

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

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27

28 **Abstract**

29

30 The Jack Rabbit II (JR II) chlorine field trials in 2015 and 2016 involved nine 5 to 20
 31 ton releases of pressurized liquefied chlorine from a tank mounted 1 m above a broad flat
 32 desert sand surface. A model comparison study was initiated, where 17 widely-used

33 dense-gas dispersion models were run by scientists in seven countries. Predictions were
34 submitted following specified formats, using specified emissions and meteorology inputs.
35 To compare with the model predictions, sets of observations were defined for the arc-
36 maximum 1-3 s averaged concentrations (arc max C) and for cloud widths and heights (to
37 20 ppm and 200 ppm contours) at distances from 0.2 to 11.0 km from the release. The
38 initial focus is on the three field trials (1, 6, and 7) that have the highest observed concen-
39 trations and that have detailed emissions information.

40 It is found that these models are able to satisfactorily simulate (generally within a fac-
41 tor of two) the observed arc max C's and their variation with downwind distance at this
42 flat desert site. At each downwind distance, the scatter in the arc max C predictions co-
43 vers about 1 ½ orders of magnitude, but the observed arc max C is within the range of the
44 predictions. The median of the cloud width predictions is about 50 % larger than the
45 observed value for the three trials. The median of the cloud height predictions is within
46 about 10% of the observed value. For both cloud width and/or height, there are a few
47 models with large (factor of 3 or higher) overpredictions.

48 Of the 17 models, when compared to observations, there is a core group of 5 or 6 with
49 consistently (across all three trials and all distances) less mean error and scatter in their
50 predictions of arc max C and cloud width and height. However, as a group, the 17 mod-
51 els are performing adequately (using the "factor of two" rule of thumb). An important
52 caveat is that, at the JR II desert site, chlorine deposition is minimal. At a site with vege-
53 tation and/or organic-rich soil, the effects of removal of chlorine by deposition are ex-
54 pected to be significant.

55

56 **Keywords:** Jack Rabbit II chlorine field experiment, dense gas dispersion, model
57 evaluation

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59

60 **1 Introduction**

61

62 The Jack Rabbit I (in 2010) and II (in 2015 and 2016) field experiments, at a
63 flat desert site within Dugway Proving Ground (DPG) in Utah, were initiated be-
64 cause there had been much concern about the possible effects of pressurized liq-
65 uid chlorine and anhydrous ammonia released from storage tanks and transporta-
66 tion vessels (e.g., see Hanna et al., 2008, 2012 and 2016). A prime contributor to
67 the concern was the finding that, for the Macdona and Graniteville chlorine railcar
68 accidents, the available models predicted concentrations that, when combined
69 with exposure and health effects models, were suggesting that there would be
70 large numbers of casualties. Yet, at both accident sites, there were far fewer cas-
71 ualties than expected by the model systems. This discrepancy could be caused by
72 several factors, such as overestimates of emissions to the atmosphere, biased dis-
73 persion models, limited knowledge of deposition to the surface, and limitations to
74 the health effects modules. JR II addresses the first and second factors – the
75 emissions and dispersion models. In the current paper, though, we make use of
76 the emissions model testing and improvements resulting from detailed observa-
77 tions of the JR II tank and releases (Spicer and Tickle 2020) and provide all of the
78 modelers with the optimized emissions estimates. We had hoped to also test the
79 deposition modules at JR II, but discovered that it was not possible due to the
80 chlorine-containing salt that was naturally present in the desert surface at the test
81 site. In fact, the chlorine deposition is minimal for these releases, thus the JR II
82 field tests are best for evaluating the dispersion models.

83

84 Observations from three of the JR II trials (1, 6, and 7) are used in the current
85 paper to compare with the predictions of 17 dense gas model runs, from the U.S.,
86 Canada, five European countries, and the European Commission (see Table 1).
87 The models are briefly described in the next section. To avoid confusion, note
88 that two of the model runs were for the same model (SLAB) run by different per-
89 sons at different groups (SLAB-I by INERIS in France and SLAB-R by RAND

90 Corp in the US). An overview of the JR II field experiment and a description of
91 the model evaluation exercise are given by Fox et al. (2020) as an introduction to
92 the special JR II issue of Atmospheric Environment.

93
94 Many of the modelers who are listed in Table 1 participated for three or four
95 years in the JR II Modeling Working Group, which was advising the project
96 managers. These modelers ran test cases to assist in guiding the placement of
97 samplers in the field test experiments. In contrast, other modelers in Table 1 had
98 seen only limited subsets of the JR II data prior to this exercise. All modelers were
99 sent a set of recommended inputs for emissions (Spicer and Miller, 2017) and for
100 meteorology (Hanna, 2018) and were asked to send model outputs of the arc-
101 maximum concentrations (arc-max C) for averaging times of 1 s, and cloud
102 widths and heights (to the 20 ppm and 200 ppm concentration contours) at
103 distances of 0.2 0.5, 1, 2, 5, and 11.0 km from the release. This is summarized in
104 the Jack Rabbit II Model Inter-Comparison Specification (Mazzola, et al. 2019).
105 More details on the recommended emissions and meteorology are given by Spicer
106 and Tickle (2020) and Hanna (2020), respectively, in this special issue. Further
107 discussions on the concentration observations are given by Chang and Mazzola
108 (2020) and on the cloud width and height observations by Mazzola (2020).

109
110 We briefly summarize the model inputs in Table 2 (meteorology) and in Table
111 3 (emissions). Hanna (2020) and Spicer and Tickle (2020) have full details
112 supporting these tables. In addition, for models which can treat these, we specified
113 a surface roughness of 0.5 mm, and a chlorine deposition velocity assumption of
114 0.04 cm/sec, for the Dugway desert playa.

115
116 An over-arching goal for this model inter-comparison exercise is to facilitate
117 assessment and improvement of all models used for analysis of hazardous gas

118 releases. It is intended to generate collaborative studies involving experts in the
 119 field, and the test data from JR II have been widely distributed and hopefully will
 120 generate additional research. With continuing collaboration, it is hoped that
 121 scientific gaps related to modeling of hazardous gas releases will be identified,
 122 leading to future research, and that all models can become more accurate.

123

124 **Table 1.** List of models being compared and organizations running the models.

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126

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

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128

129 **Table 2.** Basic recommended meteorological inputs for trials 1, 6 and 7 (mixing
 130 height, wind speed, 1/L, Pasquill stability class). L is determined by observations at 2 or
 131 2.5 m.

Trial	Date	Release time	Time of observation	Mixing height	Wind speed at z = 2 m	1/L	Pasquill stability class
		MDT = UTC -6	UTC	m	m/s	1/m	
1	8 24 15	1336	1335	1000	1.5	0.0678	E or F
6	8 31 16	1424	1430	1000	2.4	0.056	E
7	9 2 16	1356	1356	1000	4.0	0.0229	D or E

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133

134 **Table 3.** Averaged simplified emission rates and parameters for Trials 1, 6 and 7 for both
 135 single source and dual source assumptions.

	Trial 1	Trial 6	Trial 7
Single source, tank release into atmosphere			
Primary release			
Discharge rate (kg/s)	224.	260.	259
Discharge period (s)	20.3	32.2	33.3
Temperature (°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
Dual source, tank release with rainout and evaporation			
Primary release modified for rainout			
Discharge rate (kg/s)	146	168	162
Discharge period (s)	20.3	32.4	33.6
Temperature (°C)	-37.3	-37.4	-37.4
Vapor fraction	0.262	0.266	0.274
Density (kg/m ³)	11.96	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 (°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

136

137

138 **2 Overview of Models**

139

140 Most of the 17 models have been routinely run by members of the JR II mod-
141 eling working group. A few models were added in order to have broader cover-
142 age. The models can be divided into two groups – publicly-available and proprie-
143 tary. Publicly-available models include those that are widely distributed around
144 the world (such as SLAB) and those that are used only within the country or la-
145 boratory of development (e.g., PUMA). Proprietary models generally do not
146 make their source code available and also charge a fee to users.

147 Some models include only a transport and dispersion module. Other models
148 also include a meteorological processing module, an emissions module, and/or an
149 exposure and health effects module. In the current exercise, we do not include
150 health effects estimates, and we provide suggestions for input meteorology and
151 emissions. However, modelers were given the option of using their own emis-
152 sions and/or meteorological modules.

153 Below we provide brief summaries of each model and references where further
154 details can be found. Some models (ADAM, B&M, DRIFT, HPAC, IDDM,
155 PUMA, and PMSS) have papers in the current special issue.

156 2.1 Publicly available models

157 ADAM (Fabbri et al., 2017 and 2020, Fabbri and Wood, 2019) is a conse-
158 quence assessment tool, recently developed by the Joint Research Centre of the
159 European Commission. Its atmospheric dispersion module is an in-house modified
160 version of SLAB, which introduces several modeling improvements such as the
161 exact calculation of the average concentration for instantaneous releases, the cal-
162 culation for time-varying releases, the inclusion of the contribution from pool
163 evaporation in case of rainout, and the extension of the calculation for downward
164 jets.

