Jack Rabbit II Inter-model Comparison Exercise

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Outlines

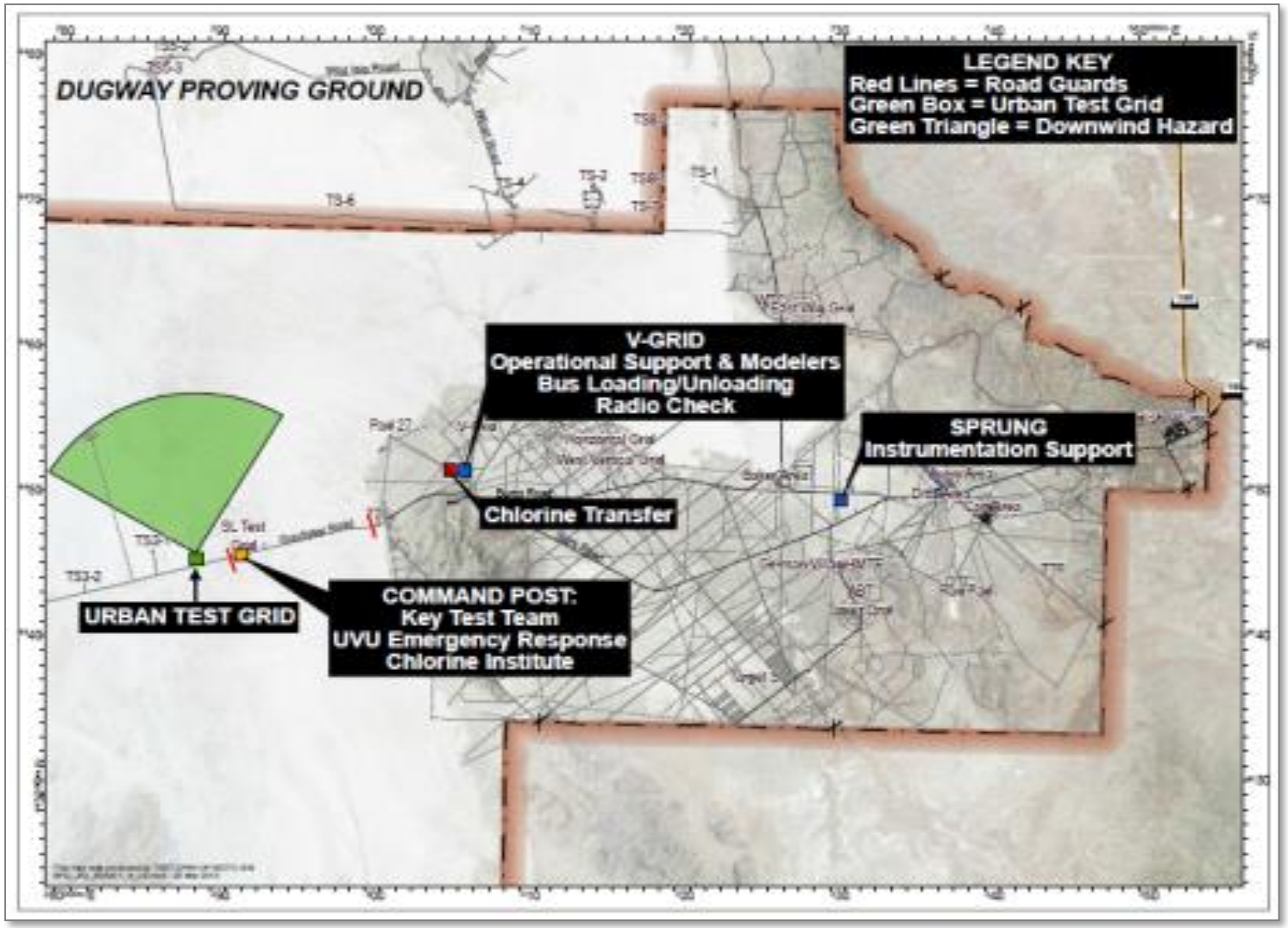
- Jack Rabbit II (JR II) introduction
- Inter-model comparison protocols and participants
- Comparisons of arc max concentrations
- Comparisons of cloud widths and heights
- Conclusions and next steps

Jack Rabbit – Context & Research Questions

- Many accidental releases of toxic industrial chemicals occurred (e.g., Festus, MO; Macdona, TX; Graniteville, SC)
- Maximum casualties < 10, but model predictions often much higher
- Are models wrong, or do we run models wrong?
- Do first responders have enough guidance in responding to such incidents? Is equipment still effective in a chlorine cloud?

Jack Rabbit II Test Site

- Dugway Proving Ground, Utah
  - Flat salt playa
- Five trials in 2015
  - With mock urban array
- Four trials in 2016
  - Without mock urban array



