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

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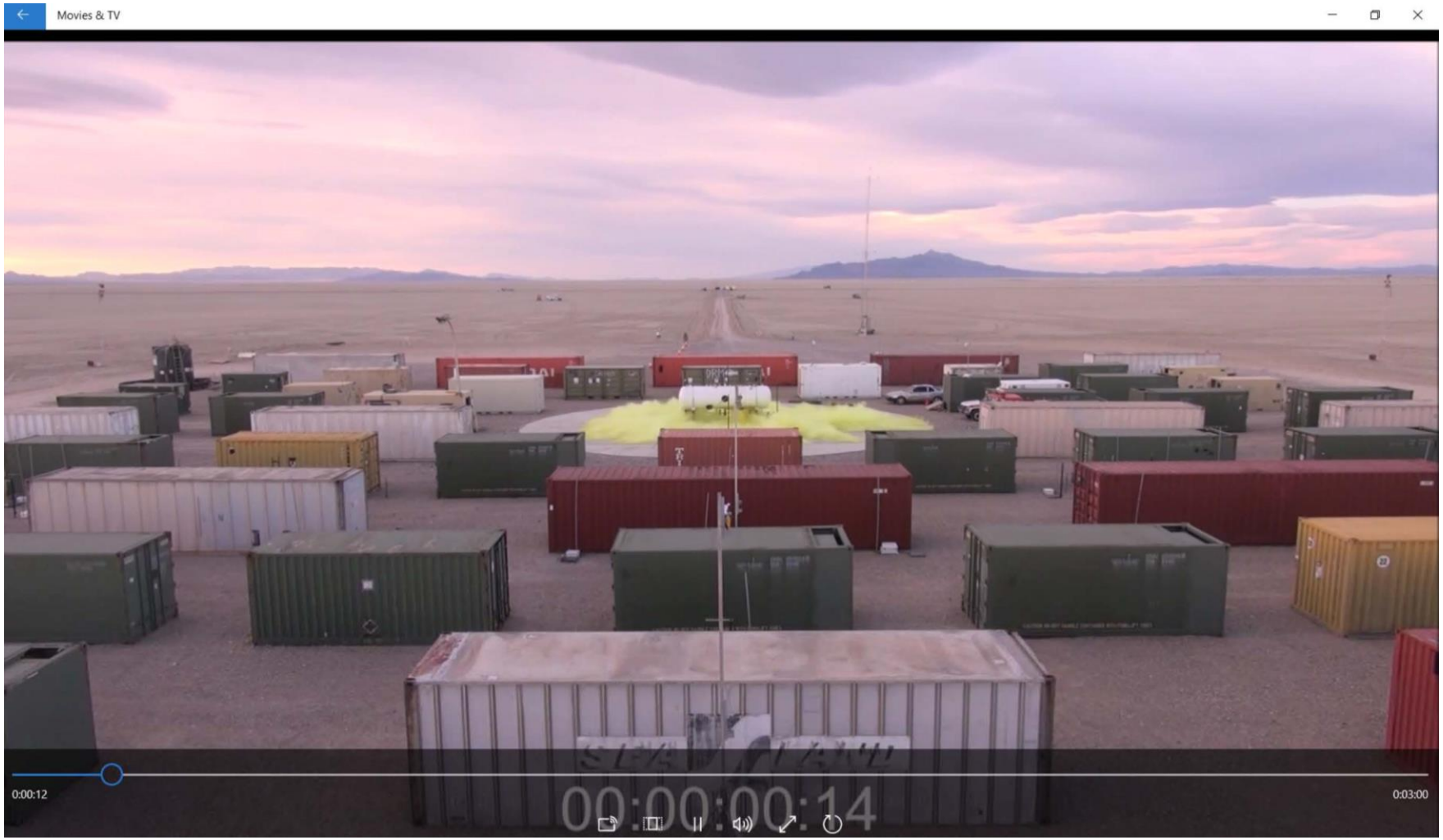
JR II 2015 cloud, looking south (upwind) 0.5 sec after release starts. Hole is at tank bottom



Side to side dimension of obstacle array = 100 m

Broad Goals

- Improve all models used for analysis of hazardous gas releases
- Generate collaborative studies so experts are talking to each other
- Widely distribute field data from JR II, thus generating additional research
- Identify gaps to be addressed in future theoretical analyses and field studies

Description of JR II

- Overview of nine JR II trials
- Summary of trials 1, 6, and 7, selected for model comparison
- Modeled and observed “endpoints” for comparisons (arc max ***C***, cloud width ***W*** and height ***H***) in this paper
- Sampling arcs used (0.2, 0.5, 1, 2, 5, and 11 km); saturation issues
- Use of lidars and sampler data on arcs to estimate width ***W*** and height ***H***