165 ALOHA (NOAA/EPA 1992) is a comprehensive dispersion model for hazard-
166 ous gasses that is part of the CAMEO modeling software distributed by the US
167 EPA and NOAA to emergency responders. Its passive (neutral) gas algorithm is
168 based on the Gaussian plume model and its dense gas algorithm is based on
169 DEGADIS (Havens and Spicer, 1990).

170 The B&M model is based on the Britter and McQuaid (1988) Workbook for
171 Dense Gas Dispersion. It consists of two nomograms (one for instantaneous re-
172 leases and one for continuous releases) where dimensionless concentration varia-
173 tions with downwind distance are presented as a function of a dimensionless cloud
174 stability (depending on cloud excess density and size). Field and laboratory data
175 are used to develop the curves. A crucial assumption for the current chlorine re-
176 lease trials regards specification of the initial cloud density and dimension scale
177 (see the Hanna 2020 paper in this special issue).

178 The Canadian Urban Dispersion Modelling (CUDM) system was developed in
179 a collaboration involving Environment Canada, the University of Alberta, Water-
180 loo University, and the Canadian Department of Defence. The system consists of
181 a wind model and a plume model component. The former is a high-resolution
182 Reynolds-averaged Navier-Stokes (RANS) model with k-epsilon closure, that
183 computes detailed winds around explicitly-resolved urban-scale streets and build-
184 ings provided from databases of 3D city building layouts. Inflow boundary condi-
185 tions are supplied either from larger-scale 3D NWP analyzed or forecast fields or
186 from single wind profiles that assume neutral vertical stability. An optional hori-
187 zontally-uniform k-eddy wind configuration with no obstacles is also available.
188 The plume model component of the CUDM is the well-mixed 3D Lagrangian sto-
189 chastic particle trajectory model of Thomson (1987). The urban Lagrangian sto-
190 chastic (urbanLS) model is based on Wilson et al. (2009) and uses passive scalar
191 particles with dry deposition on surfaces parameterized by a deposition velocity. It
192 does not account for plume density effects.

193 DRIFT (Gant et al 2018 and 2020) is a widely-used dense gas dispersion model
194 developed by the UK Health and Safety Executive (HSE). It is an integral model
195 similar in basic principle to DEGADIS, HEGADAS, and SLAB, and has been
196 widely validated with available dense gas field experiment observations.

197 The ESCAPE model (Expert System for Consequence Analysis and Preparing
198 for Emergencies) was developed at the Finnish Meteorological Institute and can
199 be used for evaluating the releases of toxic and flammable gases into the atmos-
200 phere, their source terms, atmospheric dispersion and the effects on humans and
201 the environment. Kukkonen et al. (2017) have presented the mathematical treat-
202 ments of this model and an evaluation of the model against selected experimental
203 field data. The treatments for atmospheric heavy gas and passive dispersion are
204 modified versions of the DRIFT model. The operational implementation of the
205 ESCAPE modelling system can be accessed anywhere using internet browsers, on
206 laptop computers, tablets and mobile phones. The model has been adapted to be
207 able to automatically use the real time predictions and forecasts of the numerical
208 weather prediction model HIRLAM, “High Resolution Limited Area Model”.

209 The HPAC/SCIPUFF (Hazard Protection Assessment Capability/Second Order
210 Closure Puff) model system was developed for US Department of Defense scenar-
211 ios (DTRA 2008, Sykes et al. 2014, Simpson et al. 2020). The dispersion model
212 can be described as a Lagrangian puff model. It can treat clouds with positive or
213 negative buoyancy, and has been validated with a broad array of hazardous gas
214 release field experiments.

215 IDDM (Integral Dense-gas Dispersion Model), developed at the US National
216 Center for Atmospheric Research (NCAR) accounts for source momentum, densi-
217 ty effects, and boundary layer processes in predicting the transport, growth, and
218 maximum concentrations due to dense gas releases. An early version called the

219 “NCAR” model was presented in Gant et al. (2018, Appendix A) with the more
220 recent IDDM form given by Weil (2019) and Weil and Alessandrini (2020).

221 PUMA is a real-time Gaussian puff model, developed by the Swedish Defence
222 Research Agency, with the purpose of providing support during ongoing emer-
223 gencies (Sigg et al., 2018). It operates on the local scale with meteorological
224 properties described by similarity theory and it has dense gas capabilities de-
225 scribed by Björnham and Burman (2016).

226 RAILCAR was originally developed by the US Navy to simulate emissions of
227 hazardous gases released from railcars. It uses basic physics and chemistry, along
228 with observations from several railcar accidents, to parameterize emissions condi-
229 tions for input to dispersion models. RAILCAR also includes a basic dispersion
230 model. See (Bauer 2013 and 2015, Bauer et al. 2018) for details. The US Navy
231 also funded the linking of RAILCAR with two dense gas dispersion models,
232 ALOHA and QUIC. The current model comparison exercise used RAILCAR-
233 ALOHA and RAILCAR-QUIC. However, the model outputs that we compare
234 here are from previous applications by the model developer to the JR II Trials 1,
235 6, and 7, using their own assumed emissions and meteorology, rather than the
236 inputs suggested by us.

237 SLAB (Ermak, 1990) is perhaps the most widely-used dense gas dispersion
238 model in the public domain. As its name infers, it is an integral slab model. Here
239 we include SLAB runs by two groups, INERIS (called SLAB-I) and RAND
240 (called SLAB-R). This exemplifies the typical differences encountered when the
241 same model is run by two expert users in different organizations.

242 VDI (1990) is a German regulatory model that is used to simulate dense gases.
243 The VDI Guideline 3783, Part 2 “Dispersion of Heavy Gas Emissions by Acci-
244 dental Releases” was released in 1990. The Guideline is based on results which
245 have been gained by systematic wind tunnel experiments. In these experiments the

246 release type was varied between an instantaneous release and a continuous gas
247 source. Overall 26 generic dispersion areas were investigated, ranging from a free
248 field without any buildings to different built up situations. By the application of
249 dimensional analysis relations, the results which have been gained in the small-
250 scale model can be transferred directly to fullscale released masses and to the en-
251 vironmental and ambient conditions, which are of practical interest. The guideline
252 is designed for the near field dispersion, where heavy gas effects are dominating,
253 down to a minimum concentration of 1 Vol.%. For estimations of the far field
254 effects, the VDI 3783 Part2 can be coupled with Part 1 of this guideline, enabling
255 us to estimate the gas dispersion down to ppm values.

256 2.2 Proprietary models

257 Phast is a commercial package developed by DNVGL containing a wide range
258 of models for consequence and risk assessment. The dispersion model (Witlox
259 and Holt, 1999) allows a range of source terms (evaporating pools, instantaneous
260 releases, finite duration and time-varying releases). It accounts for dense and
261 buoyant gases, 2-phase releases, droplet modelling and rainout. For cases that
262 rainout, an integrated pool spreading and evaporation model is included. Plumes
263 may evolve through one or more different stages: initial expansion, momentum
264 jet, heavy gas, and passive. In its most recent versions it includes enhancements to
265 model along-wind spreading for short duration and time-varying releases (Witlox
266 and Harper, 2014). Phast is widely-used by the chemical processing industry and
267 by many government agencies.

268 PMSS (Parallel Micro-SWIFT-SPRAY) combines algorithms developed by
269 public research agencies such as the French Atomic and alternative Energies
270 Commission (CEA) and by a commercial company, Aria Technologies. The
271 model was run for this exercise by Aria Technologies. PMSS aims to provide a
272 simplified but rigorous CFD solution of the flow and dispersion in built up envi-

273 ronments in a moderate amount of time. It is the efficiently parallelized version of
274 MSS (Oldrini et al., 2017). MSS encompasses the local scale versions of SWIFT
275 and SPRAY. Micro-SWIFT is a mass-consistent diagnostic model taking account
276 of obstacles (such as the CONEX array). In its recent version, it also includes a
277 RANS momentum solver. Micro-SPRAY is a Lagrangian Particle Dispersion
278 Model able to account for obstacles (Tinarelli et al., 2012). It is also able to deal
279 with the dispersion of a dense gas (Anfossi et al. 2010, Gomez et al. 2020).
280 PMSS has been thoroughly validated against numerous wind tunnel and field ex-
281 periments in complex environments, especially in the framework of the COST ES
282 10006 project (Trini Castelli et al., 2017).

