Overview of Jack Rabbit II (JR II) field experiment and summary of the methods used in the dispersion model comparisons

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Abstract This paper provides an introduction to the special *Atmospheric Environment* issue on comparisons of 17 widely-used dense-gas dispersion models using observations from the 2015-2016 Jack Rabbit II (JR II) chlorine release experiments. Other papers will describe specific aspects of the JR II field experiment, results of individual dispersion model runs for the models, and comparisons of model predictions with JR II observations and other models. Here we provide a general overview of the field experiment and a brief summary of the model comparison goals and methods.

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1. Introduction and Overview of JR II

The Jack Rabbit II (JR II) field experiments were the second in a series of large-scale outdoor hazardous gas release trials that have been conducted at the United States Army Dugway Proving Ground (DPG), Utah, over a ten year period. Jack Rabbit I took place in 2010 and involved 10 trials with 1 to 2 ton releases of pressurized liquefied chlorine and anhydrous ammonia (see Fox and Storwold 2011, Bauer 2013, Hanna et al. 2012 and 2016, Hearn et al.

2012 and Spicer and Miller 2018). JR I was followed, in 2015 and 2016, by a set of nine trials with releases of approximately five to 20 tons of pressurized liquefied chlorine. Led by the U.S. Department of Homeland Security Science & Technology (DHS S&T) Chemical Security Analysis Center (CSAC) and collaborative team of partners from government, industry, and academia, these field trials were performed to fill critical data and knowledge gaps in atmospheric transport and dispersion modeling, emergency response, industrial safety, and hazard and risk mitigation. Phase 1 of the JR II testing was completed in September 2015, with the execution of five chlorine release trials ranging from approximately five to 10 tons each. Phase 2 was completed in September 2016, with four additional chlorine release trials ranging from approximately 10 to 20 tons each. The atmospheric transport and dispersion modeling gaps addressed in JR II included: large-scale releases; effects of obstacles and buildings; source-term mass-balance for initial conditions; validation of models beyond 0.5 km; investigation of rapid phase transitions and limited soil chemical reactivity. The DPG final test report by Nicholson et al. (2017) describes the characteristics of the JR II field experiments and results. Further details are given in several other papers in the current JR II special issue on model comparisons.

1.1 *Test Site*

The field experiments were performed at the DPG testing installation located in the Utah desert approximately 75 miles southwest of Salt Lake City (see Nicholson et al., 2017). DPG consists of over 1,250 square miles of encroachment-free terrain, including nearly a half million acres of salt flats with mountain ranges on the west, east, and south edges, as shown in the Google Earth image in Figure 1. The site selected for the JR II test grid, shown in Figure 2 as a green wedge, is an extremely isolated part of the desert playa where the salt flats extend to the north for nearly 90 miles with a less than 1/10,000 slope. This area is completely uninhabited and nearly devoid of vegetation, which made it a suitable location to release of tons of chlorine while minimizing the environmental impacts and risks to safety and health.

Figure 1 – Satellite photo (Google Earth) of western Utah including DPG. Mountains are visible as a dark color, while the light color is the desert area, which is about 100 km wide (W-E) at its widest point. The Jack Rabbit II Test Grid was approximately in the middle of the lower left lobe of the desert

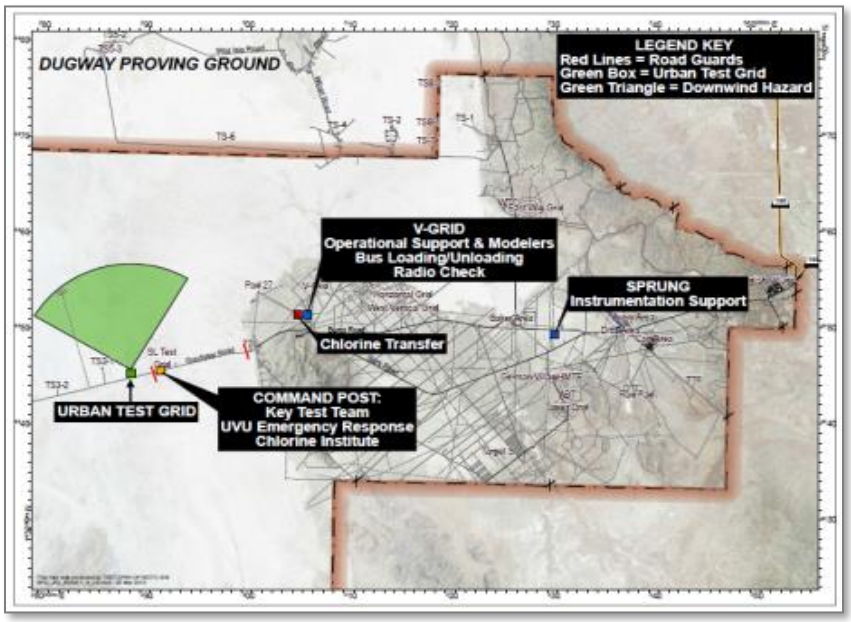

Figure 2. Portion of Dugway Proving Ground, Utah, showing sites used for the JR II field experiment. The green wedge encompasses the sampling grid.

For Trials 1-5, conducted in 2015, a staggered grid of over 80 CONEX containers was set up in a square array called the "Urban Test Grid" atop a 122 m x 122 m (400 ft. x 400 ft.) gravel foundation, which was constructed to support these structures and test activities on the relatively soft desert playa. The source tank was located about 25 m inside the upwind edge of this array as depicted in Figure 3. An additional 61 m x 122 m (200 ft. x 400 ft.) portion of the gravel base was constructed upwind to mix and condition the air as it flowed from the playa to the 0.61 m (24 in.) high foundation, which had a 20 degree slope at all the edges.