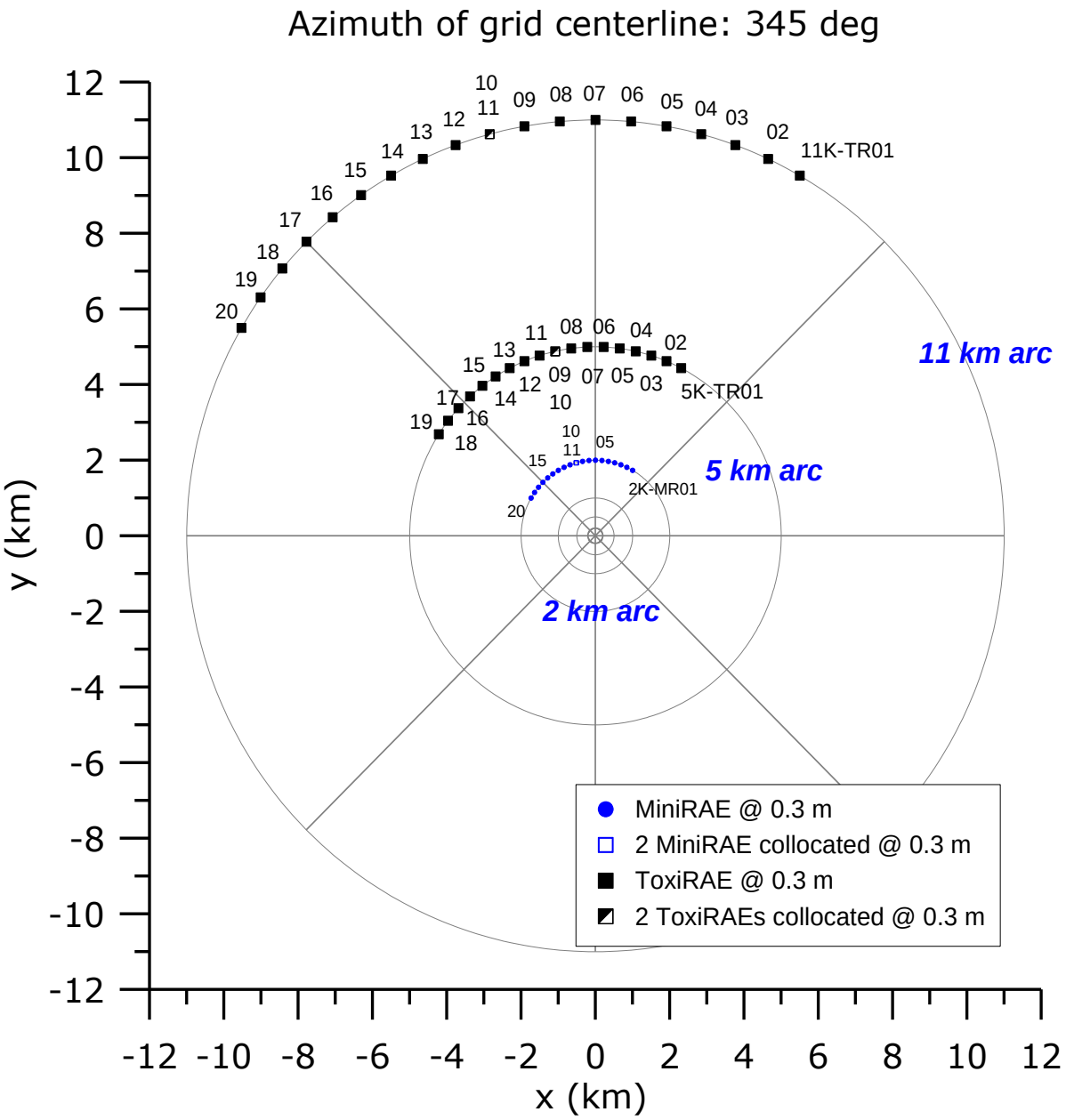
Overview of Trials 1, 6, 7 (Used for Model Comparisons)

Trial	Time (UTC)	Mass released	Duration of release	Mass release rate	Wind speed at z = 2 m	Wind dir at z=2 m	1/L	Pasquill stability class
	(MDT=UTC–6)	kg	s	kg/s	m/s	deg	1/m	
1	24 Aug 2015 1336	4,547	20.3	224	1.45	147.4	0.068	E or F
6	31 Aug 2016 1424	8,372	32.2	260	2.42	146.9	0.056	E
7	2 Sep 2016 1356	8,625	33.3	259	3.98	149.6	0.0229	D or E

Further details of Trials 1, 6 and 7

- These three trials have a downwards (trials 1 and 6) or 45° downwards (trial 7) jet, large observed concentrations, and relatively steady winds. The plume was not on the edge of the sampler network.
- We did not consider samplers at x < 200 m, since many of the models cannot simulate the initial dense momentum jet.
- For trials 1-5, in 2015, there was a 122 m square array of 80 CONEX containers around the source location. For trials 6-9, in 2016, the CONEX array was removed.

