker[3]

[1]Health and Safety Executive (HSE), Harpur Hill, Buxton, SK17 9JN, UK

[2]GT Science & Software, 29 Mount Way, Waverton, Chester, CH3 7QF, UK

[3]Health and Safety Executive (HSE), Redgrave Court, Merton Rd, Bootle, L20 7HS, UK

*Corresponding author. E-mail address: simon.gant@hse.gov.uk

Abstract

In 2015 and 2016, the US Army conducted nine large-scale chlorine releases at the Dugway Proving Ground in Utah, known as the Jack Rabbit II trials. The purpose of these experiments was to improve our understanding of pressure-liquefied chlorine releases and atmospheric dispersion, and to provide useful practical knowledge for emergency responders. Data from three of the Jack Rabbit II trials (Trials 1, 6 and 7) were subsequently selected for an international model inter-comparison exercise, which included modelling contributions from the US, UK, Canada, France, Germany, Sweden, Finland and the European Commission. This paper provides details of one of the UK contributions to that exercise, using the DRIFT integral dispersion model. Participants in the exercise were given a set of prescribed model input conditions. The methodology used in DRIFT to model these conditions is described here, which consisted of three runs: a baseline case and two sensitivity tests that examined the effect of variations in the modelled wind-speed profile and the dry deposition rate.

A brief review is also provided of the experimental data used for the model inter-comparison exercise. Gas concentrations were measured in the Jack Rabbit II trials using an extensive array of gas sensors arranged on arcs downwind from the release point. Four types of sensors were used, which each had calibration and/or saturation limits. In some of the trials, sensors that recorded the highest concentrations on an arc were saturated with gas and under-recorded the actual concentrations. In other cases, especially near the source, there were only a few sensors on an arc and therefore it is uncertain whether the plume maximum concentrations were recorded.

Results from DRIFT are compared to the Jack Rabbit II data in two ways. Firstly, against the full dataset of maximum arc-wise concentrations, and secondly against the subset of measurements that were unaffected by saturation issues or there being a sparse sensor array. In the first case, DRIFT gives higher concentrations than were measured on average, noting that some measurements probably under-recorded the concentration owing to the previously mentioned sensor saturation issues. In the second case, using the more reliable dataset, the statistical performance of DRIFT falls within commonly-used dense-gas model acceptance criteria.

Sensitivity tests on the wind speed profile and dry deposition rate had an effect on the DRIFT predictions in Trial 1, but little impact in Trials 6 and 7. This behaviour is likely to be due to the changing meteorology during Trial 1, and the lower wind speed and smaller chlorine mass released in that trial.

Remaining knowledge gaps and possible future directions for research are discussed. These include further work on dry deposition, modelling of the other Jack Rabbit II trials (potentially using source models as well as prescribed common source conditions), and comparisons of predicted and measured toxic load, calculated from the time-varying concentrations.

Keywords

DRIFT; Jack Rabbit II; chlorine; flashing jet; dense-gas dispersion; model validation

Highlights

- DRIFT configuration for Jack Rabbit II model-inter-comparison exercise is presented
- Experimental data for Trials 1, 6 and 7 are briefly reviewed
- DRIFT results fall within criteria for dense gas model acceptance
- Predictions sensitive to wind speed profile and dry deposition in Trial 1

1. Introduction

The regulatory framework in Great Britain for controlling major accident hazards at sites handling large quantities of toxic or flammable material (such as refineries and chemical plants) requires the site operator to carry out a risk assessment and prepare emergency response plans, which are documented in their safety report (HSE, 2015). In preparing this document, the site operator (or usually, their consultant) uses dispersion models to predict the consequences of potential incident scenarios involving the release of hazardous substances into the atmosphere. One of HSE's roles as a competent authority is to examine the safety report and raise issues that require further investigation. The goal of the risk assessment and emergency plan is ultimately to put measures in place to protect workers and the public from harm in the event of an incident.

In addition to this activity, HSE uses dispersion models to assess the risks posed by major hazards sites and (based on these results) it provides public safety advice in the form of three-zone risk maps to local planning authorities (HSE, 2017). The planning authorities are responsible for using this land-use planning advice to control developments such as schools and housing around major hazards sites.

It is critically important that dispersion model predictions are accurate in order to have confidence in these risk assessments, emergency plans and land-use planning advice. Model inter-comparison exercises provide a valuable opportunity to test the accuracy of dispersion models and benchmark their performance against each other. They help assess the strengths and weaknesses of different models and understand the effects of user-variability, i.e. the potential for one model user to obtain a different result from another user for the same scenario. Model inter-comparison exercises also bring together the dispersion modelling community to study a set of experiments in-depth, to discuss the findings and develop improved modelling approaches.

Perhaps one of the earliest model inter-comparison exercises in the field of major accident hazards that demonstrated the benefit of this activity was undertaken by Havens (1977), who analysed the dispersion of Liquefied Natural Gas (LNG) vapour from ship tankers. The work came at a time when there was significant interest in the bulk import of LNG into the USA through ports, which were in some cases surrounded by high-population areas (e.g. Boston harbour). Havens (1977) reviewed predictions from several different dispersion models and found that they gave predictions of the flammable cloud size ranging from 0.75 miles to several tens of miles for the same spill scenario. To address uncertainties in these hazard predictions, a program of large-scale LNG release experiments was subsequently undertaken, including the Burro, Coyote and Falcon trials (Koopman *et al*., 1982, Goldwire *et al*., 1983, Brown *et al*., 1990) and models such as DEGADIS were developed (Havens and Spicer, 1985, 1988). The analysis of LNG dispersion models continues to the present day, although the focus is now on LNG *export* from the USA. Details of the model evaluation protocol currently used by the USA regulator PHMSA (the Pipelines and Hazardous Materials Safety Administration) for LNG vapour dispersion models can be found on the National Fire Protection Association's website[1].

Other notable model inter-comparison exercises on major accident hazards that involved HSE over the last few decades include those accompanying the Thorney Island dense-gas release experiments (McQuaid and Roebuck, 1985), the URAHFREP trials on hydrogen fluoride (Porter and Nussey, 2001), the SMEDIS project on dense-gas dispersion (Carissimo *et al*., 2001) and the more recent HySAFE project on hydrogen releases[2].

Model inter-comparison exercises on major accident hazards have been undertaken elsewhere in Europe in recent years, notably in France. Following the devastating explosion at the AZF factory in Toulouse in 2001, a new technological risk prevention plan (the Plan de Prévention des Risques Technologiques, PPRT) was implemented by the French Ministry, which included new requirements for the prediction of major accident hazards. To evaluate the capabilities of Computational Fluid Dynamics (CFD) dispersion models for application to the PPRT, a French working group of modellers from the energy and chemical industries, consultants, regulators and academia, led by INERIS (Institut National de l'Environnement Industriel et des Risques), compared predictions for several relevant major hazard scenarios involving dense, passive and buoyant gas dispersion. The modellers' results showed significant differences, with more than an order-of-magnitude range in predicted concentrations for the same scenario. As a result of that work, the group developed a prescriptive approach to the use of CFD dispersion models in PPRT studies (INERIS, 2015). In parallel, INERIS is also leading the European SAPHEDRA project, which aims to build a European platform for evaluation of consequence models

[1] http://www.nfpa.org/news-and-research/fire-statistics-and-reports/research-reports/hazardous-materials/lng-model-evaluation-protocol-and-validation-database-update, Accessed date 9 December 2019.
[2] http://www.hysafe.org/, Accessed date: 9 December 2019.

dedicated to emerging risks[3]. One of the outputs of the project, to date, has been a review of protocols for evaluating major hazards consequence models (Coldrick, 2017).

The projects mentioned above have mostly concentrated on industrial hazards, often involving dense gases. There have been numerous other dispersion model inter-comparison exercises aimed more at addressing Chemical, Biological, Radiological and Nuclear (CBRN) threats and air quality issues. In nearly all cases, these have studied passive dispersion. Notable projects include the two European COST Actions 732[4] and 1006[5] on microscale meteorological models and local-scale emergency prediction for airborne hazards in built environments. Both of these projects involved model inter-comparison exercises and developed good practice guidelines for modellers. Work in the USA has included the Joint Urban 2003 study in Oklahoma City (Hanna *et al*., 2018) and the Midtown Manhattan trials in 2005 (Flaherty *et al*., 2007). The UDINEE project[6] has also recently examined models suitable for simulating releases from Radiological Dispersion Device (RDD) events in urban areas. Many other initiatives on dispersion model evaluation have been presented at the conferences on "Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes", which also provides on its website (www.harmo.org) access to the Model Validation Kit and some classic experimental datasets. Another, seminal, model inter-comparison study is the work of Hanna *et al*. (1993), which led to the creation of the Modelers Data Archive (Chang and Hanna, 2010) and the BOOT software (Chang and Hanna, 2005).