Source: Dugway Proving Ground

2015 JR II

With CONEX Container Array

All five trials 90°downward

Source: Dugway Proving Ground

2016 JR II

Without CONEX Container Array

Trial 6:
90°downward

Trial 7:
45° downward

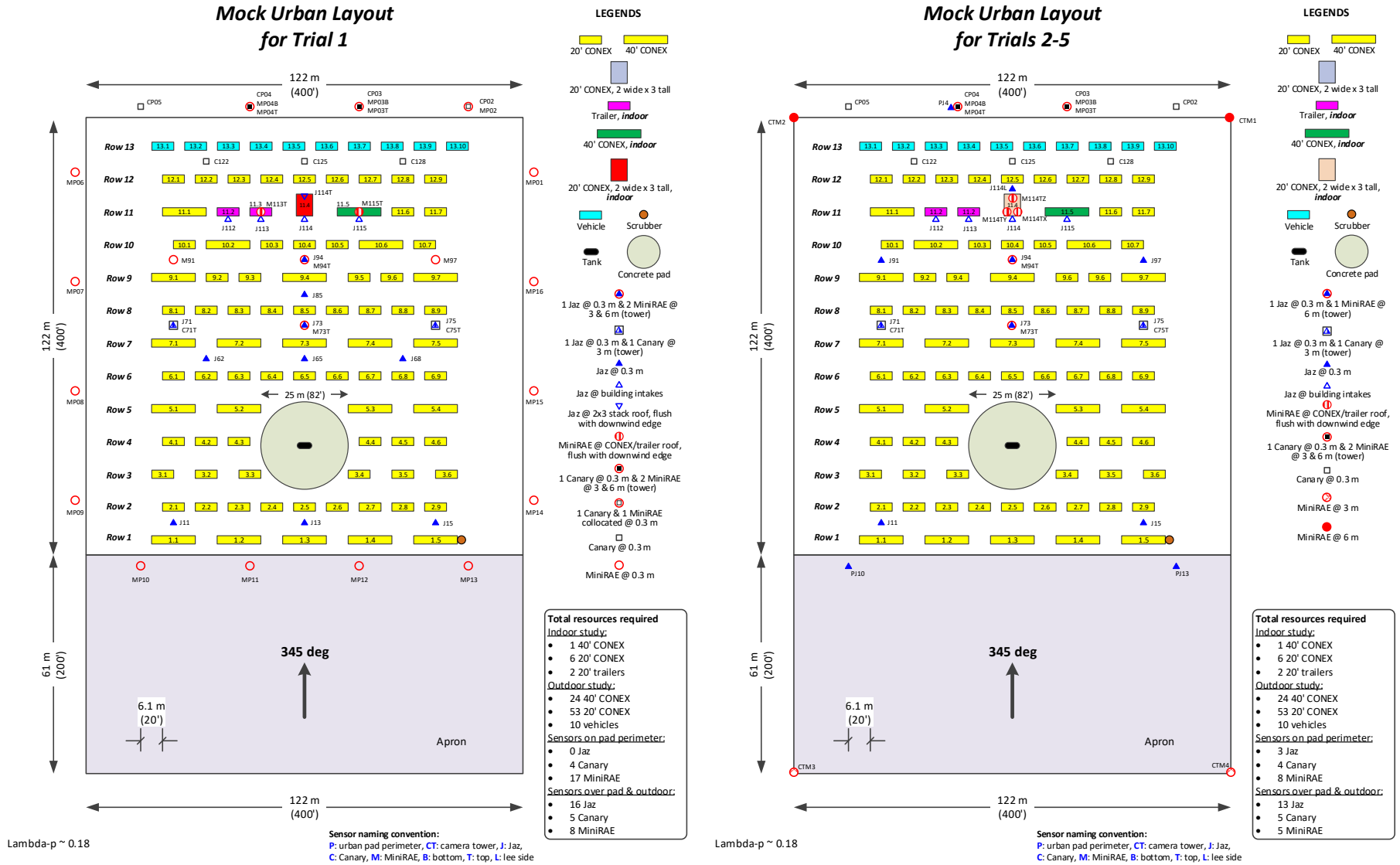
Trial 8:
90°upward

Trial 9:
90° downward

Source: Utah Valley University

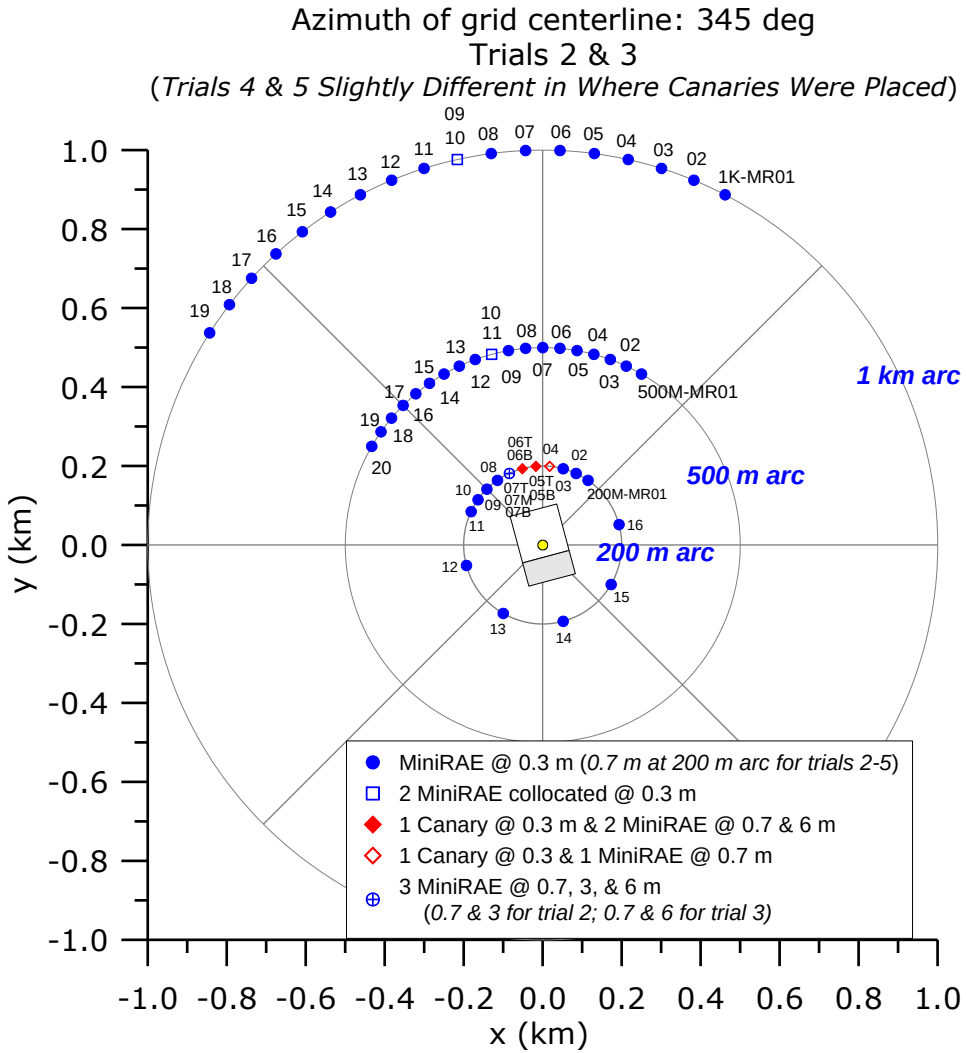
2015 JR II Sensor Layout, Mock Urban Pad

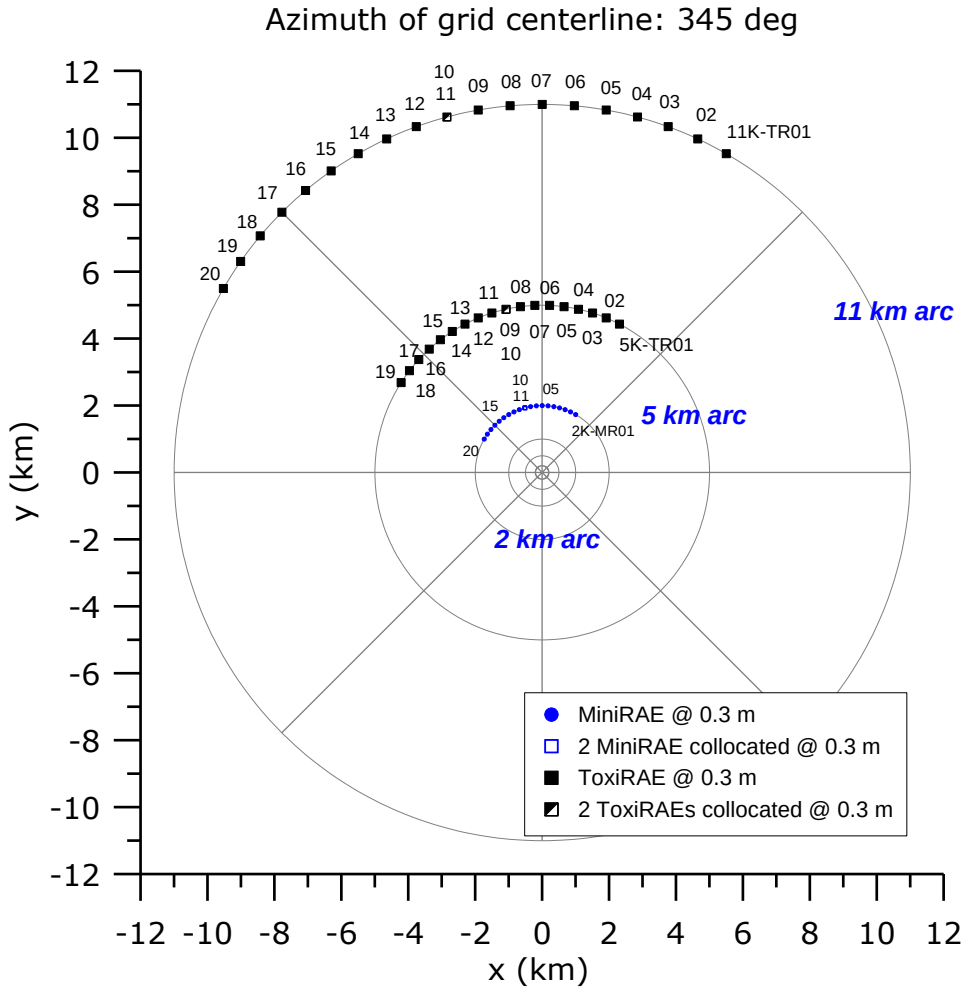
- CONEX array meticulously placed to mimic urban conditions