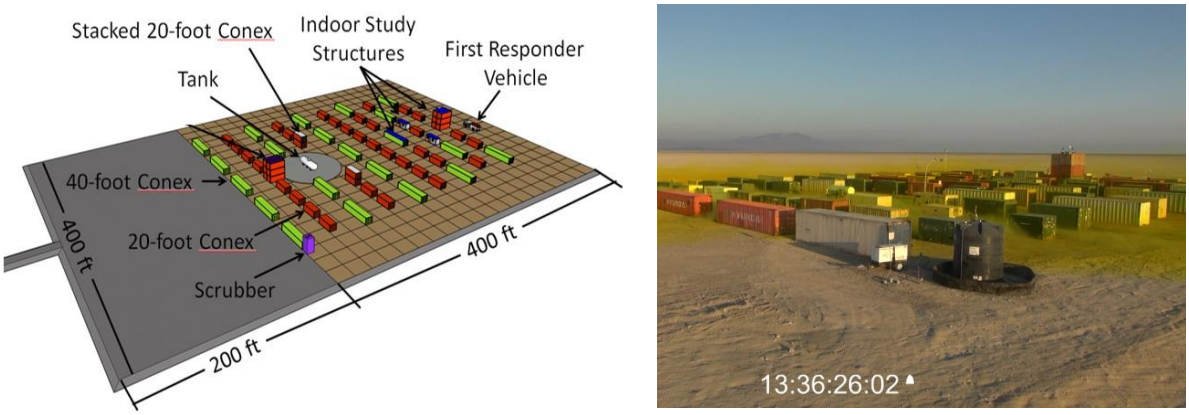

Figure 3 – The Urban Test Grid (UTG) test site configuration used in JR II Trials 1-5 is shown in the illustration (left) indicating the locations of the release tank, Conex containers, and vehicles corresponding to the photo of the UTG (right) approximately 30 seconds after the Trial 1 release.

Within the UTG, the release tank was positioned on top of a rebar-reinforced circular concrete pad that was 25 m (82 ft.) in diameter and 15.2 cm (6 in.) thick. The concrete pad was also constructed with a 2.5 cm (1 in.) high perimeter lip in order to contain any liquid pooling on the ground during a release. This enabled the liquid phase to be observed and quantified, and it avoided permeation of liquid chlorine into the ground where it could have persisted for days and delayed additional trials. Spicer and Tickle (2020) provide details of the release tank and the concrete pad.

A combination of 86 Conex containers were deployed to the UTG that were between 5.48 m to 12.19 m (18 ft. to 40 ft.) long, and 2.44 m (8 ft.) high. During Trials 1 through 5, most of the Conex containers were placed on the UTG as single unstacked units. One structure, seen at

the far right in both panels of Figure 3, was erected using six 6.1 m (20 ft.) long containers stacked in a 2 × 3 configuration. This structure, along with one additional 12.2 m (40 ft.) Conex container and two trailers, were modified to include installation of indoor instrumentation to measure and characterize the infiltration of chlorine during the experiments (see Sohn et al. 2019 for a description of the results of the indoor measurements). The dimensions of the trailers were approximately 6.1 m × 3 m × 2.4 m (20 ft. × 10 ft. × 8 ft.). Additionally, three fire trucks, one ambulance, and three cars were placed at various positions on the UTG to support several experiments and objectives from partners in the Emergency Response community (see Byrnes et al. 2017 and Byrnes and Noll 2019).

For Trials 6 through 9, conducted in 2016, the array of Conex containers at the UTG was removed, as shown in Figure 4, leaving only two structures used for indoor infiltration studies (see Sohn et al., 2019). Two emergency response vehicles were also deployed in Trials 6 through 9 to assess the operational impact, damage, and interior survivability of exposure to a high-concentration (10,000 to 100,000 ppm) chlorine cloud.

Figure 4 – The test site configuration of the 2016 JR II release trials is shown from drone footage captured by Utah Valley University Emergency Services partners. Conex containers were removed from the UTG for Trials 6-9, leaving only two vehicles and two structures.

1.2 *Chlorine Release Tank, Mechanism, and Procedures*

As described by Spicer and Tickle (2020), a purpose-built 7.70 m^3 tank was used to contain and disseminate the chlorine for the 5 to 10-ton (4,540 to 9,070 kg) release experiments in Trials 1-8. The tank was reused for each trial, and was refilled from a 20-ton (18,100 kg) chlorine tanker truck vessel between experiments. For Trial 9, the tanker truck vessel itself was breached to release 20 tons (18,100 kg) of chlorine in the final experiment. Before all trials, the release tank was filled with chlorine and pressurized to approximately 100 psi (6.9 barg), which is consistent with the pressures used when transporting liquefied chlorine in bulk domestically via rail car or tanker truck.

Releases from the tank were achieved by remotely firing explosive bolts to remove a flange covering a 15.2 cm (6 in.) diameter hole at various ports on the tank. The tank was designed with four dissemination ports, each oriented differently as follows: 0 degrees (upwards), 90 degrees (horizontal), 135 degrees downwards, and 180 degrees downwards. A photo of the tank is shown in Figure 5, with the black circular ports visible as described.

Figure 5 – The tank used to disseminate chlorine in JR II Trials 1-8 is shown with four different 6-inch circular ports (black) from which a breach could be generated to conduct a release.

