

# DENSE GAS PLUME RISE AND TOUCHDOWN FOR JACK RABBIT II TRIAL 8 CHLORINE FIELD EXPERIMENT

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**Abstract:** The series of nine Jack Rabbit II (JR II) chlorine release field experiments in 2015 and 2016 involved releases of pressurized liquefied chlorine from tanks containing 5 to 20 tons of liquid. This paper concerns JR II Trial 8, where the release hole (15.2 cm diameter) was oriented upwards at the top of the tank. To our knowledge, this is the only full-scale vertically-directed release of pressurized liquefied chlorine that is available for detailed analysis. Our aim is to improve understanding of the characteristics of the dense jet trajectory (e.g., maximum plume rise, downwind distance where the dense plume first touches the ground, and maximum concentration at touchdown). The chlorine emission rate was measured by instruments in the tank, and the plume rise geometry was estimated from photographs, videos, and lidar scans taken from several angles. During the first 10 seconds of the release, the videos show that the dense jet rises up to about 40 m, then sinks towards the ground, touching down at a distance of about 60 m. The portion of the plume that sinks to the ground then spreads out about 30 to 40 m in all directions due to gravity slumping. Due to the decrease with time of the momentum jet mass release rate, the jet gradually becomes less dense and less powerful and the plume remains aloft after about 30 to 60 s. However, the dense cloud that touched down in the early phases moves downwind as a typical dense cloud. The observed dense jet plume rise and touchdown distance are shown to approximately agree within about a factor of two with integral model predictions by 1) the analytical dense gas plume formulas suggested for vertical jets in 1973 by Hoot, Meroney, and Peterka (HMP), 2) the analytical formula for buoyant (positive or negative) plume trajectory suggested by Briggs in 1969, and 3) the DRIFT dispersion software, which is an integral model. Also, HMP and DRIFT model predictions of concentration at touchdown agree with Trial 8 observations within a factor of about two. It is concluded that the dense jet plume models are able to simulate the Trial 8 plume trajectory and ground level maximum concentration within acceptable ranges (i.e., most of time, within a factor of two).

**Key words:** *dense gas dispersion; chlorine releases; plume rise of dense jet; touchdown of dense jet plume, Jack Rabbit II field study*

## INTRODUCTION

The Jack Rabbit field experiments in 2010, 2015, and 2016 were initiated because there had been much concern about the possible effects of pressurized liquid chlorine released from storage tanks and transportation vessels. The JR I field experiments, which took place at Dugway Proving Ground (DPG) in the U.S. in 2010, addressed one and two ton releases of pressurized liquefied chlorine or ammonia from a tank mounted about 1 m above ground, with the initial jet pointed downward (Fox and Storwold 2010, Bauer 2013, Hanna et al. 2012 and 2016). JR II took place in 2015 and 2016, also at DPG, and involved nine chlorine release trials, with released amounts of about 5 to 20 tons (Fox et al., 2021).

50 A special virtual issue of this journal (in which the current manuscript is placed)  
51 contains papers related to a 17-model comparison exercise that used observations from  
52 JR II trials 1, 6, and 7, which all involved downward-directed jets. Several of the  
53 special issue papers are general (i.e., apply to all nine trials), covering topics such as a  
54 comprehensive project overview (Fox et al., 2021), a discussion of source emissions  
55 (Spicer and Tickle, 2020), recommendations on meteorological inputs (Hanna, 2020), a  
56 description of concentration observations (Chang et al, 2020), and a summary of the  
57 results of the 17-model comparison study (Mazzola et al., 2020). Because these general  
58 papers are available, we will refer the reader to those papers for comprehensive  
59 discussions of some topics.

60  
61 The current paper analyzes the dense gas plume observed during JR II Trial 8, the  
62 only trial with an upward directed release. Trial 8 received only limited attention in the  
63 multi-model comparison, which focused on downwards-directed releases. The main  
64 novelty is that JR Trial 8 is the only extensively controlled and measured full-scale  
65 field trial in existence involving pressure-liquefied chlorine where the discharge is  
66 upwards from the top of the vessel. The outflow exhibits complex behavior with a very  
67 short (one or two seconds) duration initial gas venting stage, followed by about 30 s of  
68 two-phase venting (due to liquid swell within the vessel – the champagne effect),  
69 through to the final stage of gas-phase venting, which approached negligible discharge  
70 rate at about 100 s. Several models that are commonly used for industrial risk  
71 assessments do not account for this complex physics, and, instead, would simulate Trial  
72 8 as a purely gaseous release (as a consequence, it is likely that such models would  
73 under-predict the hazard at ground level). There are therefore important practical  
74 reasons to study this experiment, since it provides risk assessment specialists and  
75 emergency responders with some insight into what would happen in this release  
76 scenario. It also provides useful scientific data that can be used to assess the accuracy  
77 of dispersion models. Models have not been tested against the Trial 8 observations  
78 previously. It is therefore useful to disseminate in the scientific literature the data from  
79 this unique experiment to enable others to test their models against the measurements.  
80 Plus, we have examined the performance of three integral dispersion models against the  
81 data.

82  
83 Our aim is not to describe the experimental set-up in significant detail, since, as  
84 mentioned above, there are already published papers in the special issue that describe  
85 the JR II details. Because this is the only available field data set for large upwards-  
86 directed dense jets, it is of initial interest to determine whether the dense jet plume  
87 trajectory and maximum ground level concentration are consistent with the physical  
88 principles assumed by integral dispersion models. The models solve for the variation  
89 with downwind distance of the cross-wind integral of concentration, which is described  
90 by a simple shape function. For the Briggs (1969) and the Hoot-Meroney-Peterka  
91 (HMP, 1973) models, the cross-wind shape is a top hat. For DRIFT (Tickle and  
92 Carlisle 2013), the cross-wind distribution is a Gaussian profile (for the momentum-jet  
93 phase). Integral models are routinely used when assessing hazards for regulatory and  
94 safety purposes. It is therefore of practical interest to compare the observed plume  
95 behavior in Trial 8 with predictions from this class of models. A benefit of integral

96 dispersion models, as well as their execution speed, is that they provide insights into the  
97 dominant physics controlling the bulk behavior of the plume.

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99 The three dense gas plume models for vertical releases that we use here are based on  
100 early seminal studies of dense gas plumes by Bodurtha (1961) and Turner (1966).  
101 Bodurtha (1961) carried out wind tunnel tests with dense plumes and focused on  
102 determining how far from the source the dense cloud touched the ground, and the  
103 magnitude of the maximum ground level concentration. Empirical formulas were  
104 suggested. Turner (1966) focused more on analytical solutions to the fundamental  
105 governing equations. Briggs (1969) looked at a large amount of plume rise literature,  
106 for both positive and negative buoyant plumes, developed a set of universal  
107 dimensionless equations based on fundamental science, and used available laboratory  
108 and field data to determine the scaling constants in his equations. His suggested plume  
109 rise trajectory formula is used in the current paper.

110  
111 Hoot et al. (1973) and Hoot and Meroney (1974) carried out a new set of wind  
112 tunnel experiments for vertically-oriented dense jets. Building on Briggs' (1969)  
113 approach, they developed some simple science based analytical formulas that produced  
114 good fits to their observations. We use those formulas here.

115  
116 At about the same time as the Hoot et al. experiments, Ooms and his colleagues  
117 began a comprehensive theoretical analysis of dense jets and carried out a series of  
118 wind tunnel experiments (Ooms et al. 1974, Ooms and Duijm 1984, Xiao-Yun et al.  
119 1985). Cleaver and Edwards (1990) suggest an alternate dense gas jet model and  
120 compare it with experimental data. A few years later, Schatzmann et al. (1995a and  
121 1995b) report results of EPA wind tunnel experiments involving heavy gas jets and  
122 used the data to calibrate and further test a dense jet model. The above wind tunnel  
123 experiments verified the accuracy of the investigators' models.

124  
125 Other more recent papers (e.g., Allason et al., 2014) include dense gas jets as one  
126 component of a more comprehensive research study. They carried out small-scale  
127 experiments with dense jets "outdoors" and compared the results with the predictions of  
128 the Cleaver and Edwards (1990) model.

129  
130 In the above papers on dense gas vertical jets, the photographs and figures all show a  
131 similar behavior, with the dense jet initially rising quickly to a maximum plume rise,  
132 followed by a more gradual descent to the ground. Of course, if the initial negative  
133 buoyancy is not large enough, the plume will not sink down to the ground. This too is  
134 accounted for by the models. When we sent Dr. Robert Meroney (coauthor of the 1973  
135 HMP model) the photographs of the JR II Trial 8 plume, he remarked in a 6 March  
136 2021 e-mail message: "This photo looks remarkably like the dense gas plumes Tom  
137 Hoot visualized in our wind tunnel. The arc and spread of the plume, the impact with  
138 the ground, and the pancake-like spreading up and downstream after the impact. We  
139 tried to document the height of rise, the impact location, and the maximum  
140 concentration at impact, as well as the subsequent down and upwind decay of the  
141 ground concentrations".

142 To compare the three models' predictions with the JR Trial 8 observations, a  
143 challenge arises with two-phase releases that is not present in the wind tunnel and the  
144 small-scale outdoors experiments reviewed above. The difficulty is that the dense two-  
145 phase jet exiting the hole on the Trial 8 tank has a pressure that is several times larger  
146 than atmospheric pressure. However, it is common for models to require initial inputs  
147 of plume volume flux, radius, vertical velocity, and density to be at atmospheric  
148 pressure. Therefore, an "expansion model" is needed to calculate the initial conditions  
149 for the models. Fortunately, for Trial 8, the pressure in the jet decreases to atmospheric  
150 pressure within about 2 to 3 m of travel, which is much less than the observed plume  
151 rise of about 40 m and observed touchdown distance of about 50 m. Here, we use two  
152 alternate widely-used expansion models to define the initial inputs to the models.