λ_p=ratio of plan area to lot area

2015 JR II Sensor Layout, Downwind Arcs



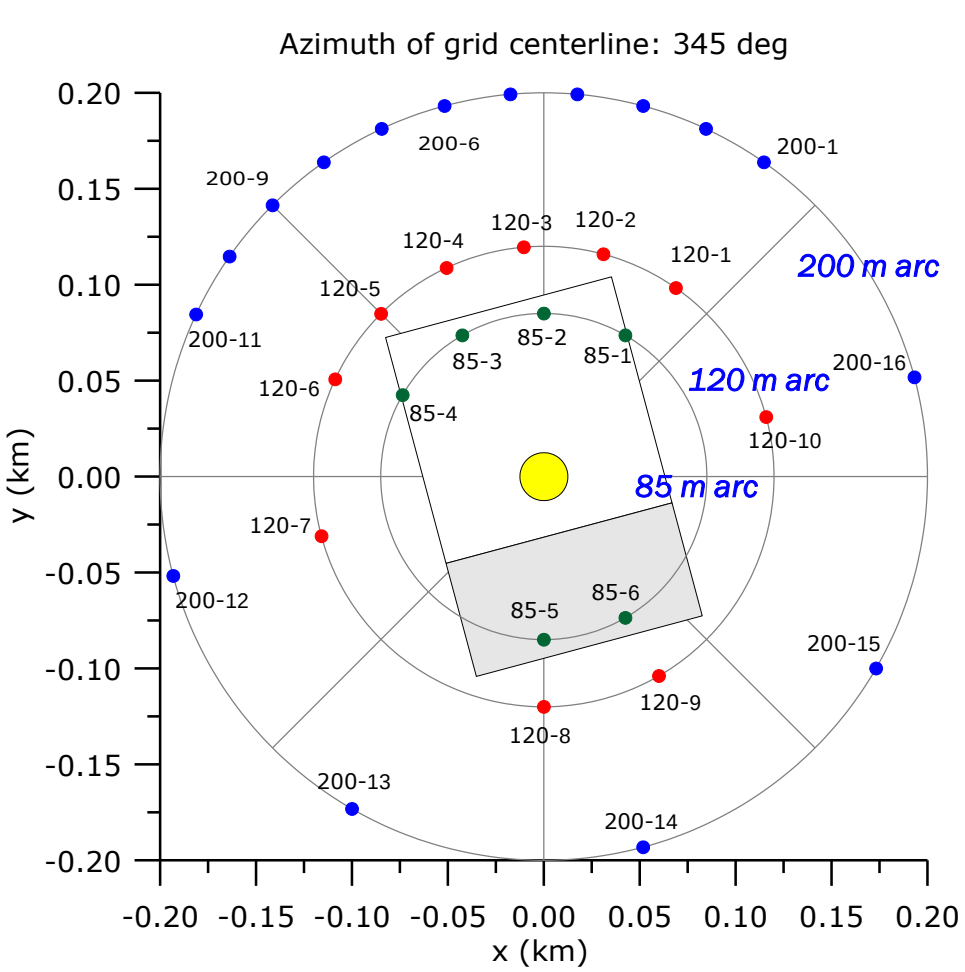


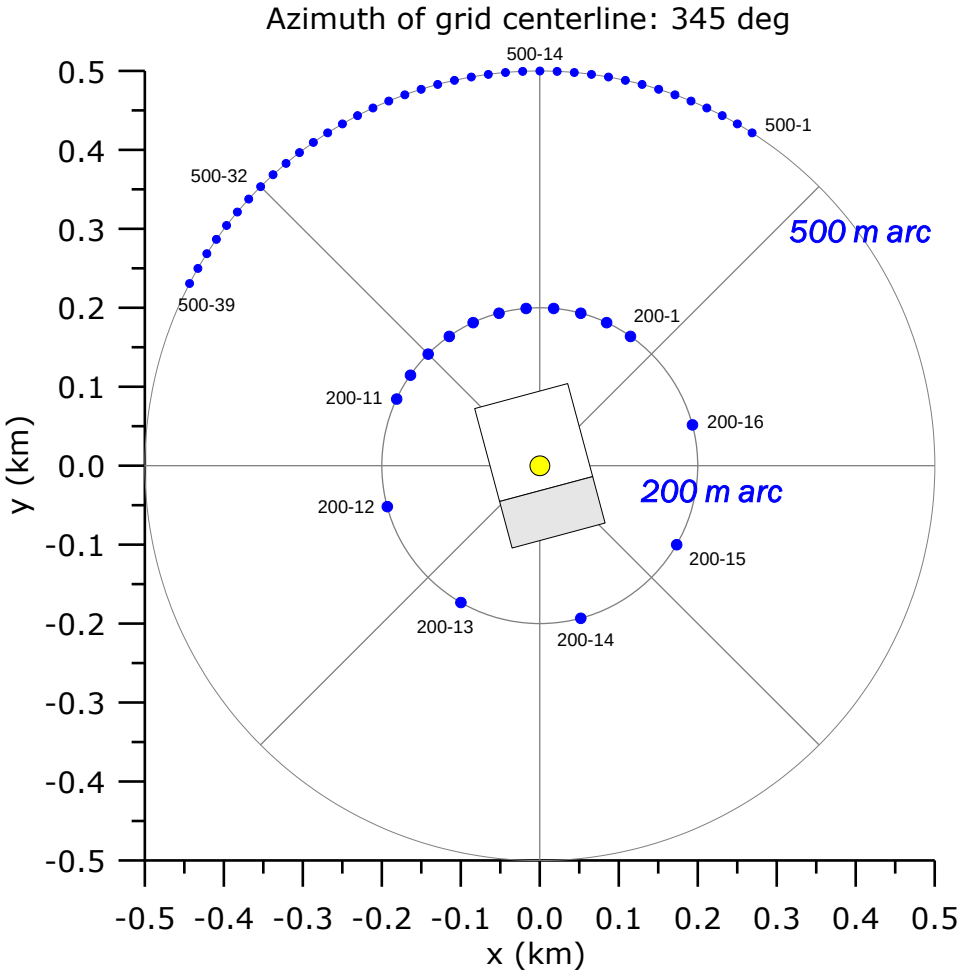
- Four types of point sensors with different dynamic ranges (before calibration)
  - Jaz: 1,000-100,000 ppmv
  - Canary: 100-10,000 ppmv
  - MiniRAE: 10-2,000 ppmv
  - ToxiRAE: 1-50 ppmv

Lidars, stand-off instruments, also deployed

Generic 2016 JR II Sensor Layout, Close-in Arcs

(Actual Sensor Allocation Depends on Trial)