A suite of instrumentation was deployed inside and outside of the tank to capture data needed to characterize mass flux and other critical source term data. The tank was mounted on a support system that incorporated seven load cells and 14 flexors to measure the dynamic mass of chlorine as it exited the tank and also account for the forces generated by the escaping jet of liquid and gas. Vertical liquid temperature profiles were dynamically measured inside the tank with bare wire thermocouples on two separate arrays. Absolute and differential pressures were measured and reported in real time during filling operations and releases. Immediately outside the tank, guided wave radar (GWR) instruments were deployed on the circular concrete pad to measure the depth of any liquid chlorine that pooled. Additionally, 36 type K 24 American Wire Gauge (AWG) wiring thermocouple arrays were deployed to measure the temperature at three locations surrounding the release tank both above and below grade (imbedded in the concrete pad).

For all trials, the releases of pressurized liquefied chlorine took place in the early morning, where the field test director was aiming for about 7:30 to 8:00 am local time (Mountain Daylight Time, or MDT, which is Greenwich Mean Time minus six hours). Climatological analysis by DPG meteorologists of several years of data from routine local observations near the planned release site had suggested that the dominant wind direction during the hour or two after sunrise was from the south-south-east (165°), so the sampling grid (an arc encompassing 90°) was set up along that direction (see Figures 8, 9, and 10). On planned release days, the DPG test director consulted the observed local winds and WRF model predictions, and proceeded with the release only if the wind direction was "on the sampling grid" (between 120° and 210°) and the wind speed was between 2 and 6 m/s at a height of 2 m.

1.3 *Instrumentation Grid and Data Collection*

As part of the field experiment, chlorine concentrations were observed by over 200 point detection instruments in the near field ($x < 100$ m) and at sampling arcs at distances of 120 m, 200 m, 500 m, and 1 km, 2 km, 5 km, and 11 km downwind. Detectors were deployed on the outer arcs spanning 90 degrees (from 300 to 30 degrees). Chang et al. (2020) provide details of the chlorine samplers.

Chlorine concentrations in the near field to the 200 m arc were measured primarily by portable ultraviolet (UV) Differential Optical Absorption Spectroscopy (DOAS) instruments. This included the UV Canary (Cerex Monitoring Solutions, Inc., Atlanta, Georgia) with a calibrated chlorine detection range of 10 to 15,000 ppm, and UV Jaz™ instruments (Signature Science, Inc., Houston, Texas) with a calibrated chlorine detection range of 100 to 100,000 ppm. Concentrations at the 500 m, 1 km, and 2 km arcs were primarily measured by MiniRAE 3000 (Honeywell Analytics / RAE® Systems, San Jose, California) handheld photoionization detectors with a detection range of 100 to 2000 ppm. At the long range sampling arcs at 5 km and 11 km, handheld ToxiRAE Pro electrochemical detectors were primarily deployed to measure the concentration with a detection range of 0 to 50 ppm.

Chlorine concentration and chlorine cloud tracking data were also collected by several standoff detectors and instruments deployed by the testing team and partners, including portable UV Sentry (Cerex Monitoring Solutions, Inc., Atlanta, Georgia) UV-DOAS instruments, and 6 different Light Detection and Ranging (LIDAR) instruments positioned up to 2 km away from the release tank.

Meteorological data were collected from more than 200 separate instruments deployed throughout the test grid and area, and included near-surface measurements as well as vertical profiles up to 2 km. The DPG meteorology team deployed 49 Portable Weather Information Display Systems (PWIDS) which measured wind speed, direction, temperature, humidity, and pressure at multiple test site locations and elevations. PWIDS were also collocated on 32-meter meteorological towers with ultrasonic anemometer to collect data that were processed to produce wind and turbulence statistics and fluxes of heat and momentum. Data to characterize horizontal and vertical wind profiles were collected using Sonic Detection and Ranging (SODAR) instruments, Doppler radar wind profilers, and weather balloons released during Trials 6 through 8. Hanna (2020) presents analyses of the JR II meteorological data and recommendations for surface and aloft meteorological profiles for use in the dispersion model comparison that is the subject of this special issue.

A variety of high-definition (HD), high-speed (HS), and IR video cameras were also deployed throughout the test grid during all trials to visualize and record the chlorine releases, and thousands of high-resolution photographs were taken before, during, and after every test to document each trial to the greatest extent possible. In total, over 2 terabytes (TB) of data were generated and acquired, enabling analysis and characterization of multi-ton chlorine releases to an unprecedented degree. These data have undergone rigorous quality assurance and quality control measures and were archived into the JR II final data package, which is maintained in mirrored archives by DHS S&T CSAC, DTRA, and DPG.

1.4 *Trial Summary and Observations*

All nine field trials took place in the early morning, with releases of about 5 to 20 tons of pressurized liquefied chlorine from a hole of about 15 cm diameter in the tank. These masses are typical of what might be released during a road tanker-truck accident, and are about 10 to 30 % of what would be released from a railcar. These field experiments are unique in that no previous field experiments have come even close to using this large of a mass release of chlorine. The chlorine release times and basic characteristics of the nine total JR II trials are listed in Table 1.

Table 1. Basic characteristics of the nine JR II release trials.

