Jack Rabbit II update

Chlorine Release Experiments and Modelling

Chlorine Covenant Steering Group
HSE Sheffield Office, UK
Wednesday 4 December 2019

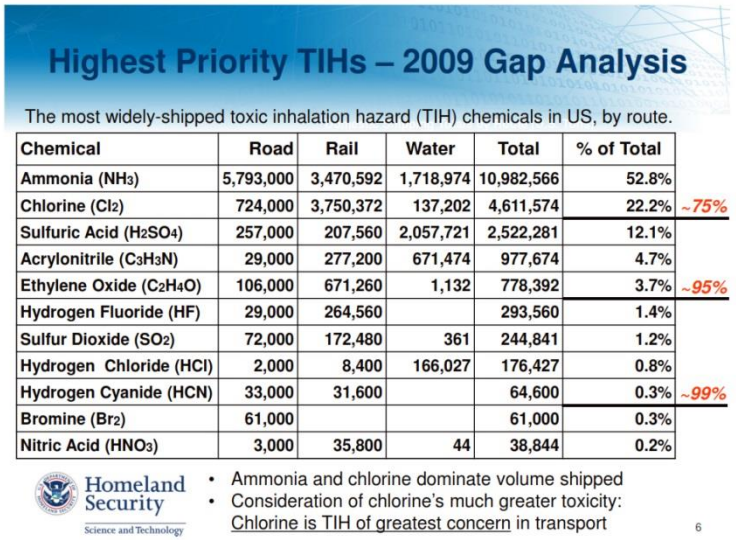
Dr Simon Gant, Fluid Dynamics Team
HSE Science Division, Buxton

Outline

- Background
- Aims of HSE involvement
- Jack Rabbit II
  - 2015 tests: 5 – 10 ton releases in mock urban array
  - 2016 tests: 10 – 20 ton releases in open terrain
- Results from model inter-comparison exercise
- Ongoing work
- Future Directions

Background: Motivation

- Mid-2000s, US Congress expresses concerns for risks to public from accidents or terrorist attacks on railcars containing chlorine and other Toxic Inhalation Hazard (TIH) chemicals passing through metropolitan areas[1]
- 4 million tons of chlorine transported by railcar annually in the US[2]
- Previous incidents, e.g. Graniteville (2005): railcar collision, 9 fatalities, 554 injured, 5400 evacuated[3]



Highest Priority TIHs – 2009 Gap Analysis

The most widely-shipped toxic inhalation hazard (TIH) chemicals in US, by route.

Chemical	Road	Rail	Water	Total	% of Total	
Ammonia (NH_3)	5,793,000	3,470,592	1,718,974	10,982,566	52.8%	
Chlorine (Cl_2)	724,000	3,750,372	137,202	4,611,574	22.2%	~75%
Sulfuric Acid (H_2SO_4)	257,000	207,560	2,057,721	2,522,281	12.1%	
Acrylonitrile (C_3H_3N)	29,000	277,200	671,474	977,674	4.7%	
Ethylene Oxide (C_2H_4O)	106,000	671,260	1,132	778,392	3.7%	~95%
Hydrogen Fluoride (HF)	29,000	264,560		293,560	1.4%	
Sulfur Dioxide (SO_2)	72,000	172,480	361	244,841	1.2%	
Hydrogen Chloride (HCl)	2,000	8,400	166,027	176,427	0.8%	
Hydrogen Cyanide (HCN)	33,000	31,600		64,600	0.3%	~99%
Bromine (Br_2)	61,000			61,000	0.3%	
Nitric Acid (HNO_3)	3,000	35,800	44	38,844	0.2%	

Homeland Security
Science and Technology

- Ammonia and chlorine dominate volume shipped
- Consideration of chlorine's much greater toxicity: Chlorine is TIH of greatest concern in transport

