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DRIFT DISPERSION MODEL PREDICTIONS FOR THE JACK RABBIT II MODEL INTER-COMPARISON EXERCISE

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Abstract: In 2015 and 2016, the US Army conducted a series of 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, involving thirteen models 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 model-inter-comparison exercise, using the DRIFT integral dispersion model. Participants in the model inter-comparison exercise were given a set of prescribed input conditions. The methodology used in DRIFT to model these conditions is described here. Three sets of results from DRIFT are presented. These included a baseline case plus two sensitivity tests to examine the effect of variations in the modelled wind speed profile and the dry deposition rate. The results show that the DRIFT baseline configuration performs reasonably well across the three trials, with around 60% of the predicted maximum arc-wise concentrations within a factor of two of the measurements. The sensitivity tests had a significant effect in Trial 1, but little impact in Trials 6 and 7.

Key words: *DRIFT, Jack Rabbit II, chlorine, dense gas, model validation*

INTRODUCTION

The Jack Rabbit II model inter-comparison exercise was initiated in March 2018, coordinated by Tom Mazzola (Engility Corporation), Steven Hanna (Hanna Consultants) and Joseph Chang (RAND Corporation). Three of the nine Jack Rabbit II experiments were selected for the initial phase of the inter-comparison exercise: Trials 1, 6 and 7. The mass of pressure-liquefied chlorine released in these trials was 4.5 tonnes, 8.4 tonnes and 8.6 tonnes, respectively. The orifice in each case was 6-inches (0.152 m) in diameter. In Trials 1 and 6, the orifice was on the underside of the vessel and the released jet was directed vertically downwards onto a concrete pad from a height of 1 m. In Trial 7, the orifice was on the lower half of the tank in a position where the jet was angled 45-degree downwards from the horizontal. Since the orifice was not on the underside of the tank in Trial 7, approximately 446 kg of cold chlorine liquid remained in the vessel at the end of the release (the initial chlorine mass in Trial 7 was 9.1 tonnes).

In Trial 1, there was a grid of Conex shipping containers around the release point to simulate an urban array of buildings. In Trials 6 and 7, these containers were removed so that the dispersing cloud could spread unobstructed in all directions around the release point. Concentrations in all of the trials were measured in arcs downwind from the release point at various distances out to 11 km. Further details of the trials can be found in various presentations and publications, notably from the Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling (e.g. Fox *et al*., 2017). The Jack Rabbit II dataset can be requested by emailing: Jack.Rabbit@st.dhs.gov, and a selection of photos and videos taken by Utah Valley University can be found on their project website (https://www.uvu.edu/esa/jackrabbit/).

HSE's involvement in the Jack Rabbit II project dates back to April 2015, when it was invited to participate in the Modelers Working Group (MWG) coordinated by the principal sponsors of the project (the US Chemical Security and Analysis Center and the Defense Threat Reduction Agency). The main motivation for HSE's participation was to validate the DRIFT dispersion model (Tickle and Carlisle, 2013), which HSE uses for its regulatory work in the UK. Over the last four years, HSE has collaborated with two other members of the MWG: the US National Center for Atmospheric Research (NCAR) and DNV GL. Together, the three organisations published a preliminary analysis of the 2015 experiments (Trials 1 to 5) and their development and testing work on integral models (DRIFT, PHAST and NCAR's new model) and a CFD model (Gant *et al*., 2018). HSE is keen to continue its participation in the ongoing model inter-comparison exercise to help analyse the strengths and weaknesses of different modelling approaches, to further validate DRIFT and work towards harmonisation of modelling methodologies.

DRIFT MODEL CONFIGURATION

The coordinators of the Jack Rabbit II model inter-comparison exercise provided a set of prescribed model input conditions to the participants and requested that all of the modellers use these values to ensure that models could be compared on a like-for-like basis. Details of how these conditions are implemented in different models may differ. For example, some models (like DRIFT) contain sub-models for rainout and evaporation of droplets in the two-phase jet, whereas other models can only simulate the dispersion of vapour. Also, some models use a wind speed at a reference height to set the meteorological conditions, whereas other models use the friction velocity.

Table 1 provides a detailed breakdown of the inputs provided to the modellers. Entries are colour-coded to identify which specified inputs were used to configure DRIFT, and which inputs were modified in DRIFT from the specified values. The three inputs that were modified were the initial two-phase jet temperature, the atmospheric pressure, and 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 Dugway test site, 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.