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### OVERVIEW OF JR II TRIAL 8

156 The nine JR II field trials took place over an extensive dry lake bed (salt playa) with  
157 minimal vegetation at DPG, where the surface roughness was determined to be about  
158 0.5 mm (Fox et al., 2021). The release was initiated between about 7 to 9 AM  
159 (depending on when the wind speed and direction were within prescribed bounds) in  
160 late August and early September of both 2015 and 2016. The release tank containing  
161 pressure liquefied chlorine was at the center of a 25 m diameter concrete pad. Identical  
162 15.2 cm (6.0 inch) holes were located at the bottom, the top, and at a 45 degree  
163 downwards angle on a horizontal ten-ton tank (Nicholson et al. 2017 and Spicer and  
164 Miller 2018). The bottom of the tank was located 1 m above ground level (agl) and the  
165 tank was 1.37 m (54 inches) in diameter. The hole was at the top of the tank for Trial 8,  
166 as identified in Figure 1. The Trial 8 release on 11 September 2016 began at 9:01:45 am  
167 Mountain Daylight Time (LDT); or 15:01:45 GMT. The initial chlorine mass in the  
168 tank was 9100 kg, the release duration (two phase jet phase) was about 30 s and total  
169 mass released in the jet was 2400 kg.

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**Figure 1.** Photo of JR II ten ton release tank. The arrow depicts the upward jet release location at the top of the tank used in Trial 8. The bottom of the tank is 1 m above ground level.

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176 The observed air temperature was 15.8 °C and estimated air density was 1.05 kg m<sup>-3</sup>.  
177 Winds were observed by a network of about 35 portable 2 m towers, supplemented by  
178 three 32 m towers with sonic anemometers at heights of 2, 4, 8, 16, and 32 m; one of  
179 the towers was less than 100 m upwind of the JR II release tank. For the 10-minute  
180 period after the release, wind speed at a height of 2 m near the source location was 2.1  
181 m s<sup>-1</sup>, and wind direction was from 120° (Hanna, 2020). Wind speed increased to 2.9 m  
182 s<sup>-1</sup> at z = 16 m and 3.9 m s<sup>-1</sup> at z = 100 m. Wind direction veered to about 165° between  
183 z = 32 and 100 m. Over the next 20 minutes, the surface wind direction near the source  
184 slowly veered to about 155° and the mean 10 minute averaged wind speed at 2 m first  
185 increased to 2.9 m s<sup>-1</sup> and then decreased to about 1.5 m s<sup>-1</sup>.

186

187 As is typical in the early morning, the boundary layer stability varied significantly in  
188 time and space. A deep (hundreds of meters) stable layer had formed during the night  
189 (see plots of temperature profiles in Hanna, 2020) and persisted in the early morning.  
190 For example, temperatures at 100 m were about 2 or 3 °C higher than at the surface at  
191 the time of the release. However, the morning sun had warmed the surface enough that  
192 a weak upward sensible heat flux was observed by sonic anemometers at 2 m, and a  
193 shallow (4 to 8 m) unstable layer had formed. Above the 8 m level, the boundary layer  
194 remained slightly stable. Thus, the boundary layer is not steady-state, and standard  
195 Monin-Obukhov formulas for wind and temperature and turbulence profiles are not  
196 strictly applicable. Also, the so-called “mixing depth” is not well-defined.

197

198 As was done for all nine JR II trials, concentrations (at 0.3 m) and winds (at 2 m)  
199 were measured at all directions around the circle for downwind distances of about 50 to  
200 120 m, and on 90° arcs at distances of 0.2, 0.5, 1, 2, 5, and 11 km (see Chang et al.,  
201 2021). The 360° coverage in the near field was intended to capture the gravity slumping  
202 in all directions, which extended about 50 to 100 m in most trials. The 90° arcs were  
203 centered on the expected dominant wind direction (from 165°).

204

205 Still photos and videos were taken by cameras located at several near-ground sites to  
206 the side of the expected cloud direction and from the rear. These were essential for  
207 estimating the maximum plume rise and touchdown distance for the plume in Trial 8.  
208 In addition, a drone, operated by Utah Valley University, was used to take videos from  
209 above the chlorine cloud. Since the hole was at the top of the tank during Trial 8, over  
210 70 % of the chlorine liquid remained in the tank after the momentum jet decreased to  
211 nearly zero after about 100 s. This remaining liquid was “dumped” onto the concrete  
212 pad about 10 minutes later and subsequently evaporated over 10 to 20 minutes.  
213 Chlorine samplers continued to collect data during this period, thus effectively creating  
214 an additional “trial” that could be used to test evaporating pool models. The current  
215 paper deals only with the jet release component, not the subsequent liquid dump.

216

217 Fox et al. (2021) and Mazzola et al. (2021) include tables of basic characteristics  
218 (e.g., mass released, start time, duration, wind speed and direction, ambient temperature  
219 and a measure of stability) of the releases for all JR II trials. Here, though, we include  
220 additional details for Trial 8, such as the variation of mass emission rate with time, and

221 we calculate the initial conditions needed for input to the models. As mentioned at the  
222 end of the previous section, the conditions at the exit hole could not be used as initial  
223 conditions because the effluent is overpressured at the hole. We use two alternate  
224 expansion models to estimate the initial cloud density, vertical velocity, and radius at  
225 the point (about 2 m from the hole) where the pressure drops almost to ambient.

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## 227 **OBSERVATIONS OF DENSE JET RISE IN TRIAL 8**

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229 Spicer and Miller (2018) and Spicer and Tickle (2020) used observations inside the  
230 tank to explain that the vapor release during Trial 8 lasted only one or two seconds,  
231 followed by a two-phase jet that lasted about 30 s. This was followed by a steadily  
232 diminishing gas jet for another 60 or 70 s. The videos from the side showed a brief  
233 initial yellow-green vapor cloud, followed by a white two-phase cloud in the rise phase  
234 until about 25 to 30 s after the release started. After the plume centerline rose to a  
235 height of about 40 m at a distance of about 20 m downwind, the plume's excess density  
236 caused it to sink to the ground, reaching the ground at a downwind distance of about 50  
237 m. The sinking yellow-green cloud appeared to be gas phase only (without aerosol  
238 droplets) as it was approaching the ground. The videos indicated that, over a period of  
239 about 30 s, the plume "touchdown" distance increased from about 50 m initially to  
240 about 100 m. After that, due the decrease in density of the plume, the visible green  
241 plume remained aloft.

242

243 The observations that we use in the analysis of the dense jet are mostly based on  
244 scaling of photographs. There were no in situ measurements in the chlorine plume aloft.  
245 As discussed by Chang et al. (2021), the only in situ concentration measurements  
246 within 100 m of the source were at near-ground sensors in the closest 100 m from the  
247 source. Those measurements were used to test the models' predictions of maximum  
248 ground level concentration at ground level at the distance of plume touchdown. The  
249 available observations for determining the plume trajectory aloft were still photographs  
250 and videos, and limited lidar data. The photos and videos were taken by high quality  
251 cameras set up at several locations by Dugway Proving Ground. The lidar observations  
252 were scans of the plume taken from a distance of about 1.5 km, on either side of the  
253 plume (Ponsardin, 2017). Because the lidar could not penetrate very far into the plume,  
254 only the edges of the plume could be seen.

255

256 Measured distances from the images (still and video) were obtained by setting a  
257 distance scale based on the known height of the camera scaffold towers (21 ft = 6.4m)  
258 shown in Figure 2 (with arrows drawn to show the measurements taken from these  
259 particular image frames). For the horizontal distances, a small correction has been  
260 included to account for the fact that the plume axis is not aligned exactly perpendicular  
261 to the camera line of view. The plume axis direction was estimated from overhead  
262 drone video footage.