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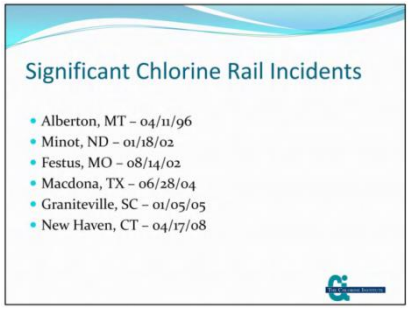
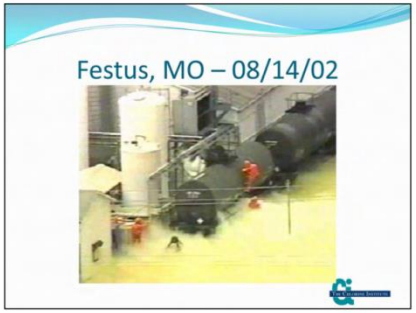


Significant Chlorine Rail Incidents

- Alberton, MT – 04/11/96
- Minot, ND – 01/18/02
- Festus, MO – 08/14/02
- Macdona, TX – 06/28/04
- Graniteville, SC – 01/05/05
- New Haven, CT – 04/17/08



Festus, MO – 08/14/02

Chlorine release in Festus, Missouri, about 30 miles south of St. Louis.
Caused by unloading line corrosion and poor maintenance of emergency shutdown equipment.

BBC NEWS

Syria conflict: Aleppo 'chlorine gas attack' investigated

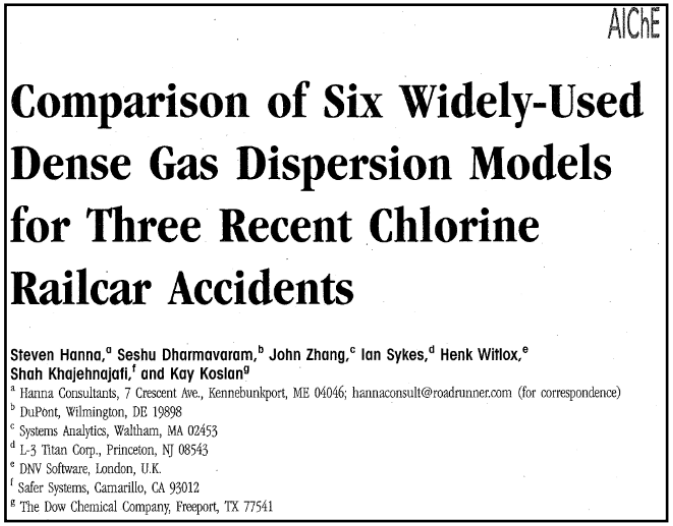
Top Stories

Features

[1] https://www.dhs.gov/science-and-technology/csac
[2] http://clorosur.org/seminar2016/presentation/18/04-DHS-CSAC.pdf
[3] Source: Chlorine Institute

Background: Motivation

- In 2008, scientific papers published on evaluation of six commonly-used dense gas dispersion models for three chlorine incidents
- All models significantly over-predicted the hazard
  - Predicted AEGL-3 (life threatening) > several km
  - No casualties in the incidents beyond around 100 m
- Concerns raised about accuracy of models
- Uncertainties:
  - Source terms: release rates
  - Dispersion
  - Terrain effects (vapour “hold up”?)
  - Deposition and chemical reactions
  - Infiltration into buildings/vehicles
  - Toxic effects