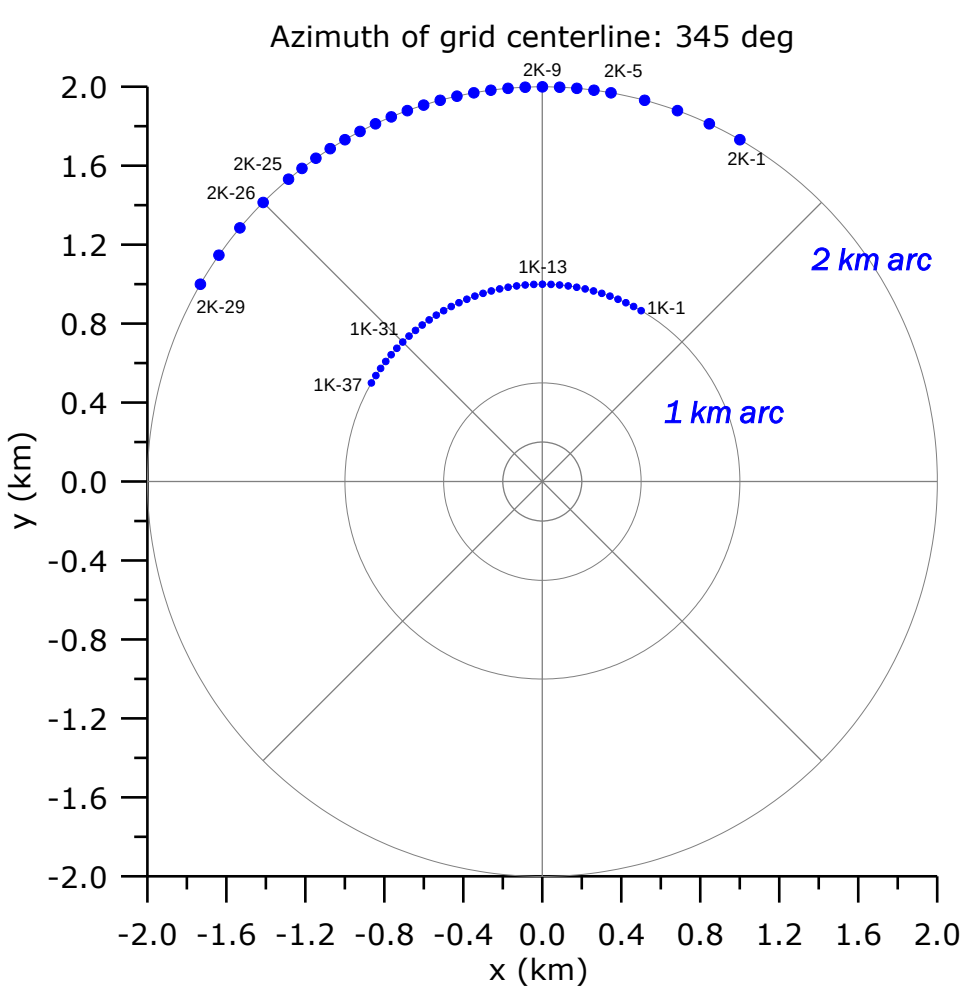


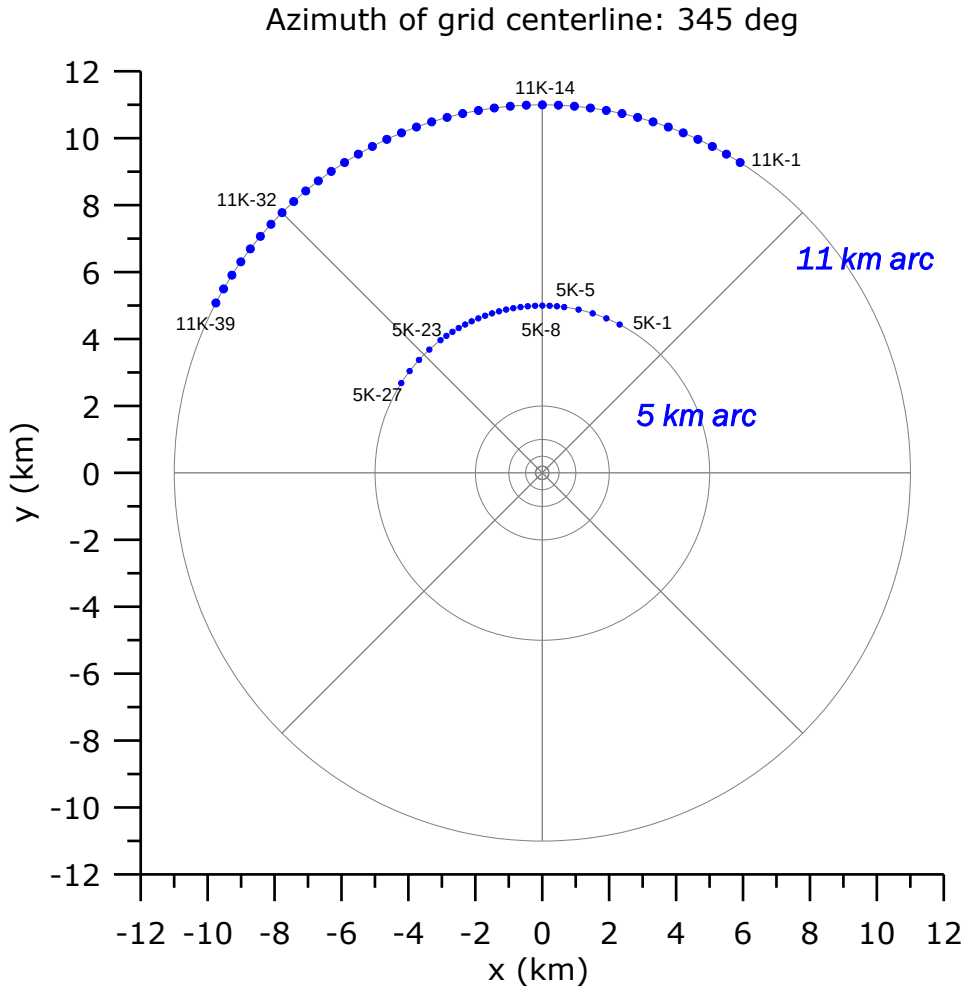


Lidars, stand-off instruments, also deployed

Generic 2016 JR II Sensor Layout, Far-away Arcs

(Actual Sensor Allocation Depends on Trial)





Lidars, stand-off instruments, also deployed

Inter-model Comparison Protocols

- Three trials
  - 1 (90° downward), 6 (90° downward), and 7 (45° downward)
  - Exclude sensors on mock urban pad and close-in arcs (85 and 120 m)
- Recommended standard model inputs
  - Source configuration, emissions, surface roughness, CONEX positions, meteorology (profiles), boundary layer parameters (heat flux, friction velocity, Obukhov length, stability, etc.)
  - Participants allowed to modify inputs (e.g., run own source emission model)
- Model outputs requested
  - Arc max concentrations (C) at distance (x) = 0.2, 0.5, 1, 2, 5, and 11 km
  - Cloud widths (W) and heights (H) to 200 and 20 ppmv at 0.5, 1, and 2 km
  - Contour plots at various times after release
  - C time series at sensor locations
- ***Exercise not a competition, but in spirit of collaboration to improve quality of modeling tools***

17 Models

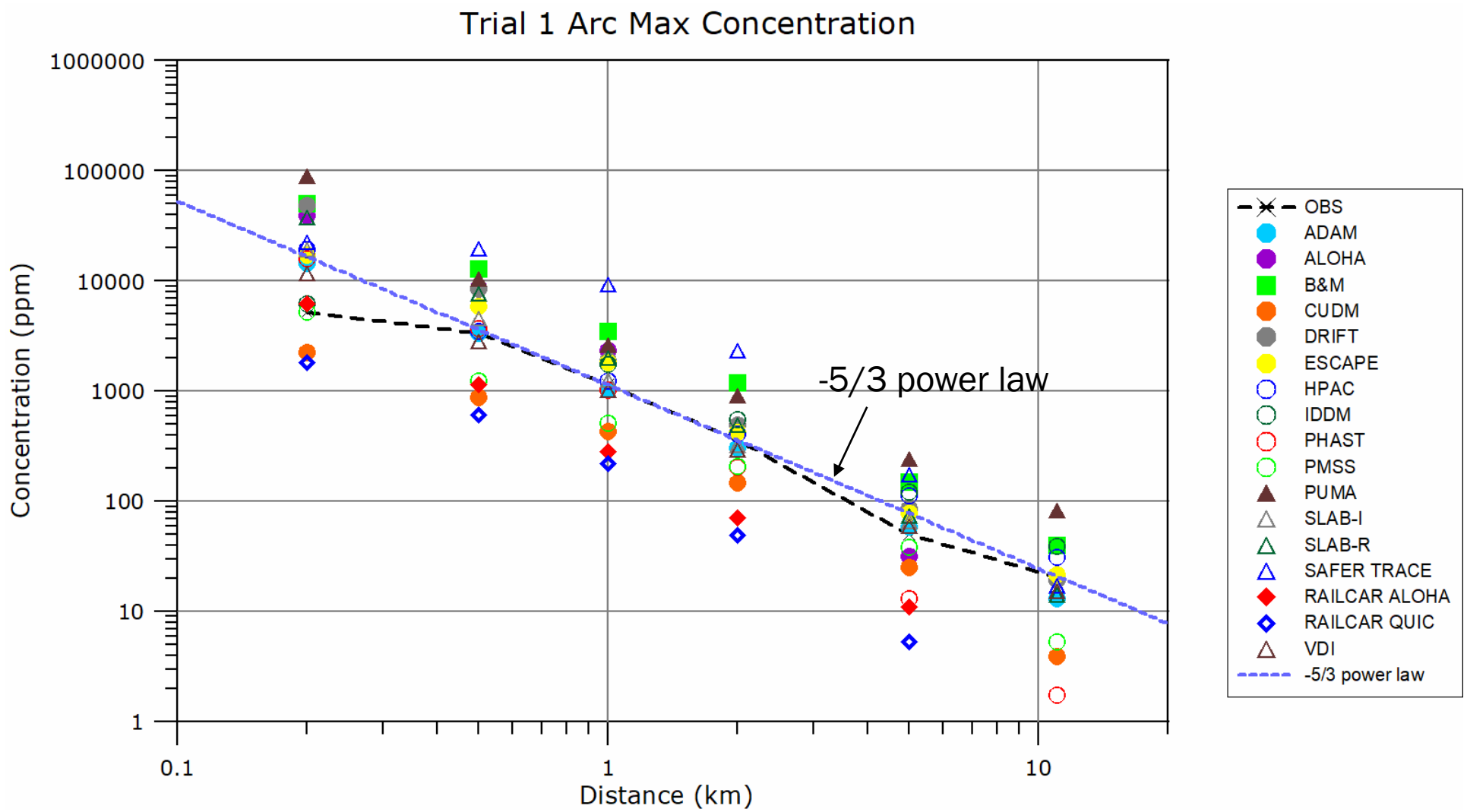
- Most models do not directly treat some specific JR II phenomena, e.g.,
  - Obstacle array
  - 90° or 45° downward pointing jets hitting ground
- But these effects should dissipate farther downwind

