Results of comparisons of the predictions of 17 dense gas dispersion models with observations from the Jack Rabbit II chlorine field experiment

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Abstract

The Jack Rabbit II (JR II) chlorine field trials in 2015 and 2016 involved nine 5 to 20 ton releases of pressurized liquefied chlorine. A model comparison study was initiated, where 17 widely-used dense-gas dispersion models were run by scientists in seven countries. Predictions were submitted following specified formats, using specified emissions and meteorology inputs. To compare with the model predictions, sets of observations were defined for the arc-maximum 1-3 s averaged concentrations and cloud widths and heights (to 20 ppm and 200 ppm contours) at distances from 0.2 to 11.0 km from the release. The initial focus is on the three field trials (1, 6, and 7) that have the highest observed concentrations and that have detailed emissions information. It is found that, of the 17 models, there is a core group of 5 or 6 with less bias (under about 50 %) and scatter (under a factor of five) in arc max C. The cloud widths tend to be overpredicted and the cloud heights tend to be underpredicted by most models, although a few models exhibit less bias.

1 Introduction

The Jack Rabbit I (in 2010) and II (in 2015 and 2016) field experiments, at Dugway Proving Ground (DPG) in Utah, were initiated because there had been much concern about the possible effects of pressurized liquid chlorine and anhydrous ammonia released from storage tanks and transportation vessels (e.g., see Hanna *et al.*, 2008, 2012 and 2016). The current paper uses observations from three of the JR II trials (1, 6, and 7) to compare with the predictions of 17 dense gas models, from the U.S., Canada, five European countries, and the European Commission (see Table

1). All modelers were sent a set of recommended inputs for emissions (Spicer and Miller 2017) and for meteorology (Hanna, 2018) and were asked to send model outputs of the arc-maximum concentrations (arc-max C) for averaging times of 1 s, and cloud widths and heights (to the 20 ppm and 200 ppm concentration contours) at distances from 0.2 to 11.0 km from the release.

Table 1. List of models being compared.

Model(s) run	Organization
Accident Damage Analysis Module (ADAM)	European Commission Joint Research Centre (JRC), Italy
ALOHA, SLAB-R	Rand, USA
Britter & McQuaid workbook (B&M)	Hanna Consultants, USA
Canadian Urban Dispersion Model (CUDM)	Environment and Climate Change, Canada
DRIFT	Health & Safety Executive (HSE), UK
ESCAPE	Finnish Meteorological Institute (FMI)
HPAC 6.5	Defense Threat Reduction Agency (DTRA), USA
Integral Dense-gas Dispersion Model (IDDM)	National Center for Atmospheric Research, NCAR, USA
PHAST	DNV GL Ltd, UK
PMSS	Aria, France
PUMA	Swedish Defence Research Agency (FOI)
RAILCAR-ALOHA, RAILCAR-QUIC	Naval Surface Warfare Center, USA
Safer Trace	Safer Systems, USA
SLAB-I	INERIS, France
VDI 3783 Parts I & II	BAM, Germany

2 JR II brief description

JR II took place over a broad flat desert at DPG. Releases were initiated between about 7 to 9 AM local time in late summer. The pressurized liquid chlorine tank was at the center of a 25 m diameter concrete pad. The main release was a two-phase momentum jet from a 15.2 cm diameter hole, with duration of about 20 to 40 seconds. The hole was at the tank's bottom for Trials 1-6, at its top for Trial 8, and pointing 45° downwards and downwind for Trial 7. During 2015, the source location was within a mock urban array of about 80 CONEX shipping containers set up on a packed gravel area 122 m square. For 2016, the CONEX obstacle array was removed. Concentrations were measured in the area containing by the obstacle array, and also on 90° arcs at distances of 0.2, 0.5, 1, 2, 5, and 11 km. Continuous (with 1 to 3 s averaging time) samplers were used, as well as several UV lidars and still photography and videos. Table 2 lists the general characteristics of the three JR II trials used in the current paper. The details of the tank and the pressurized releases are described by Nicholson *et al.* (2017) and Spicer and Miller (2017).

Table 2. Summary of Trials 1, 6, and 7 in JR II.

Trial	Time UTC (MDT = UTC - 6)	Mass released kg	Duration of release s	Mass release rate kg/s	Wind speed at z = 2 m m/s	Wind direction z = 2 m	1/L 1/m	Pasquill stab class
1	8 24 15 1336	4547	20.3	224	1.5	147	0.068	E or F
6	8 31 16 1424	8372	32.2	260	2.4	147	0.056	E
7	9 2 16 1356	8625	33.3	259	4.0	150.0	0.0229	D or E

3 Model comparison methodology and examples of results

After the 17 models were run for the three JR II Trials in Table 2, two types of methodologies for comparing model predictions with observations were used. The first type is a simple "look and see" approach using tables and scatter plots. There are few enough numbers that they can be easily seen in a single table or scatter plot. The second type is application of the BOOT model evaluation software (Chang and Hanna 2004), where performance measures such as FAC2 (fraction of C_p within a factor of 2 of C_o), and FB (fractional mean bias) are calculated.