JR II C Samplers on 2, 5, and 11 km arcs

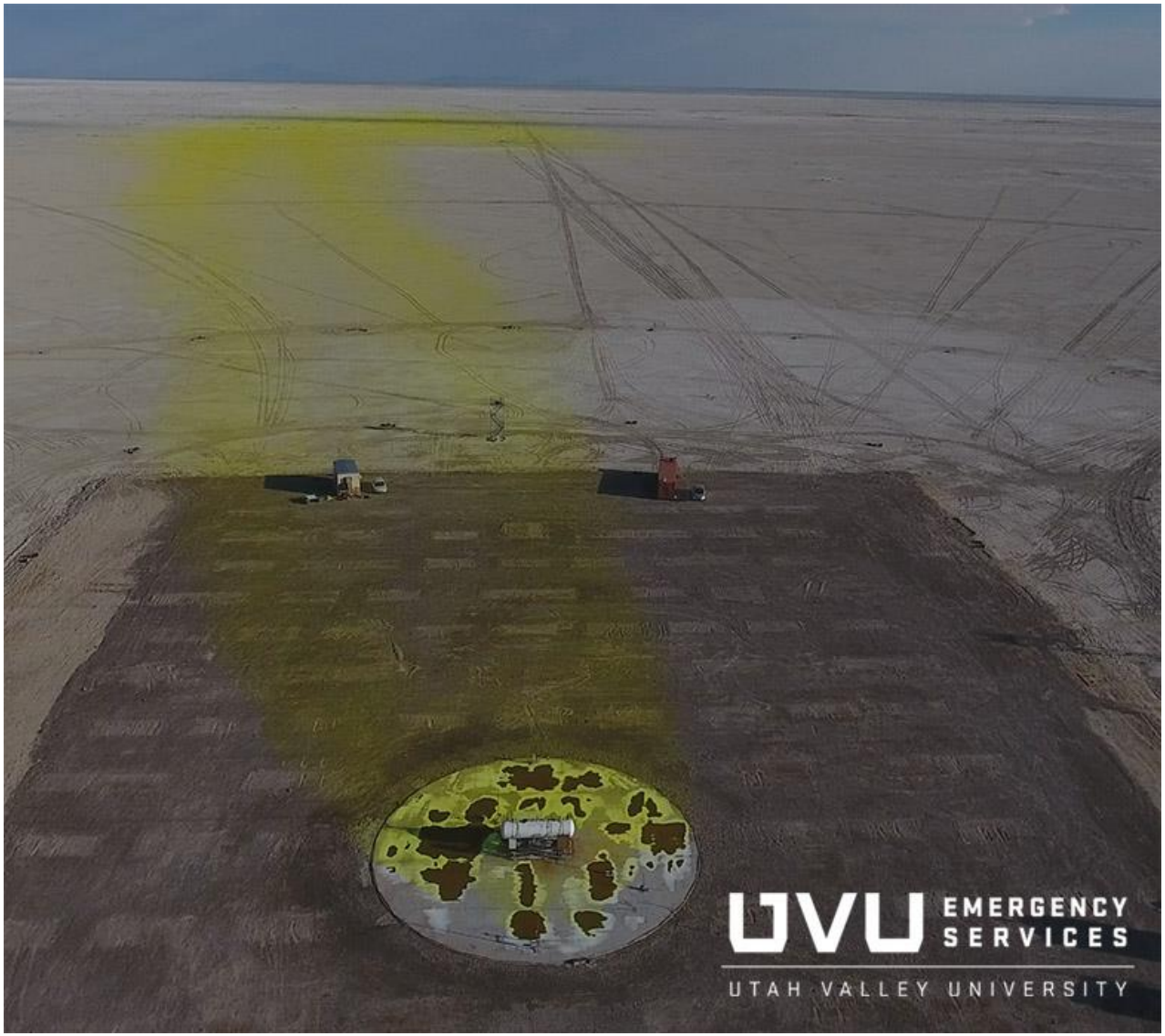


Trial 1, 30 s after release starts. Hole is at bottom of tank. Wind is blowing towards the left. Dense cloud moves 40 m upwind of source.

Trial 6 Hole at tank bottom. Photo taken by UVU drone about 10 min after release starts

Dark spots on pad are liquid that is still evaporating

Broader cloud in distance is from initial 2-phase jet.



Trial 7 – Hole is pointed 45 downwards towards downwind direction. Photo taken by UVU drone 30 s after release starts

Arc max *C* observations

- We use the 1 to 3 sec basic averaging time (resolution) of the samplers.
- Some (6 out of 18) samplers reporting arc max ***C*** are saturated, and as a result the actual concentration is likely larger than that reported.
- e.g., the MiniRae readings in trials 1 and 6 at 0.5 km are saturated at about 3300 ppm. The ToxiRae ***C***'s of 50 ppm at 5 or 11 km are saturated.
- We kept the saturated data in the model comparison exercise.