Model(s)	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

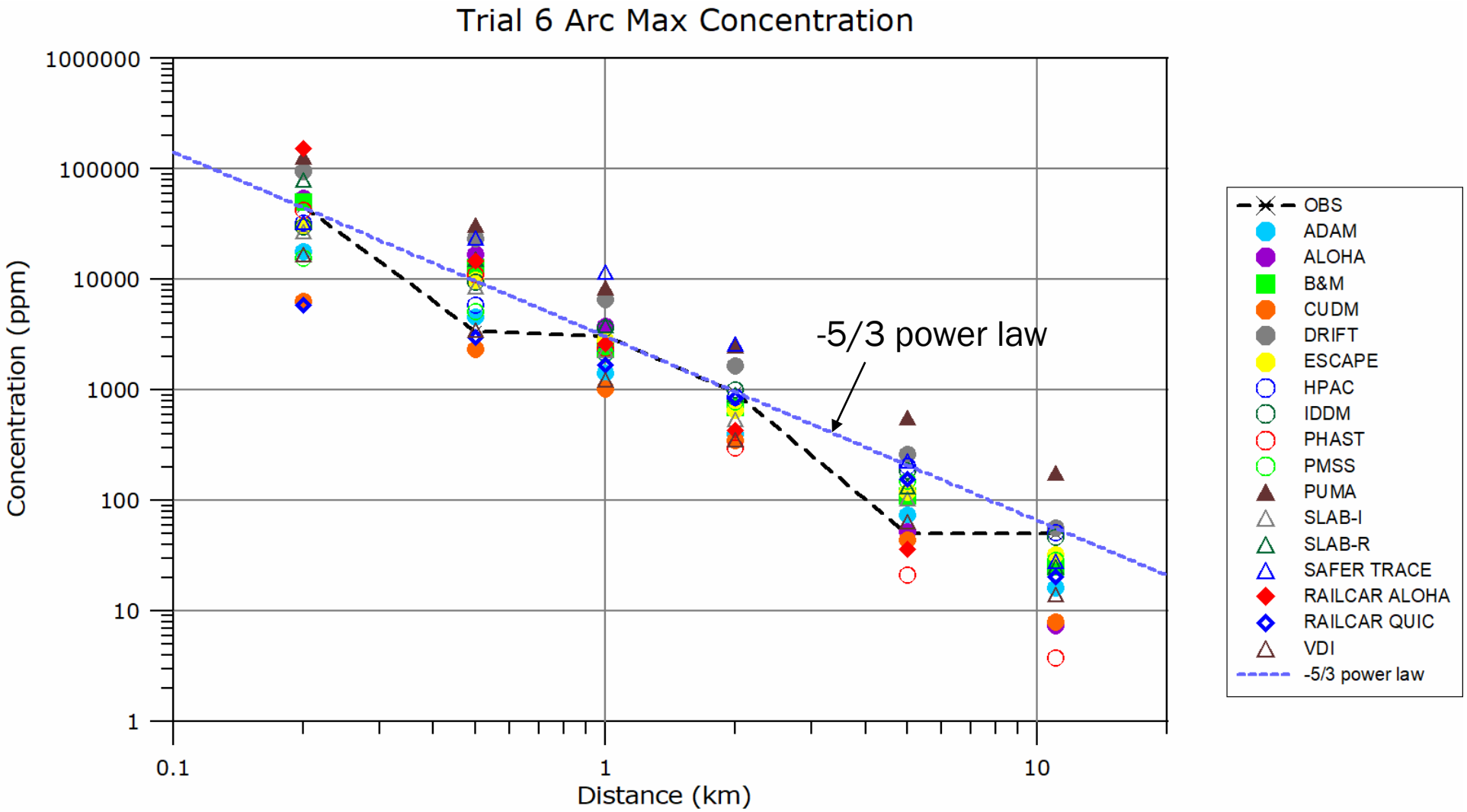
Arc Max *C* Observations

- 1 to 3-s basic averaging time (resolution) of sensors used
- QA/QC'ed and calibrated based on test gases
- Some (6 out of 18) sensors reported arc max *C* saturated, so actual *C* likely > reported
  - MiniRAE readings in Trials 1 and 6 at 0.5 km saturated at ~3,300 ppmv
  - ToxiRAE readings of 50 ppmv at 5 or 11 km saturated
  - Saturated data retained in model comparison