Regarding the modification to the friction velocity, the DRIFT baseline case used the specified values of the mean wind speed at the 2 m reference height, the surface roughness and the Monin-Obukhov length to define the wind speed profile. DRIFT used a standard log-law velocity profile with modifications for neutral, stable and unstable conditions in the surface layer from Businger (1973). From the shape of this profile, it was possible to back-calculate the friction velocity that DRIFT used internally. In Trials 1, 6 and 7, the calculated friction velocities were u^* = 0.054 m/s, 0.096 m/s and 0.164 m/s. The specified values given to the participants of the model inter-comparison exercise were 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. Figure 1 compares the wind speed profiles calculated by DRIFT using either the specified reference velocity or the specified friction velocity (in both cases using the inverse Monin-Obukhov length given in Table 1). The differences shown in Figure 1 relate to the complex meteorology at the Dugway test site. 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 over this period 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 (in comparison, it took around 60 minutes for the chlorine cloud to reach the furthest arc at 11 km in Trial 1).

	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

	Trial 1	Trial 6	Trial 7
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 Class	E/F	E	D/E

Table 1. 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.

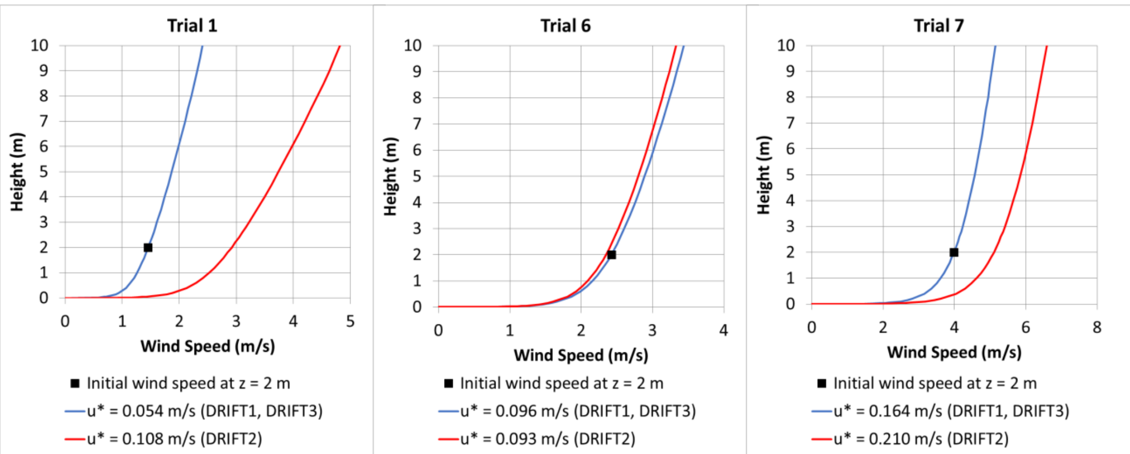

Figure 1. Wind speed profiles for the three trials and the specified wind speed at 2 m reference height.

It is challenging to take into account such large changes in the atmospheric conditions when defining the constant conditions needed by dispersion models. The reference velocity 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 was based on a longer 30 minute average. Participants had the choice when setting up their models to use either of the two values. HSE chose to use the reference velocity as it was considered to provide a better indication of the wind speed driving the chlorine cloud dispersion near the ground at the time of the release. However, it was acknowledged that this was a significant source of uncertainty. To address this issue, a set of DRIFT results were produced using the friction velocity instead of the reference wind speed to define the wind speed profile in the model.

Another potentially important source of uncertainty in the models is the deposition rate. Previous work has shown that large values of the dry deposition velocity 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*., 2017). Participants in the model inter-comparison exercise were requested to use a deposition velocity of v_d = 0.04 cm/s. The baseline configuration of DRIFT used this value. However, many other dispersion models (including PHAST) are currently unable to take deposition into account. To help compare models on a like-for-like basis, another set of DRIFT runs were submitted to the model inter-comparison exercise using a deposition velocity of zero. In summary, the three sets of DRIFT results submitted to the model inter-comparison exercise were:

- **DRIFT1** Baseline case, using an atmospheric wind profile based on values of the initial wind speed at z = 2m, surface roughness and inverse Monin-Obukhov lengths given in Table 1
- **DRIFT2** Sensitivity test, using an atmospheric wind profile based on the specified friction velocity (u*) value, instead of the initial wind speed at z = 2 m, with the same surface roughness and inverse Monin-Obukhov length values taken from Table 1
- **DRIFT3** Sensitivity test, which is the same as the DRIFT1 baseline case, except that dry deposition is 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).