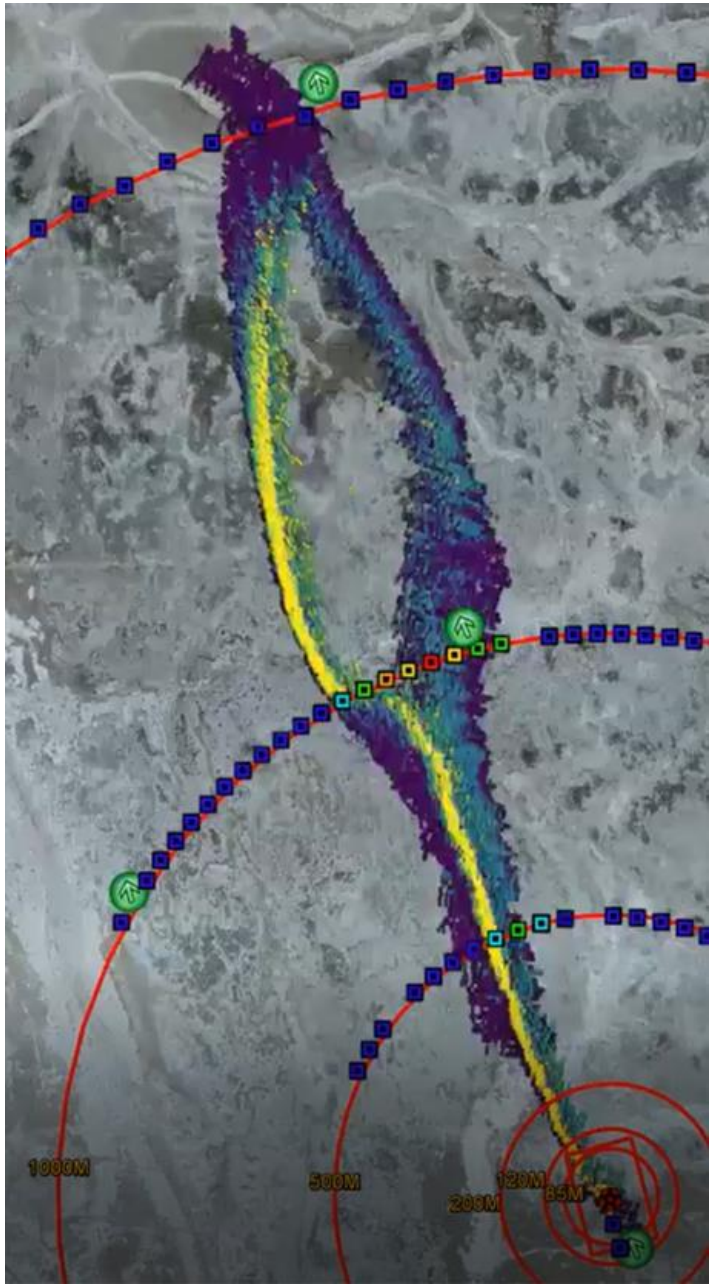
Cloud width (*W*) and height (*H*) observations

- ***W*** and ***H*** are observed and modeled based on 20 ppm and 200 ppm contours
- This is different from $\boldsymbol{\sigma_y}$ and $\boldsymbol{\sigma_z}$
- Obs ***W*** is based on 1) MiniRae samplers on arcs, and 2) lidar data
- ***H*** is mostly based on MiniRae obs on a few 6 m towers, with some use of lidars

Lidar observations of plume edges

- Lidars were set up by DPG on either side of the expected plume.
- The operators use a predetermined relation between signal and concentration
- However, the lidar cannot “see” very far into a dense chlorine plume.
- Example on next slide.

Lidar observations of Trial 7 cloud edge where the colored pattern is an example snapshot at ~4.6 min. Such data is reviewed to determine width ***W*** at times of arc max ***C*** on arcs of 0.5 km (2.25 min), 1 km (4.15 min) and 2 km (7.4 min). Colored dots on arcs are sampler locations.