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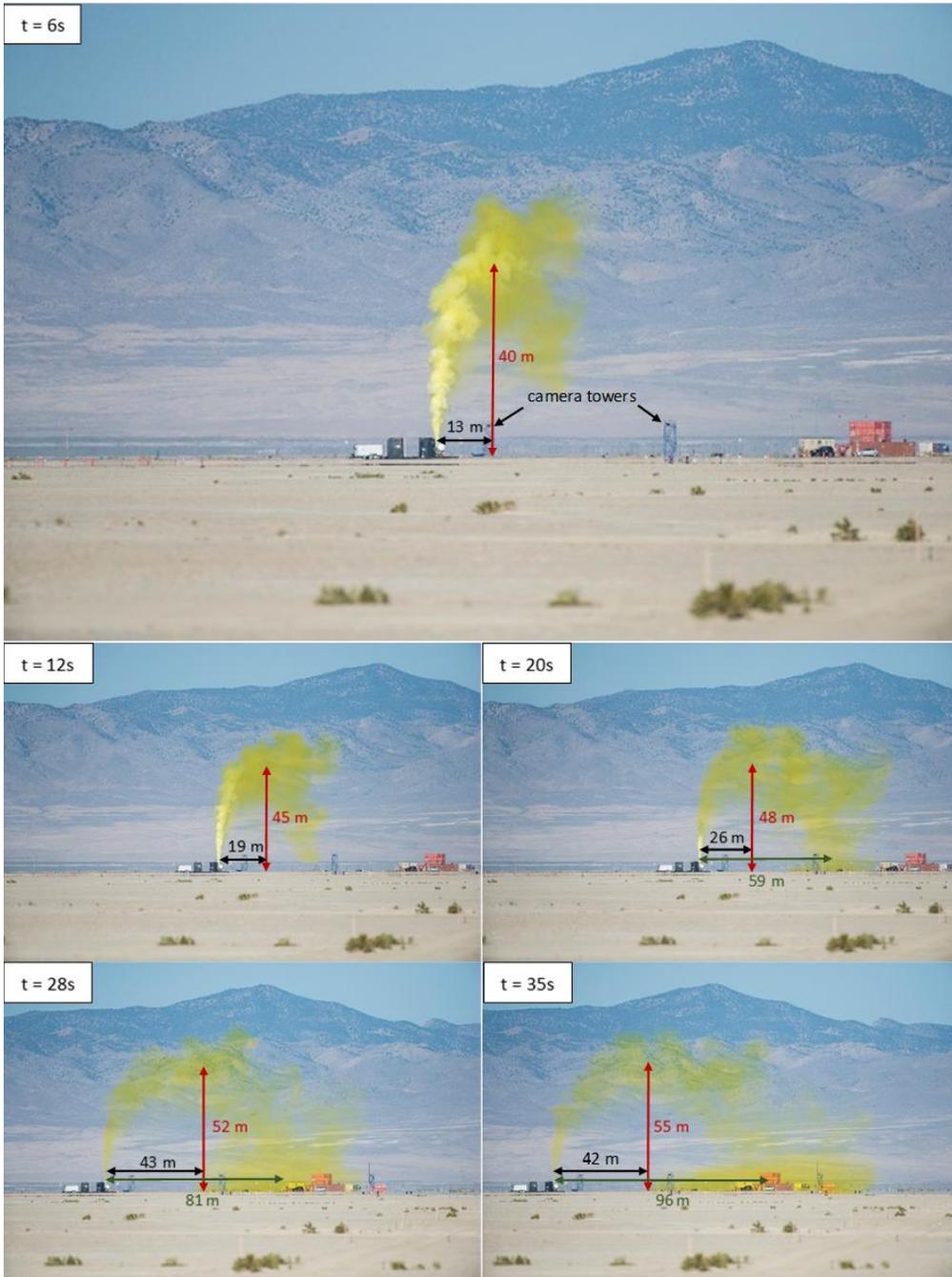
264 The plume centerline location was estimated visually by following the plume path  
265 on the video frames. The measurements of distances from the frames were made using  
266 freely available software, which sets a scale on an image and takes further

267 measurements with that scaling applied. The main uncertainty was in judging the  
268 centerline of a sometimes-billowing plume structure. Our estimates of these distances  
269 have an uncertainty of approximately 20% in the horizontal and vertical distances to the  
270 maximum plume centerline height, and a larger uncertainty of approximately 30% in  
271 the horizontal distance at which the center of the plume touches down. The touchdown  
272 uncertainty is larger due to the visual complexity caused by gravity induced spreading  
273 of the grounded portion of the cloud.  
274

275 Although these methods of determining the centerline from analysis of photographs  
276 and videos may seem approximate, it is judged sufficiently accurate for the present  
277 purposes. Commonly, when dispersion models are compared to data from large-scale  
278 field trials, they are judged to be acceptable if the errors are less than a factor of two.  
279

280 Figure 2 contains a time sequence of photos of the Trial 8 plume, illustrating how the  
281 plume maximum rise, the distance to maximum rise, and the distance to touchdown were  
282 estimated. The camera towers used for distance scaling are indicated. There are five  
283 panels, showing the plume from the side, for times after release of 6, 12, 20, 28, and 35 s.  
284 These times were chosen to show the progression of the visible plume behavior. It is  
285 important to recognize that the observed plume at a distance of 100 m downwind in a  
286 photo represents the chlorine that was released about 30 seconds earlier, since the cloud  
287 is travelling downwind at approximately the speed of the wind ( $2$  to  $3$  m s<sup>-1</sup>). In the near  
288 field, the high-velocity jet rapidly projects the chlorine upwards, which is then  
289 transported by the wind and simultaneously entrains ambient air. Times of 12 and 20 s  
290 are included in Figure 2 because the videos suggest that the first plume “touchdown”  
291 occurred during that time period after release. After touchdown, the ground-based cloud  
292 seen in the photos at 28 and 35 s spreads out about 30 or 40 m in all directions, and is  
293 advected downwind by the ambient wind.  
294

295 Videos and photos were also analyzed for times after release exceeding 100 s.  
296 However, at those larger times, two different clouds are seen – One hugging the ground  
297 and containing plume material that touched down during the first 30 or 40 s after the  
298 release, and another at an elevation of about 30 to 50 m resulting from chlorine gas  
299 released after 30 or 40 s, that remained aloft (i.e., did not sink to the ground)  
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306 **Figure 2.** Sequence of still images of Trial 8. Times are seconds after the release was initiated  
307 and are approximate, having been estimated from the times indicated on videos. The camera  
308 towers used for setting the vertical length scale are indicated on the first image. The estimated  
309 maximum plume height, distance to maximum plume height, and distance to touchdown are  
310 indicated. The portion of the plume with a whitish tinge is where there are two phases (i.e.,  
311 aerosols imbedded).

312

313 The maximum centerline rise height increased from approximately 40 m at 10 s to  
314 approximately 60 m at 40 s. Similarly, the horizontal distance to the maximum plume  
315 rise increased from approximately 20 m at 10 s to approximately 50 m at 40 s. Over  
316 this time period, the emission was two-phase and the emission mass flux, emission  
317 momentum flux and the emission density decreased by large factors. However, the  
318 emission velocity increased due to the increased vapor fraction over time. These are  
319 competing effects that could have different effects on the plume behavior. Increasing  
320 the vertical velocity and decreasing the density would be expected to increase the  
321 plume rise, whereas reducing the mass flux would be expected to diminish the plume  
322 rise. The observed trajectory behavior suggests that the net effect was to initially  
323 increase the rise during the two-phase venting period. After about 60 s, when the vessel  
324 was venting only vapor, the maximum rise height was observed to decrease slightly  
325 with time, which is consistent with a diminishing emission velocity as the pressure in  
326 the vessel decreased.

327

328 The observed plume touchdown distance is estimated to be about 50 m at about 10 s  
329 and about 100 m at about 40 s. The observed maximum concentration for the jet  
330 release in Trial 8 is 12080 ppm at a distance of 85 m (Chang et al., 2021).

331

332 As confirmatory evidence of these video and photo observations, Ponsardin (2017)  
333 describes lidar observations of the aerosol content of the Trial 8 plume. The two lidars  
334 were 1.5 km to the side of the plume. Only the edges of the plume could be seen. The  
335 lidar data confirm a first touchdown point for aerosols as 50 m, though somewhat later  
336 in time than the vapor plume touchdown from Figure 2. Also, the lidar detected  
337 aerosols at heights extend to 42-43 m above ground at times after release of 6-8 s,  
338 further confirming the video and photo estimates of maximum plume rise at a time of  
339 about 10 s.

340

341 As mentioned earlier, the values of observed maximum plume rise and distances to  
342 maximum rise and touchdown are based on snapshots at certain times after the release  
343 began. However, the part of the cloud that is seen to be touching down on the photo  
344 may have been emitted 10 to 40 s earlier. This complicates our comparisons of  
345 observations with model predictions, which are produced assuming steady-state  
346 conditions and using inputs (e.g., initial density, radius, and vertical velocity) based on  
347 5 or 10 s time increments after release.

348

349 It is possible that, when the plume is not sufficiently dense, a horizontal plume (i.e.,  
350 with approximately constant plume centerline height) may visually appear to  
351 “touchdown” by virtue of its bottom edge touching the ground, despite the plume  
352 centerline remaining aloft. This does not mean that the plume center has reached  
353 ground level. Also, over sufficient travel distance and in the presence of a mixing  
354 depth (a cap to upwards dispersion), even in the absence of downward gravitational  
355 motion, vertical mixing will result in a nearly constant concentration from ground level  
356 to the mixing depth.

357

358 When we view the various videos for Trial 8, including a Utah Valley University  
359 drone video that was taken from about 100 m above the plume, it appears that the  
360 ground-level cloud passes over and around the few obstacles (small trailers and Container  
361 Express (CONEX) shipping containers) in its path, even having a clear zone in the wake  
362 behind the obstacles. This is consistent with the typical recirculating wake flow around  
363 an obstacle, first “piling up” in front of the obstacle, then passing around and over the  
364 obstacle. If most of the cloud is at heights less than the obstacle height, there often is a  
365 partially clear area of length about 5 or 10 m visible in the wake immediately behind the  
366 obstacle. These phenomena are better seen in the videos for the other trials, which had  
367 downward-directed releases.