The focus of the present paper is the Jack Rabbit II chlorine trials and one of the drivers for the project was a model inter-comparison study published in 2008 that compared hazard estimates from six widely used dense-gas dispersion models for three chlorine railcar incidents in the USA (Hanna *et al*., 2008). An important finding of that study was that all of the models over-predicted the number of casualties in the incidents by an order of magnitude or more. Five of the six models tested in that study (ALOHA, SLAB, SCIPUFF, PHAST and TRACE) were also used in the Jack Rabbit II model inter-comparison exercise presented in this journal special edition. The reasons for the models' over-predictions in the 2008 study are discussed further in the accompanying paper by Mazzola *et al*. (2020).

2. Aims

The principal motivation for HSE's involvement in Jack Rabbit II was to assess the strengths and weaknesses of the dispersion model that HSE uses for regulatory purposes in Great Britain, namely the DRIFT model (Tickle and Carlisle, 2013). HSE was also interested to develop an understanding of the capabilities of the DNV GL model, PHAST, which is used by many of the site operators and consultants in Great Britain to produce risk assessments and emergency-response plans, as required by the Control of Major Accident Hazards (COMAH) regulations (HSE, 2015). A third aim was to collaborate with other experts involved in Jack Rabbit II, to work together to ensure the success of the project, and to share knowledge and expertise.

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[3] https://projects.safera.eu/project/14, Accessed date: 9 December 2019.
[4] https://mi-pub.cen.uni-hamburg.de, Accessed date: 9 December 2019.
[5] http://www.elizas.eu/index.php/cost-action-es1006-summary.html, Accessed date: 9 December 2019.
[6] https://udinee.jrc.ec.europa.eu/, Accessed date: 9 December 2019.

HSE's involvement in Jack Rabbit II started in April 2015. In advance of the trials, HSE contributed model predictions from DRIFT and PHAST to help the experimental team select the positions for concentration sensors. Following the trials, HSE analysed the measurement data and shared findings with the Jack Rabbit II Modelers' Working Group. HSE also sponsored work on analysis of the chlorine source term, which is described in the accompanying paper by Spicer and Tickle (2020) in this journal special issue. Details of HSE's initial analysis of the Jack Rabbit II 2015 trials and its collaboration with the modelling teams at DNV GL and the US National Center for Atmospheric Research (NCAR) are described by Gant *et al*. (2018a). HSE has given numerous presentations on its work at the annual George Mason University (GMU) conferences[7], the European Harmo conference and the UK Hazards conference (Gant *et al*., 2015, 2017a, 2017b, 2018b, 2019; McKenna *et al*., 2016a, 2016b, 2017a, 2017b).

The purpose of this paper is to describe the configuration of DRIFT for the Jack Rabbit II model inter-comparison exercise and to present the results from sensitivity tests performed using DRIFT, which are not reported in the overall summary paper by Mazzola *et al*. (2020). A brief review of the Jack Rabbit II trials and the model inter-comparison exercise is first presented, since some people may read the current paper in isolation. For a more thorough overview of the Jack Rabbit II trials, the reader is directed to the accompanying paper by Fox *et al*. (2020) in this journal special issue.

3. Background to the Jack Rabbit II Model Inter-Comparison Exercise

The Jack Rabbit II trials were conducted at Dugway Proving Ground in two phases. In the first phase, five tests were conducted in August and September 2015 (Trials 1 – 5), which consisted of 5 to 9 ton releases of chlorine from a specially-designed 10-ton capacity vessel. The release mechanism involved a flange on the underside of the tank fitted with a blanking plate held on by explosive bolts, which were fired to remove the plate and initiate the discharge. In all five of the tests in 2015, the jet was directed vertically downwards through a 6-inch (0.152 m) diameter orifice onto a concrete pad from a height of 1 m. A grid of Conex shipping containers was placed around the release point to simulate an urban array of buildings. Concentrations were measured in arcs downwind from the release point at various distances out to 11 km.

The second phase of experiments in August and September 2016 was conducted without the grid of Conex containers and with several different release orientations. The first three tests (Trials 6, 7 and 8) involved the jet being angled either vertically downwards (180 degrees), 45 degrees downwards from horizontal (135 degrees) or vertically upwards (0 degrees). In all three tests, the same 10-ton vessel was used as in the earlier 2015 tests. The final test in 2016 (Trial 9) involved an explosive charge being used to cut a 6-inch hole in the underside of a 20-ton chlorine road tanker to produce a downwards-directed jet.

A summary of the nine trials is given in Table 1. In Trials 7 and 8, where the release was either 45 degrees downward or vertically upwards, the release points were respectively on the side and top of the 10-ton vessel. Following the primary release, some liquid chlorine remained in the vessel (below the

[7] http://camp.cos.gmu.edu/, Accessed date: 10 December 2019.

height of the orifice), which had cooled down through auto-refrigeration to the chlorine boiling point. In both trials, a secondary release of this cold liquid chlorine was performed a few minutes after the primary release, using a discharge valve on the underside of the vessel. In effect, this means that Trials 7 and 8 involved two releases: a primary release of pressurized chlorine and a secondary release of cold liquid chlorine.

Table 1. Summary of the release conditions, configuration and weather data for the Jack Rabbit II 2015 and 2016 trials

Trial	Initial Chlorine Mass (kg)	Release Angle	Mock Urban Array Present?	Wind Speed at height of 2 m (m/s)	Pasquill Stability Class	Notes
1	4,545	Vertically down	Yes	1.5	E or F	Wind speed and direction changed during plume dispersion
2	8,192	Vertically down	Yes	4.7	C or D	
3	4,568	Vertically down	Yes	3.8	D or E	Narrow plume may have bypassed furthest downwind sensors
4	7,017	Vertically down	Yes	1.8	E	Plume passed outside sensor array at 1 km
5	8,346	Vertically down	Yes	1.5	E	Plume passed outside sensor array on some arcs beyond 1 km
6	8,391	Vertically down	No	2.4	E	Analysis of chlorine liquid rainout undertaken for this trial by Spicer *et al*. (2019)
7	9,072	45-degree down	No	4.0	D or E	Primary jet release followed later by secondary release of auto-refrigerated liquid chlorine
8	9,120	Vertically up	No	2.1	D	Primary jet release followed later by secondary release of auto-refrigerated liquid chlorine
9	17,700	Vertically down	No	2.6	E	Release from truck tanker, no load cell data for chlorine release rate, release orifice may have been partially obstructed

Key: Unshaded cells are the 2015 trials, shaded cells are the 2016 trials

Over the period from 2014 to 2017, various dispersion modelling groups performed simulations of the Jack Rabbit II trials, both to help configure the experiments and to evaluate models using the data. Following completion of Jack Rabbit II in September 2016, plans were initiated for a model comparison exercise. The task of simulating all nine trials was considered too onerous (since most organisations would be self-funding) and it was decided to focus efforts on a smaller subset of trials. The debate over which trials to choose centred around the need to consider a range of conditions, both with and without the mock urban array, and the desire to use the “best” data, unaffected by measurement issues or other uncertainties.

Of the five trials conducted in 2015, Trial 3 was a 5 ton chlorine release in relatively high wind speeds and it produced a narrow plume that appeared to pass in between sensors on the arcs furthest downwind. In Trials 4 and 5, the changing wind direction blew the cloud out of one side of the sensor array at some downwind arcs. Of the remaining two 2015 trials, Trial 1 was a 5 ton release in stable conditions (Pasquill Class E or F) whilst Trial 2 was a larger 9 ton release in neutral to unstable conditions (Pasquill Class D or C). Analysis showed that the measured maximum concentration divided by the chlorine mass released (C_{max}/M_{total}) was higher for Trial 1 than Trial 2, and therefore Trial 1 was selected for the model inter-comparison exercise.

Of the four trials conducted in 2016, it was important to use Trial 6 for the model inter-comparison exercise, since there was good video footage for this trial that enabled source conditions for the jet and evaporating pool to be calculated (Spicer *et al*., 2019). Trial 9 (the truck trailer release) did not use load cells to measure the release rates, and there were concerns that the disc of metal that had been removed by the explosive charge on the underside of the tanker had partially-blocked the orifice. Given the uncertainties in the source term for this trial, it was decided against using it for the exercise. The remaining two trials consisted of the 45-degree downwards release (Trial 7) and the vertically-upwards release (Trial 8). There was greater interest in simulating Trial 7, given that it produced high concentrations on the downwind arcs of sensors and was the closest case to the horizontal release scenario that is often considered in risk assessments. The final decision was therefore to use Trials 1, 6 and 7 for the model inter-comparison exercise.