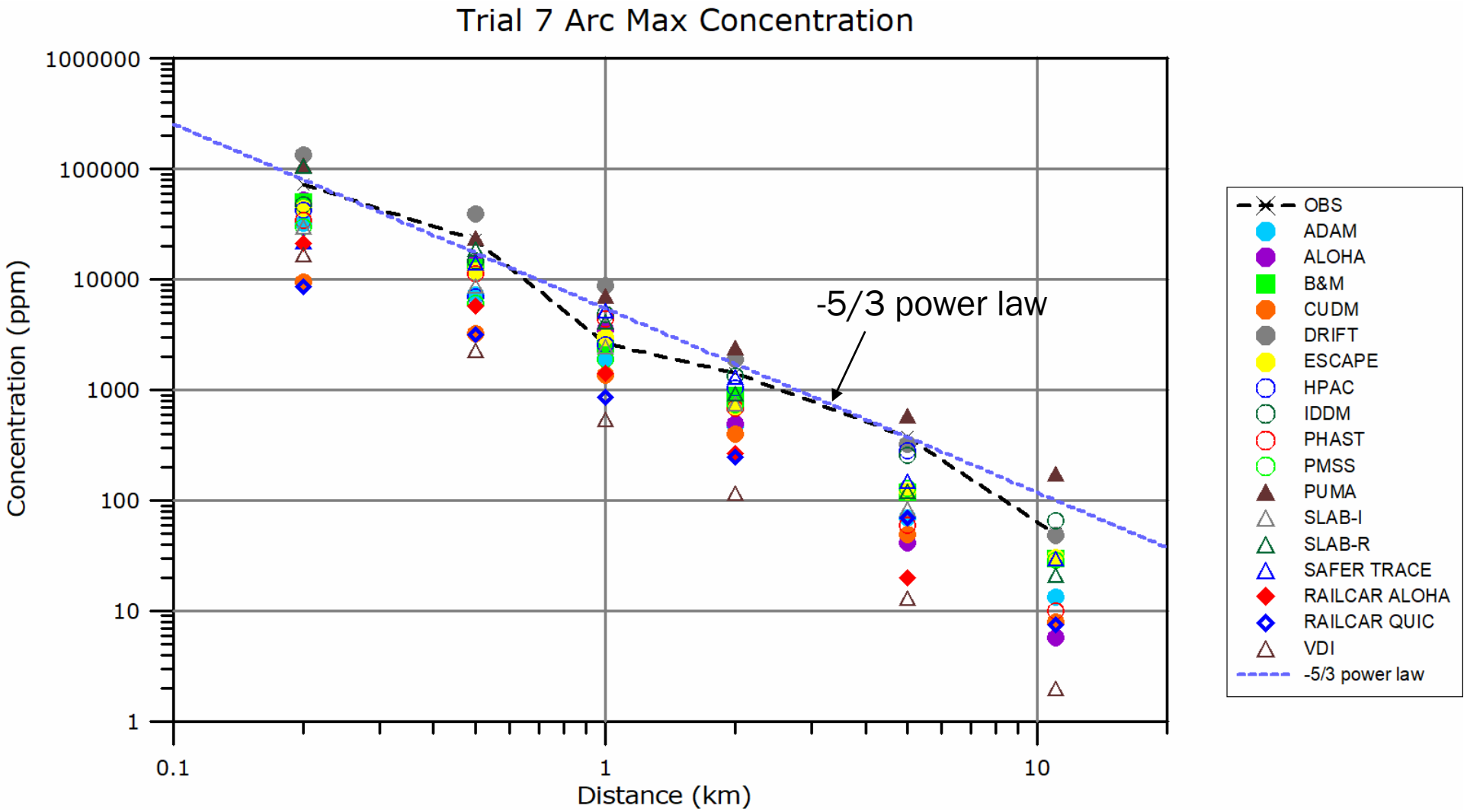
Trial 1 – Arc Max *C*



Trial 6 – Arc Max *C*



Trial 7 – Arc Max *C*



Results of $C(x)$ Plots

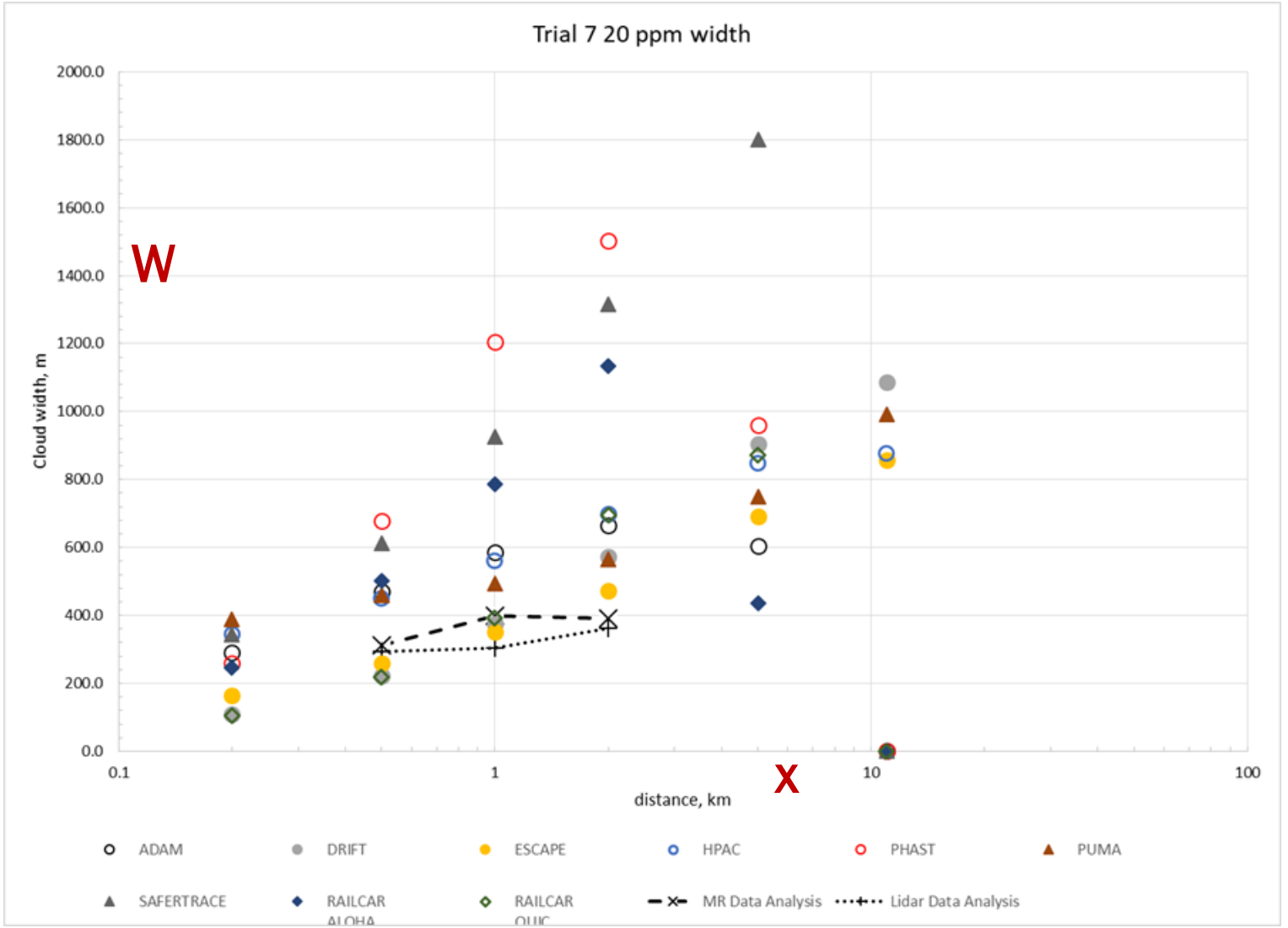
- For any trial and any x, range of model predictions about 1 to 1½ orders of magnitude
- Scatter slightly larger for Trial 1, which may be due to influence of CONEX array
  - Many models do not treat obstacle array
- Observations always inside range of model predictions
  - More models overpredicted Trial 1 at 200 m, possibly due to difficulty for models to model sharp concentration decrease from urban pad to 200 m arc
  - More models underpredicted Trial 7, possibly due to 45° rather than 90° downward release (larger impact anticipated for 45° release)
- ***Observations and predictions closely follow $x^{-5/3}$ power law***
- See backup slides for detailed results of statistical evaluation

Comparison of Cloud Widths *W* and Heights *H*

- Focus on 0.5, 1 and 2 km arcs
- Focus on *W* and *H* to 20 and 200 ppmv
- *W* and *H* observations from combination of
  - Fixed sensors (usually MiniRAEs)
  - Lidars
- Generally more difficult to estimate *W* and *H* from observations due to limited observations

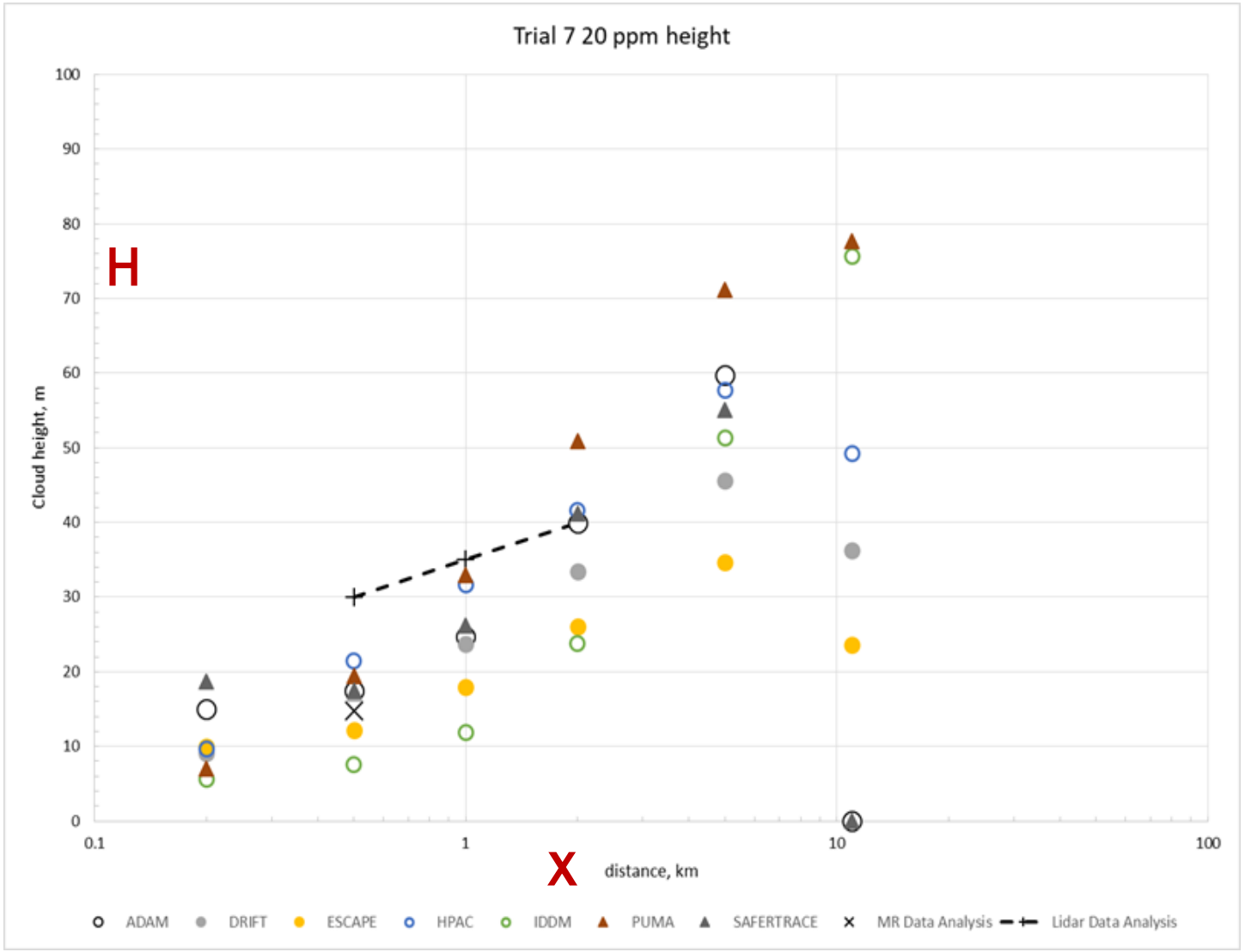
Modeled and Observed *W* to 20 ppmv for Trial 7