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## 370 **MASS EMISSION RATE AND OTHER SOURCE INPUTS**

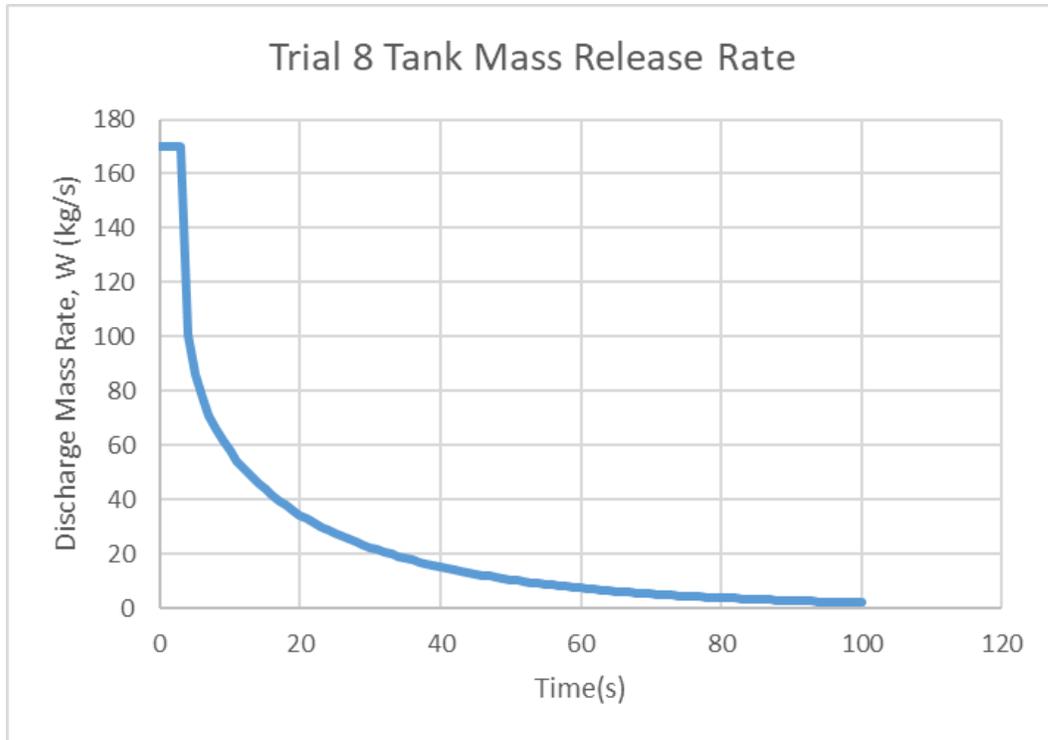
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372 To calculate the Trial 8 plume trajectory and concentrations at plume touchdown,  
373 models require specification of conditions at the location where the jet leaves the  
374 storage tank. Some models can treat the complex thermodynamics that occur in the  
375 first few meters after the jet passes through the hole, when the jet is depressurizing and  
376 approaching ambient pressure. This is often called the expansion zone. However, most  
377 dense jet models require that initial conditions be specified assuming that the jet is at  
378 ambient pressure. Spicer and Miller (2018) and Spicer and Tickle (2020) have  
379 determined these input conditions at ambient pressure for the JR II releases. Based on  
380 their analysis of the observed tank conditions during Trial 8, they suggest the mass  
381 emission rate variation with time after the release begins, as plotted in Figure 3. Note  
382 the constant release rate for the first two seconds (all vapor), the rapid decrease with  
383 time (e.g., a factor of about 3 decrease by 10 s), and also the long “tail” where the mass  
384 emission rate is slowly decreasing. For the first 1 or 2 s, the release was all-vapor, then  
385 switched to two-phase. The presence of liquid aerosols after a few seconds is evident  
386 from the visual appearance of the plume – droplets in the plume make the cloud opaquer  
387 and more reflective (white appearance). A chlorine vapor plume appears yellow-green  
388 and is not opaque. The observed transition in appearance of the Trial 8 plume is also in  
389 good correspondence with the transition predicted by modelling the discharge rate over  
390 time (Spicer and Tickle, 2020).

391

392 No droplet size measurements are available for this particular release. However, the  
393 fraction of the chlorine mass in the initial jet that is in liquid phase will likely consist of  
394 very small aerosol drops with a mass mean diameter of about 50  $\mu\text{m}$  (Britter et al.,  
395 2011). This size range is expected because the same liquid break-up mechanisms are  
396 expected to hold as in flashing releases of other chemicals. After expanding to  
397 atmospheric pressure, but before mixing with air, the jet temperature will be close to  
398 the chlorine boiling point of  $-34\text{ }^{\circ}\text{C}$ .

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401

402 **Figure 3.** Mass emission rate as a function of time after the release was initiated (from Spicer  
 403 and Tickle, 2020).

404

405 A few models can simulate the plume behavior starting at the hole on the tank, when  
 406 the jet has a pressure much larger than the ambient pressure. However, as mentioned  
 407 earlier, most models cannot simulate the plume behavior within the depressurizing jet  
 408 itself (within about the first 2 or 3 m from the hole in this case), but instead apply  
 409 pseudo-source conditions once the jet has expanded to reach atmospheric pressure. In  
 410 our analysis of Trial 8, the initial conditions were defined as a function of time (in  
 411 piecewise blocks) after the release started, since the mass flux significantly decreased  
 412 over time.

413

414 Spicer and Tickle (2020) discuss methods of estimating plume conditions after  
 415 depressurization (expansion). Pseudo-source expansion models bridge this expansion  
 416 zone by making certain simplifying assumptions applied to a control volume. Typical  
 417 assumptions are that during expansion, heat transfer with surroundings is ignored,  
 418 mixing with air is ignored, equilibrium is restored between phases. There are  
 419 alternative assumptions relating to the velocity change on expansion - two alternative  
 420 approaches are considered for this study:

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422 Expansion Model 1. Velocity increases above the exit value due to acceleration  
 423 by excess pressure at the exit. This is also referred to as a momentum  
 424 conservation model (e.g., Britter et al., 2011)

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Expansion Model 2. Velocity unchanged from exit velocity (e.g., Ewan and Moodie, 1986)

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Although DRIFT’s default modeling (Tickle and Carlisle, 2013) corresponds with Expansion Model 1, both expansion models are tested with DRIFT in the current exercise. Thus, the Expansion Model 1 and Model 2 inputs are used for all three models (HMP, Briggs, and DRIFT). Witlox et al. (2017) found that the conservation of momentum approach (Model 1) gave slightly better agreement with their experimental observations data when using their dispersion model (PHAST).

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Because the HMP and Briggs models are steady-state models, we define 11 “steady-state” time segments covering the first 100 s of the Trial 8 release. The time segments (periods) are shorter in the initial periods, when the mass emission rate is more rapidly decreasing with time. Table 1 lists the conditions determined for each time period using Expansion Model 1 and Model 2. The listed time in the first column is the end of the period (e.g., the listed time of 10 s corresponds to averaging over the time period from 5 to 10 s after release). The listed duration of release refers to the averaging time for the numbers listed in subsequent columns. The average mass flux  $Q_c$ , initial cloud temperature  $T_c$ , and mass fraction vapor apply to both Models 1 and 2. Initial cloud density ( $\rho_c$ ), volume flux ( $V_c$ ), vertical velocity ( $w_o$ ), and radius ( $R_o$ ) are outputs of both Expansion Models 1 and 2. The exit conditions used as input to Expansion Models 1 and 2 have been determined by adjusting the vapor mass fraction in the two-phase nozzle discharge model of Leung (1990) to match the time-dependent emission rate in Spicer and Tickle (2020). The measurements within the vessel show that during two-phase discharge, the pressure in the vessel is well approximated by the saturated vapor pressure. During vapor discharge, the upstream stagnation pressure is adjusted to match the observed emission rate. The vapor mass fraction at the vent exit is assumed to be the same as that inside the vessel; this amounts to a ‘frozen flow’ discharge

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**Table 1.** Initial plume conditions assumed for 11 time periods after the release is initiated. The mass flux  $Q_c$ , the temperature  $T$  and the mass fraction of vapor represent conditions at the exit hole. The effective cloud density  $\rho_c$ , volume flux  $V_c$ , vertical velocity  $w_o$  and plume radius  $R_o$  represent conditions after the plume pressure decreases to ambient.

Release time ending	Duration of release	$Q_c$		Mass fraction vapor	$\rho_c$		$Q_c/\rho_c$		$w_o$		$R_o$	
		observed	observed		Model 1	Model 2	Model 1	Model 2	Model 1	Model 2	Model 1	Model 2
s	s	kg/s	K		kg/m <sup>3</sup>	kg/m <sup>3</sup>	m <sup>3</sup> /s	m <sup>3</sup> /s	m/s	m/s	m	m
5	5	139.4	286.2	0.19	16.71	16.35	8.34	8.53	84.6	51.0	0.177	0.231
10	5	66.8	283.7	0.31	10.11	9.71	6.61	6.88	148.2	87.1	0.119	0.159
15	5	48.8	281.0	0.42	7.57	7.23	6.45	6.75	182.3	108.1	0.106	0.141
20	5	37.8	277.9	0.53	5.96	5.66	6.34	6.68	210.0	126.4	0.098	0.130
25	5	30.1	274.9	0.66	4.80	4.56	6.27	6.60	234.2	143.7	0.092	0.121
30	5	24.3	271.8	0.81	3.93	3.73	6.18	6.51	255.8	160.7	0.088	0.114
40	10	18.1	267.4	0.98	3.21	2.88	5.64	6.28	263.3	176.0	0.083	0.107
50	10	12.4	262.0	1	3.16	2.84	3.92	4.37	221.1	175.3	0.075	0.089
60	10	8.64	257.4	1	3.16	2.89	2.73	2.99	164.3	161.0	0.073	0.077
80	20	5.24	252.3	1	3.08	2.95	1.70	1.78	97.9	97.9	0.074	0.076
100	20	2.71	247.2	1	3.05	3.01	0.89	0.90	49.7	49.7	0.075	0.076

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462 assumption. The advantages of applying the model of Leung (1990) are its simplicity of  
 463 computation, useful when fitting to measured flow rates, together with its applicability to  
 464 both the two-phase and subsequent vapor venting regimes. Reassuringly, the predicted  
 465 time of transition from two-phase venting to vapor venting using the Leung (1990)  
 466 discharge model agrees with the estimated transition time from visual observations.

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## 469 DESCRIPTION OF DENSE GAS PLUME RISE MODELS TESTED

470

471 Three models for vertical jets of dense gases are compared with the Trial 8  
 472 observations of maximum plume rise, distance to maximum plume rise, distance to  
 473 plume touchdown, and concentration at plume touchdown. The first two models (Hoot,  
 474 Meroney and Peterka (HMP, 1973); and Briggs 1967) are one-line analytical formulas.  
 475 The third model, DRIFT, is a comprehensive dispersion modelling program for  
 476 estimating the effects of a variety of hazardous releases to the atmosphere (Tickle and  
 477 Carlisle, 2013). The basic assumptions for each model are summarized below.