283 SAFER/TRACE (SAFER Systems, 2014) is similar to Phast in that it is wide-
284 ly-used in the chemical processing industry. TRACE algorithms cover a ground-
285 based or elevated release of dense or non-dense gasses. It can handle dispersion of
286 gas or vapor/aerosol streams. It has comprehensive algorithms for release rate
287 estimation from tank, pipe, and liquid pool (e.g., Meel and Khajehnajafi 2012 and
288 Khajehnajafi and Pourdarvish 2011). Users have the ability to create gaseous or
289 liquid mixtures. The liquid mixture model includes popular equation of state mod-
290 els (e.g., Peng Robinson, Soave, Redlich-Kwong) for hydrocarbon mixtures and
291 Antoine, and Wilson for non-ideal solutions. Its chemical database covers most of
292 the chemicals used in Industry. The TRACE fire model includes pool fire, jet fire,
293 fireball, and flashfire. The explosion model includes vessel burst, BLEVE, and
294 unconfined vapor cloud explosion. SAFER TRACE™ incorporates an intelligent
295 wizard feature that allows the user to easily and rapidly build a scenario, create
296 backs up and share scenarios with other users. Results can be viewed in tabular or
297 graphical formats. Output information can be exported to other applications like
298 word processors, spreadsheets and presentation managers, and Google Earth.
299

300 **3 JR II brief description**

301

302 As described by Fox et al. (2020), JR II took place over a broad flat desert at
 303 DPG. Releases were initiated between about 7 to 9 AM local time in late sum-
 304 mer. The pressurized liquid chlorine tank was at the center of a 25 m diameter
 305 concrete pad, and the tank's bottom was 1 m above the surface. The main release
 306 was a two-phase momentum jet from a 15.2 cm diameter hole, with duration of
 307 about 20 to 40 seconds. The hole was at the tank's bottom for Trials 1 and 6, and
 308 pointing 45° downwards and downwind for Trial 7. During 2015, the source loca-
 309 tion was within a mock urban array, consisting of about 80 CONEX shipping con-
 310 tainers set up on a packed gravel area 122 m square. For 2016, the CONEX obsta-
 311 cle array was removed. Concentrations were measured in the area containing the
 312 obstacle array, and also on 90° arcs at distances of 0.2, 0.5, 1, 2, 5, and 11 km.
 313 Continuous (with 1 to 3 s averaging time) samplers were used, as well as several
 314 UV lidars and still photography and videos. Table 4 lists the general characteris-
 315 tics of the three JR II trials used in the current paper. The details of the tank and
 316 the pressurized releases are described by Nicholson *et al.* (2017), Spicer and Mil-
 317 ler (2017), and Spicer and Tickle (2020). Further discussion of the JR II field
 318 tests and model inter-comparisons is found in Fox *et al.* (2020).

319

320 **Table 4.** General characteristics of Trials 1, 6, and 7 in JR II.

321

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

322

323

324 Trials 1, 6 and 7 were chosen as initial representative trials. They have
325 downwards (Trials 1 and 6) or 45° downwards (Trial 7) jet directions, relatively
326 large observed concentrations, and relatively steady winds. Because the plume
327 was not on the edge of the sampler network, full definition of peak concentra-
328 tion and plume width was possible. In the future, the six additional JR II trials
329 may be evaluated by some modelers as further research funding allows. Alt-
330 hough there were samplers at distances less than 200 m, these were not consid-
331 ered here as many models cannot simulate the initial dense momentum jet or the
332 detailed effects of the obstacle array. The samplers used for arc max concentra-
333 tions were located at a height of 0.3 m. To estimate cloud height, a few short
334 towers were available with observations at 0.3, 3, and 6 m. See Chang and Maz-
335 zola (2020) for more information on the sampler arrays.

336

337 **4 Results of model comparisons**

338

339 After the 17 model runs were completed for the three JR II Trials in Table 4,
340 two types of methods for comparing model predictions with observations were
341 used. The first type is a simple visual inspection approach using tables and scatter
342 plots. There are few enough numbers that they can be easily seen in a single table
343 or scatter plot. In addition to the visual inspections, we generated some simple
344 comparisons, such as the fractions of cases when a model would overpredict or
345 underpredict by more than a factor of 2. The second type is application of the
346 BOOT model evaluation software (Chang and Hanna 2004), where performance
347 measures such as FB (Fractional mean Bias), MG (Geometric Mean bias), NMSE
348 (Normalized Mean Square Error), VG (Geometric Variance, FAC2 (fraction of
349 predictions within a factor of 2 of observations), and FAC5 and FAC10 are calcu-
350 lated, and statistical significance tests are applied. The first four performance
351 measures are defined as follows:

352

$$353 \quad \text{FB} = (\langle C_o \rangle - \langle C_p \rangle) / (0.5(\langle C_o \rangle + \langle C_p \rangle))$$

354

$$355 \quad \text{MG} = \exp(\langle \ln C_o \rangle - \langle \ln C_p \rangle)$$

356

$$357 \quad \text{NMSE} = \langle (C_o - C_p)^2 \rangle / (\langle C_o \rangle \langle C_p \rangle)$$

358

$$359 \quad \text{VG} = \exp(\langle (\ln C_o - \ln C_p)^2 \rangle)$$

360

361

362 where C_o and C_p are observed and predicted variables (arc max concentrations in
 363 the below applications), respectively, and the $\langle \rangle$ brackets indicate an average. A
 364 perfect model, with C_o and C_p always equal to each other, has $\text{FB} = \text{NMSE} = 0$,
 365 MG and $\text{VG} = 1$, and $\text{FAC2} = 1$.

366

367

368 **4.1 Arc max C**

369

370 First, we will consider the maximum peak concentration (arc max C) on each
 371 of the sensor arcs. The sensor data have undergone extensive quality assurance
 372 and control. Some sensors saturated (exceeded their calibration limits), but we
 373 still include such peaks with qualification. Although the sensors used to determine
 374 the arc max C observation were all located at a height of 0.3 m, some models pre-
 375 dicted concentrations at a height of 0 m (ground level). At the downwind distanc-
 376 es of these sensors (x greater than or equal to 200 m), the differences in predicted
 377 concentration between heights of 0 and 0.3 m are expected to be less than a few
 378 per cent. Chang and Mazzola (2020) further describe these sensor data.

379

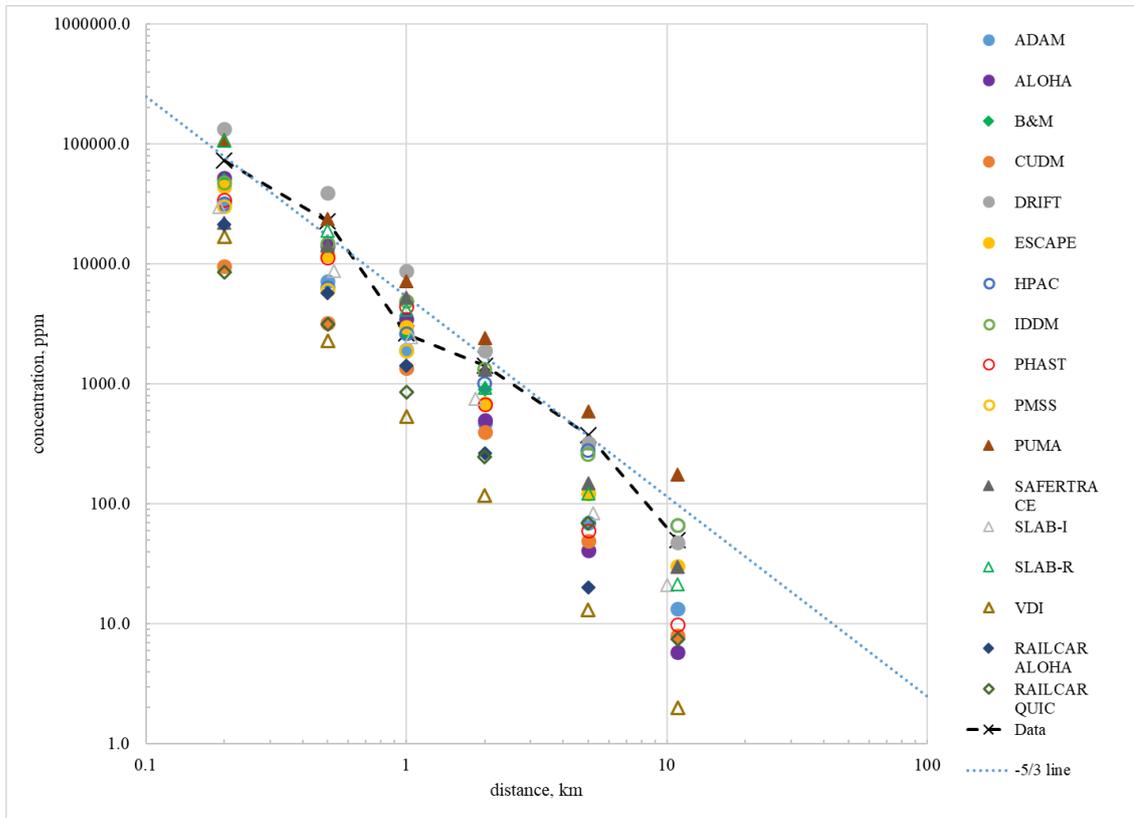
380 Figure 1 is a plot containing model predictions and observations of arc max C
381 as a function of distance for Trial 7. Of the three trials, Trial 7 has the largest
382 observed concentrations, and there is more of a tendency for slight model under-
383 prediction. In this figure, eight of the models are within a factor of 2 of the ob-
384 servations at more than half of the downwind distances. The other models tend to
385 underpredict by more than a factor of two at most downwind distances. At most
386 distances, the range of the 17 model predictions covers about $1\frac{1}{2}$ orders of mag-
387 nitude. It is also seen that a $-5/3$ power law reasonably fits the data from unsatu-
388 rated sensors. Dense gas modelers have recognized for almost 50 years that the
389 arc max C from a ground-level dense gas source will tend to follow an approxi-
390 mate $-5/3$ power law (e.g., see Hoot and Meroney 1974, whose wind tunnel data
391 yielded a -1.68 power law). In order to see individual model points more clearly, a
392 zoomed-in plot for just the outer four arcs is presented in Figure 2. Here the ten-
393 dency to underpredict by most models is clearer. For example, we can see that all
394 but one of the models underpredict at 5 km distance, and most of the models un-
395 derpredict by more than a factor of 2.