Trial	Date (MDT)	Start Time (MDT)	Release Duration (s)	Average Emission Rate (kg/s)	Jet or Pool Mass (kg)	Wind Speed Near Source at z = 2 m (m/s)	Wind Direction Near Source (deg)	Temp. Near Source (C)
1	8/24/2015	7:35:46 AM	20.3	224.0	4,547	1.5	147	17.5
2	8/28/2015	9:24:21 AM	32.4	252.8	8,192	4.7	176	23.0
3	8/29/2015	7:56:55 AM	20.3	225.0	4,568	3.8	170	22.9
4	9/1/2015	8:39:33 AM	28.8	243.6	7,017	1.8	196	22.6
5	9/3/2015	7:29:09 AM	33.6	248.4	8,346	1.5	242	21.5
6	8/31/2016	8:23:35 AM	32.2	260.0	8,372	2.4	147	22.3
7	9/2/2016	7:56:00 AM	33.3	259.0	8,625	4.0	150	18.7
8	9/11/2016	9:01:45 AM	30.0	78.93	2,368	2.1	120	15.8
9	9/17/2016	8:05:00 AM	132.6	133.5	17,700	2.6	162	11.2
7 dump	9/2/2016	8:11:00 AM	300	1.507	452	4.0	150	18.7
8 dump	9/11/2016	9:16:45 AM	300	22.51	6,754	2.9	129	15.8

In all five of the 2015 trials, the chlorine was released downward through a hole in the tank, as shown in Figure 6. In two additional trials in 2016 (Trials 6 and 9), the chlorine releases were also directly downward through a hole in the bottom of the tank, which assured that all of the tank contents were evacuated rapidly during the experiment. The bottom of the tank was about 1 m above ground level.

Figure 6. Photographs of JR II 2015, showing the CONEX array, when Trials 1-5 took place. The 10 ton release tank is visible in the top photo, 47 s after the Trial 5 release. The photo on the bottom was taken during Trial 1, 27 s after the release, with the wind blowing towards the left of the photo.

In Trial 7, the hole was at a 135° angle downward (relative to 0° at the top of the tank) and directed downwind, and in Trial 8, the hole was in the top of the tank at 0°, which oriented the release directly upwards (see Figure 7). Therefore, in these two trials, there was some liquid chlorine left in the tank as the tank rapidly depressurized, cooling the remaining chlorine to a temperature below the boiling point. That liquid was "dumped" to the surface about 5 minutes after the initial momentum jet ceased. The resulting liquid pool subsequently evaporated in 5 to 10 minutes. Thus, in Trials 7 and 8, in addition to the main release trial, there was another release, from an evaporating pool, which was detected by the concentration sampling network.

Figure 7. Photographs of the chlorine releases in Trials 6-9 of the JR II 2016 field experiment. Source: drone footage captured by Utah Valley University Emergency Services partners.

For the first 30-60 seconds of the JR II trials, the release is two-phase, with about 20 % of the mass in the gas phase, and the remainder in the liquid phase in the form of small (50 to 100 μm) drops. About 30 to 40 % of the released mass was observed to "rain-out", or deposit on the surface of the 25 m diameter concrete pad directly beneath the tank. The rained-out liquid was observed to evaporate in approximately 20 to 25 minutes. Spicer and Tickle (2020) make specific recommendations on the quantitative recommendations for mass emission rate, and rainout, and liquid pool evaporation. Initially, the effective density of the two-phase mixture following the release is about 10 or 20 times that of air, and, after the drops evaporate, the density is about 2.5 that of air. Therefore, a dense gas dispersion model is needed to assess the downwind concentration variations.

As mentioned earlier, Nicholson et al. (2017) describe JR II in their DPG Final Test Report. More details on the JR II emissions, the meteorology, the chlorine concentrations, and the cloud width and depth observations are given in other papers in this special issue (Spicer and Tickle 2020, Hanna 2020, Chang et al. 2020, Mazzola 2020, and Mazzola et al. 2020).

2. Inputs for model comparison

Many dense gas dispersion models exist, but not all are widely-used. For this special issue, describing the results of comparisons of 17 dense gas dispersion models with three of the JR II trials (1, 6, and 7), many members of the international community have joined together to run their models and compare the results. Because most of the groups running their models are doing the work as volunteers, depending on their organizations' internal funding, we tried to make the work as easy as possible. We provided some simplified model input files (emissions and meteorology), by carrying out analyses of the extensive available data and condensing the information into data sets consistent with the models' needed inputs. This initial model comparison exercise used the three trials (1, 6, and 7) that had the highest observed concentrations. The wind direction in these trials also aligned the plume to disperse within the sampling grid.

As mentioned above, the 17 models being compared with the JR II field data have slightly different requirements for inputs. Not wanting to bury the modelers in Gigabytes of JR II field data, but still provide enough information for everyone to run their models, we analyzed the complete set of field data and developed a simplified, optimized set of inputs that can be used by all models. For the three trials being modeled (1, 6, and 7), the standard recommended model inputs covered:

- Source configuration and simplified emissions (Spicer et al. 2020)
- CONEX positions and all concentration and meteorological observation positions (Chang et al. 2020, Hanna 2020)
- Meteorological inputs, such as boundary layer parameters (near surface wind speed and direction, heat flux, friction velocity, Monin-Obukhov length, etc.), surface roughness length z_o, CONEX morphology parameter Λ_p, and vertical profiles of temperatures and winds (Hanna 2020)

Participants were allowed to modify the above-provided inputs (e.g., run their own source emission model, or choose different meteorological inputs). All modelers were asked to submit the following outputs, where C is chlorine gas concentration:

- Arc max C (raw and 20- and 60-s averages) at 0.2, 0.5, 1, 2, 5, and 11 km
- Cloud widths and heights to 200 and 20 ppmv at same distances
- C contour plots at various times after release
- C time series at sampler locations

However, in some cases (e.g., the two RAILCAR options), the modeler provided slightly different outputs and/or used slightly different inputs, since they had run their model prior to the start of the current model comparison study, and did not have resources to rerun with the updated inputs.