478

479 **HMP:** The Hoot, Meroney and Peterka (1973) model contains analytical one-line  
 480 formulas (also see p 57 of Hanna et al. 1996) for the maximum plume rise, downwind  
 481 touchdown, and concentration at touchdown, for dense gasses released vertically  
 482 upwards. In the 1970s there was much concern and research about dense gases released  
 483 from vents. Hoot et al. (1973) carried out wind tunnel experiments with dense plumes  
 484 in cross-winds and used basic dimensional analysis principles to decide which  
 485 dimensionless variables to plot and use to develop empirical relations. Extensive details  
 486 and tables and plots of experimental data are in the 1973 Hoot et al. report; a briefer  
 487 summary is in the conference paper by Hoot and Meroney (1974). The HMP model  
 488 equations are given below.

489

490 Maximum plume rise  $\Delta h$  above source:

491

$$492 \Delta h/2R_o = 1.32 (w_o/u)^{1/3} (\rho_o/\rho_a)^{1/3} [w_o^2/(2R_o g')]^{1/3} \quad (1)$$

493

494 where  $g' = g(\rho_o - \rho_a)/\rho_o$ ;  $g$  is acceleration of gravity ( $9.8 \text{ m s}^{-2}$ ),  $\rho_a$  is ambient air density,  
 495  $u$  is wind speed, and  $\rho_o$ ,  $R_o$ , and  $w_o$  are initial plume density, radius and vertical  
 496 velocity after depressurization.

497

$$498 \text{Distance to maximum plume rise } x/2R_o = w_o u / (2R_o g') \quad (2)$$

499

500 Plume touchdown distance  $x_g$  downwind:

501

$$502 x_g/2R_o = w_o u / (2R_o g') + 0.56 \{ (\Delta h/2R_o)^3 [(2 + h_s/\Delta h)^3 - 1] u^3 / (2R_o w_o g_a') \}^{1/2} \quad (3)$$

503

504 where  $g_a' = g(\rho_o - \rho_a)/\rho_a$  and  $h_s$  is elevation of the stack or vent opening above the ground  
 505 (2 m for JR II Trial 8). Air density  $\rho_a$  is assumed to be  $1.055 \text{ kg m}^{-3}$  based upon the  
 506 measured air pressure and temperature.

507

508 The HMP model also has a formula for the ratio of the maximum concentration,  
509  $C_{\max}$ , at plume touchdown to the initial concentration,  $C_o$ , after depressurization:

$$511 \quad C_{\max}/C_o = 2.43 (w_o/u) [(h_s + 2\Delta h)/(2R_o)]^{-1.95} \quad (4)$$

512  
513 where  $h_s$  is height of the source above ground (2 m for Trial 8).

514  
515 **Briggs:** The Briggs (1969) model is based on his equation for the trajectory of a  
516 buoyant (or negatively buoyant) plume as a function of distance,  $x$ , downwind of the  
517 release point:

$$519 \quad \Delta h = [(19(\rho_o/\rho_a)(M_o/u^2)x - 4.2 (B_c/u^3)x^2)]^{1/3} \quad (5)$$

520  
521 where  $M_o = w_o^2 R_o^2$  is proportional to the initial momentum flux and  $B_c = g[(\rho_o -$   
522  $\rho_a)/\rho_a]w_o R_o^2$  is proportional to the initial buoyancy flux (here assumed positive for a  
523 dense cloud). The maximum rise occurs at the distance where  $d(\Delta h)/dx = 0$ . This  
524 equation is most often used for positively buoyant plumes, but is also valid for  
525 negatively buoyant clouds. The plume touchdown distance can be calculated as the  
526 distance where  $\Delta h = 0$  (i.e., the first term in the equation equals the second term). That  
527 is,  $x_g = 4.52(\rho_o/\rho_a)uM_o/B_o = 4.52 w_o u/[g(\rho_o - \rho_a)/\rho_a]$ . Briggs does not include a formula  
528 for maximum ground level concentration,  $C_{\max}$ .

529 **DRIFT:** This is a commercially-available integral dispersion model that is used by  
530 HSE for its regulatory work in the UK. While DRIFT was originally conceived as a  
531 dense-gas dispersion model, it has subsequently been adapted to model dispersion of  
532 passive and buoyant sources (Tickle and Carlisle, 2008). DRIFT incorporates a  
533 momentum-jet model to simulate pressurized releases, which includes both single and  
534 two-phase jet models, where the latter assumes homogeneous equilibrium between the  
535 gas phase and the dispersed liquid droplet phase. The thermodynamic models in  
536 DRIFT are able to account for multi-component mixtures and humidity effects  
537 (condensation and evaporation of water droplets, and associated latent heat transfer),  
538 including their effect on cloud buoyancy (Tickle, 2001). Releases can be modelled at  
539 different angles to the vertical (including the vertically-upwards case in Trial 8) and  
540 also for different lateral cross-wind directions.

541  
542 DRIFT assumes that the boundary layer is steady state and can be characterized by  
543 Monin-Obukhov similarity. Based on observed wind speed at 2 m, the derived  
544 roughness length ( $z_o = 0.5$  mm) for the DPG salt playa, and a measure of upward heat  
545 flux, the model calculates the friction velocity  $u^*$ , the eddy dissipation rate  $\varepsilon$  ( $m^2 s^{-3}$ ),  
546 and the Monin-Obukhov length  $L$ . From these inputs, a vertical profile of wind speed  
547 and turbulence is estimated. Plume dispersion is parameterized by passive entrainment  
548 terms dependent upon the eddy dissipation rate and K-theory diffusivity. A measure of  
549 lateral wind fluctuation is used to parameterize passive spreading. The dispersion of the  
550 plume is modelled as a volumetric air entrainment rate per unit length along the plume  
551 trajectory (the product of the entrainment velocity and open perimeter length of a  
552 section through the plume). For the elevated plume, the entrainment velocity is  
553 parametrized as a sum of terms representing the entrainment due to: shear as a result of

554 the excess velocity component along the axis of the jet, cross-flow induced entrainment  
555 associated with the component of ambient velocity perpendicular to the plume, and  
556 ambient turbulence that is proportional to the cube root of the atmospheric kinetic  
557 energy dissipation rate.

558

559 For the ground-based dense plume after touchdown, the entrainment is split into top  
560 entrainment (the product of the top entrainment velocity and plume width) and edge  
561 entrainment (the product of the edge entrainment velocity and plume height). The top  
562 entrainment velocity is proportional to the atmospheric friction velocity with a  
563 suppression factor due to stable density stratification in the dense cloud. The edge  
564 entrainment velocity includes a term dependent upon the lateral gravitational spreading  
565 velocity of the cloud and the lateral ambient velocity fluctuation, which is taken be  $2u^*$ .  
566 An additional lateral spread is included to represent the effect of larger scale motions  
567 resulting in lateral plume meander.

568

569 As stated earlier, DRIFT assumes steady state meteorology. However, the JR II  
570 Trial 8 release occurred in the early morning, when conditions are changing from stable  
571 to unstable. In addition, the shallow near-surface unstable layer during the Trial 8  
572 release is capped by a deep inversion layer above about 16 or 32 m, and so the  
573 treatment within DRIFT is at best an approximation. Surface meteorological conditions  
574 during the 10 minute period after the release began have been assumed based upon the  
575 recommendations in Hanna (2020): 2.1 m/s wind speed at 2 m height, inverse Monin-  
576 Obukhov length of  $-0.1632 /m$ , surface roughness length of 0.5 mm, relative humidity  
577 of 26.5%. Despite the non-steady conditions, DRIFT's predictions of the plume  
578 trajectory are in reasonably good agreement with the observations – possibly because  
579 the trajectory is mainly affected by the mixing induced by the plume itself, rather than  
580 depending in detail upon the atmospheric turbulence.

581

582 Further details of DRIFT are discussed in Tickle and Carlisle (2013), and  
583 applications to JR II Trials 1, 6 and 7 are described in Gant et al. (2021). DRIFT  
584 Version 3.7.17 has been used for this study. The model is run “as-is” without any  
585 modifications.

586

587 Approximate account of the time-dependence of the discharge is taken by  
588 undertaking multiple runs of DRIFT's steady continuous dispersion model using  
589 release conditions corresponding to the time segments in Table 1 DRIFT predicts the  
590 centerline trajectory, which has been used to estimate the maximum height and  
591 downwind distance at which this occurs. For the touchdown point, the predicted  
592 ground-level concentration as a function of downwind distance has been examined to  
593 determine the downwind distance at which the maximum ground-level concentration  
594 occurs – this is taken to be the touchdown distance.

595

596 In addition to its steady continuous dispersion model, which neglects along-wind  
597 diffusion, DRIFT also includes dispersion models for instantaneous, finite-duration and  
598 time-varying releases which include along-wind diffusion effects. It is increasingly  
599 important to account for along-wind diffusion when considering greater downwind

600 distances where the cloud travel time exceeds the release duration. For the purpose of  
 601 comparing concentration predictions with measurements at 85 m and beyond, DRIFT's  
 602 finite-duration model has been used based upon the average release over the first 30s,  
 603 corresponding approximately with the two-phase discharge region.

604  
 605

## 606 RESULTS

607

608 The HMP, Briggs, and DRIFT model predictions of maximum plume rise, distance  
 609 to maximum plume rise, and distance to plume touchdown are compared with  
 610 observations in Table 2, for assumed initial conditions at times after the release begins,  
 611  $t$ , equal to 10 and 40 s. In all cases, the models are compared for both expansion  
 612 models (Model 1 and Model 2). As mentioned earlier, the observed values are  
 613 estimated from videos and photos from “snapshots” at 10 s and 40 s after the release  
 614 starts. However, the modeled values are assuming steady state conditions with  
 615 emissions inputs from the times of 10 s and 40 s after the release starts. The HMP and  
 616 Briggs models can only treat steady-state releases. The DRIFT model can treat some  
 617 aspects of time-variable releases; however, it was run here in steady-state mode, to be  
 618 consistent with the HMP and Briggs models.