In March 2018, the first of several teleconferences took place to discuss the exercise. An open invitation to participate in the exercise was extended internationally, on the understanding that participants would need to be self-funding, but in return would get access to the measurement data and have an opportunity to benchmark their models against other participants' results. During the group's telecons, the practicalities of the exercise were discussed.

Participants in the model inter-comparison exercise planned to use a range of models of different complexity. Some models like HPAC could accept complex inputs, such as time-varying meteorological files, whilst others like PHAST and DRIFT could only accept a single set of meteorological conditions. Similarly, for the source conditions, some models could only accept a vapour source, whereas others could handle more complex two-phase source conditions. To resolve these issues, a common set of meteorological and source model inputs were provided to model participants that represented the "lowest common denominator" set of conditions, which could be used by all models, consisting of constant weather conditions and a vapour-only source. Hanna (2020) also provided a set of more detailed meteorological conditions that some models could use. Spicer and Tickle (2020) similarly provided additional two-phase source conditions for models capable of simulating droplet evaporation. The aim was to provide some flexibility for modellers to use their model as they would do in practice (e.g. for risk assessment or emergency response), whilst still providing a common framework for comparing models on an equal basis. The choice of modelling approach was left to the modeller. It was also recognized that there could be limitations to certain models which meant that changes to the prescribed conditions were necessary. The coordinators of the model inter-comparison exercise requested that whatever set of conditions were modelled were fully documented and a description of the modelling methodology was included with the submission of results to the coordinators of the exercise.

Participants in the model inter-comparison exercise were requested to produce the following outputs from their model in a standardised format:

- Maximum near-ground concentrations (at a nominal height of 0.3 m) at the downwind distances of the sensor array (0.2, 0.5, 1, 2, 5 and 11 km) for three averaging times: the raw data resolution (1-3 seconds), 20 and 60 seconds
- Cloud widths and heights at set concentrations and positions
- Contour plots of the chlorine concentration at defined times and positions, using a common contour scale
- Concentration time series at the locations of sensors

Most of the analysis to date has focussed on the first two outputs (maximum concentrations and cloud widths), mainly for the short averaging time of 1-3 seconds. Preliminary analysis showed that the effect of the averaging time was fairly minor in the near-field and negligible at the furthest downwind arcs, at least in the 2015 trials (see Gant *et al*., 2019).

Further background to the Jack Rabbit II trials and details of the modelling outputs are provided in the papers by Fox *et al*. (2020) and Mazzola *et al*. (2020) in this special issue of *Atmospheric Environment*.

4. DRIFT model

DRIFT is a commercially-available integral dispersion model produced by ESR Technology. The model was originally developed by the Safety and Reliability Directorate (SRD) of the UK Atomic Energy Authority (UKAEA) (Webber *et al*., 1992), but much of its development over the last 15 years has been sponsored by HSE. The version of DRIFT used in the present work was 3.7.11.

Whilst DRIFT was originally developed as a dense-gas dispersion model, it has subsequently been adapted to model dispersion of passive and buoyant sources (Tickle and Carlisle, 2008). DRIFT incorporates a momentum-jet model to simulate pressurized releases and is capable of simulating both single and two-phase jets, where the latter model assumes homogeneous equilibrium between the gas phase and the dispersed liquid droplet phase. The jet can be angled in any direction vertically and horizontally (including in a lateral cross-wind direction). The model accounts for condensation of water vapour from the air and its subsequent evaporation downwind in the dispersing cloud.

DRIFT can model various types of dispersing clouds, resulting from instantaneous, continuous, finite-duration and time-varying releases. The finite-duration model was used for the Jack Rabbit II simulations presented here. It is based on the physics of the continuous release model, where the front and back edges of the cloud are tracked over time as the cloud drifts downwind. A smoothing operation is applied to the cloud concentrations at these edges to account for along-wind diffusion. In common with most other integral models, DRIFT assumes that the terrain is flat with a uniform surface roughness.

4.1 Configuration for Jack Rabbit II model inter-comparison exercise

Table 2 provides a detailed breakdown of the prescribed model input conditions that were provided to participants of the model inter-comparison exercise. The inputs are colour-coded to identify which specific inputs were used to configure DRIFT, and which inputs were modified by DRIFT from the specified values.

The three inputs that were modified were: 1.) the atmospheric pressure, 2.), the initial two-phase jet temperature and 3.) the friction velocity. DRIFT is only able to model a standard atmospheric pressure of 101,325 Pa, which is appropriate for HSE's regulatory work in the UK, but it means that the model was unable to account for the lower atmospheric pressure at the high-altitude US Army Dugway Proving Ground, where the atmospheric pressure was between 86,850 Pa and 87,370 Pa. This limitation also affected the initial jet temperature, which DRIFT assumed to be equal to the chlorine boiling point at standard atmospheric pressure (-33.7 °C), whereas in the experiments it was around -37.4 °C. The result of the higher atmospheric pressure and higher chlorine boiling point is that DRIFT is expected to slightly overpredict the persistence of the chlorine liquid aerosol. The effect on the downwind dispersion of the cloud, once the aerosol droplets have all evaporated, is not expected to be significant. Modification of the friction velocity is discussed below in the section on sensitivity studies.

4.2 Modelling of the Jack Rabbit II source conditions

A three-stage modelling approach was used to simulate the Jack Rabbit II trials with DRIFT, as summarized in Figure 1. The DRIFT Stage 1 model simulated the jet discharging from the vessel up to the point where the jet impinged on the ground. The source conditions for this calculation were the "primary release" conditions given in Table 2. The DRIFT Stage 1 model calculated the entrainment of air into the jet with the associated evaporation of chlorine droplets and condensation of water vapour, but only up to the point where the jet impinged on the ground. Conditions from this impingement point were then used as inputs to the second stage calculation. The modelled jet was angled vertically downwards in Trials 1 and 6, and 45°downwards from the horizontal in Trial 7, to match the conditions in the experiments.

The DRIFT Stage 2 model simulated the conditions after the jet impinged on the ground and comprised two separate calculations with different sources: an area source that represented the jet conditions after impingement (Stage 2a) and an evaporating pool source (Stage 2b). The post-impingement jet source term (Stage 2a) was determined from the source in Stage 1 with the liquid fraction adjusted to account for chlorine rainout into the pool. This rainout rate was calculated from the specified "primary release" discharge rate minus the specified "primary release modified for rainout" given in Table 2. For example, in Trial 1, the "primary release" mass flow rate was 224 kg/s and "primary release modified for rainout" was 145 kg/s, so the rainout rate was 224 – 145 = 79 kg/s. This 79 kg/s of liquid chlorine was removed from the two-phase jet conditions in the Stage 1 calculation (at the point where the jet impinged on the ground) before it was input into the Stage 2a calculation as post-impingement jet source conditions. The amount of chlorine liquid rainout in the DRIFT source conditions was therefore exactly the same as that given in the prescribed model inputs in Table 2. A fraction of the water that had condensed into the two-phase jet in Stage 1 was also removed from the source in Stage 2a, in proportion to the amount of liquid chlorine removed for rainout. Air entrained into the jet in Stage 1 was fully retained in the Stage 2a source. DRIFT's area source model was used to model the Stage 2a source, which involve a circular source at ground level with diameter equal to that of the jet in the Stage 1 calculation at the point when it impinged on the ground. One of the limitations of this approach was that the momentum of the jet and the enhanced turbulence in the impingement zone were not taken into account in the area source in Stage 2a.

The evaporating pool source in the Stage 2b model was specified using the conditions given in Table 2, i.e. for Trial 1 the evaporation rate was 43.2 kg/s. Dispersion from the impinged jet and evaporating pool sources were modelled by DRIFT as separate cloud 'segments'. In the final stage of the calculation process (Stage 3), the concentrations from the cloud segments from the Stage 2a and 2b calculations were combined (i.e. added together) to give the predicted concentration output from DRIFT.