Models being compared

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

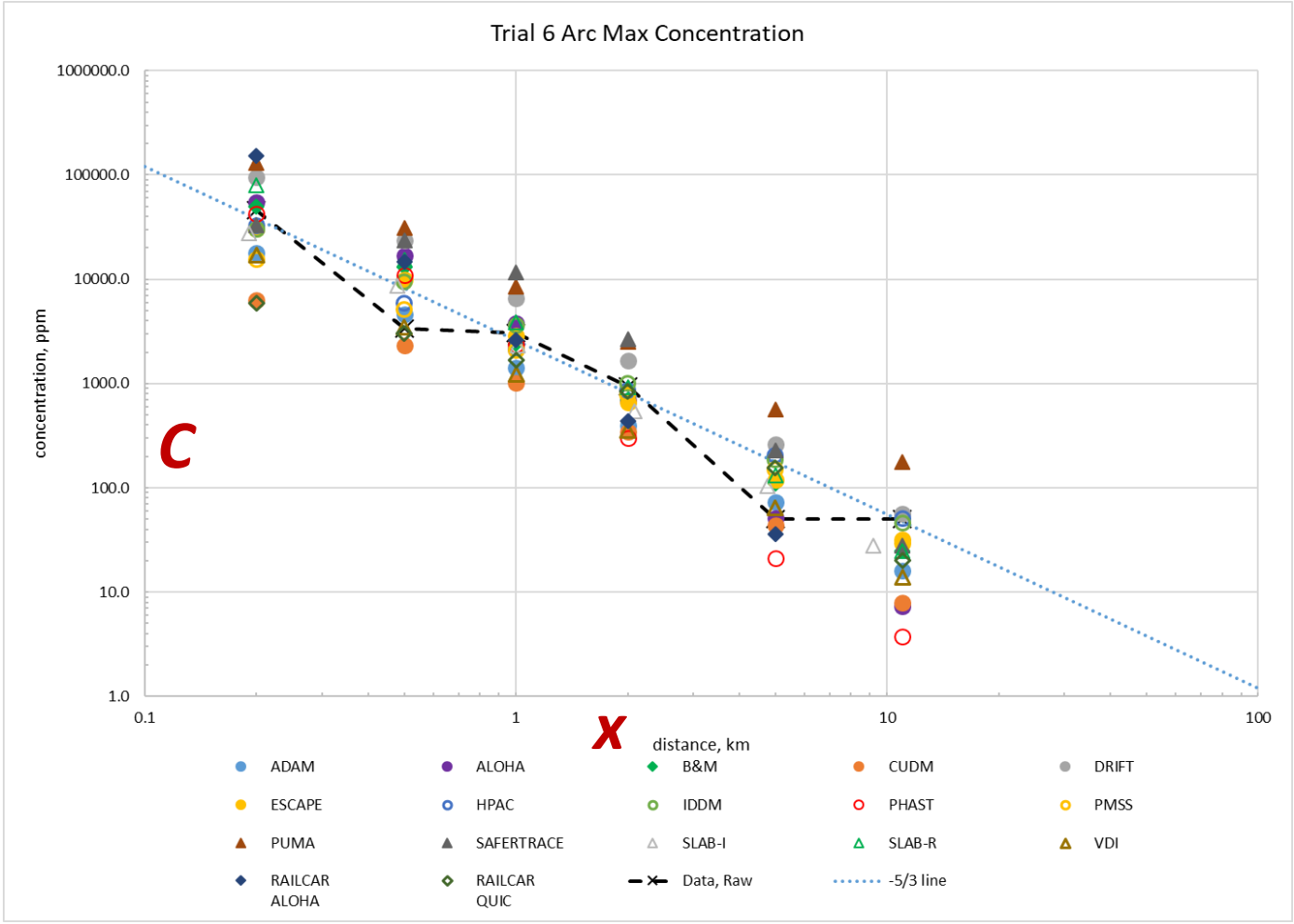
Materials sent to modelers for comparison exercise

- Our recommendations for emissions and meteorology inputs
- Source, sampler, CONEX, and meteorological measurement locations.
- The comprehensive JR II data archive, which also contains concentration observations, is available on request.
- Modelers were allowed to modify the provided inputs

Model comparison methods

- This is not a horse race. We want every model to be a winner
- Plots (***C***, ***W***, and ***H*** vs ***x*** for all models) reveal patterns and degree of agreement with observations.
- Tallies are made of numbers of times that the modeled value is within a factor of two of the observed value, and larger and smaller.
- The BOOT model evaluation software is applied.

Arc max *C* vs *x* plot for trial 6, for all 17 models, for the observations (dashed line), and showing a -5/3 line best fit to the unsaturated data



Conclusions from $C(x)$ plots for Trials 1, 6, and 7

- For any trial and any $\boldsymbol{x}$, the range of model predictions is about 1 to 1 ½ orders of magnitude
- The scatter is slightly larger for Trial 1, which may be due to the influence of the CONEX array
- The observed $\boldsymbol{C(x)}$ values are always inside the range of the predictions

Summary of BOOT calculations of performance measures for arc max C for trials 1, 6, and 7

- In general the 17 models' arc max **C** predictions are within FAC2 about half of the time. There are about as many over as under. Models with more within FAC2 are ESCAPE, HPAC, and IDDM.
- A few models tended to overpredict and others tended to underpredict over all three trials.
- Some models did well on two trials and not as well on the other trial
- Although most models' bias did not vary with ***x***, some models showed a variation in bias with ***x***.