2.1 *Emissions Inputs*

The estimated JR II emissions durations and rates and total mass released are based on analyses by Spicer and Miller (2018) and Spicer et al. (2019). In addition to summarizing previous work, Spicer and Tickle (2020) developed simplified source specifications for the purpose of making a fair comparison between atmospheric dispersion model predictions and observed concentrations. Two simplified sources were developed for Trials 1-7. In one case, a single (constant) mass rate was specified based on the primary (essentially constant) aerosol release rate. This rate was chosen because it is the fastest rate that chlorine could move downwind and would represent an upper bound, especially for near field measurements. In the second case, the release was divided between an initial aerosol release and an evaporating liquid release. The aerosol rate accounted for the primary release as well as rainout on and re-evaporation of chlorine on the concrete pad. The duration of this phase was the duration of the primary release from the tank. The evaporating liquid release rate was taken to be the pool evaporation rate at the end of the aerosol release. This case was developed to represent the rate chlorine was estimated to move downwind during the primary release as well as the evaporating pool. In both cases (single rate and two-period rate), the final duration was chosen so that the total amount of chlorine released was included in the dispersion model simulations.

2.2 *Locations of CONEXs, concentration samplers, and meteorological instruments*

The modelers were provided with locations (lat-long and elevations) of all instrumentation. The 3D geometry data for the CONEXs were provided. For example, Figure 8 shows the CONEX positions for the 2015 trials 1 -5. Concentration sampler positions are also shown.

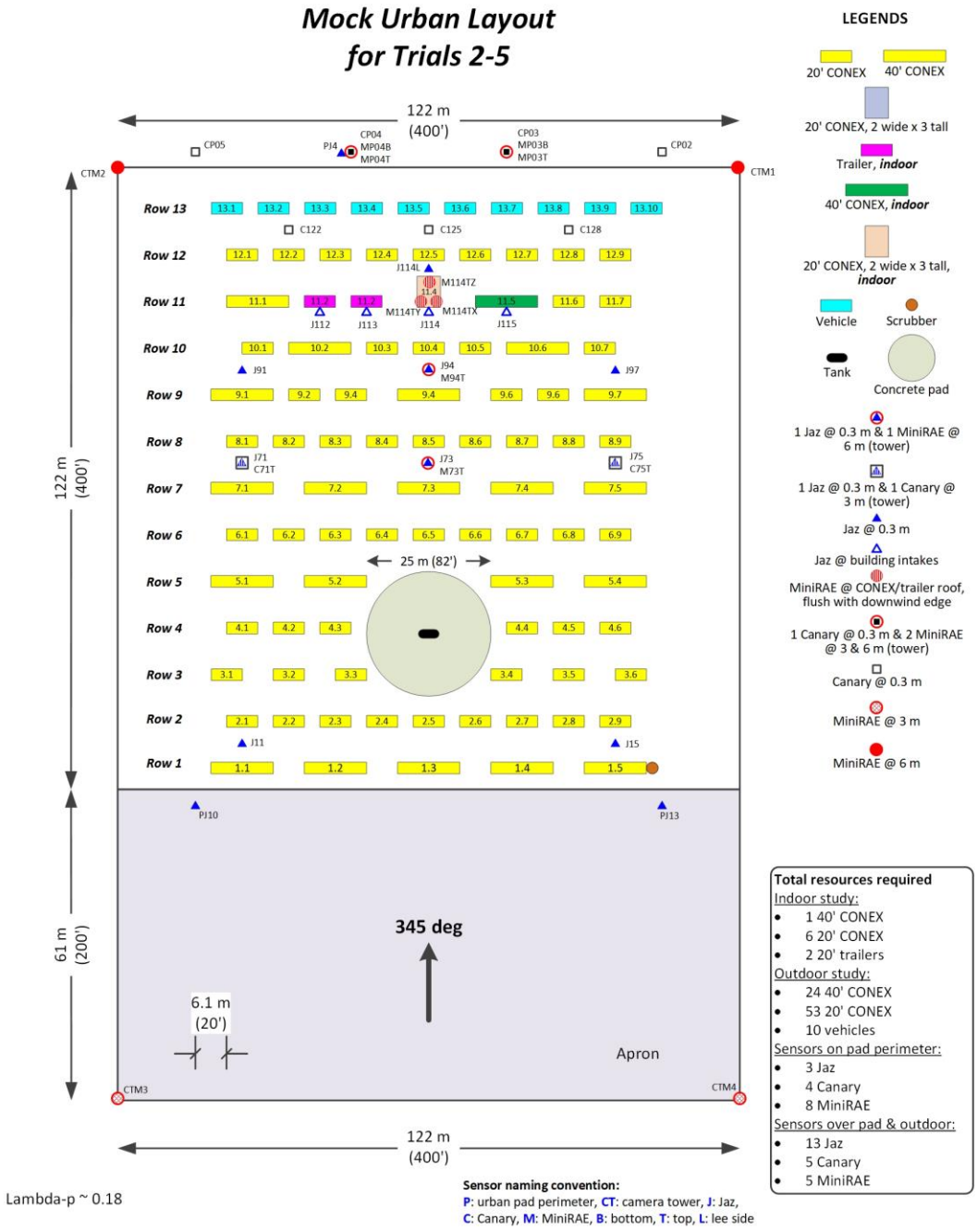

Figure 8 – Mock Urban CONEX array and chlorine samplers within the array for Trials 2-5. The 25 m diameter concrete pad on which the tank was placed can be seen.