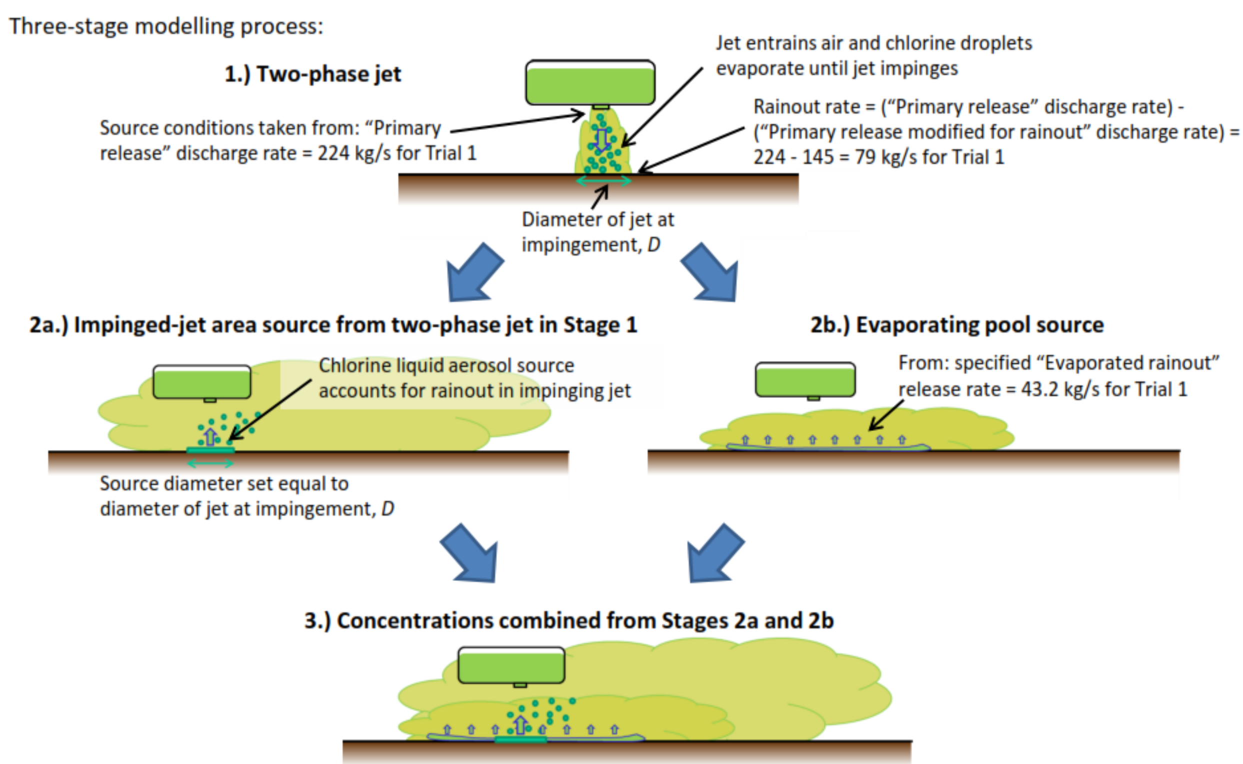

Figure 1 Summary of three-stage DRIFT model for the Jack Rabbit II model inter-comparison exercise

Videos of the Jack Rabbit II Trials 1 and 6 showed that the impinging jet produced a momentum-driven wall-jet that rapidly dispersed the cloud radially outwards from the impingement point across the concrete pad (see Figure 2)[8]. In Trial 7, where the release was angled downwards at 45 degrees from horizontal, a momentum-driven V-shaped wall-jet was produced in the near-field. DRIFT does not currently have the capability to model these momentum-driven jets and instead the area source model was used to simulate the jet component in the Stage 2 calculation. The area source model (illustrated in Figure 3) was originally intended to model dense-gas dispersion from ground-based, low momentum, area sources such as vaporizing pools. The model feeds material into the overlying cloud at a specified rate and the initial configuration of the cloud is assumed to be cylindrical – the same as in DRIFT's instantaneous puff model. Radial spreading of the cloud is determined from the maximum of either the gravitational or passive spreading rates, and there is mixing through the top face of the cloud that is driven by air entrainment. This radial spreading means that for large release rates the model expands the initial source diameter and allows the edge of the cloud to move upwind from the source. The spreading of the cloud over the area source ceases when the vertical cross-sectional area of the cloud becomes sufficiently large to enable downwind transport of the cloud at a rate equal to the source rate. This then specifies the source for DRIFT's subsequent finite-duration dispersion model, as illustrated in Figure 3. In situations where the source ceases before steady source conditions are established, DRIFT uses its instantaneous puff dispersion model instead.

[8] Videos from the trials can be viewed on the Utah Valley University website: https://www.uvu.edu/es/jack-rabbit/, Accessed date: 10 December 2019.

Figure 2 Images taken from the videos of the Trial 1 and 7 releases showing the wall jet produced when the two-phase chlorine jet impinged on the ground

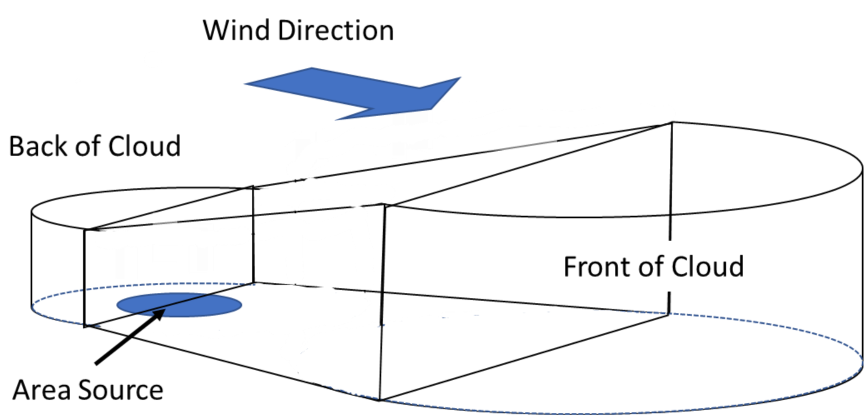

Figure 3. Schematic diagram of DRIFT's area source option

	Trial 1	Trial 6	Trial 7
Primary release			
Discharge rate (kg/s)	224	260	259
Discharge period (s)	20.3	32.2	33.3
Temperature (^{o}C)	-37.3 (-33.7)	-37.4 (-33.7)	-37.4 (-33.7)
Vapor fraction	0.171	0.172	0.172
Density (kg/m^3)	18.32	18.15	18.12
Velocity (m/s)	50.8	44.2	44.2
Area (m^2)	0.241	0.324	0.323
Primary release modified for rainout			
Discharge rate (kg/s)	145	168	162
Discharge period (s)	20.4	32.4	33.6
Temperature (^{o}C)	-37.3	-37.4	-37.4
Vapor fraction	0.264	0.266	0.274
Density (kg/m^3)	11.89	11.79	11.41
Velocity (m/s)	50.8	44.2	44.2
Area (m^2)	0.240	0.323	0.322
Evaporated rainout			
Discharge rate (kg/s)	43.2	34.0	34.0
Discharge period (s)	36.8	86.4	93.4
Temperature (^{o}C)	-37.3	-37.4	-37.4
Vapor fraction	1	1	1
Density (kg/m^3)	3.160	3.152	3.144
Area (m^2)	491	491	491
Meteorological conditions			
Atmospheric pressure (mbar)	873.7 (1013)	871.1 (1013)	868.5 (1013)
Initial wind speed (m/s) at z = 2 m	1.45	2.42	3.98
Initial wind direction at z = 2 m	147.4	146.9	149.6
Initial temperature (^{o}C) at z = 2 m	17.5	22.3	18.7
Surface roughness (mm)	0.5	0.5	0.5
Friction velocity, U* (m/s)	0.108 (0.054)	0.093 (0.096)	0.210 (0.164)
Sensible heat flux, Hs, (K-m/s)	-0.012	-0.0034	-0.0160
Inverse Monin-Obukhov length (m^{-1})	0.124	0.056	0.0229
Pasquill Stability Class	E/F	E	D/E

Table 2. Source and meteorological conditions provided to participants of the Jack Rabbit II model inter-comparison exercise. Coloured values indicate the following: **Blue** = Used for DRIFT input; **Red** = DRIFT used a different value (shown in brackets); **Green** = Calculated internally by DRIFT (not used as input to DRIFT); **Black** = Not used.

4.3 Baseline case and sensitivity tests

Three sets of DRIFT simulations were performed for the model inter-comparison exercise using different inputs, which are referred to as a baseline case (DRIFT1) and two sensitivity tests (DRIFT2 and DRIFT3). In summary, the configuration of these three models was as follows:

- **DRIFT1**: Baseline case with an atmospheric wind profile based on values of the initial wind speed at *z* = 2m (U_{ref}), surface roughness (z_0) and inverse Monin-Obukhov length ($1/L$) given in Table 2. It is these baseline DRIFT1 results that are presented in the model inter-comparison by Mazzola *et al*. (2020).
- **DRIFT2**: Sensitivity test with an atmospheric wind profile based on the friction velocity (*U**), surface roughness (z_0) and inverse Monin-Obukhov length ($1/L$) given in Table 2
- **DRIFT3**: Sensitivity test with the same conditions as the DRIFT1 baseline case (i.e. using U_{ref}, z_0 and $1/L$ from Table 2), except that dry deposition was switched off, by changing the deposition velocity from v_d = 0.04 cm/s (in DRIFT1 and DRIFT2) to v_d = 0.0 cm/s (in DRIFT3).