619

620 **Table 2.** Comparison of observed and modeled maximum plume rise, distance  $x$  to  
 621 maximum plume rise, and plume touchdown distance (all in meters) for times after  
 622 release of 10 and 40 s.

623

	Obs	HMP Model 1	HMP Model 2	Briggs Model 1	Briggs Model 2	DRIFT Model 1	DRIFT Model 2
Maximum rise $t = 10$ s	40	63	45	83	59	46	31
Maximum rise $t = 40$ s	60	60	51	87	66	45	40
$x$ at maximum rise $t = 10$ s	20	36	20	70	50	26	14
$x$ at maximum rise $t = 40$ s	50	84	60	200	150	84	67
Touchdown $t = 10$ s	50	120	70	200	100	90	55
Touchdown $t = 40$ s	100	270	198	500	300	260	220

624

625 Table 2 shows that, for  $t = 10$  s, the predicted maximum plume rise is largest for the  
 626 Briggs model and smallest for the DRIFT model. There are six values of predicted  
 627 maximum plume rise. Here, we define the median predicted value as the average of the  
 628 3<sup>rd</sup> and 4<sup>th</sup> ranked values. Thus, the observed maximum rise is 40 m and the median  
 629 predicted maximum rise is 52 m (a 30 % overprediction). The three models' best

630 individual predictions of maximum rise are 45 m (about 12 % too large) for HMP  
631 Model 2, 59 m (about 50% too large) for Briggs Model 2, and 46 m (about 15% too  
632 large) for DRIFT Model 1. This agreement is good, considering all the uncertainties.  
633 For  $t = 40$  s, the maximum plume rise predictions have about the same fractional error  
634 as for  $t = 10$  s. The observed value is 60 m and the median of the predictions is 55 m.  
635

636 Table 2 shows that, in all cases, the Model 1 expansion option produces larger plume  
637 rise predictions than the Model 2 option. The major reason for this is that (as seen in  
638 Table 1) the initial vertical velocity,  $w_0$ , is greater (by about 40 to 60 % in the first 40 s)  
639 for Model 1 than Model 2. Briggs' formula (eq. 5) indicates that, for a given volume  
640 flux, the momentum flux is larger as  $w_0$  increases. Because the distance downwind to the  
641 maximum rise and the touchdown distance will increase as maximum rise increases,  
642 those predicted distances are also larger for the Model 1 expansion option than for the  
643 Model 2 option in all cases.  
644

645 The distance ( $x$ ) to maximum rise is also addressed in Table 2 for the models for  $t =$   
646 10 s and 40 s. The observed distance was 20 m and 50 m, respectively, based on the  
647 snapshots. The median overprediction of this distance by the models was about 60 to  
648 70 %. However, for  $t = 10$  s, where the observed distance is 20 m, the HMP Model 2  
649 and the DRIFT Model 2 predictions are 20 m and 14 m. The DRIFT Model 1  
650 prediction is 26 m, which means that the two DRIFT predictions bracket the observed  
651 value of 20 m. The HMP and DRIFT Model 2 predictions are about 15 to 20 % too  
652 large for  $t = 40$  s. The Briggs model tends to overpredict this distance by a factor of 2  
653 to 4 for both  $t = 10$  and 40 s.  
654

655 The touchdown distance (observed to be 50 m for  $t = 10$  s and 100 m for  $t = 40$ s) is  
656 important because that is where the maximum ground concentration is likely to be.  
657 Table 2 shows that the median model overprediction of touchdown distance is about a  
658 factor of 2 for  $t = 10$  s and a factor of 2.6 for  $t = 40$  s. DRIFT Model 2 is the closest  
659 for  $t = 10$  s (observed 50 m vs predicted 55 m) and HMP Model 2 is the closest for  $t =$   
660 40 s (observed 100 m vs predicted 198 m). The Briggs model produced overpredictions  
661 of a factor of 2 to 5. .  
662

663 It is concluded from Table 2 that the three models with the two alternate expansion  
664 models can predict maximum plume rise, distance to maximum rise, and touchdown  
665 distance within a factor of two most of the time. Often the models' predictions are  
666 within 20 or 30 % of the observations. There is no evidence whether Expansion Model  
667 1 or 2 performs better.  
668

669 Figures 4, 5, and 6 contain plots of observations and predictions of these three  
670 variables versus release time. They include the same data as Table 2, but more clearly  
671 show the trends of the different models. As discussed before, the observations listed for a  
672 certain time are based on snapshots of the plume at that time, whereas the predictions  
673 listed for that time are steady-state solutions using the mass emission rate and other initial  
674 conditions for that time after the release starts. For example, a dot at a time of 40 s for a

675 given model represents a steady-state calculation using inputs (from Table 1) averaged  
676 from 30 to 40 s.

677

678 Observed and predicted maximum plume rise are plotted in Figure 4 as a function of  
679 release time,  $t$ , from 0 to 100 s. Each dot represents the middle of a time period (of  
680 duration 5, 10, or 20 s) when emissions and other inputs are assumed constant. It is  
681 clearly seen that Briggs Model 1 produces the largest plume rise and DRIFT Model 2  
682 usually produces the smallest plume rise. HMP tends to be “in the middle”. The trend in  
683 maximum plume rise with time for all models is an increase with time until about 30 to  
684 40 s, and then a decrease with time. This trend may seem counterintuitive, since the mass  
685 emission rate is continually decreasing, by a factor of about 10, over the 40 s time period.  
686 The Briggs’ formula for plume rise (eq 5) can explain this. There are two terms – the  
687 first is proportional to the momentum flux, and the second is negative and proportional to  
688 the total cloud excess density. As time increases, the first term decreases in magnitude,  
689 but the second term also decreases in magnitude. Earlier, we postulated that, initially, the  
690 second term has a large effect and the cloud excess density holds the plume rise down.  
691 As time increases and approaches about 40 s the momentum flux term has more influence  
692 and the cloud excess density effect decreases. Thus, the maximum plume rise increases  
693 even though the mass flux has decreased. After about 40 s, the initial jet is “all gas” and  
694 its excess density is decreased due to the fact that imbedded chlorine aerosol drops are no  
695 longer present, so the effects of the second term diminish, and the maximum plume rise  
696 decreases as the momentum flux decreases.

697

698 The red dots in Figure 4 are the observed maximum plume rise (40 and 60 m) at times  
699 after release starts of 10 and 40 s. We can look at the figure and see that HMP Model 2  
700 and DRIFT Model 1 produce best agreement with the observation at  $t = 10$  s, and all six  
701 models bracket (within plus and minus about 20 to 25 m) the observation at  $t = 40$  s.

702

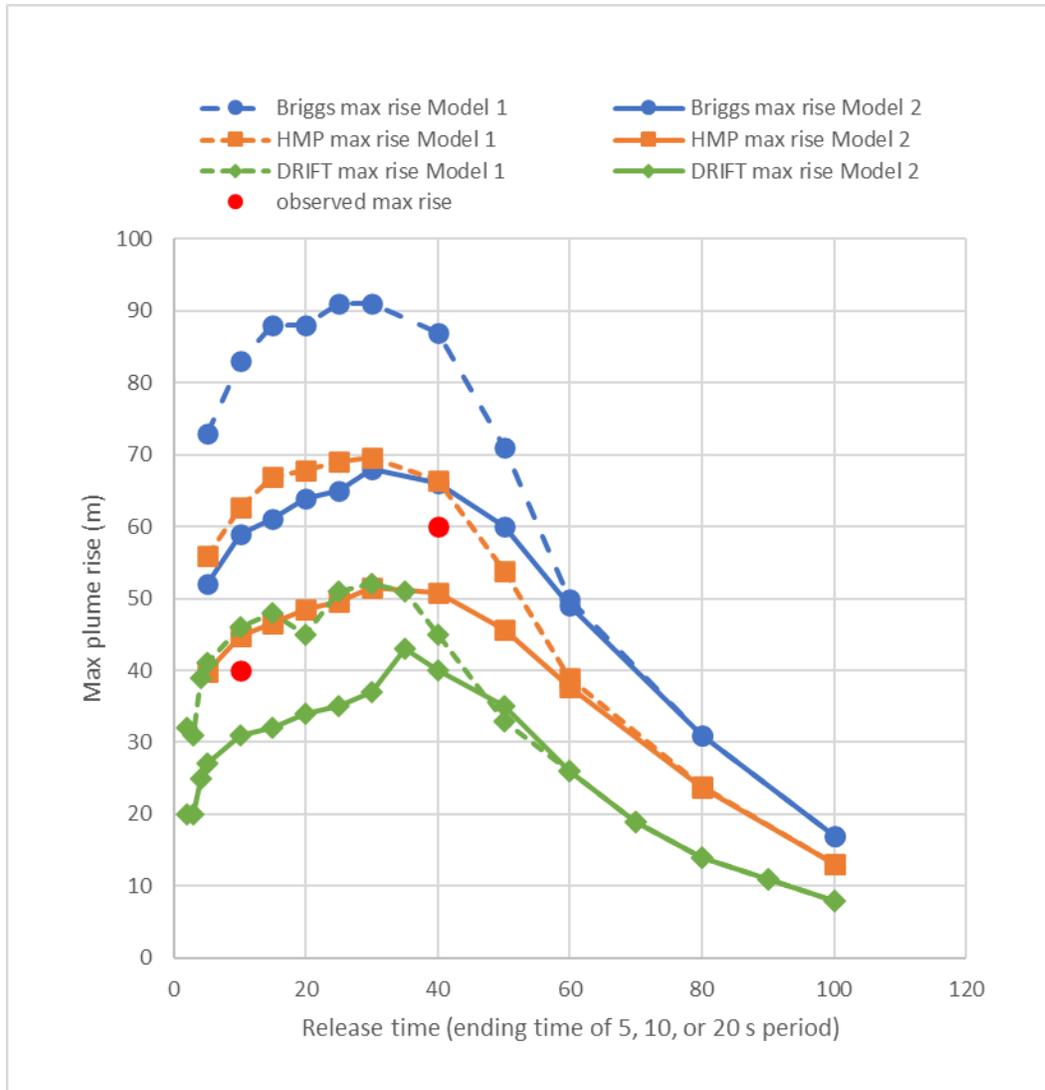
703 The distance to maximum plume rise is plotted in Figure 5. The predicted trend with  
704 time follows the trend seen in Figure 4 for maximum plume rise, with a maximum at  
705 about 40 s. This is expected, since the distance to maximum plume rise is positively  
706 correlated with the maximum plume rise. As stated in the discussion of Table 2, the  
707 models tend to mostly overpredict the observed distance, especially at  $t = 40$  s. However,  
708 the overprediction at  $t = 40$  s is only 20 to 30 % for HMP Expansion Model 2 and DRIFT  
709 Expansion Model 2. At  $t = 10$  s, the two DRIFT versions bracket the observation of 20 m,  
710 and HMP Expansion Model 2’s prediction is 20 m.