There were four types of concentration samplers (photo-ionization detectors or PiDs) used – Jaz (about 1,000 to 100,000 ppm), Canary (about 200 to 15,000 ppm), MiniRaes (about 10 to 2000 ppm), and ToxiRaes (about 1 to 50 ppm). They provided data with resolution of about 1 to 2 s. Most were located at a height of 0.3 m; they were low to the ground because a dense chlorine cloud is known to be shallow.

In Figure 9, the sampler locations on arcs at 85, 120, and 200 m are shown on the left side. and the locations on arcs at 200 and 500 m are shown on the right side. At a few locations, vertical profiles of concentration were measured on 3 or 6 m towers.

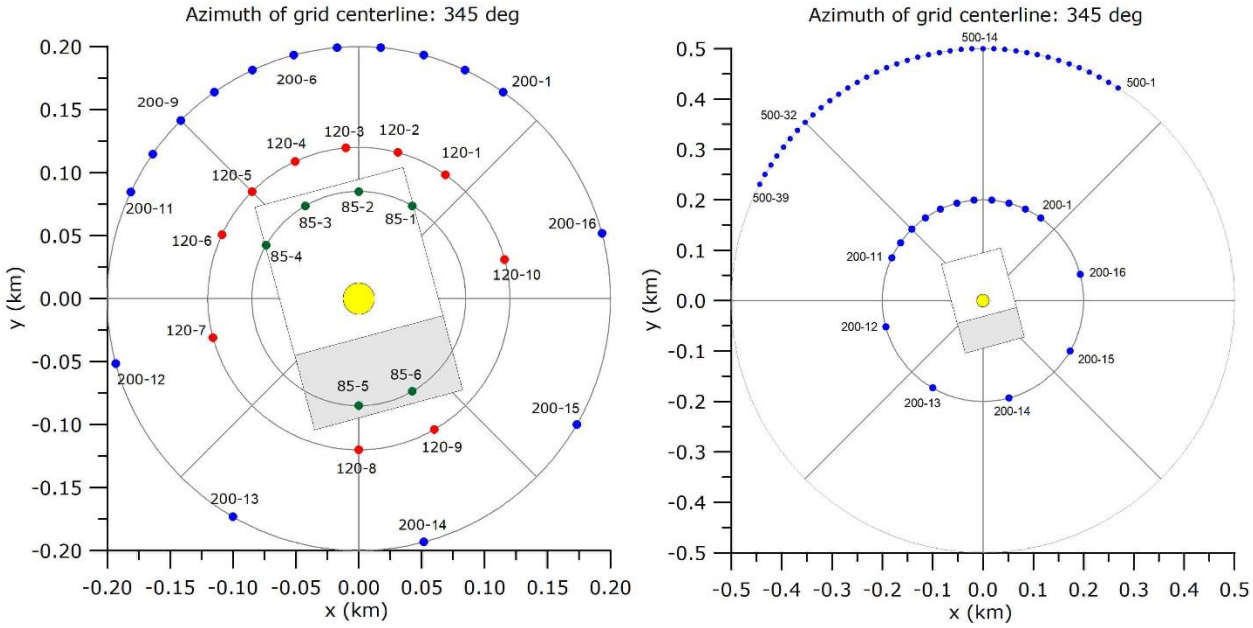

Figure 9. Sampler locations for arcs at 500 m and less for 2016.

Figure 10 shows the sampler locations at 1, 2, 5, and 11 km. Note that the sampler arcs cover 90 degrees in Figure 7, and are centered on a wind direction from 165 degrees (or towards 345 degrees), which is the dominant wind direction in late August in the early morning at the site. The samplers were placed sufficiently close to each other so as to help assure that at least 3 or 4 samplers on each arc would be "hit" by the chlorine cloud.

To determine cloud widths and depths to the 20 ppm and 200 ppm contours, the in situ (fixed) samplers were used, as well as three DPG LIDARs. The LIDARs used theoretical absorption techniques so that a concentration could be estimated based on the signal returning to the LIDARs (see Mazzola, 2020).

The farthest arc was at 11 km, which is equal to about 7 miles.