The motivation for performing the DRIFT2 simulations was to investigate the effect of uncertainties in the atmospheric boundary-layer profiles that were provided to participants in the model inter-comparison exercise. A description of the method used to calculate these inputs is given in the accompanying paper by Hanna (2020). DRIFT only requires three of the four inputs (U_{ref}, z_0, $1/L$, and U^*) to specify its wind speed profile. Internally within DRIFT, it uses a standard log-law velocity profile and modifications for neutral, stable and unstable conditions in the surface layer from Businger (1973).

The baseline case (DRIFT1) used the specified mean wind speed at the reference height of 2 m (U_{ref}) to specify the boundary-layer profile (rather than the friction velocity, U^*), since it was considered to provide a better indication of the wind speed driving dispersion of the chlorine cloud near the ground at the time of the release. From the prescribed values of U_{ref}, z_0, and $1/L$, it was possible to back-calculate the U^* value that DRIFT was using internally, from its wind speed profile. In Trials 1, 6 and 7, these calculated friction velocities were U^*_{DRIFT} = 0.054 m/s, 0.096 m/s and 0.164 m/s. In comparison, the specified values given to the participants of the model inter-comparison exercise were U^* = 0.108 m/s, 0.093 m/s and 0.210 m/s, respectively. Clearly, there were significant differences between the U^* values in Trial 1, and to a lesser extent in Trial 3. To assess the impact of this uncertainty on the dispersion model predictions, the DRIFT2 configuration used the prescribed values of U^*, L and z_0 to specify the wind speed profile (and not U_{ref}).

Figure 4 compares the two wind speed profiles calculated by DRIFT using either the specified reference velocity, U_{ref} (i.e. DRIFT1), or the specified friction velocity U^* (i.e. DRIFT2), in both cases using the z_0 and $1/L$ values given in Table 2. The cause of the differences between the profiles is the complex meteorology at Dugway Proving Ground. The trials all took place in early morning, when the sun was rising and the atmosphere was transitioning from stable to neutral or unstable conditions. The wind speed near the ground often increased during this period, whilst the trials were taking place, and the wind direction changed. For example, in the first 30 minutes after the release started in Trial 1, the wind speed increased by around a factor of two (see Figure 5). The reference velocity, U_{ref}, provided to participants in the model inter-comparison exercise was based on a 10 minute average, starting at the time of the release. The friction velocity, U^*, was instead based on a longer 30 minute average, and it consequently gave a higher mean wind speed in Trials 1 and 3. Participants had the choice when setting up their models to use either the U_{ref} or U^* values.

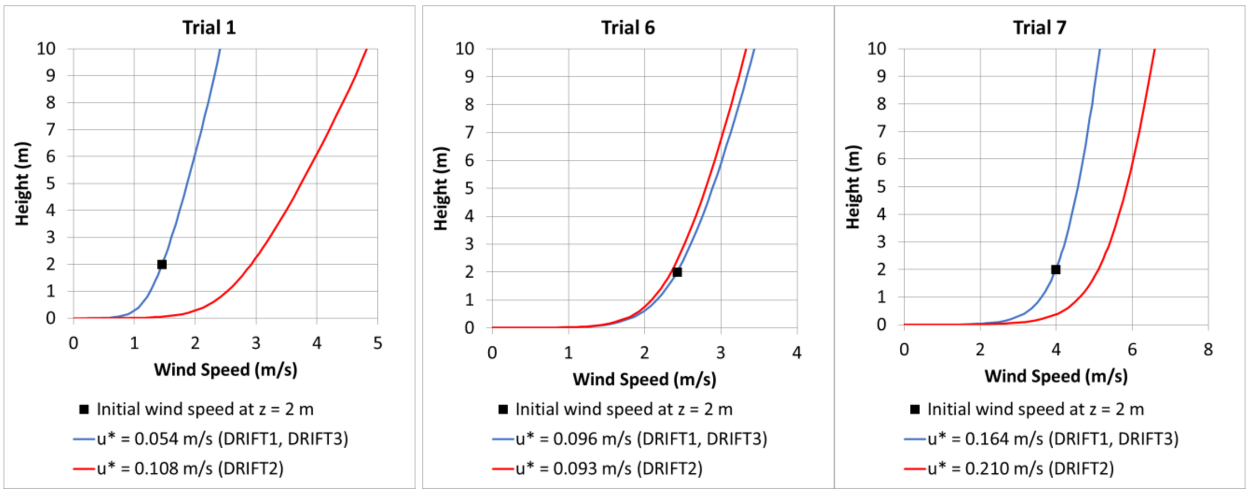

Figure 4. Wind speed profiles for the three trials and the specified wind speed at 2 m reference height.

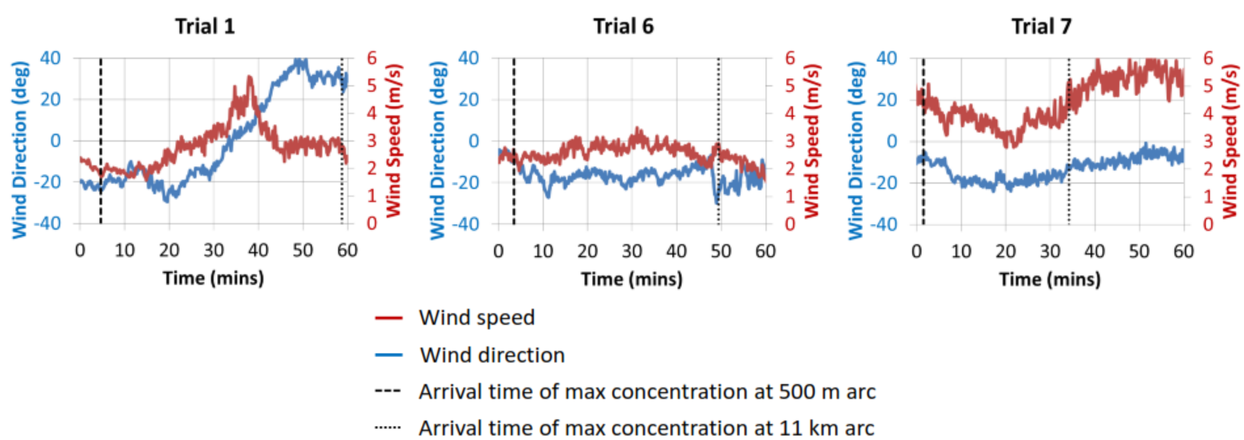

Figure 5 Wind speed and direction measurements taken by Portable Weather Instrumentation Data System PWIDS 19, located 100 m upwind of release point. The wind direction is given relative to the centreline of the arcs of downwind sensors (i.e. 0° is along the centreline of the array)

Another potentially important source of uncertainty in the model predictions is the deposition rate. Previous work has shown that large values of the dry deposition velocity, v_d, (of the order of a few centimetres per second) can significantly reduce downwind chlorine concentrations, particularly in low wind speeds, when the cloud moves more slowly and deposition occurs over a longer time period (Hanna and Chang, 2008; McKenna *et al*., 2017b). Participants in the model inter-comparison exercise were requested to use a deposition velocity of v_d = 0.04 cm/s to represent the low chlorine reactivity with the bare salt playa at Dugway Proving Ground, and the DRIFT1 and DRIFT2 model configurations used this value. However, many other dispersion models (including PHAST) are currently unable to take deposition into account (i.e. they assume a deposition velocity of zero). To help compare models on a like-for-like basis, the DRIFT3 runs were performed using a deposition velocity of zero. In all other respects, the DRIFT3 model configuration was identical to DRIFT1.

The deposition model used in DRIFT calculated the deposition rate from the product of the local chlorine concentration and the deposition velocity. The model had no upper limit on the amount of chlorine that was deposited at a given location, due to the surface becoming saturated. This effect is currently being investigated experimentally in a purpose-built deposition wind tunnel at Arkansas University (Spicer and Feuvrier, 2017). Consideration was given to how to include such saturation effects in DRIFT, but this was found not to be straightforward, since the structure of integral models like DRIFT makes it difficult to couple conditions within the cloud to those outside the cloud that are dependent upon the location's earlier exposure time-history. This matter may need further investigation in due course.