396

397 It is worth pointing out that, of the three trials being studied here, Trial 7, with
398 a 45° downward jet, was likely the most challenging for the models. For instance,
399 the ADAM model can simulate either downward or horizontal jet directions, but
400 not an angle in-between. For this comparison we simply averaged results for
401 these two geometries in ADAM.

402

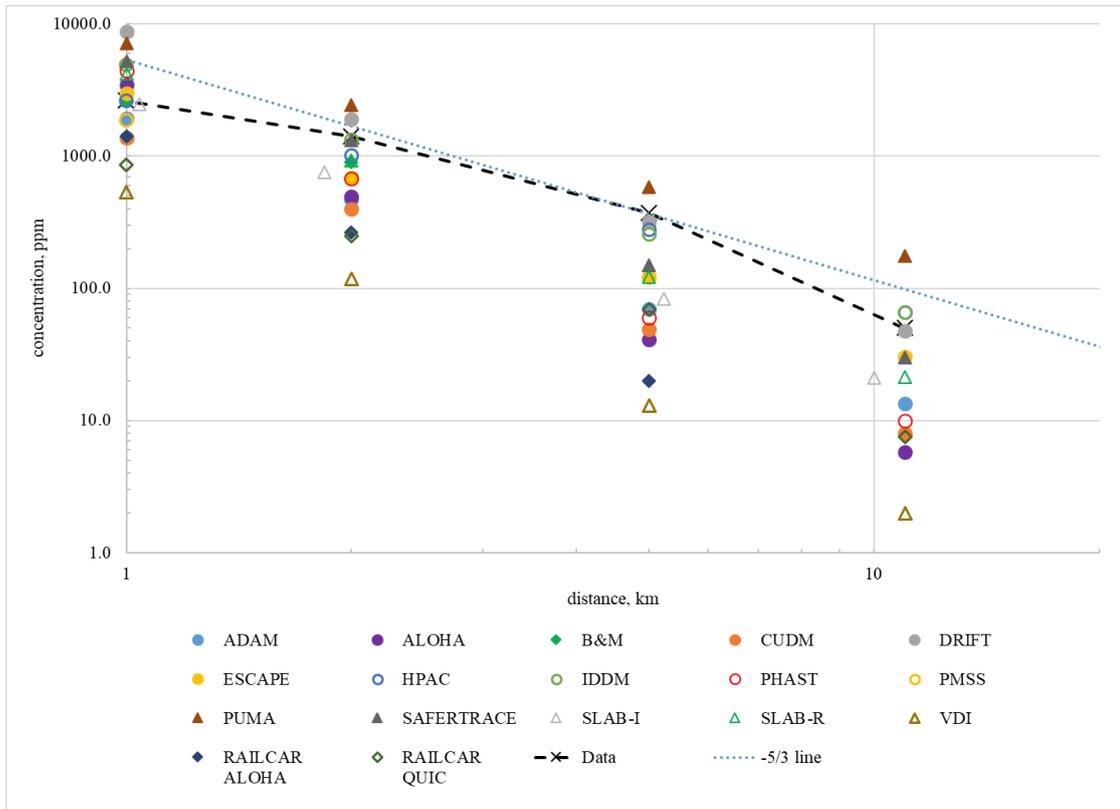
403



404
405

406 **Figure 1.** Plot of predicted and observed arc max C for all models for Trial 7. The ob-
407 served observations (averaging times of 1s-3s) are the X's connected by a dashed line. Saturated
408 observations (at 1 and 11 km) have a light gray box around the X. The straight blue-
409 dotted line represents a $-5/3$ slope.

410
411



412

413 **Figure 2.** Zoomed plot of predicted and observed arc max C as a function of distance for
 414 all models for Trial 7 for the most distant four arcs at 1, 2, 5 and 11 km. Otherwise, as for
 415 Figure 1.

416

417 For Trial 7, tallies (counts) have been made of the numbers of times that the
 418 modeled arc max C is larger by more than a factor of two, smaller by more than a
 419 factor of two, and within a factor of two of the observed arc max C. The counts
 420 are displayed in Table 5. Of the 101 model entries, 49 are within a factor of two
 421 (black), 49 underpredict by greater than a factor of two, and only 3 overpredict.

422

423

424 **Table 5.** 17 model predictions and observations of arc max C for Trial 7 for the six
 425 downwind distances. **Black** indicates prediction and observation within a factor of 2;
 426 **Blue** indicates underprediction larger than a factor of two; **Red** indicates overprediction

427 larger than a factor of two. For the observed concentrations, **Orange** indicates observed
 428 value is saturated.

x (km)	0.2	0.5	1	2	5	11
ADAM	32368	7192	1923	471	69	13
ALOHA	52300	14100	3470	497	41	6
B&M	50000	13000	2600	900	120	30
CUDM	9560	3230	1365	396	49	8
DRIFT	132908	38929	8694	1892	321	48
ESCAPE	44044	11833	3001	685	122	30
HPAC	31372	6314	2633	1005	278	66
IDDM	47472	14738	4886	1336	257	66
PHAST	34153	11304	4418	681	60	10
PMSS	30216	6044	1878	743	128	29
PUMA	108480	23835	7163	2428	586	176
SLAB-I	29800	8750	2460	750	83	21
SLAB-R	107047	18793	4185	925	121	21
TRACE	22154	14110	5198	1312	149	30
RAILCAR ALOHA	21290	5729	1417	266	20	
RAILCAR QUIC	8598	3138	861	248	69	8
VDI	16823	2277	537	117	13	2
Observed	72580	22686	2621	1417	373	50

429

430

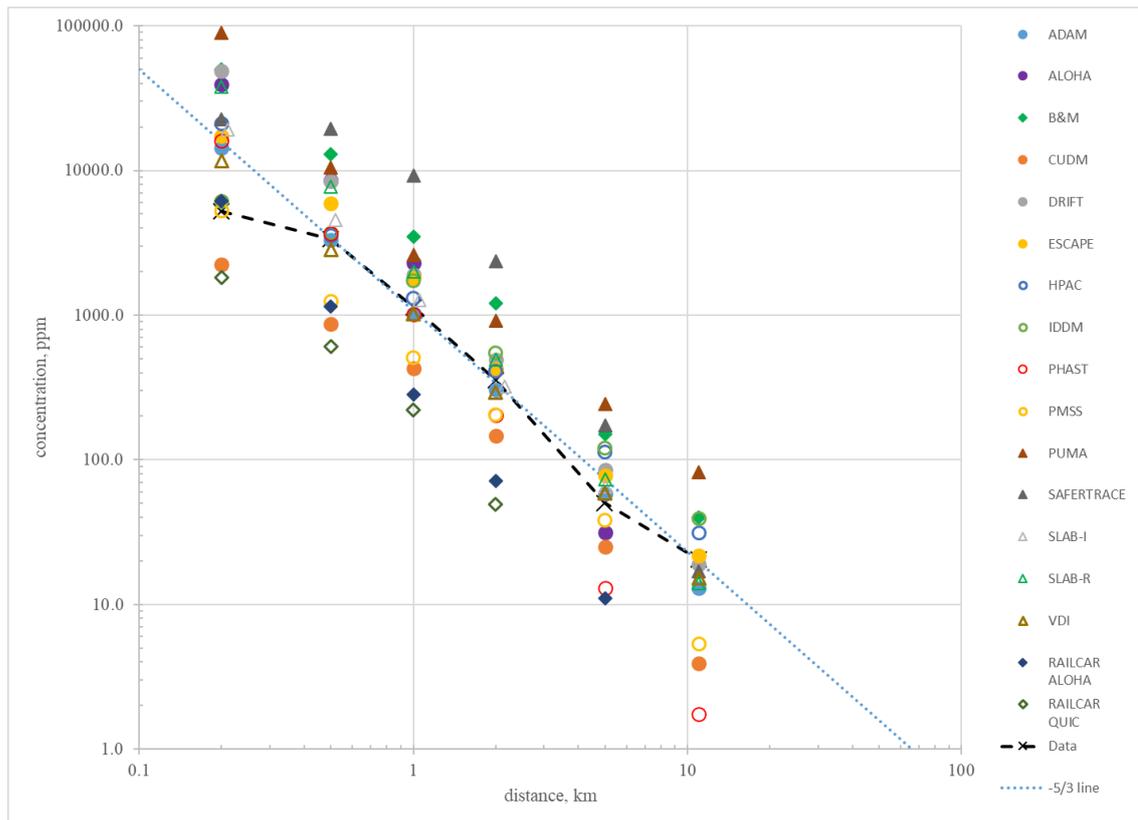
431 Arc max C summary plots, similar to that for Trial 7 in Figure 1, are given in
 432 Figures 3 and 4 for Trials 1 and 6, respectively. For the three JR II trials being
 433 analyzed (1, 6, and 7), some differences in mean bias and scatter in arc max C
 434 model predictions and observations are expected. For example, the observed arc
 435 max C values are seen to generally fall below the median of the range of model

436 predictions for Trial 1, near the median for Trial 6, and above the median for Trial
 437 7, There are many rational scientific explanations, such as variations in the mass
 438 released, the wind speed, the ambient stability at the time of release, the presence
 439 of the CONEX array, and the location of the hole. A few of the differences can be
 440 explained by basic science principles, such as the fact that both modeled and ob-
 441 served concentrations approximately scale with mass of chlorine released.