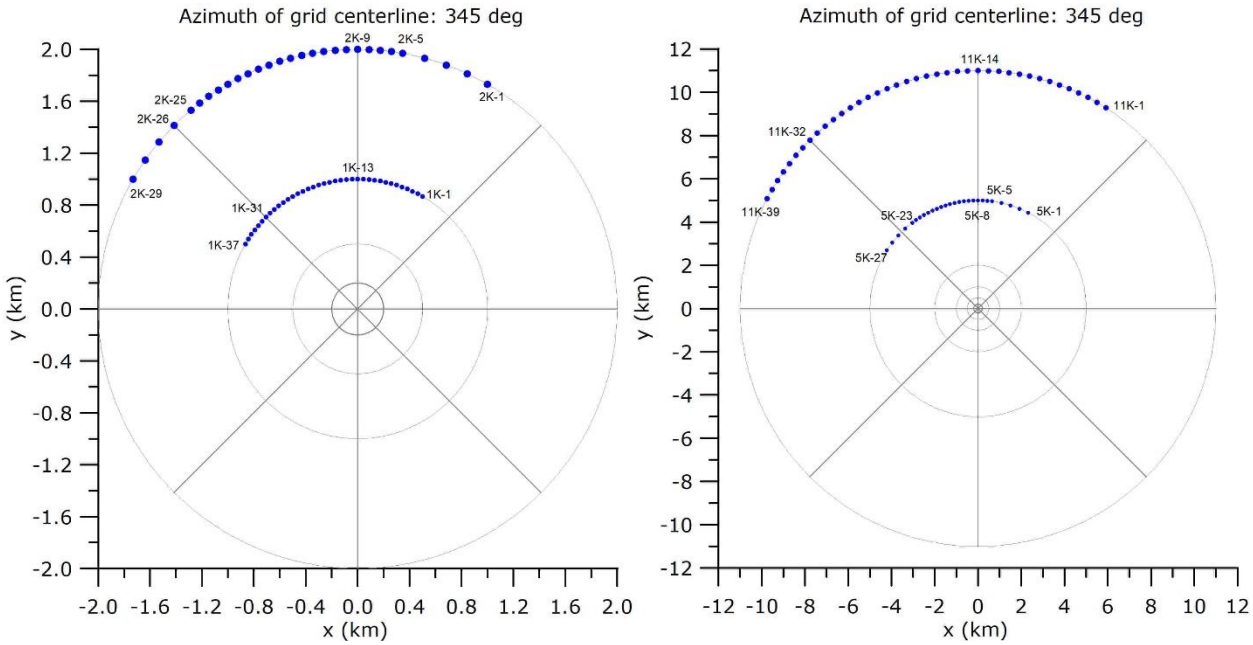

Figure 10. Sampler locations for 1, 2, 5, and 11 km arcs for 2016.

2.3 *Meteorological Inputs*

The meteorological instruments at the JR II experiment site included a meso-network of about 35 surface wind sites, a surface energy balance site, three 32 m towers located 1 km apart, and several vertical sounding instruments. The challenge was to determine a single set of meteorological inputs for the dispersion models. The specific recommendations for meteorological inputs for the model comparison exercise are described by Hanna (2020).

It is assumed that the recommended meteorological conditions should be representative of the flat desert about 100 m upwind of the chlorine release location. Recommendations of surface

momentum and sensible heat fluxes for each field trial are based on 30 minute averages of sonic anemometer observations at 2 m on the upwind 32 m tower and at 2.5 m on a nearby "Energy Balance" station, for the period during which the chlorine release took place. Wind speed and direction are 10-minute averages of aerovane observations at 2 m on the same upwind 32 m tower and a nearby 2 m tower. Wind profiles on the same 32 m tower during nearly neutral conditions were used to estimate that the surface roughness length, z_o, for the flat desert equals 0.5 mm.

Some of the dispersion models can parameterize the wind flow in the "street canyons" of the CONEX array used in 2015. For this purpose, the height of the CONEXs (H = 2.6 m) and the morphology parameters λ_p (ratio of obstacle plan area to total lot area) and λ_f (ratio of obstacle frontal area facing the wind to total lot area) are often used. Since the CONEXs width and height are approximately the same, it can be assumed that $\lambda_p = \lambda_f$, which are calculated to equal 0.18.

Single vertical profiles of wind speed, wind direction, and temperature were specified for a time close to the chlorine release time, based on observations at five levels on the three 32 m towers, a radiosonde, a minisodar, and two wind profilers (449 MHz and 921 MHz). A RASS system measured temperature profiles at the 449 MHz profiler location. The nine chlorine releases began at times ranging from about 7:30 am to 9:30 am MDT (local time). The boundary layer was stable for releases before about 8:30 and was marked by a shallow mixed layer (about 8 to 16 m) for later releases. Above the 32 m tower tops, the atmosphere was stable up to elevations of a few hundred meters. Large wind direction shears were usually found in this layer, since the near-surface flow was a drainage (katabatic) down-valley flow (from about 165 degrees), while the synoptic flow above 100 m was from the west.

Another important caveat is that JR II took place in a broad flat valley where drainage winds were occurring in the early morning. There were often mesoscale variations in winds observed in time and space. For example, Trials 1, 5, and 8 were marked by variations in observed wind speeds (up to a factor of two) and/or directions (up to about 60°) with periods of about 10 to 20

minutes in the near field. These relatively slow trends show up as increased u* and increased turbulence intensities, which also do not agree with Monin-Obukhov similarity.

2.4 *Examples of model inputs*

Here we provide examples of the detailed model input specifications sent to all modelers. Mazzola et al. (2020) provide details. Table 2 is a broad overview of model inputs, and Table 3 addresses the source emission rate details.

Table 2. Recommended model inputs for model comparisons for Trials 1, 6, and 7.