5. Brief review of experimental data

Figure 6 presents a summary of the measured maximum concentrations in Jack Rabbit II Trials 1, 6 and 7. The six graphs present the data across the arcs of sensors, located at distances of 200 m, 500 m, 1 km, 2 km, 5 km and 11 km downwind from the release location. Details of the equipment used to measure the concentrations are given in the accompanying paper by Fox *et al*. (2020). Several points are worth noting from Figure 6 with respect to the model inter-comparison exercise:

- Sensors saturated at several arcs, namely: at 5 km in Trial 1; at 500 m, 5 km and 11km in Trial 6; and at 1 km and 11 km in Trial 7. The ToxiRAE saturation limit was 50 ppm and the MiniRAE limit was 2,000 ppm. The sensor readings in Trial 1 were corrected to account for their calibration, which caused some of the MiniRAE values shown in Figure 6 to exceed their saturation limit of 2,000 ppm.
- There was a sparse array of sensors in the near-field at 200 m and 500 m, and therefore uncertainty that the actual maximum concentrations were recorded. For example, in Trial 7 there was only one working Canary sensor at 500 m, which recorded the maximum concentration on that arc.
- In Trial 1, there were twin peaks in the concentration at the 200 m arc. CFD model predictions by Los Alamos National Laboratory and HSE (Gowardhan, 2015; Gant *et al*., 2018a) showed that this behaviour was due to the chlorine cloud being directed preferentially along street canyons in the mock urban array (rather than directly downwind), which produced a crescent-shaped structure to the cloud in the near-field. Integral models like DRIFT and PHAST are unable to take this behaviour into account, nor do they even account for the presence of the urban array. In previous work, Gant *et al*. (2018a) used a higher roughness length in the near-field to account for the presence of the urban array, but in the simulations for the model inter-comparison

exercise presented here, a uniform roughness length of $z_0 = 0.5$ mm was used throughout (in accordance with the specified model input conditions given to participants of the exercise).

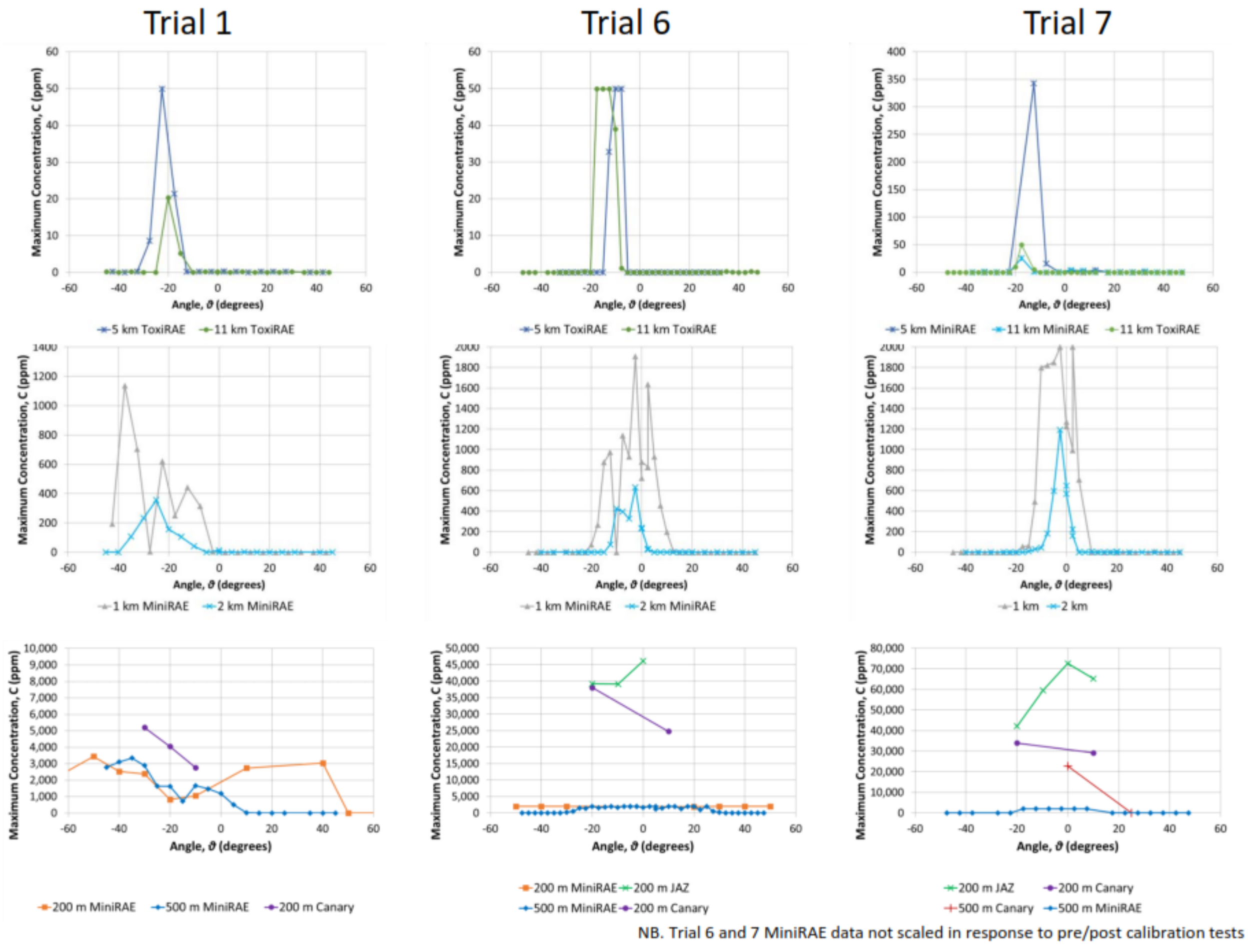

Figure 6 Measured maximum chlorine concentrations in the Jack Rabbit II Trials 1, 6 and 7. Three graphs are shown for each trial with the concentrations at 200 and 500m (bottom), 1 and 2 km (middle) and 5 and 11 km (top). The horizontal scale shows the angle across the arc of sensors.

6. Results

Maximum arc-wise concentrations for the three trials are presented in Figure 7. All of the results are for the "raw" sensor data, which was equivalent to a short averaging time of approximately 1-3 seconds. Three model results are shown (for model configurations: DRIFT1, DRIFT2 and DRIFT3), and the experimental data (Chang *et al.*, 2020) is shown as either square symbols or triangles. The triangles represent data points where it is likely that the measurements under-reported the actual concentrations, due to sensors saturating at their maximum threshold concentration, or there being too few sensors on that arc to provide a reliable indication of the maximum concentration on that arc. Over-prediction of these values should therefore not necessarily be taken as an indication of poor model performance. The experimental data shown in square symbols were not affected by these issues of sensors saturating or there being too sparse an array of sensors.

Figure 7 shows that the baseline DRIFT1 results are in reasonable agreement with the measurements. A scatter plot comparing measured to predicted concentrations for DRIFT1 across all of the data from Trials 1, 6 and 7 is shown in Figure 8. Most of the data points shown as square symbols in the plot, which are unaffected by issues of sensors saturating or clouds bypassing sensors, fall within the factor of two lines. Table 3 presents the statistical performance measures of geometric mean, geometric variance, fractional bias, normalised mean square error and factor-of-two for the three DRIFT models, using either the full set of measured maximum arc-wise concentrations or the subset of more reliable data. These results are also plotted in Figure 9 against the acceptance criteria proposed by Ivings *et al*. (2013) for LNG vapour dispersion models (shown as dashed lines in Figure 9). These acceptance criteria are the same as those proposed by Carissimo *et al*. (2001) for use with dense-gas dispersion models. Table 3 also lists the criteria given by Hanna and Chang (2012) for passive dispersion in rural and urban areas, for comparison purposes.

The results show that when compared against the full dataset of maximum arc-wise concentrations DRIFT1 gives higher concentrations than were measured on average, with 61% of maximum arc-wise concentrations within a factor of two of the measurements. Using the more reliable subset of data, the statistical performance of DRIFT1 falls within the Ivings *et al*. (2013) model acceptance criteria, with 75% of the predicted concentrations within a factor of two of the measurements and a geometric mean of 0.7.

The DRIFT2 results show that the choice of wind speed profile has a significant effect in Trial 1, but very little effect in Trials 6 and 7. The changes in wind speed profiles are largest in Trial 1 (see Figure 4), so this result is not surprising. Concentrations were higher with DRIFT2 than DRIFT1, and in worse agreement with the experiments. This trend towards increased concentrations with DRIFT2 was expected, since the wind speed was higher in that case and therefore the dense cloud was advected downstream faster and had less time to disperse and dilute before reaching the downstream positions. It is sometimes assumed that higher wind speeds give lower (not higher) concentrations downwind[9]. However, for short-duration or instantaneous releases the puff size is proportional to time. The puff is therefore smaller when it reaches a given distance if the wind speed is higher, which leads to higher concentrations (see Hanna and Chang, 2017).