442

443

444

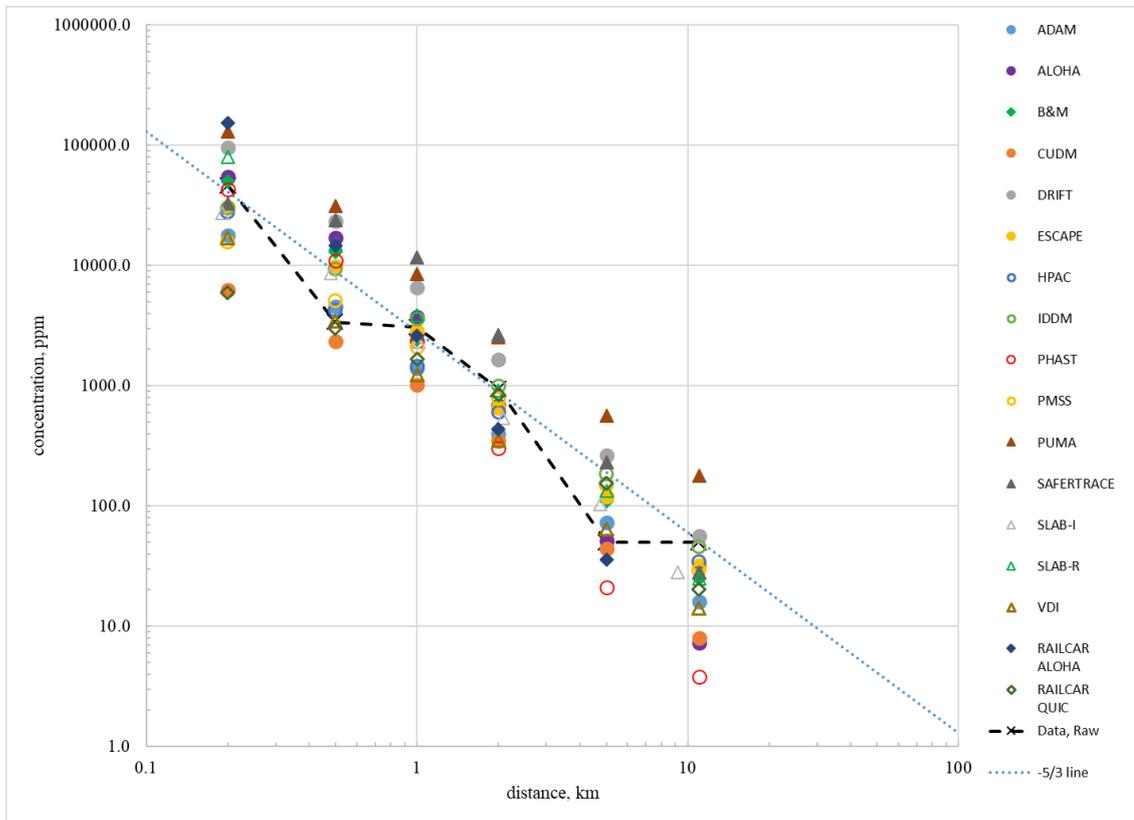


445

446 **Figure 3.** Plot of predicted (for all models) and observed arc max C for Trial 1. The
 447 observations (averaging times of 1 – 3 s) are indicated by the X's connected by a dashed
 448 line. Saturated observations are at 0.2 and 5 km. The straight blue-dotted line represents
 449 a -5/3 slope.

450

451



452

453 **Figure 4.** Plot of predicted (for all models) and observed arc max C for Trial 6. The
 454 observations (averaging times of 1 – 3 s) are the X's connected by a dashed line. Saturat-
 455 ed observations are at 0.5 and 5 km. The straight blue-dotted line represents a $-5/3$ slope.

456

457 Considering all 17 model predictions of arc max C for all 3 trials and at 6
 458 downwind distances, the range of model predictions for any trial or distance is
 459 consistently about 1 to 1 ½ orders of magnitude in Figures 1 through 4. The ob-
 460 served arc max C values are always inside the range of the 17 model predictions.
 461 A comparison of the magnitudes of the arc max C's along the best fit $x^{-5/3}$ lines
 462 for the three trials suggest some empirical conclusions. At any x, the ratio of con-
 463 centrations on the best fit line during Trial 1 to those during Trial 6 is 0.39, and
 464 the ratio during Trial 6 compared to Trial 7 is 0.52. Thus, the ratio for Trial 1 to
 465 Trail 7 is 0.20. Trial 1 likely has the smallest concentrations because of two major

466 reasons mentioned earlier: (1) its mass released was about half of that for Trials 6
467 and 7, and (2) the CONEX array would increase turbulence and therefore increase
468 rates of dispersion in the first 100 m. Trial 7 likely has the largest concentrations
469 because of two major reasons: 1) its 45° downward and along-wind jet orienta-
470 tion, thus decreasing the width of the initial jet, and 2) the wind speed was more
471 than twice as large as that for Trials 1 and 6, causing the cloud to move downwind
472 faster with less total dispersion at any downwind distance. Britter and McQuaid
473 (1988) provided further details of the rationale for why the short-term arc max C
474 can be larger (a worst case) for large wind speeds. This is the opposite of what
475 happens for continuous releases.

476

477 Table 6 extends the factor of two analyses for Trial 7 in Table 5 to Trials 1 and
478 6. Counts of the over, under and within factor of two predictions by all models
479 for these three trials and for all distances are listed. It is seen that about half of
480 the model predictions are within a factor of 2 of the observations and there are a
481 few less overpredictions than underpredictions by greater than a factor of 2.
482 Models with more arc max C comparisons within a factor of two of observations
483 include ESCAPE, HPAC, and IDDM. It was found that there are 6 models that
484 have less mean bias and scatter for all three trials. Some models have larger mean
485 biases for one trial, and smaller mean biases for the other two trials. A few models
486 show consistent under or over predictions by a factor of 2 for all three trials.

487

488

489 **Table 6.** Summary of numbers of times the observed arc max C is overpredicted (**red**) or
 490 underpredicted (**blue**) by more than a factor of two, or predictions were within a factor of
 491 two (**black**) of observations for the three trials and the six downwind distances. Percent-
 492 ages for each model's predictions are in parentheses.
 493

	number red (overpredicted)	number black (within factor of 2)	number blue (underpredicted)
ADAM	1 (5.6%)	8 (44.4%)	9 (50%)
ALOHA	3 (17.6%)	10 (58.8%)	4 (23.5%)
B&M	7 (38.9%)	10 (55.6%)	1 (5.6%)
CUDM	0 (0%)	4 (22.2%)	14 (77.8%)
DRIFT	7 (38.9%)	11 (61.1%)	0 (0%)
ESCAPE	3 (16.7%)	13 (72.2%)	2 (11.1%)
HPAC	3 (16.7%)	12 (66.7%)	3 (16.7%)
IDDM	3 (16.7%)	15 (83.3%)	0 (0%)
PHAST	2 (11.1%)	7 (38.9%)	9 (50%)
PMSS	1 (5.6%)	10 (55.6%)	7 (38.9%)
PUMA	14 (77.8%)	4 (22.2%)	0 (0%)
SLAB-I	3 (17.6%)	10 (58.8%)	4 (23.5%)
SLAB-R	4 (22.2%)	12 (66.7%)	2 (11.1%)
TRACE	9 (50%)	7 (38.9%)	2 (11.1%)
RAILCAR ALOHA	2 (13.3%)	4 (26.7%)	9 (60.0%)
RAILCAR QUIC	1 (5.9%)	3 (17.6%)	13 (76.5%)
VDI	1 (5.6%)	7 (38.9%)	10 (55.6%)
Sum	64 (21.3%)	147 (49.0%)	89 (29.7%)

494

495

496 Despite the biases and scatter discussed above, it is clear that these widely-
 497 used dense gas models are all able to simulate the basic behavior of the observa-

498 tions of arc max C. There is not a consistent mean bias one way or another. The
499 scatter also is consistent over the three trials and six downwind distances. There is
500 no general trend in bias or scatter with distance.

501

502 In order to assess the significance of model performance differences in their
503 predictions of arc max C, the BOOT statistical analysis methods were applied
504 (Chang and Hanna 2004). Table 7 presents the performance measures VG, MG,
505 FAC2, and FAC5 for the 17 models for Trials 1, 6, and 7, and for all arcs except
506 the 11 km arc. Not all models produced predictions on the 11 km arc. The medi-
507 ans across all 17 models can be determined: 2.69 for VG, 1.04 for MG, 0.47 for
508 FAC2 and 0.93 for FAC5. Recall that for a perfect model, all of these perfor-
509 mance measures will equal 1.0. $MG < 1.0$ indicates an overprediction mean bias
510 and $MG > 1.0$ indicates an underprediction mean bias. The ranges across all 17
511 models are 1.4 to 11.9 for VG, 0.31 to 3.55 for MG, 0.2 to 0.8 for FAC2, and 0.4
512 to 1.0 for FAC5.