- x: MiniRAE observations
- +: Lidar observations



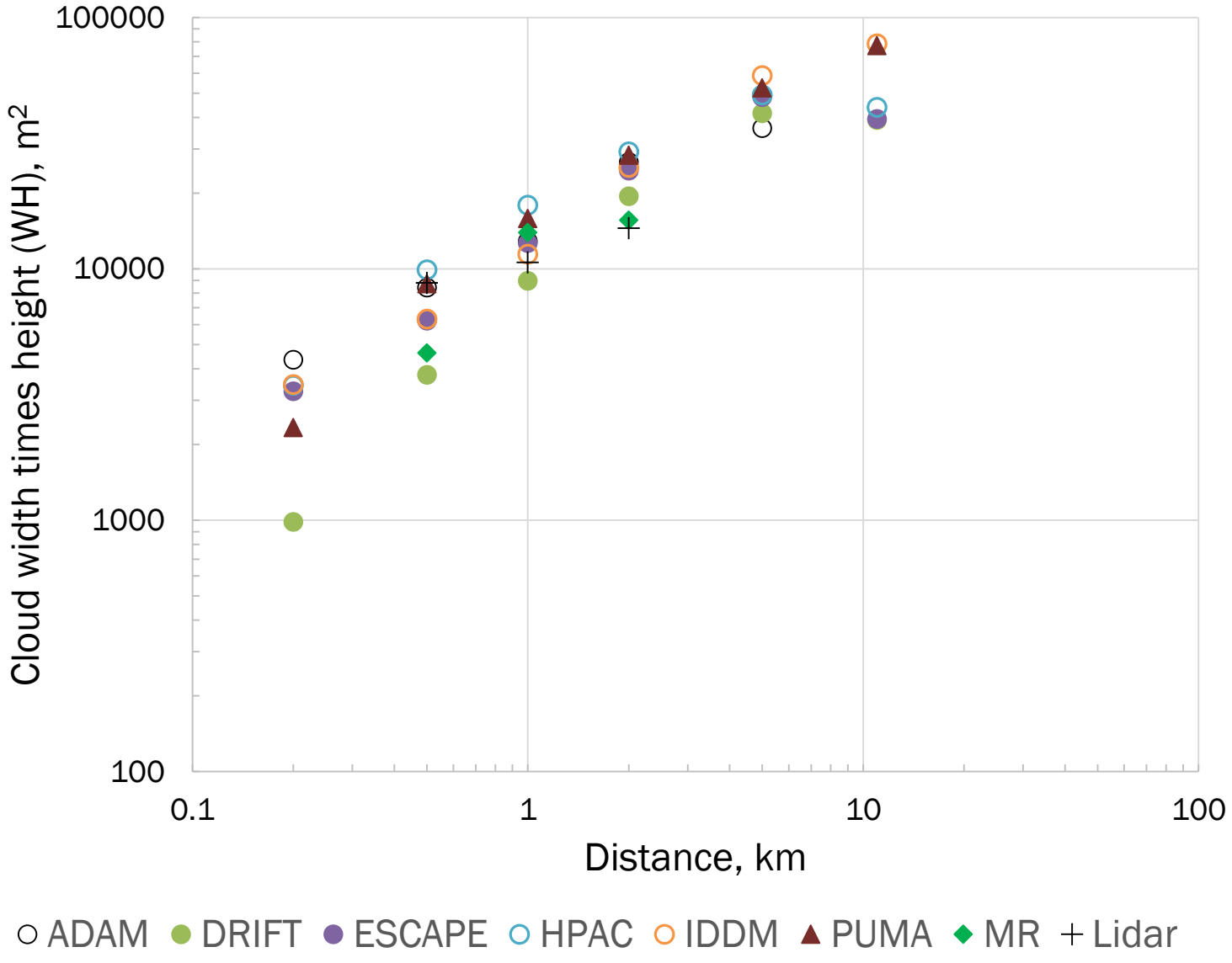
Modeled and Observed *H* to 20 ppmv for Trial 7

- x: MiniRAE observations
- +: Lidar observations



Modeled and Observed *WH* for 20 ppmv for Trial 7

- Green diamonds: MiniRAE observations
- +: Lidar observations



Results of *WH* Plots

- On average, models overpredict *W*, underpredict *H*, but unbiased for *WH* (cloud cross-sectional area)
- Caveats
  - Observations of arc max *C*, *W* and *H* close to instantaneous
  - *W* and *H* are determined at the time when arc max *C* passes a sampling arc
  - At large *x*, *W* and *H* go to zero since arc max *C* becomes < 20 or 200 ppmv

Conclusions

- Arc max concentrations:
  - Model predictions span ~1 to 1½ orders of magnitude
  - Observations always inside range of predictions
  - Observations and predictions closely follow $x^{-5/3}$ power law
- Models generally overpredict width, underpredict height, but unbiased for cloud cross-sectional area
- So, dispersion model predictions generally OK
- However,
  - Source terms for actual accidents often not well known
  - Deposition of chemicals on surfaces still unclear, and can play an important role
  - Health effects highly uncertain (even when models do a good job in predicting concentrations)

Next Steps

- Add the other six trials
  - Some have variable winds
  - Trial 8 is an upward vertical jet followed by a liquid “dump” with pool evaporation – in fact two releases
- A special issue of *Atmospheric Environment* on JR II model comparison organized
- *C* time series produced at fixed sensors, allowing key timing information to be estimated such as time after release at which max *C* is observed

Questions?

Backup Slides

Model Comparison Participants

- Modeling Working Group (MWG) was established for JR II planning and analysis in 2012-2018
- Most modelers in comparison exercise were on MWG, which had biweekly conference calls
- Several modelers ran test cases to assist in planning field experiment and saw JR II data
- Other modelers had not seen JR II data
- So, not all modelers are on equal footing
- ***Exercise not a competition, but in spirit of collaboration to improve quality of modeling tools***

Basic Characteristics of JR II Trials

Trial	Date	Start Time	End Time	Release Duration	Average Emission Rate	Jet or Pool Mass	Wind Speed Near Source at z = 2 m	Temp Near Source
	(MDT)	(MDT)	(MDT)	(s)	(kg/s)	(kg)	(m/s)	(C)
1	8/24/2015	7:35:46	7:36:44	20.3	224.0	4,547	1.5	17.5
2	8/28/2015	9:24:21	9:25:10	32.4	252.8	8,192	4.7	23.0
3	8/29/2015	7:56:55	7:57:31	20.3	225.0	4,568	3.8	22.9
4	9/1/2015	8:39:33	8:40:16	28.8	243.6	7,017	1.8	22.6
5	9/3/2015	7:29:09	7:29:59	33.6	248.4	8,346	1.5	21.5
6	8/31/2016	8:23:35	8:24:10	32.2	260.0	8,372	2.4	22.3
7	9/2/2016	7:56:00	7:56:35	33.3	259.0	8,625	4.0	18.7
8	9/11/2016	9:01:45	9:02:45	30.0	78.93	2,368	2.1	15.8
9	9/17/2016	8:05:00	8:08:00	132.6	133.5	17,700	2.6	11.2
7 dump	9/2/2016	8:11:00	8:16:00	300	1.507	452	4.0	18.7
8 dump	9/11/2016	9:16:45	9:21:00	300	22.51	6,754	2.9	15.8