Switching off the deposition model (i.e. the DRIFT3 results) also had the greatest effect in Trial 1, although the differences were relatively modest. The effects were greatest in Trial 1 due to the lower wind speed in this trial as compared to the other trials and the smaller chlorine mass released in Trial 1 (around half the mass released in Trials 6 and 7).

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[9] This behavior is generally true for *continuous* releases. For that reason, risk assessment methods often adopt stable atmospheric conditions and low wind speeds (typically “F2” conditions: Pasquill class F and 2 m/s winds) for representative worst-case dispersion (e.g. NFPA, 2001).

One possible reason for the high predicted concentrations in Trial 1 is that DRIFT did not take into account the presence of the mock urban array. In future work, it would be useful to revisit these simulations and apply the same methodology as used in previous DRIFT studies by Gant *et al*. (2018a) with enhanced roughness to account for these obstacles. The mock urban array was not present in Trials 6 and 7.

Another possible source of uncertainty arises from DRIFT's use of a higher atmospheric pressure than was present at Dugway. As mentioned earlier, this could potentially lead to aerosol droplets persisting further downwind in the model than in the experiments. The furthest extent reached by the modelled aerosol was 422 m in Trial 7. The aerosol was composed of a mixture of chlorine and condensed atmospheric water, and was probably mainly water at that point. Any effect on the predicted concentrations would principally affect the results at the 200 m arc, since the aerosol had evaporated completely before reaching the next downwind arc at 500 m. Concentrations output from DRIFT included contributions from both the chlorine vapour and droplet phases, and so the presence of some chlorine in the liquid phase should not have led to under-prediction of the concentrations at 200 m. Since the modelled source conditions, in terms of liquid fraction, were prescribed from measurements made at Dugway, the main effect of the higher atmospheric pressure was to give the chlorine aerosol droplets a higher initial temperature (-33.7 °C) than in the experiments (-37.4 °C). As the cloud dispersed downwind, it will have cooled due to the latent heat of vaporisation of the chlorine aerosol. When all the liquid had evaporated, the effect of the different initial temperature on the heat balance is considered likely to have been insignificant.

The above discussion has focused on the maximum arc-wise concentrations, which are commonly examined in model inter-comparison exercises. In addition to these values, predictions were obtained from DRIFT for the plume width and height, and also time-varying concentrations at the sensor positions, which were all provided to the coordinators of the model inter-comparison exercise. To help provide a visual picture of the DRIFT predictions, Figure 10 compares concentration contours from DRIFT1 to the maximum measured concentrations at each of the sensors. The results show that the predicted plume widths are generally of a similar magnitude to those indicated by the measurements. The higher wind-speed in Trial 7 is clearly shown by the advection speed of the cloud shown in these plots and the more elongated shape to the cloud.

Further comparisons of DRIFT to predictions from other models and the measurements, including results for cloud width and height, are provided in the paper by Mazzola *et al*. (2020) in this special issue of *Atmospheric Environment*.

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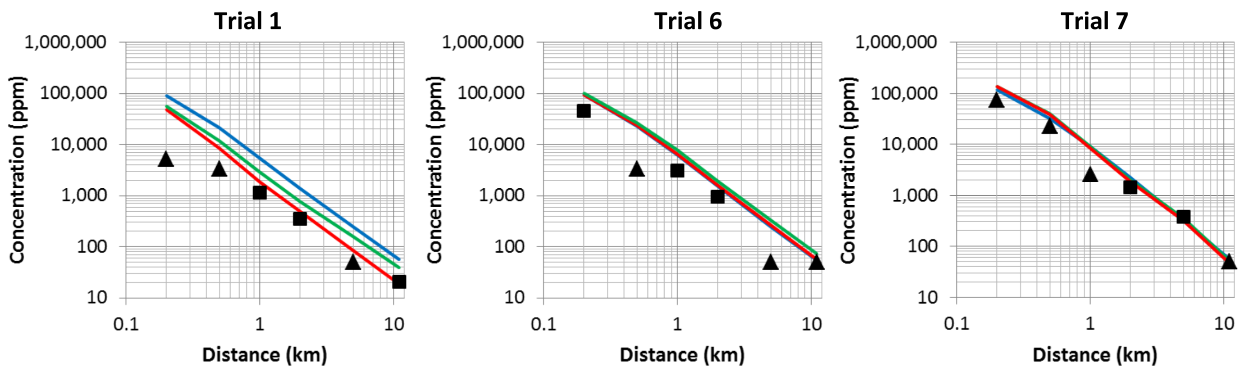

Figure 7 Maximum arc-wise concentrations for: DRIFT1, DRIFT2, DRIFT3, symbols: experiments (▲ sensors saturated or plume centreline may have bypassed sensors, ■ sensors unaffected by these issues)

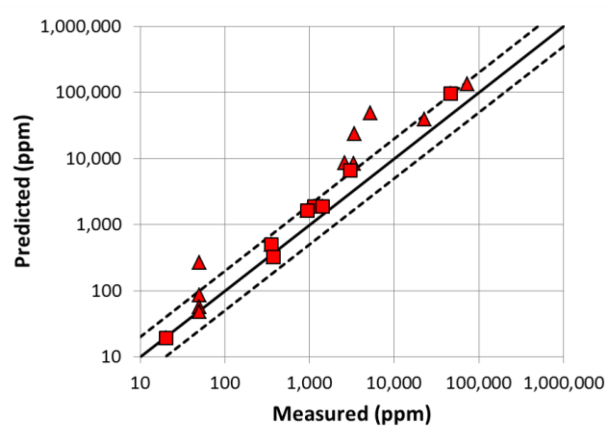

Figure 8 Scatter plot comparing measured and predicted concentrations in Trials 1, 6 and 7 for DRIFT1. Symbols: ▲ sensors saturated or plume centreline may have bypassed sensors, ■ sensors unaffected by these issues. Dashed lines show factor of two under- and over-prediction.

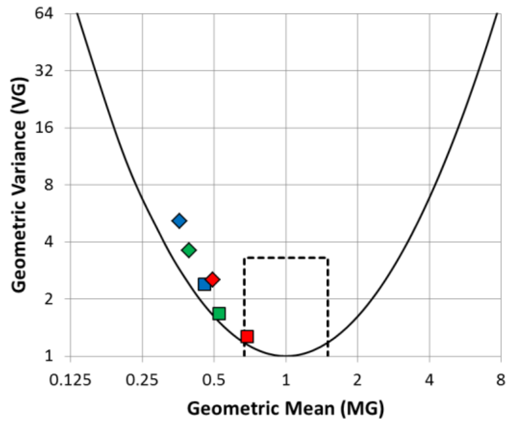

Figure 9 Geometric mean versus geometric variance. Symbols: ◆ ■ DRIFT1, ◆ ■ DRIFT2, ◆ ■ DRIFT3, where diamond-shaped ◆ symbols indicate all of the data was used to calculate MG and VG, whilst square-shaped ■ symbols use the subset of data unaffected by saturation issues or plumes bypassing sensors. The solid line indicates the lower bounding value of VG for a given MG and dashed lines show the bounds of an "acceptable" model according to the criteria given by Ivings *et al*. (2013).

		MG	VG	FB	NMSE	FAC2
DRIFT1	All data	0.49	2.5	-0.77	2.6	61%
	More reliable data	0.69	1.3	-0.68	3.4	75%
DRIFT2	All data	0.36	5.1	-0.85	3.4	39%
	More reliable data	0.46	2.4	-0.70	3.0	38%
DRIFT3	All data	0.39	3.6	-0.84	3.0	39%
	More reliable data	0.52	1.7	-0.75	3.9	38%
Acceptance criteria (Ivings *et al.*, 2013; Carissimo *et al.*, 2001)		0.67 < MG < 1.5	VG < 3.3	-	-	> 50%
Acceptance criteria – rural		-	-	|FB|< 0.3	NMSE < 3	> 50%
Acceptance criteria – urban (Hanna and Chang, 2012)		-	-	|FB|< 0.67	NMSE < 6	> 30%

Table 3 Statistical performance measures of Geometric Mean (MG), Geometric Variance (VG), Fractional Bias (FB), Normalised Mean Square Error (NMSE) and Factor-of-Two (FAC2) for the three DRIFT runs using the maximum arc-wise concentrations. Each model run is compared using full set of maximum arc-wise concentration data and also the subset of data that is not affected by issues of sensors saturating or there being a sparse array of sensors.