513

514 Chang and Hanna (2004) and Hanna and Chang (2012) suggested some “ac-
515 ceptance criteria” for the model performance measures for rural and for urban
516 scenarios, respectively. For example, if $FAC2 > 0.6$ a model is “acceptable” for
517 rural areas. The criterion is $FAC2 > 0.3$ for urban areas where modeling has more
518 uncertainties. These criteria were developed based on results of many model
519 evaluation exercises with many research-grade field experiments. The Jack Rab-
520 bit II field study took place over a flat desert playa for downwind distances > 100
521 m. For the 2015 trials, with the mock urban array (CONEXs) in place at $x < 100$
522 m, there might be some effect at distances beyond the end of the array. Also, the
523 above acceptance criteria were developed without consideration of dense gas ex-
524 periments. Nevertheless, in Table 7, $FAC2 > 0.3$ for 12 of the 17 models, and
525 $FAC2 > 0.6$ for 3 of the models.

526

527

528 Table 7. BOOT calculations of the model performance measures Geometric Variance
 529 VG, Geometric Mean MG, FAC2 and FAC5 for the arc max concentration for the three
 530 trials and for arcs at 0.2, 0.5, 1, 2, and 5 km.

531

	VG	MG	FAC2	FAC5
ADAM	1.91	1.50	0.47	0.93
ALOHA	2.69	0.92	0.60	0.87
B&M	2.80	0.66	0.47	0.93
CUDM	5.34	3.16	0.27	0.73
DRIFT	3.04	0.43	0.53	0.80
ESCAPE	1.58	0.93	0.67	1.00
HPAC	1.65	1.04	0.60	1.00
IDDM	1.40	0.79	0.80	1.00
PHAST	2.24	1.44	0.40	0.93
PMSS	1.81	1.59	0.53	1.00
PUMA	6.89	0.31	0.27	0.80
RC/ALOHA	6.24	2.20	0.27	0.80
RC/QUIC	11.87	3.55	0.20	0.40
SLAB-I	1.74	1.13	0.60	1.00
SLAB-R	2.03	0.65	0.67	0.93
TRACE	5.97	0.45	0.27	0.73
VDI	7.92	2.43	0.40	0.80

532

533

534 The reader can see that, for each performance measure in Table 7, there are
 535 several models with values of, say, MG or FAC2 that are close to each other (say,
 536 within plus or minus 10 or 20 %). The question therefore arises whether the mod-
 537 els with similar MG or FAC2 are significantly different, using the statistical defi-
 538 nition. This question can be answered by BOOT, since one of the outputs is an
 539 indication about whether or not it can be concluded, with 95% confidence, that
 540 there is a significant difference in a performance measure for two models. The
 541 results for the Geometric Mean MG are recorded in Table 8, where 'X' means

542 that the difference in the natural logarithm (\ln) of the geometric mean MG for two
543 models is significantly different from 0, at the 95 % confidence level. This table
544 was developed using the 17 models whose performance measures are in Table 7,
545 and shows that there is no significant difference in $\ln(\text{MG})$ for the five models
546 with MG closest to 1; ALOHA, ESCAPE, HPAC, IDDM, and SLAB-I. However,
547 the same holds true for the four models with the largest underpredictions and
548 MG greater than 2; CUDM, RAILCAR/ALOHA, RAILCAR/QUIC, and VDI;
549 and for the three models with the largest overpredictions and MG less than 0.5;
550 DRIFT, PUMA and TRACE. Considering all 17 models compared with each
551 other, only about 20 % of the pairs in Table 8 show no significant difference.

552

553 **Table 8.** Summary of significance of model performance differences based on differ-
554 ences in \ln of geometric mean bias in arc max C for the three trials and the five closest
555 downwind distances. An X indicates a model pair where there is a significant difference
556 at the 95% confidence level. Beige indicates those models with MG closest to 1; yellow
557 those with $\text{MG} > 2$; and blue with $\text{MG} < 1/2$. Note that the table is symmetric but the
558 bottom half is not shown for visual simplicity.

559

560

	ADAM	ALOHA	B&M	CUDM	DRIFT	ESCAPE	HPAC	IDDM	PHAST	PMSS	PUMA	RC/ALOHA	RC/QUIC	SLAB-I	SLAB-R	TRACE	VDI
ADAM		X	X	X	X	X	X	X			X		X	X	X	X	X
ALOHA			X	X	X				X	X	X	X	X		X	X	X
B&M				X	X	X	X		X	X	X	X	X			X	X
CUDM					X	X	X	X	X	X	X			X	X	X	
DRIFT						X	X	X	X	X	X	X	X	X	X		X
ESCAPE									X	X	X	X	X	X	X	X	X
HPAC										X	X	X	X		X	X	X
IDDM									X	X	X	X	X			X	X
PHAST											X	X	X		X	X	X
PMSS											X		X	X	X	X	
PUMA												X	X	X	X		X
RC/ALOHA														X	X	X	
RC/QUIC														X	X	X	
SLAB-I															X	X	X
SLAB-R																	X
TRACE																	X
VDI																	

561

562

563

564 **4.2 Cloud width and height**

565

566 As described by Mazzola (2020), cloud width and height were estimated using
567 a combination of samplers and lidars at distances of 0.5, 1, and 2 km. The ob-
568 served cloud width and height were estimated at the time when the arc max C oc-
569 curred at each arc. The cloud edges were defined at two concentration levels: 20
570 ppm and 200 ppm. Videos from a drone showed that the instantaneous visible
571 cloud at distances of 0.5 to 2 km had a “mushroom” shaped footprint, with a
572 broad leading “head” due to the initial momentum jet release and associated dense
573 gas horizontal spreading, and a narrower trailing cloud due to evaporation from
574 liquid rainout from the concrete pad around the source (see Fox et al. 2020). Since

575 the “head” had the largest concentrations, the cloud widths and heights correspond
576 to that part of the visible cloud. For example, Figure 5 shows the predicted versus
577 observed cloud widths and heights for Trial 7. Note that observations are plotted
578 for samplers (dashed line with X symbol) and for lidar (dotted line). As explained
579 by Mazzola (2020), observed cloud height was estimated from lidars where avail-
580 able plus a few instances where there was a short tower with samplers at heights
581 of 0.3, 3, and 6 m.

582

583 Predictions of cloud width and height are available from only about half to 2/3
584 of the models. It is seen in Figure 5 that most of the models overpredict the cloud
585 width, sometimes by as much as a factor of 3 or 4. The median of the biases cal-
586 culated for all the models indicates about 70 % overprediction. However, two of
587 the models have a bias less than about 25 % at distances of 0.5 and 1 km. At dis-
588 tances of 5 and 11 km, where there were no observations, the expected decrease in
589 cloud width at a fixed edge concentration is evident among about half of the mod-
590 el predictions.

591

592 Regarding cloud height during Trial 7, at a distance of 1 km, the range of the
593 model predictions encompass the observations (uncertainty limits are shown).
594 Over all models, there is about a 30 % median bias towards overprediction. The
595 median bias across all models is near 0 at 1 km, is about 53 % at 0.5 km and about
596 33 % at 2 km.

597

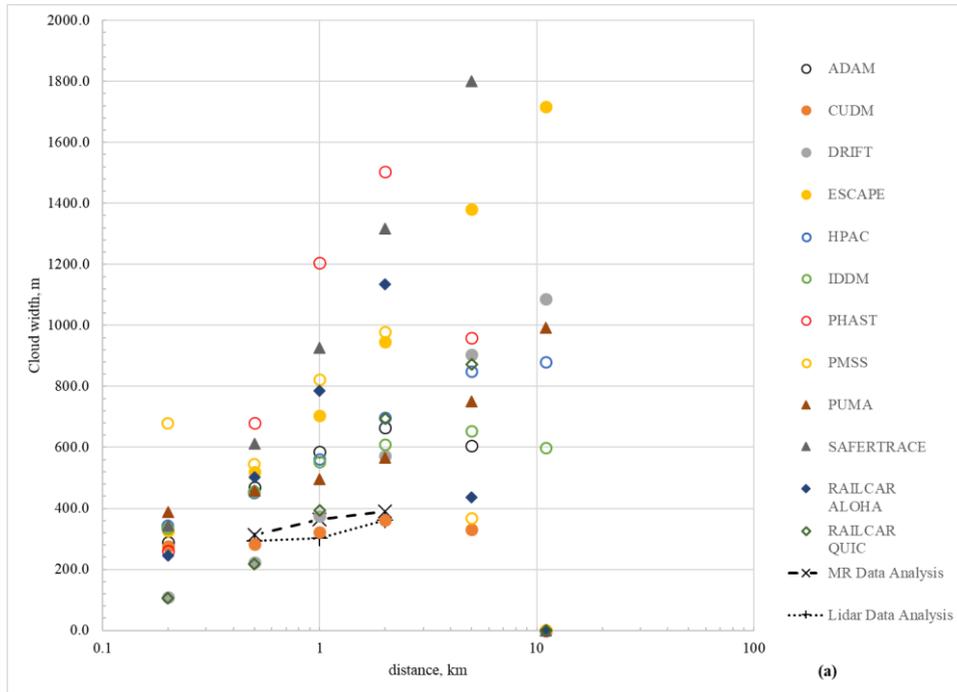
598 Similar to the format in Table 5, Table 9 provides counts of factor of 2 agree-
599 ment between model predictions and observations of cloud width and height to 20
600 ppm by distance. No models underpredict cloud width by more than a factor of 2.
601 58% of models predict within a factor of 2, while 42 % overpredict cloud width

602 by greater than a factor of 2. For cloud height, all of the models' predictions are
 603 within a factor of 2.