711

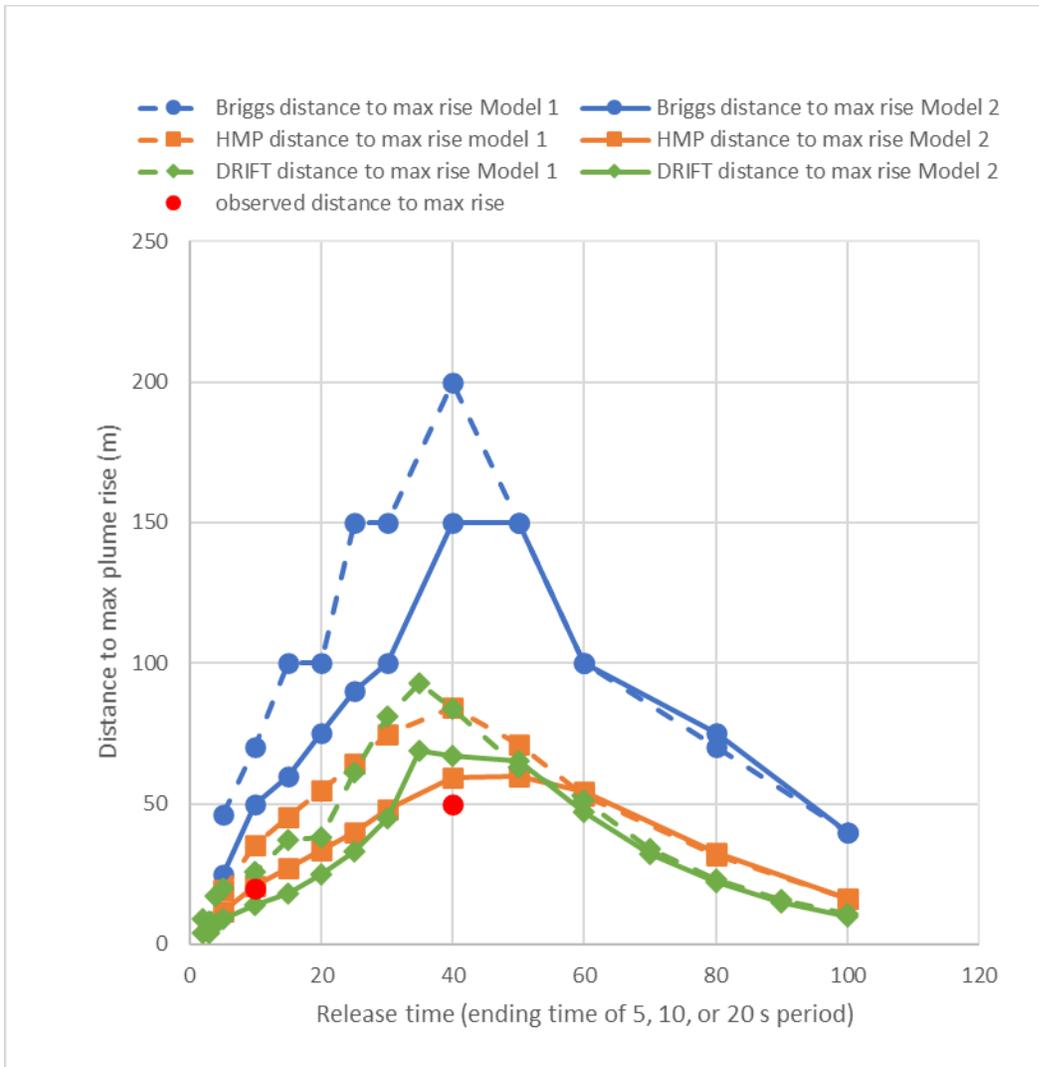
712 As seen in Figure 6, the plume touchdown distances also follow the same shape as the  
713 maximum plume rise and distance to maximum rise curves. Note in Table 1 that the  
714 vapor fraction is 1.0 (i.e., the plume is all gas) after a time of 30 or 40 s. The observed  
715 distance to touchdown also increases from 50 m at  $t = 10$  s to 100 m at  $t = 40$  s, but all six  
716 model predictions of touchdown distance are larger than these values. Agreement is best  
717 at  $t = 10$  s, where the DRIFT Expansion Model 2 predicts 55 m (10 % high) and the HMP  
718 Expansion Model 2 predicts 70 m (40 % high). All except the Briggs Expansion Model 1  
719 are within about a factor of two too large for  $t = 10$  s.

720

721 It is concluded that these models are satisfactorily capturing the basic physics and are  
 722 producing predictions of maximum plume rise and distances that are usually within a  
 723 factor of two of the Trial 8 observations. It is likely that better performance would be  
 724 found for models that can simulate the time-variable source conditions and plume  
 725 behavior, as well as account for the fact that, in the presence of wind speed shear, the  
 726 elevated plume (resulting from smaller emissions after 30 or 40 s) might overtake the  
 727 ground-based cloud (resulting from larger two-phase emissions in the first 10 or 20 s).  
 728  
 729

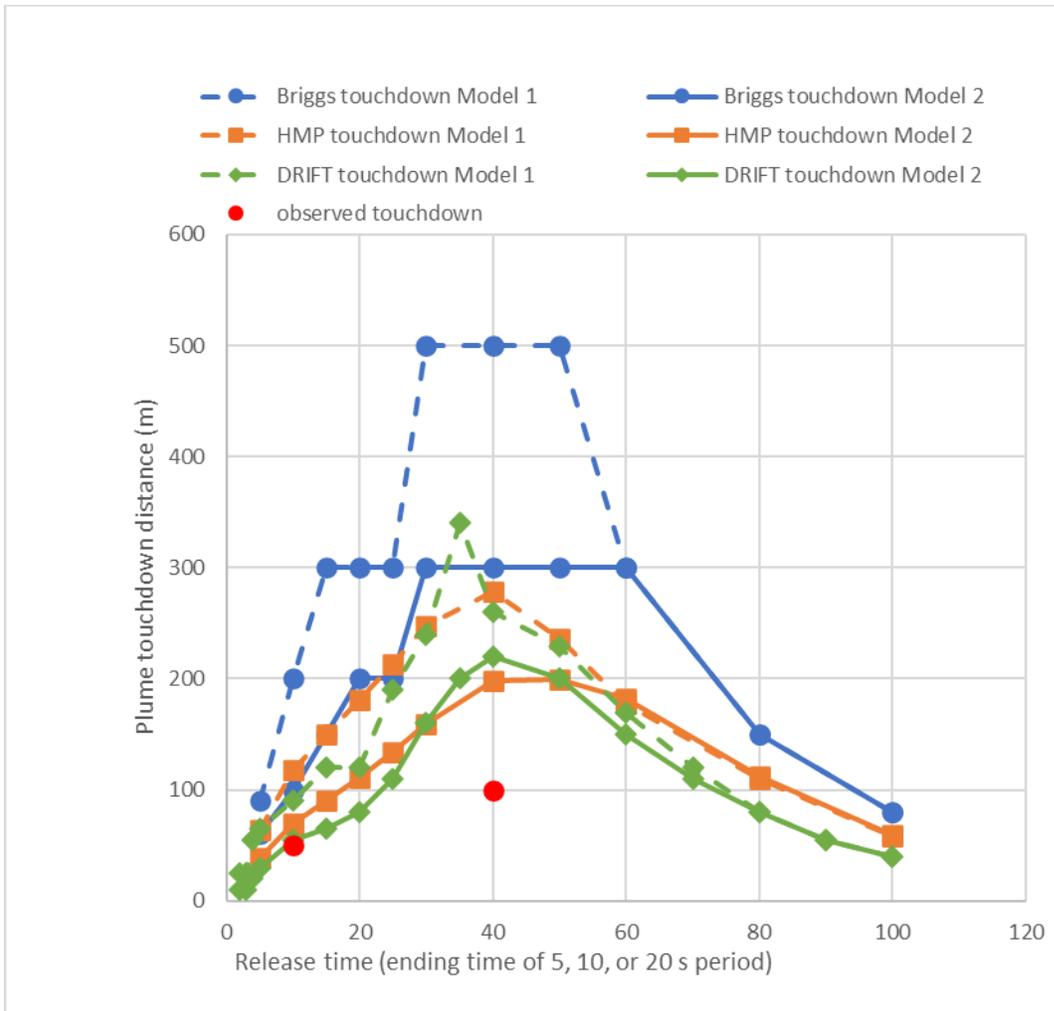


730  
 731 **Figure 4.** Observed and modeled maximum vertical plume rise, calculated using emissions  
 732 rates for 11 time segments after release was initiated.  
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**Figure 5.** Observed and modeled horizontal distance to maximum plume rise, calculated using emissions rates for 11 time segments after release was initiated.