3.1 Arc max C

Figure 1 is a plot containing model predictions and observations of arc max C as a function of distance for Trial 7. Of the three trials, Trial 7 has the largest observed concentrations, and there is more of a tendency for model underprediction. In this figure, 8 of the models are within a factor of 2 at more than half of the downwind distances. The other models tended to underpredict by more than a factor of two at most downwind distances. At most distances, the range of the 17 model predictions covers about 1 ½ orders of magnitude. For Trials 1 and 6, some differences in arc max C predictions and observations are expected, due to variations in the mass released, the wind speed, the presence of the CONEX array, and the location of the hole. Indeed it is found that concentrations approximately scale with (mass)/(wind speed), and that the 45°downwards angle in Trial 7 resulted in slightly larger concentrations. It was also found that concentrations were slightly less when the CONEX array was present. In general, the observed arc max C's were closer to the middle of the range of the 17 models for Trials 1 and 6. Considering all 17 model predictions of arc max C at all 3 trials and 6 downwind distances, about half of the predictions are within a factor of 2 of the observations and there are about as many over and underpredictions by a factor of 2. It was found that there are 5 or 6 models that have less mean bias and scatter for all three trials.

3.2 Cloud width and height

Cloud width was estimated using a combination of samplers and lidars at distances of 0.5, 1, and 2 km. Observed cloud height was estimated mainly from lidars plus a few instances where there was a short tower with samplers at heights of 0.3, 3, and 6 m. Videos from drones showed that the instantaneous visible cloud at distances of 0.5 to 2 km had a "mushroom" shape, with a broad leading "head" due to the initial momentum jet release, and a narrower trailing cloud due to evaporation from liquid rainout around the source. Here we estimate the cloud width and height at the time when the arc max C occurs at each arc. Figure 2 shows the predicted vs observed cloud widths and heights for Trial 7. Note that observations are plotted for samplers (dashed line with X symbol) and lidar (dotted line). Predictions of cloud width and height from only about half of the models are available. It is seen that most of the models overpredict the cloud width, sometimes by as much as a factor of 3 or 4. However, two of the models have mean bias less than about 20 %. Regarding cloud height, at distances of 0.5 and 1 km, most of the models underpredict the cloud depth, sometimes by as much as a factor of 4. However, the underprediction tendency decreases with distance, and there is little mean bias seen at 2 km. Similar results are found for trials 1 and 6.

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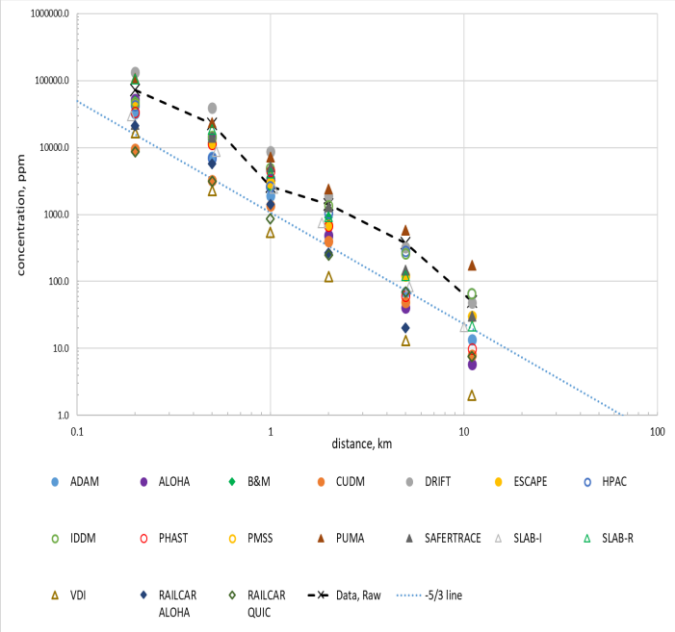

Figure 1. Scatter plot of predicted arc max C for all models for Trial 7. The observations (raw data) are the X's connected by a dashed line. The straight blue-dotted line represents a -5/3 slope

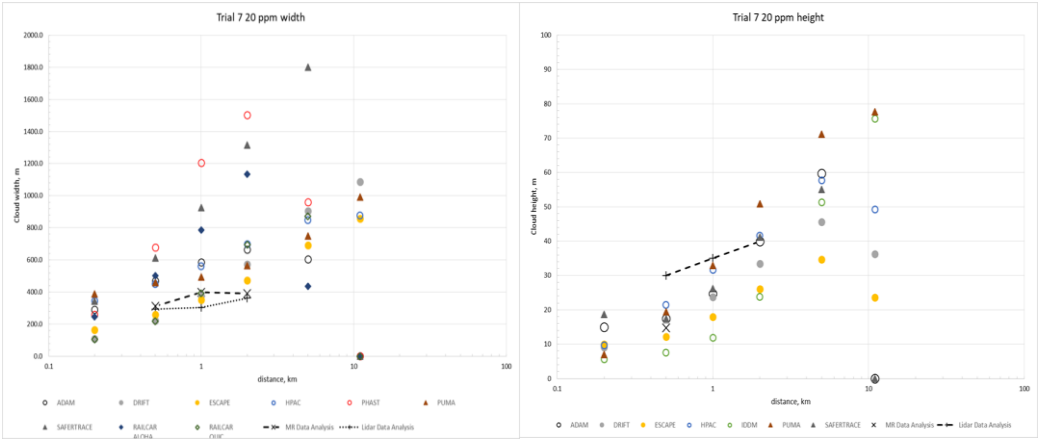

Figure 2. Comparison of model-predicted and observed cloud widths (left) and heights (right) (to 20 ppm) vs (dashed line with X is samplers and dotted line is lidars) for Trial 7.