604

605 Although the plots for width and height at a concentration edge of 200 ppm are
 606 not shown here, Table 10 provides a summary of performance. It is seen that
 607 most models predict cloud dimensions to 200 ppm within a factor of 2, while
 608 about 25 % of the models overpredict both width and height by greater than a fac-
 609 tor of 2. The overpredictions by a model are listed for either cloud width or
 610 height, but not for both.

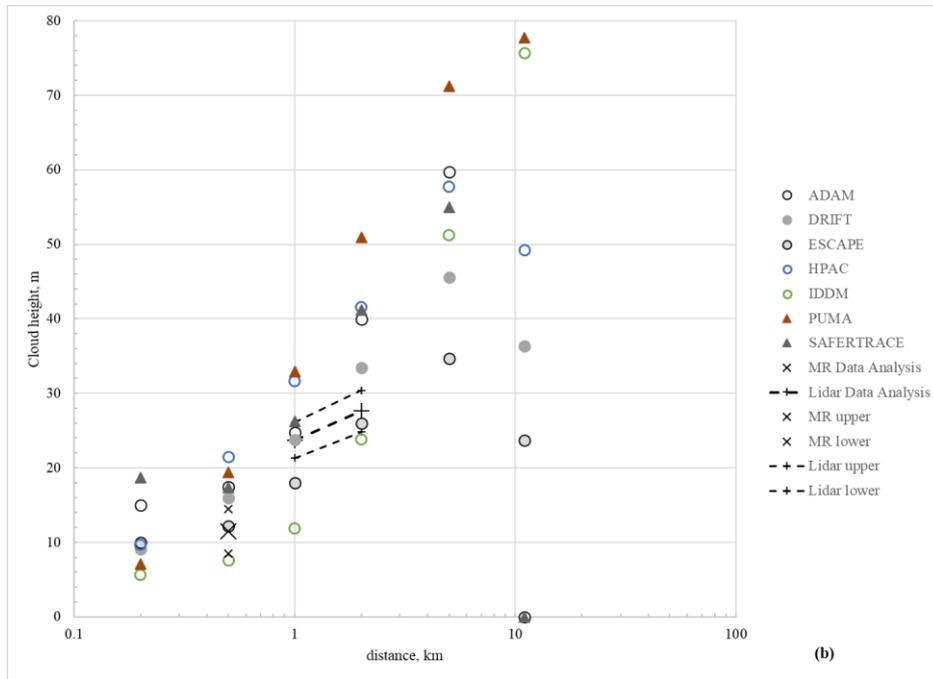
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615

616 **Figure 5.** Comparison for Trial 7 of model-predicted and observed cloud widths (a) and
 617 heights (b) (to 20 ppm) as a function of downwind distance. The X points are from sam-
 618 plers and the dashed line is from lidars, for which uncertainty estimates are shown.

619

620

621 **Table 9.** Model predictions and observations for 20 ppm cloud width (in m) (12 models)
 622 and height (in m) (7 models) at time of arc max C for Trial 7 for three downwind
 623 distances. **Black** is prediction and observation within a factor of 2; **Blue** is underpredic-
 624 tion larger than a factor of two (none shown); **Red** is overprediction larger than a factor
 625 of two.

x (km)	Width (m)			Height (m)		
	0.5	1	2	0.5	1	2
ADAM	469	586	665	17.5	24.8	39.9
CUDM	282	322	361			
DRIFT	223	374	573	15.9	23.7	33.4
ESCAPE	519	704	947	12.2	18.0	26.0
HPAC	451	561	697	21	32	42
IDDM	455	551	610	7.6	11.9	23.8
PHAST	680	1205	1503			
PMSS	545	822	977			
PUMA	459	495	566	19.4	32.9	50.9
TRACE	611	926	1317	17.4	26.2	41.2
RAILCAR ALOHA*	502	786	1134			
RAILCAR QUIC*	218	393	695			
Median for all models	464	568	680	17.6	24.2	36.6
Observed MiniRae	313	364	391	11.5		
Observed Lidar	293	303	363		23.7	27.6
Observed Avg	303	334	377	11.5	23.7	27.6

626 * - Results reported at 10 ppm, not 20 ppm used by all other models and observations

627

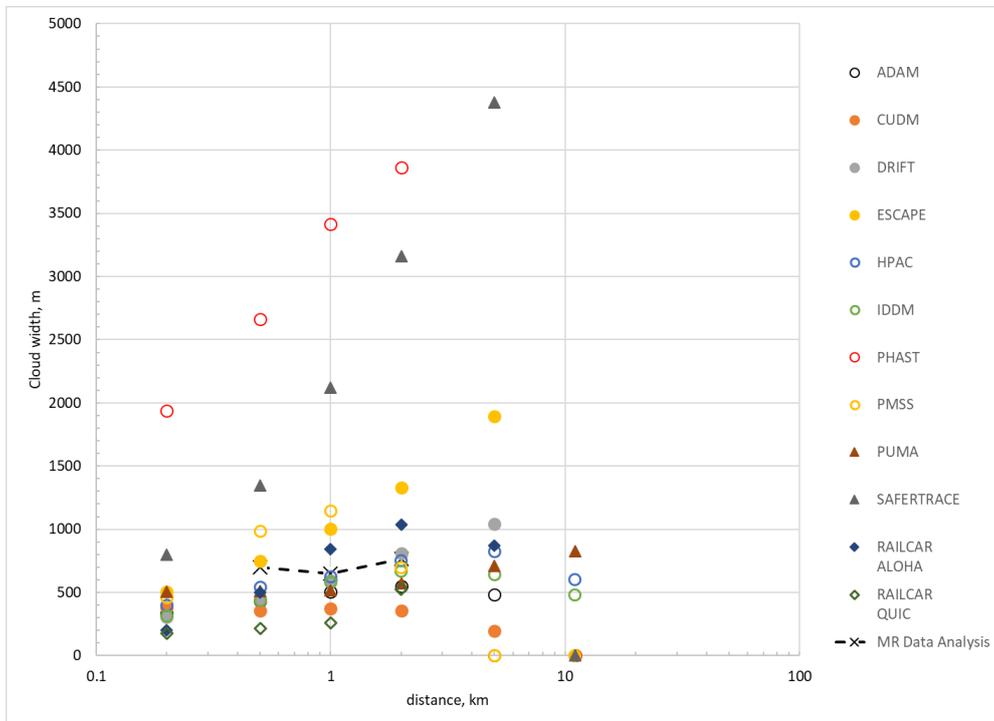
628

629 **Table 10.** Model predictions and observations for 200 ppm cloud width (in m)
 630 (10 models) and height (in m) (7 models) at time of arc max C for Trial 7 for three
 631 downwind distances. **Black** is prediction and observation within a factor of 2; **Blue** is
 632 underprediction larger than a factor of two (none shown); **Red** is overprediction larger
 633 than a factor of two.

x (km)	Width (m)			Height (m)		
	0.5	1	2	0.5	1	2
ADAM	372	415	335	12.5	16.7	19.5
CUDM	218	219	186			
DRIFT	218	351	497	10.8	15.4	19.8
ESCAPE	517	697	917	7.9	10.3	10.9
HPAC	364	431	456	17	23	27
IDDM	367	420	410	6.2	9.1	16
PHAST	536	905	870			
PMSS	504	717	170			
PUMA	381	377	395	15.4	25.1	36.9
TRACE	541	790	1027	11.7	15.7	18.3
Median for all models	377	425	433	10.3	15.6	18.9
Observed MiniRae	292	339	301	6.21	15.8	10.0

634
 635 Figure 6 shows the predicted vs observed cloud widths to 20 ppm for Trial 1.
 636 Note that observations are plotted for samplers (dashed line with X symbol) and
 637 there are no lidar observations. The bias of the models' predictions of the cloud
 638 width is less for Trial 1 than for Trial 7, since the predicted widths are scattered
 639 more evenly about the observed width. Two of the models show the largest over-
 640 predictions (by about a factor of 4 or 5). Observed cloud height was estimated
 641 only at the 0.2 km distance, where there were two short towers with samplers at
 642 heights of 0.3, 3, and 6 m. The predicted model heights and the observed height

643 (the larger of the values from the two samplers) to 20 ppm are given in Table 11.
 644 The median of the predicted heights at 0.2 km is only 6 % smaller than the ob-
 645 served value. The range of the predictions is from 0.38 to 2.30 times the observed
 646 height. The model differences may be partly caused by the different treatments by
 647 each model of the effects of the CONEX array just upwind of this arc.
 648
 649