Significant difference between models?

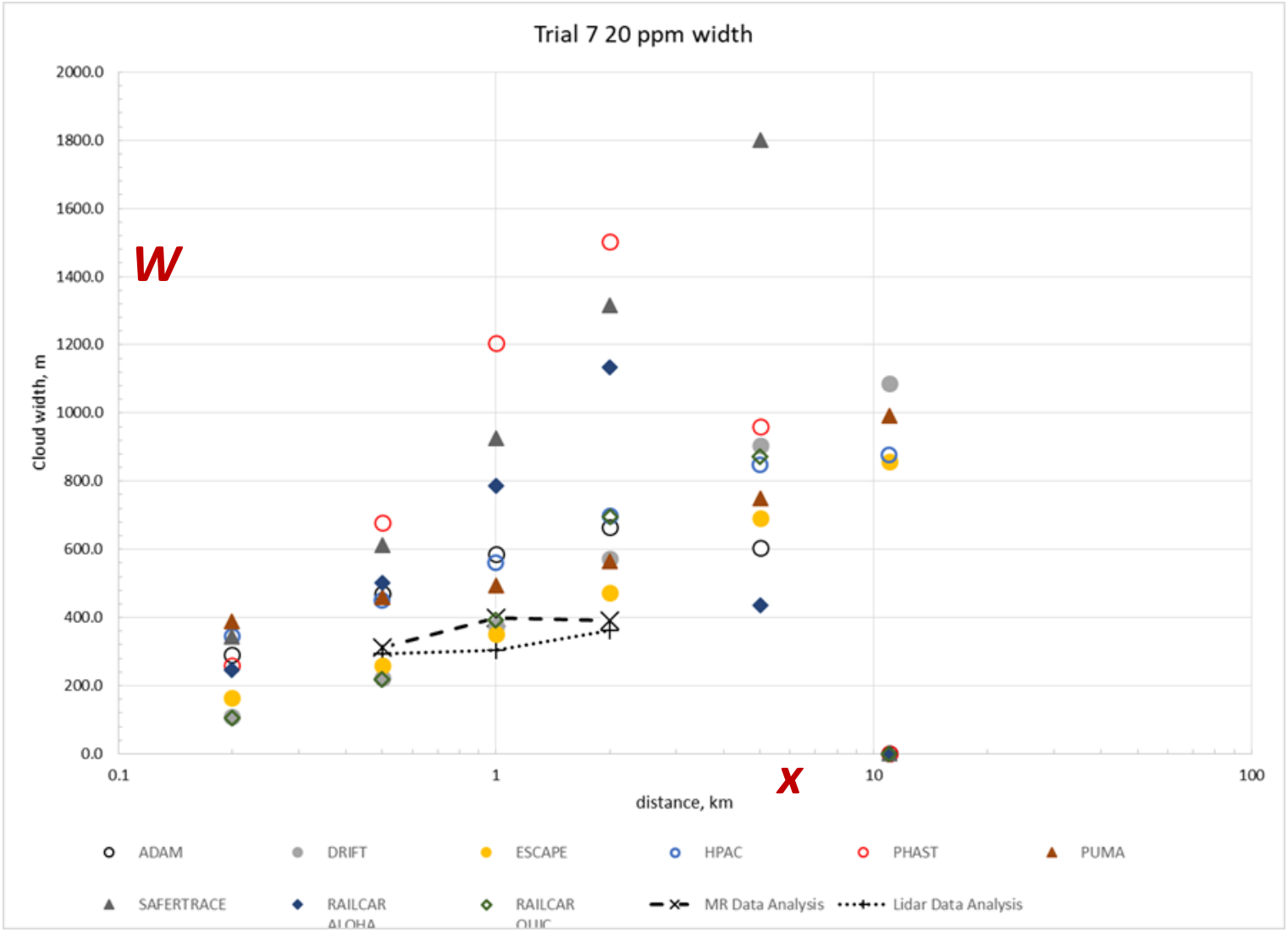
- The BOOT results for arc max ***C*** show that there is no significant difference in the geometric mean (MG) for the three top performing models.
- Therefore no one model is performing significantly better than another.
- In a few cases, a model is intending for its predictions to be “conservative” (i.e., to better assure protection of the public)

Comparisons of modeled and observed cloud widths *W* and heights *H*

- Focus on arcs at 0.5, 1 and 2 km
- Separate plots for ***C*** = 20 and 200 ppm contours
- Sometimes observations are from fixed samplers (usually MiniRaes), and sometimes they are from lidar.