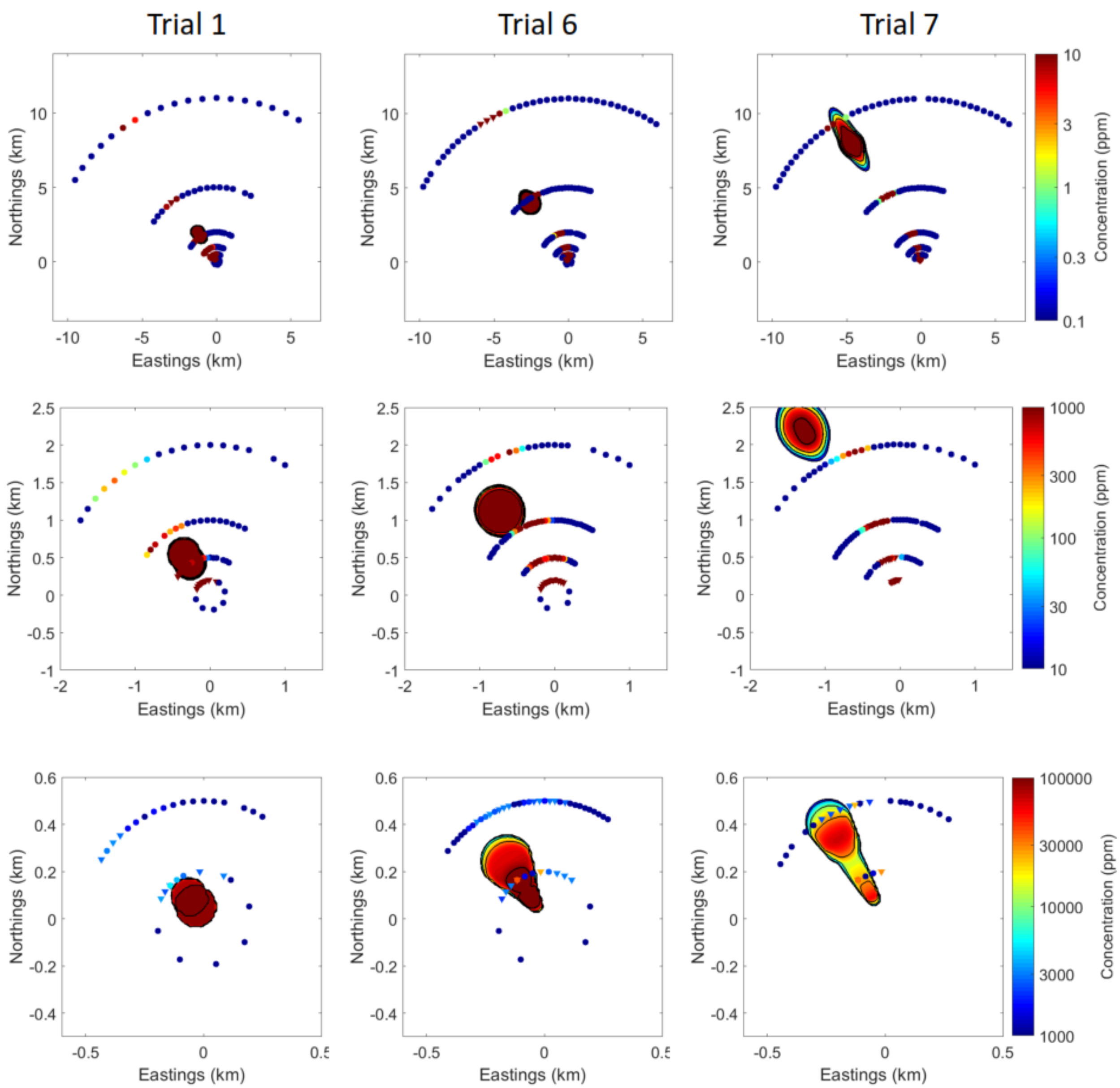

Figure 10 DRIFT1 predicted concentration contours for Trials 1, 6 and 7, at three locations: near, mid and far-field (shown in the bottom, middle and top plots, respectively). Coloured symbols show measured maximum concentrations (over all time), whereas contours show a snapshot of the predicted concentration at the time intervals of 120 s, 600 s and 1800 s in the near, mid and far-field, respectively. Triangular symbols indicate the sensor saturated, whereas round symbols indicate the sensors were unaffected by saturation issues. Both the contours and symbols use the same colour scales. Predicted concentrations below lower limit of the colour scale (e.g. 1,000 ppm in the near-field plots) are not shown, i.e. contour limits are clipped to this lower bound so that the background appears white, not blue.

7. Conclusions

The methodology used by HSE to model the Jack Rabbit II trials for the model inter-comparison exercise has been described. Three sets of results were produced using DRIFT: a baseline configuration and two sensitivity tests. The baseline model gave results that were in reasonably good agreement with the short time-averaged maximum arc-wise concentration data on six arcs, from 200 m to 11 km. In the experiments, some of the maximum arc-wise concentration measurements were affected by sensors saturating or there being too sparse an array of sensors. When compared against the full set of data (including these affected sensors), the DRIFT baseline model gave higher concentrations than were measured, with 61% of maximum arc-wise concentrations within a factor of two of the measurements. Using the more reliable subset of measurement data that were unaffected by sensors saturating or the sparse sensor array, 75% of the DRIFT baseline model predictions were within a factor of two of the measurements, the geometric mean was 0.7 and the geometric variance was 1.3. The values of the statistical performance measures were within the model acceptance criteria of Ivings *et al*. (2013).

Results from sensitivity tests showed that predictions were affected by using either the prescribed reference velocity at a 2 m height (U_{ref}) or the friction velocity (U^*) to define the wind-speed profile, particularly in Trial 1. This difference was caused by the changing meteorology at Dugway test site during the trials and the different averaging times used to calculate the two velocities. Sensitivity tests where the dry deposition model was switched off showed that this increased the predicted concentrations slightly in Trial 1 (which featured the lowest wind speed), but had practically no effect in Trials 6 and 7 (which featured higher wind speeds).

One of the aims of the model comparison exercise was, as far as practicable, to compare different models using the same source conditions and meteorology. Inevitably this involved simplification of some aspects, e.g. approximating the time-varying release as a constant release rate, so that the same inputs could be used across a wide range of models. The DRIFT results show that, despite such simplifications to the source term, a simple integral model can give reasonably good agreement with the measured concentrations.

In a real incident, measurements of the source conditions are unlikely to be available and instead it will be necessary to predict the source conditions. Similarly, in regulatory studies for land-use planning, it is necessary to predict the source conditions for a range of different potential release scenarios. To help evaluate the performance of source models, it would be useful in future work to re-run these Jack Rabbit II comparisons using source models for vessel releases, discharge and pool evaporation instead of the prescribed source conditions that were used in this model inter-comparison exercise.

Dry deposition was found to have only a relatively small effect on predictions presented here, but this was not entirely surprising given that the salt playa at Dugway Proving Ground was devoid of vegetation and a relatively low deposition velocity was used in the model. Results from previous model sensitivity tests in the literature using higher deposition velocities have shown that it can have a significant effect

(Hanna and Chang, 2008; McKenna *et al*., 2017b). However, it is unclear whether these latter results have any meaning, since they did not account for the ground becoming saturated with chlorine and the choice of deposition velocities was not based on measurement data. Until measurement data becomes available on saturation effects, this matter remains a significant source of uncertainty. Incorporating saturation effects on deposition within the DRIFT model was found not to be straightforward and it was not tested. This aspect merits further consideration in the future, once measurement data becomes available from Arkansas University.

HSE is keen to participate in further model inter-comparison exercises using data from the other Jack Rabbit II trials. In addition, in future work it would be useful to compare predicted and measured toxic loads (which can be calculated from the integral of the measured time-varying concentration raised to an appropriate toxic load exponent) since the toxic load is often the main parameter of interest in risk assessments.

The present work has provided additional evidence to support the predictive capability of DRIFT and there are plans to incorporate these experiments into the model evaluation protocol that is used to test new versions of DRIFT (Coldrick and Webber, 2017).

Without a doubt, the Jack Rabbit II trials have improved our understanding of chlorine release and dispersion behaviour, both from the scientific viewpoint of dispersion modelling and from the practical perspective of informing emergency responders. The sponsors and coordinators of the project deserve credit for this. Hopefully, the momentum generated during the Jack Rabbit II project, which led to this informative model inter-comparison exercise, will lead to further useful collaborative exercises in the future.

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