650
 651 **Figure 6.** Comparison for Trial 1 of model-predicted and observed cloud widths (to 20
 652 ppm) as a function of downwind distance. The X points are from samplers.
 653
 654

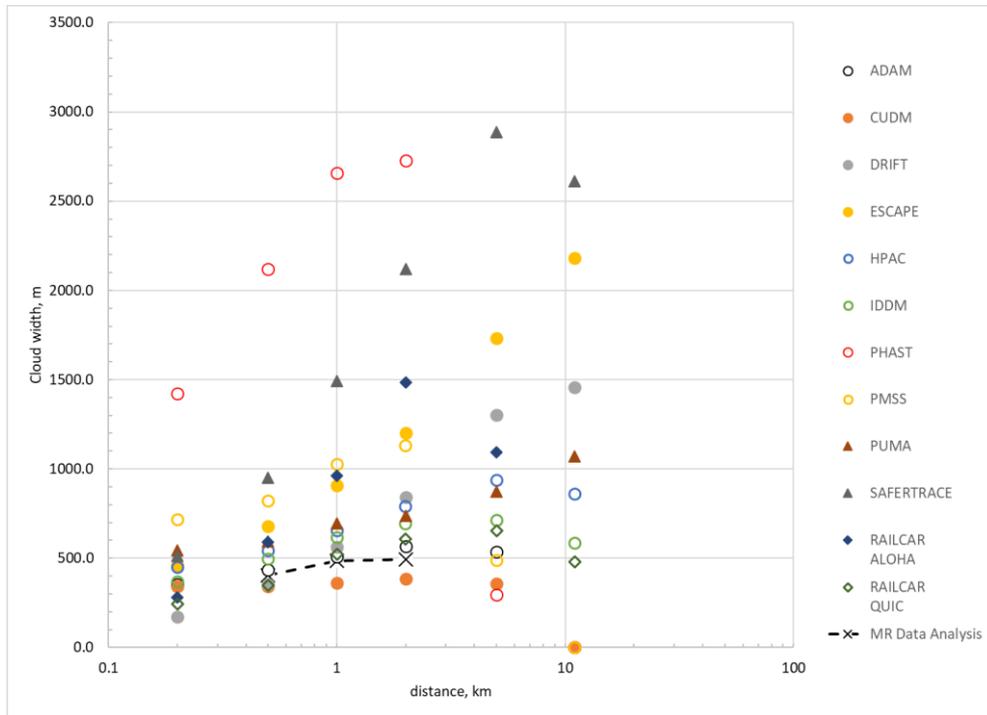
655 **Table 11.** Model predictions and observation of 20 ppm cloud height (in m) (7 models)
 656 at time of arc max C for Trial 1 for 0.2 km downwind distance. **Black** is prediction and
 657 observation within a factor of 2; **Blue** is underprediction larger than a factor of two; **Red**
 658 is overprediction larger than a factor of two.

x (km)	0.2
ADAM	3.9
DRIFT	5.1
ESCAPE	4.5
HPAC	10
IDDM	17.1
PUMA	8.5
TRACE	23.4
Median for all models	8.5
Observed MiniRae	9.2

659
 660 Figure 7 shows the predicted vs observed cloud widths to 20 ppm for Trial 6.
 661 Note that observations are based only on sampler observations (dashed line with
 662 X symbol); there were no lidar observations. All but two of the models overpre-
 663 dict the cloud widths, with two models overpredicting by more than a factor of 5.
 664 The median predicted width over all the models at 1 km is about 50 % greater
 665 than observed. Observed cloud height was estimated only at 0.5 km distance
 666 where there were two short towers with samplers at heights of 0.3, 3, and 6 m.
 667 The larger of the observed height for the two towers and the predicted heights to
 668 20 ppm by seven models are listed in Table 12. The median model-predicted
 669 height is only 8 % less than the observed height at 0.5 km, and the model predic-
 670 tions range from 0.7 to 1.9 times the observed height.

671

672



673

674 **Figure 7.** Comparison for Trial 6 of model-predicted and observed cloud widths (to 20
 675 ppm) as a function of downwind distance. The X points are from samplers.

676

677

678 **Table 12.** Model predictions and observations for 20 ppm cloud height (in m) (7 models)
 679 at time of arc max C for Trial 6 for 0.5 km downwind distance. **Black** is prediction and
 680 observation within a factor of 2; **Blue** is underprediction larger than a factor of two (none
 681 shown); **Red** is overprediction larger than a factor of two (none shown).

x (km)	0.5
ADAM	10.7
DRIFT	8.4
ESCAPE	8.1
HPAC	21.7
IDDM	8.3
PUMA	10.8
TRACE	11.6
Median for all models	10.7
Observed MR	11.6

682

683 Table 13 extends the factor of two analyses of widths and heights for Trial 7
 684 (previously presented in Tables 6 and 7) to Trials 1 and 6. The table includes data
 685 from all three trials. Counts of the over, under and within factor of 2 predictions
 686 by all models for these three trials and for all distances available are listed for
 687 both cloud width and cloud height. Note that not all models provided predictions
 688 for all combinations. It is seen that 74 % of the model predictions are within a
 689 factor of 2 of the observations (70 % for width and 84 % for height). There are
 690 more overpredictions (22 %) than underpredictions (5 %) by greater than a factor
 691 of 4. Many models mostly predict dimensions within a factor of two of observa-
 692 tions. It was found that there are 5 models that have a tendency to overpredict
 693 dimensions for 25 % or more of the comparisons. The overprediction tendency is
 694 perhaps to be expected given that the models are formulated to represent an en-

695 semble mean outcome, whereas these tests are individual realizations with no en-
696 sembles available.

697 **Table 13.** Summary of numbers of times the observed cloud width or height (to 20
698 and 200 ppm) is overpredicted (**red**) or underpredicted (**blue**) by more than a factor
699 of two, or predictions were within a factor of two (**black**) of observations for the
700 three trials and the six downwind distances. “x” means no prediction. Percentages
701 for each model’s predictions are in parentheses.

	number red (overpredicted)		number black (within factor of 2)		number blue (underpredicted)	
	Width	Height	Width	Height	Width	Height
ADAM		1 (10%)	18 (100%)	8 (80%)		1 (10%)
CUDM		x	13	x	5	x
DRIFT	1 (5.6%)		17 (94.4%)	10 (100%)		
ESCAPE	7 (38.9%)		11 (61.1%)	9 (90%)		1 (10%)
HPAC		3 (30%)	18 (100%)	7 (70%)		
IDDM		1 (10%)	18 (100%)	9 (90%)		
PHAST	16 (88.9%)	x	2 (11.1%)	x		x
PMSS	7 (38.9%)	x	7 (38.9%)	x	4 (22.2%)	x
PUMA		2 (20%)	18 (100%)	8 (80%)		
TRACE	15 (83.3%)	2 (20%)	3 (16.7%)	8 (80%)		

RAILCAR ALOHA*	3 (33.3%)	x	6 (66.7%)	x		x
RAILCAR QUIC*		x	7 (77.8%)	x	2 (22.2%)	x
Sum	49 (24.7%)	9 (12.9%)	138 (69.7%)	59 (84.3%)	11 (5.6%)	2 (2.9%)

702 * - Results reported at 10 ppm, not 20 ppm used by all other models and observations

703

704 **5. Major Conclusion and Further Comments**

705

706 In conclusion, we find that the general performance of the 17 models in this
707 comparison with JR II field observations of chlorine clouds was good. The
708 observations lie within the range of the model predictions, which cover about 1 ½
709 orders of magnitude for all trials and distances. Certainly no major biases or
710 excessive scatter are found, and there is no trend in model performance with
711 downwind distance.

712

713 This model comparison exercise focused on the dispersion models. The
714 modelers were not asked to apply emissions models or meteorological models;
715 instead, we provided emissions and meteorology inputs based on extensive
716 research by the JR II scientific team. In particular, the tank observations and the
717 rainout observations required analysis in order to optimize the emissions
718 estimates. Even in a controlled research environment, it is tricky to estimate
719 emissions for chlorine releases from holes in pressurized liquid tanks.

720

721 The deposition modules in codes could not be assessed, because, at the JR II
722 desert site (a salt playa), chlorine deposition could not be measured. Based on
723 fundamental chemistry, deposition to a dry desert such as at JR II was expected to
724 be minimal. However, at a different site with vegetation and/or organic soil, the

725 effects of removal of chlorine by deposition are expected to be significant (e.g.,
726 removing half of the chlorine in the first 1 or 2 km travel distance). The DHS is
727 currently sponsoring laboratory experiments aimed at developing better deposition
728 estimates for different vegetation and soils.

729

730 We believe that the over-arching goal to facilitate assessment and improvement
731 of all models used for analysis of hazardous gas releases is off to a very good
732 start. We encourage continued collaborative studies involving experts in the field
733 and dialog regarding lessons learned, improvement of models, and identification
734 of the most important scientific gaps related to such modeling to aid plans for
735 future research.

736

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740

741 **References**

742

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