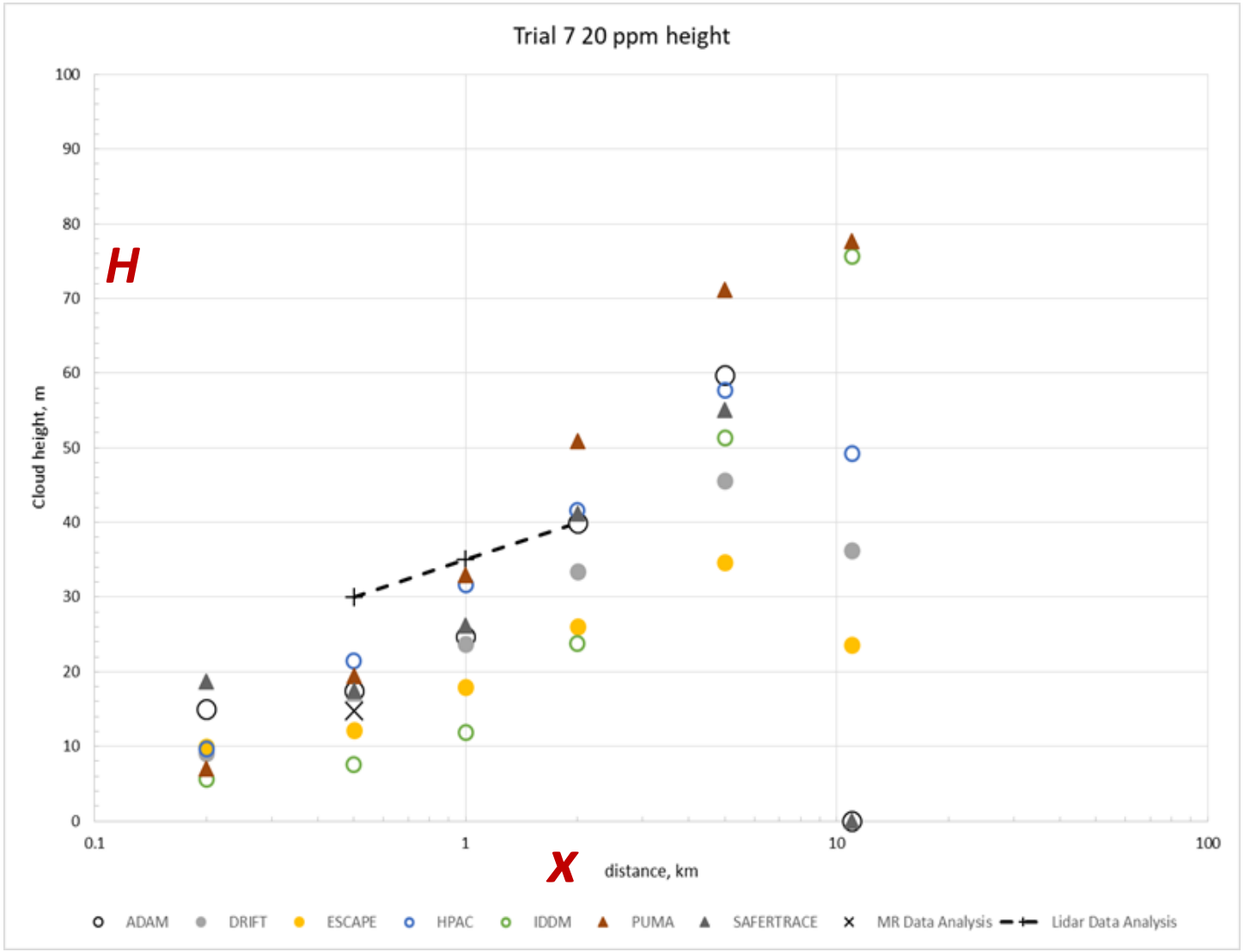
Comparison of modeled and observed cloud widths *W* (to 20 ppm) for trial 7

MiniRae obs are **X**; Lidar obs are **+**



Comparison of modeled and observed cloud heights *H* (to 20 ppm) for trial 7.