	Trial 1	**Trial 6**	**Trial 7***
Release Parameters			
Location, all at Dugway Proving Grounds; Zone 12 UTM coordinates	Northing 4445633.9 m Easting 288109.2 m Elevation 1295.5 m		
Date and Time (hh:mm:ss UTC)	24 August 2015 13:35:45	31 August 2016 14:23:35	2 September 2016 13:56:00
Tank Inventory (kg of Cl_2)	4500	8400	9100
Pressure measured at top of tank (psia)[1]	104.4	86.8	86.9
Liquid temperature (^oC)[1]	15.7	16.0	15.9
Release jet orientation (deg from tank top center)	180	180	135
Release height (m)	1.0	1.0	1.48
Hole diameter	6.0 in = 0.152 m	6.0 in = 0.152 m	6.0 in = 0.152 m
Weather/Environment			
Atmospheric pressure (mbar)	873.7	871.1	868.5
Initial wind speed[2] (m/s) at z = 2 m	1.45	2.42	3.98
Initial wind direction[2] at z = 2 m	147.4	146.9	149.6
Initial temperature (^oC) at z = 2 m	17.5	22.3	18.7
Surface roughness (mm)	0.5	0.5	0.5
Friction velocity[3], u_* (m/s)	0.108	0.093	0.210
Sensible heat flux[3], Hs, (K-m s^{-1})	-0.012	-0.0034	-0.0160
Vertical profiles of wind speed and direction and temperature[4]			
Inverse Monin-Obukhov length (m^{-1})	0.068	0.056	0.0229
Pasquill Class[5]	E/F	E	D/E

* - Trial 7 primary release shown. Secondary or "dump" release will be defined separately.

1 – The liquid in the tank should be considered at a saturated state and these experimental best numbers adjusted to assure that as needed by the analyst

2 – Initial wind is a 10 minute average at time of release initiation. Wind direction is the direction from which the wind blows in degrees clockwise from true North.

3 – Turbulent boundary layer parameters from 30 min average data at time of release.

4 – Vertical profiles of wind speed, wind direction and temperature are discussed in Hanna (2020)

5 – If the dispersion model has an option to use either Monin-Obukhov length or Pasquill Class to specify the atmospheric stability, the Monin-Obukhov length should be used for consistency.

Table 3. Recommended averaged source emission rates for trials 1, 6, and 7.

	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	-37.4	-37.4
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

* Ignoring kinetic energy effects

3. Models involved and comparison methods

A Modeling Working Group (MWG) was established for JR II planning and analysis beginning in 2014. Most modelers in the current comparison exercise were on the MWG, which had biweekly conference calls. Several modelers ran test cases to assist in designing the sampling grid for the field experiment and have seen the preliminary JR II data. Because some other modelers had not seen JR II data, not all modelers were on an equal footing. This exercise was not a competition, but was undertaken in the spirit of collaboration, to improve the quality of toxic industrial chemical modeling tools in general. Table 4 is a listing of the model names and organizations who participated. Other papers in this special issue have been written by the persons running each model.

Table 4. Models and organizations participating.

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	Defense Threat Reduction Agency (DTRA), USA
Integral Dense-gas Dispersion Model (IDDM)	National Center for Atmospheric Research (NCAR), USA
PHAST	DNV GL, Ltd, UK
Parallel-Micro-SWIFT-SPRAY (PMSS)	Aria Technologies and Atomic and alternative Energies Commission (CEA), France
Puff model of atmospheric dispersion (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

Most models do not directly treat specific JR II configurations (e.g., obstacle array, 180^{o} and 135^{o} downward pointing jets), but these effects should dissipate farther downwind

There are some uncertainties regarding the observations of arc max C and cloud widths and depths. Of course, one major uncertainty is the likelihood that the actual cloud center (and arc max C) could occur in between the samplers. This is more likely on the 5 and 11 km arcs, where, sometimes, only three or four samplers are "hit". Another cause of uncertainty is that some (6 out of 18) samplers during Trials 1, 6, and 7 reported arc max C values that are saturated, so the actual arc max C likely exceeds the reported values. For example, the MiniRAE arc max C readings in Trials 1 and 6 at 0.5 km are saturated at about 3,300 ppm, and the ToxiRAE readings of 50 ppm at 5 or 11 km are saturated. We retained the saturated data in this model comparison, lest we lose 33% of the data. The field experiment directors shifted some samplers around from trial to trial to try to avoid saturation, but, unfortunately, there was a shortage of samplers that could provide useful data at high chlorine concentrations. See Chang et al. (2020) for more detailed discussions.

Estimated cloud widths were also affected by the limited numbers of samplers "hit" on the far arcs. Furthermore, due to cloud meandering, the instantaneous cloud width could be significantly less than the time-averaged cloud width. The LIDAR remote observations of cloud width were useful, but there were some uncertainties due to the calibration methods between the LIDAR signal and concentration.

Estimated cloud heights were obtained from the sampler towers only when there was a significant decrease of concentration with height on the 6 m towers. Otherwise, LIDAR observations were used. See Mazzola (2020) for more discussion of the cloud widths and heights.

The 17 model predictions of arc max C and of cloud width and height are compared qualitatively using plots of predictions and observations versus downwind distance for the three trials in the paper by Mazzola et al. (2020). Quantitative performance measures, such as fractional mean bias FB and fraction of predictions within a factor of two of observations, are calculated using the BOOT model evaluation software (Chang and Hanna 2004).

4. Further Comments

The Jack Rabbit II project sought to provide critical data and address knowledge gaps in atmospheric transport and dispersion modeling, emergency response, industrial safety, and hazard and risk mitigation. The experiments involved the largest releases of chlorine ever undertaken and provided a highly detailed dataset of measurements from hundreds of sensors measuring release rates, gas concentrations, meteorological conditions and other parameters. The success of the project is testament to the vision of the project coordinators, the generous support of the funding agencies and the hard work of the dedicated staff at Dugway Proving Ground and the dozens of other scientists and engineers who have participated in the project. This paper has provided an introduction to the project with a short description of the test configurations, the measurement equipment, release conditions, meteorology and model inter-comparison studies. Further details on each of these topics are provided in the papers cited within this special issue of the *Atmospheric Environment* journal.

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