- All trials pointed vertically downward, except for
  - Trial 7, 45° downward from horizontal
  - Trial 8, vertically upward
- Emission estimates still subject to change
- Trials 7 and 8 further include secondary liquid dump

Recommended Source Configuration and Weather Inputs

	Trial 1	Trial 6	Trial 7*
Release Parameters			
Location, all at Dugway Proving Grounds; Zone 12 UTM coordinates	Northing 4445633.9 m Easting 288109.2 m Elevation 1295.5 m	Northing 4445633.9 m Easting 288109.2 m Elevation 1295.5 m	Northing 4445633.9 m Easting 288109.2 m Elevation 1295.5 m
Date and Time (hh:mm:ss UTC)	24 August 2015 13:35:45	31 August 2016 14:23:35	2 September 2016 13:56:00
Tank Inventory (kg of Cl2)	4500	8400	9100
Pressure measured at top of tank (psia)[1]	104.4	86.8	86.9
Liquid temperature (C)[1]	15.7	16.0	15.9
Release jet orientation (deg from tank top center)	180	180	135
Release height (m)	1.0	1.0	1.48
Hole diameter	6.0 in = 0.152 m	6.0 in = 0.152 m	6.0 in = 0.152 m
Weather/Environment			
Atmospheric pressure (mbar)	873.7	871.1	868.5
Initial wind speed[2] (m/s) at z = 2 m	1.45	2.42	3.98
Initial wind direction[2] at z = 2 m	147.4	146.9	149.6
Initial temperature (C) at z = 2 m	17.5	22.3	18.7
Surface roughness (mm)	0.5	0.5	0.5
Friction velocity[3], u* (m/s)	0.108	0.093	0.210
Sensible heat flux[3], Hs, (K-m/s)	-0.012	-0.0034	-0.0160
Inverse Monin-Obukhov length (m^{-1})	0.068[4]	0.056	0.0229
Pasquill Class[5]	E/F	E	D/E

See notes page for footnotes

Recommended Averaged Source Emission Rates

	Trial 1	Trial 6	Trial 7
Primary release			
Discharge rate (kg/s)	224.	260.	259
Discharge period (s)	20.3	32.2	33.3
Temperature (C)	-37.3	-37.4	-37.4
Vapor fraction (ignoring KE effects)	0.171	0.172	0.172
Density (kg/m^3)	18.32	18.15	18.12
Velocity (m/s)	50.8	44.2	44.2
Area (m^2)	0.241	0.324	0.323
Primary release modified for rainout			
Discharge rate (kg/s)	145	168	162
Discharge period (s)	20.4	32.4	33.6
Temperature (C)	-37.3	-37.4	-37.4
Vapor fraction (ignoring KE effects)	0.264	0.266	0.274
Density (kg/m^3)	11.89	11.79	11.41
Velocity (m/s)	50.8	44.2	44.2
Area (m^2)	0.240	0.323	0.322
Evaporated rainout			
Discharge rate (kg/s)	43.2	34.0	34.0
Discharge period (s)	36.8	86.4	93.4
Temperature (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

Single constant release

Or

Primary release + secondary release due to rainout

Arc Max C Magnitudes Comparison

- The best fit $x^{-5/3}$ lines ($C = ax^{-5/3}$) have the following relations in magnitude:
  - C(Trial 6) = 0.48 C(Trial 7)
  - C(Trial 1) = 0.20 C (Trial 7)
  - C(Trial 1) = 0.42 C(Trial 6)
- The (Trial 1)/(Trial 6) C ratio (0.42) is close to the ratio of the total mass released (0.54)
- The (Trial 6)/(Trial 7) C ratio (0.48) is about half of the ratio of the total mass released (0.97).
- Trial 7 arc max C may be enhanced because of the 45° rather than 90° downward release (see photo of Trial 7)

Tabulation of Arc Max C

	Distance (km)	Observed	ADAM	ALOHA	B&M	CUDM	DRIFT	ESCAPE	HPAC	IDDM	PHAST	PMSS	PUMA	SLAB-I	SLAB-R	TRACE	RC/ALOHA	RC/QUIC	VDI
Trial 1	0.2	5203	14418	39200	50000	2250	48491	17330	19456	6152	16038	5242	88831	19100	37966	22576	6172	1813	11636
	0.5	**3348**	3335	8550	13000	871	8403	5909	3471	3669	3661	1246	10390	4530	7721	19528	1141	607	2832
	1	1137	1019	2310	3500	430	1899	1802	1248	1739	1011	511	2618	1270	2005	9269	284	222	1018
	2	357	305	420	1200	146	496	422	403	550	204	206	915	321	491	2351	71	49	293
	5	**50**	58	32	150	25	85	78	112	121	13	38	242	65	74	173	11	5	59
	11	20	13	n/a	40	4	19	22	31	39	2	5	83	n/a	14	17	n/a	n/a	15
Trial 6	0.2	46111	17867	54500	50000	6292	95150	30581	32350	30069	42714	15562	130000	27400	80062	32715	153424	5910	16874
	0.5	**3382**	4575	16900	13000	2333	23518	9880	5880	9423	10973	5128	31108	8660	15198	23715	14627	2994	3462
	1	3053	1407	3760	2400	1016	6594	2851	2141	3609	2354	2098	8452	2300	3833	11602	2605	1689	1227
	2	937	399	685	700	348	1648	658	852	998	302	785	2506	539	918	2639	435	840	352
	5	**50**	73	52	110	44	264	120	205	184	21	149	563	103	133	229	36	154	64
	11	**50**	16	7	25	8	57	32	51	46	4	29	177	28	25	28	n/a	20	14
Trial 7	0.2	72580	32368	52300	50000	9560	132908	44044	42459	47320	34153	30216	108480	29800	107047	22154	21290	8598	16823
	0.5	22686	7192	14100	13000	3230	38929	11833	6910	14713	11304	6044	23835	8750	18793	14110	5729	3138	2277
	1	2621	1923	3470	2600	1365	8694	3001	2576	4879	4418	1878	7163	2460	4185	5198	1417	861	537
	2	1417	471	497	900	396	1892	685	1042	1336	681	743	2428	750	925	1312	266	248	117
	5	373	69	41	120	49	321	122	282	257	60	128	586	83	121	149	20	69	13
	11	**50**	13	6	30	8	48	30	66	66	10	29	176	21	21	30	n/a	8	2

- Red numbers: saturated sensors
- Shaded shells: models did not generate results at 11 km

Performance Measures

For 5 Closest Arcs

	VG	MG	FA2	FA5
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	1.58	0.92	0.73	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

- VG: geometric variance
- MG: geometric mean bias
- FA2 and FA5: fraction of predictions within a factor 2 and 5 of observations
- Perfect model has VG, MG, FA2, and FA5 = 1.0
- ESCAPE, HPAC, and IDDM seem to have better performance

See backup slides for VG, MG, FA2, and FA5 definitions

Performance Measures

$$\mathrm{MG} = \exp\left(\overline{\ln C_o} - \overline{\ln C_p}\right)$$

Geometric mean bias

$$\mathrm{VG} = \exp\left[\overline{\left(\ln C_o - \ln C_p\right)^2}\right]$$

Geometric variance

$$\mathrm{FA2} = \text{fraction of data where } 0.5 \leq \frac{C_p}{C_o} \leq 2$$

$$\mathrm{FA5} = \text{fraction of data where } 0.2 \leq \frac{C_p}{C_o} \leq 5$$

C_o: observations; C_p: predictions; overbar: average

Significance Tests for Δ(ln(MG))

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

- Bootstrap resampling used for significance tests at 95% level
- Shaded cell means not significantly different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