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**Figure 6.** Observed and modeled distance to plume touchdown, calculated using emissions rates for 11 time segments after release was initiated.

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The HMP and DRIFT models can also predict maximum ground-level concentrations at the location of predicted plume touchdown, which ranged from 55 to 120 m for  $t = 10$  s and from 198 to 270 m for  $t = 40$  s. These can be compared with the maximum observed concentration during JR II Trial 8 on the 85 m arc, which is between the observed 50 m and 100 m touchdown distances at 10 and 40 s, respectively. There were only three JAZ concentration sensors on this 85 m arc, of which two measured concentrations in excess of 10,000 ppm. The Briggs model does not predict concentrations. Table 3 lists the observed and modeled maximum concentrations. Note that the predictions for Expansion Model 2 are greater than those for Expansion Model 1, probably because the plume rise is less for Expansion Model 2 than for Expansion Model 1 for both HMP and DRIFT. The observed maximum concentration is between the Expansion Model 1 and Expansion Model 2 predicted concentrations for HMP and DRIFT. The two expansion models are alternative approximate treatments of the expansion zone that are used here to determine the input

762 conditions required by the models. It is interesting to see the effect of these alternative  
 763 approximations on the predicted trajectory, but this is not an adjudication of correctness  
 764 of either. We conclude from Table 3 that the HMP and DRIFT model predictions of  
 765 maximum concentration are reasonably close to the observations (within plus and  
 766 minus a factor of two).

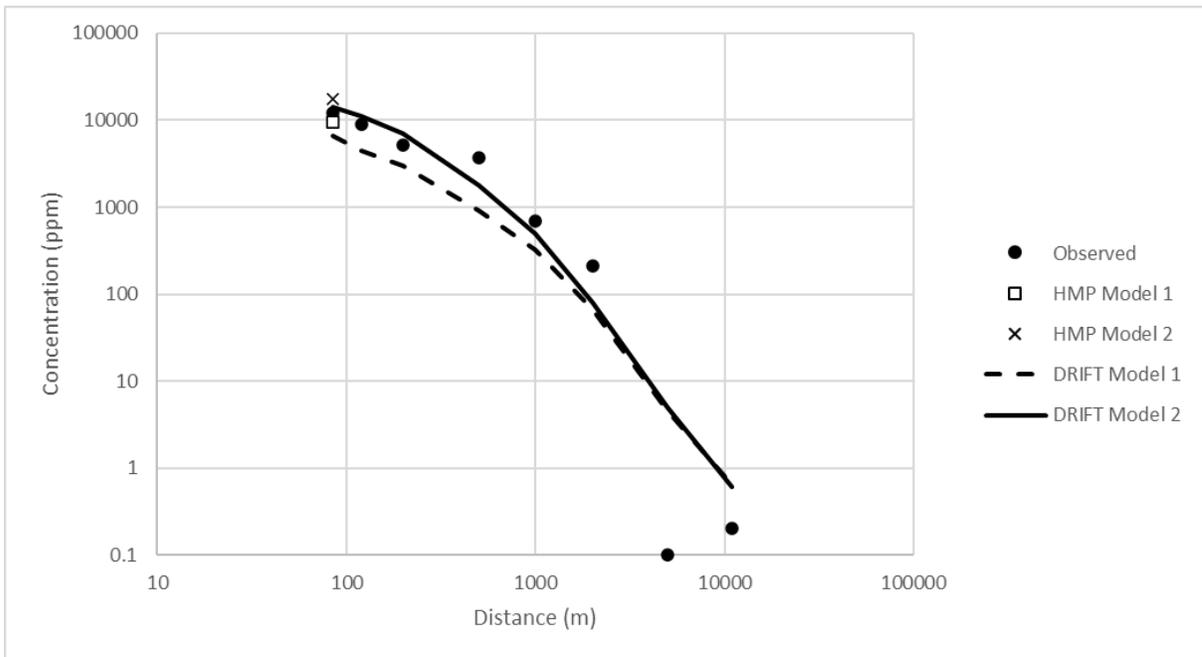
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**Table 3.** Comparison of observed and modeled maximum concentration. Model predictions are at touchdown distance.

	Observed at 85 m	HMP Model 1	HMP Model 2	DRIFT Model 1	DRIFT Model 2
Maximum C (ppm)	12080	9570	17660	6600	14000

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 782

Figure 7 shows a comparison of the observed and DRIFT model predicted arc-maximum concentrations at distances of 85 m and at seven additional sampling arcs extending to 11 km. The observations are all made at a sensor height of 0.3 m. In addition, the HMP model predictions (listed in Table 3) are shown at predicted plume touchdown distance. The observed values are from Chang et al. (2021). The DRIFT predictions with Expansion Model 2 are seen to have relatively small mean bias out to 2 km, while the DRIFT predictions with Expansion Model 1 are biased about a factor of two low, on average. The observations at the 5 and 11 km arcs are very small, less than 1 ppm, due to the cloud passing off the edge of the sampling arcs.



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 785  
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 787

**Figure 7.** Arc-maximum observed and predicted concentration as a function of distance. Observations are made at  $z = 0.3$  m. DRIFT centerline (arc-maximum) predictions are made for the sensor height. The figure also contains the HMP model predictions at plume touchdown.

788

## 789 CONCLUSIONS

790

791 JR II Trial 8 is a unique one-of-a-kind field experiment that provides useful insight  
792 into the behavior of vertically-upwards releases of pressure-liquefied chlorine from  
793 large holes in large storage vessels. Despite the hole being located on the top of the  
794 tank, i.e. in the vapor space, the release rapidly transitioned within the first few seconds  
795 from gaseous to two-phase, due to liquid swell pushing the boiling liquid out of the  
796 vessel. After expansion, the resulting two-phase plume has an effective density of about  
797 12 (five times larger than that of chlorine gas alone), due to the presence of tiny  
798 aerosols with median diameters of about 50  $\mu\text{m}$  (Britten et al, 2011). The very dense  
799 chlorine plume first rises up due to its momentum and then bends over and sinks  
800 towards the ground.

801

802 Video footage and still photographs from Trial 8 were used to examine the trajectory  
803 of the dense jet, focusing on the horizontal and vertical distances reached by the plume  
804 at different times. Distances on the photos were scaled using the known height of a  
805 camera tower near the source, and are thought to be accurate within about 20 %.  
806 During the first 10 seconds of the release, the videos showed the dense jet rising to a  
807 height of around 40 m, then sinking to the ground and touching down at a horizontal  
808 distance from the tank of about 50 m. The plume then hit the ground and spread out  
809 radially in all directions to a distance of about 30 or 40 m due to gravity slumping.  
810 Over time, the pressure in the vessel decreased, the boiling liquid level decreased below  
811 the orifice and the jet transitioned from two-phase to gaseous. Due to the reduction in  
812 density of the jet, the chlorine vapor discharged from the vessel remained aloft at later  
813 times (greater than about 30 or 40 s) and dispersed as an elevated plume, without  
814 sinking towards the ground. Meanwhile, the dense cloud that touched down in the early  
815 phase of the release continued to move downwind along the ground as a typical  
816 “pancake-shaped” dense gas cloud.

817

818 The predictions of three integral models were compared to the observed initial dense  
819 jet plume rise and touchdown distance: 1) the analytical formulas suggested in 1973 by  
820 Hoot, Meroney, and Peterka (HMP), 2) the Briggs (1969) analytical formula for plume  
821 trajectory, and 3) the DRIFT dispersion software (Tickle and Carlisle, 2013). All three  
822 models were shown to usually agree with the observed distances within about a factor  
823 of two. The Briggs model predictions of the distance to maximum plume rise and  
824 touchdown were about a factor of two to five too large. Additionally, the HMP and  
825 DRIFT models predicted chlorine concentrations near the plume touchdown position  
826 within a factor of two of the observations.

827

828 The work presented here demonstrates that integral dispersion models are able to  
829 predict the correct physical behavior for vertically-upwards directed dense jets if they  
830 are provided with suitable inputs, in terms of the discharge conditions from the orifice.  
831 The Briggs formula for plume rise provides useful insight into the physical behavior of  
832 a dense plume, namely the competition between momentum and buoyancy forces.

833

834 The other experiments in the JR II series (Trials 1-7 and 9) involved releases from  
835 the liquid space in base of the tank or a 45-degree downwards position, and they all  
836 resulted in much higher downwind concentrations than in Trial 8 (Chang et al., 2021).  
837 In emergency response or risk assessment scenarios where the release location is  
838 unknown, releases from the underside of a vessel can provide conservative estimates  
839 for the ground-level downwind concentrations. Nevertheless, there are cases where  
840 releases from the vapor space needs to be assessed. The work presented here provides  
841 useful information to help examine those scenarios.

842  
843 There are several caveats to our conclusions that concern the uncertainties in the  
844 analysis. The releases were complex, involving changes over time of phase,  
845 composition, release rate, temperature, and velocity. Our method of estimation of  
846 distances using photos has inherent uncertainties of about 20 %. Nevertheless, there is  
847 merit in comparing with measurements made from video and still images. The  
848 measurements show clear trends in the evolution of the plume trajectory which are  
849 largely matched by the model predictions. Agreement of the three models' (HMP,  
850 Briggs, and DRIFT) predictions with the observations is within margins which are  
851 generally recognized as being adequate for acceptability within the realms of major  
852 hazard consequence modelling.

853  
854  
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