MiniRae obs are **+**; Lidar obs are **X**

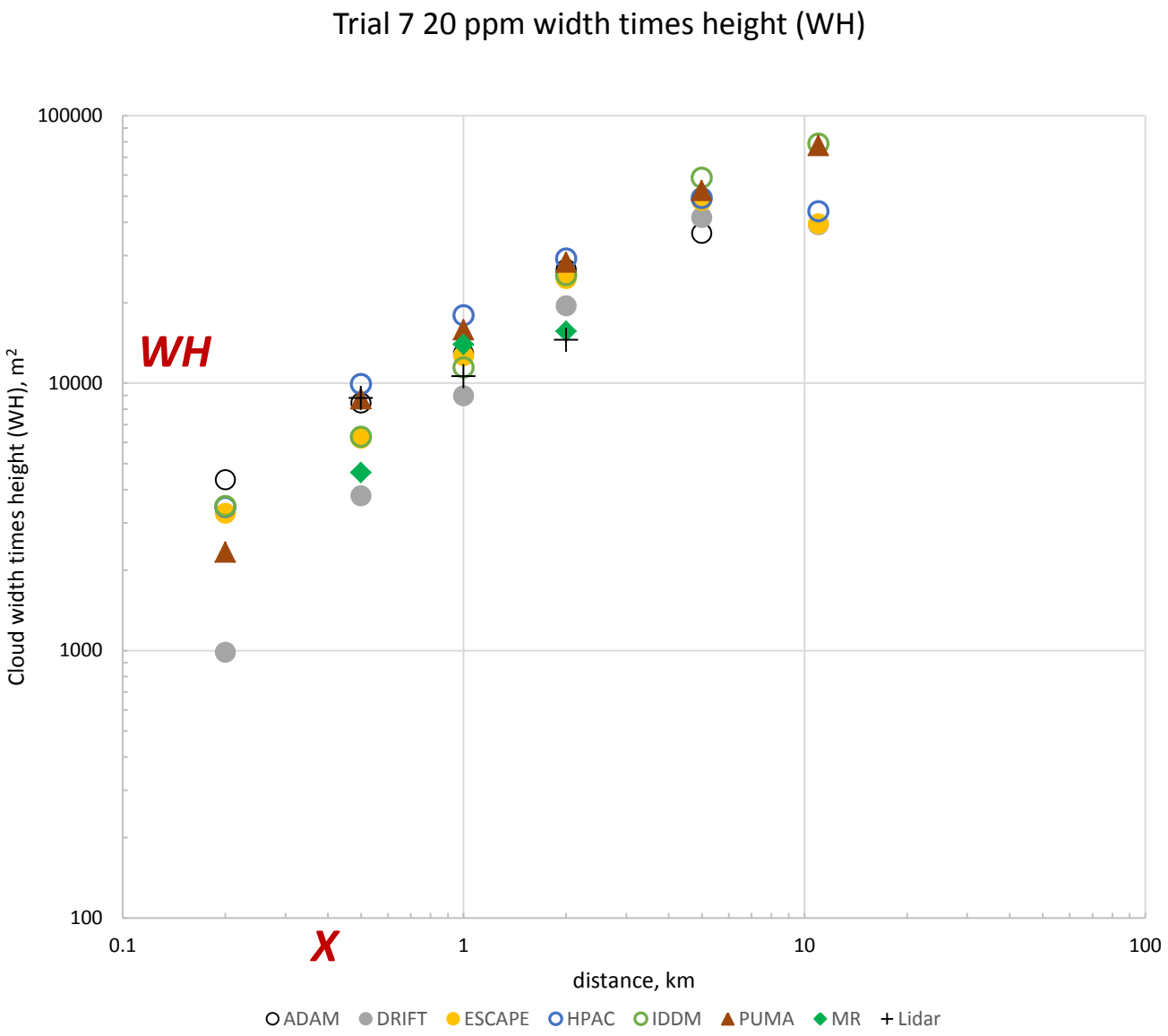


WH vs *x* plots

- On average, the models tend to over-predict cloud width ***W*** and underpredict cloud height ***H***.
- However the model predictions of arc max ***C*** have little mean bias, on average
- Knowing that the crosswind area of the cloud is proportional to ***WH***, and ***C*** is roughly inversely proportional to ***WH***, we plot ***WH*** vs ***x***.

Modeled vs observed *WH* for 20 ppm Trial 7

MiniRae obs are green diamonds; Lidar obs are **+**



Results of *WH* vs *x* plots

- On average, the models are unbiased in the ***WH*** (cloud cross-section area) comparisons.
- Obs available only at ***x*** = 0.5, 1, and 2 km.
- HPAC and DRIFT do fairly well in arc max ***C*** comparisons, but HPAC overpredicts ***WH*** and DRIFT underpredicts.
- Conclude that different models assume different cross-wind shapes.
- The spread in ***WH*** among all the models at a given ***x*** is less than that for arc max ***C***.

Caveats

- Observations of arc max ***C*** and width ***W*** and height ***H*** are close to instantaneous.
- ***W*** and ***H*** are determined at the time that the arc max ***C*** passes a sampling arc. At large ***x***, ***W*** and ***H*** go to zero since arc max ***C*** becomes < 20 or 200 ppm.
- As an alternate definition, instead of determining ***W*** as width to 20 or 200 ppm contours, we define ***W*** as the width from edge to edge as defined by 0.1 C_o where C_o is the centerline (arc max) ***C***.

Next steps

- A special issue of ***Atmospheric Environment*** on the **JR II** model comparison has been organized. Manuscripts will be submitted starting 1 Nov and ending 1 Feb. So far, 15 papers are planned.
- Time series of ***C*** are produced by the fixed samplers. These allow key timing information to be estimated such as time after release at which max ***C*** is observed.
- Add the other six trials to the analysis (some have variable winds; Trial 8 is a vertical jet followed by a liquid "dump" with pool evaporation).