RESULTS

Maximum arc-wise concentrations for the three trials are presented in Figure 2. All of the results are for the short averaging time of approximately 2 s. Three model results are shown for DRIFT1, DRIFT2 and DRIFT3, and the experimental data is shown as either square symbols or triangles. The triangles represent data points where it is known that the measurement under-represented 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 on that arc. For example, in Trial 7 there was only one working Canary sensor at 500 m, which recorded the maximum concentration on that arc. Over-prediction of these values should therefore not necessarily be taken as a poor indication of model performance. The experimental data shown in square symbols was not affected by these issues of sensors saturating or there being too sparse an array of sensors.

Figure 2 shows that the baseline DRIFT1 results are in reasonable agreement with the measurements. Using the subset of data shown with square symbols in Figure 2 (i.e. the more reliable data), around 60% of the DRIFT1 maximum arc-wise concentrations are within a factor of two of the measurements. There is a fairly consistent trend for DRIFT1 to over-predict the measurements, more so in the near-field, although a few data points are slightly under-predicted in the far field. The geometric mean is 0.63 and geometric variance is 1.3, again calculated using the more reliable subset of data.

Comparing the DRIFT2 results to the DRIFT1 results shows 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 1), 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 is expected, given that the wind speed was higher in DRIFT2, i.e. the dense cloud was convected downstream faster and had less time to disperse and dilute.

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).

In addition to the results presented in Figure 2, HSE has submitted further results for DRIFT to the model inter-comparison exercise, including maximum arc-wise concentrations for different averaging times, cloud heights and widths, contour data and time-varying concentrations at sensor positions. Further results are shown in the slides accompanying this extended abstract and in the presentation given by the coordinators of the model inter-comparison exercise.

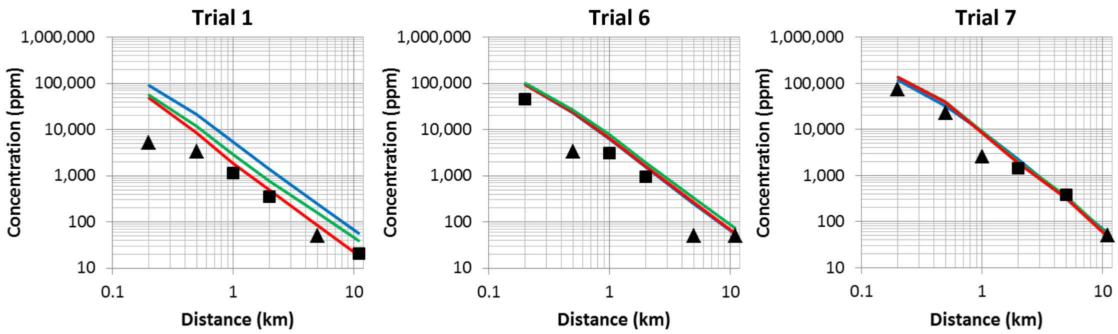

Figure 2. Maximum arc-wise concentrations for: — DRIFT1, — DRIFT2, — DRIFT3, symbols: experiments (▲ sensors saturated or plume centreline may have bypassed sensors, ■ sensors unaffected by these issues)

CONCLUSIONS

The methodology used by HSE to model three of the Jack Rabbit II trials for the model inter-comparison exercise has been discussed. Three sets of results were produced using DRIFT: a baseline configuration and two sensitivity tests. The baseline model gave results that are in reasonable agreement with the data. In the experiments, some of the maximum arc-wise concentrations were affected by sensors saturating or there being too sparse an array of sensors. When compared against the more reliable subset of this data, the DRIFT baseline model predicted around 60% of the maximum arc-wise concentrations within a factor of two. HSE is keen to participate in further model inter-comparison studies, using data from the other Jack Rabbit II trials.

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