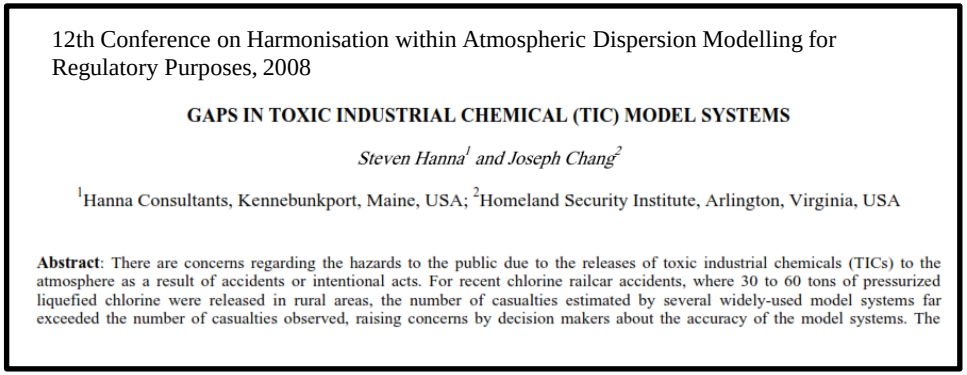


AIChE

Comparison of Six Widely-Used Dense Gas Dispersion Models for Three Recent Chlorine Railcar Accidents

Steven Hanna,[a] Seshu Dharmavaram,[b] John Zhang,[c] Ian Sykes,[d] Henk Witlox,[e] Shah Khajehnajafi,[f] and Kay Koslan[g]

[a] Hanna Consultants, 7 Crescent Ave., Kennebunkport, ME 04046; hannaconsult@roadrunner.com (for correspondence)
[b] DuPont, Wilmington, DE 19898
[c] Systems Analytics, Waltham, MA 02453
[d] L-3 Titan Corp., Princeton, NJ 08543
[e] DNV Software, London, U.K.
[f] Safer Systems, Camarillo, CA 93012
[g] The Dow Chemical Company, Freeport, TX 77541



12th Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, 2008

GAPS IN TOXIC INDUSTRIAL CHEMICAL (TIC) MODEL SYSTEMS

Steven Hanna[1] *and Joseph Chang*[2]

[1]Hanna Consultants, Kennebunkport, Maine, USA; [2]Homeland Security Institute, Arlington, Virginia, USA

Abstract: There are concerns regarding the hazards to the public due to the releases of toxic industrial chemicals (TICs) to the atmosphere as a result of accidents or intentional acts. For recent chlorine railcar accidents, where 30 to 60 tons of pressurized liquefied chlorine were released in rural areas, the number of casualties estimated by several widely-used model systems far exceeded the number of casualties observed, raising concerns by decision makers about the accuracy of the model systems. The

HSE Involvement in Jack Rabbit II

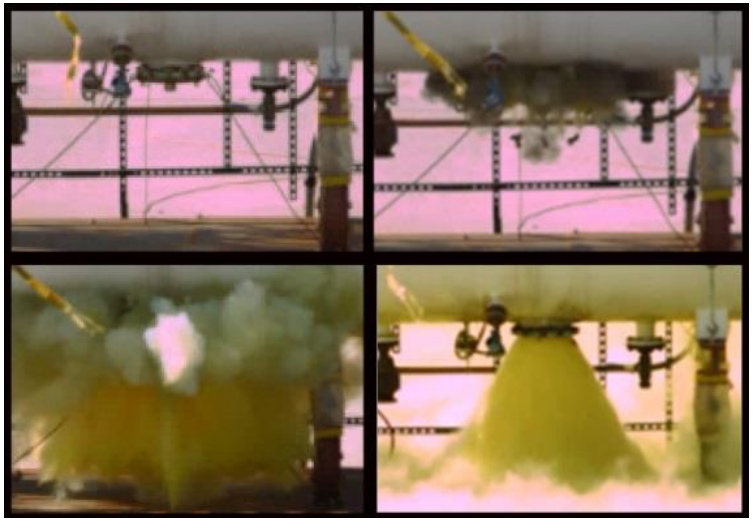
Background

- 2014 – 2015: Heath School planning inquiry – focus on chlorine dispersion modelling
- March 2015: HSE introduced to Jack Rabbit II project coordinators by DSTL
- Spring-Summer 2015/2016: Modelers Working Group telecons every two weeks
- Summer 2016: 3 week visit to NCAR and Dugway Proving Ground for VIP day
- Summer 2017: 1 week visit to NCAR to work on joint journal paper
- 2015 – 2017: Conference presentations at GMU, Harmo, IChemE Hazards, EuroChlor

Aims of HSE Involvement

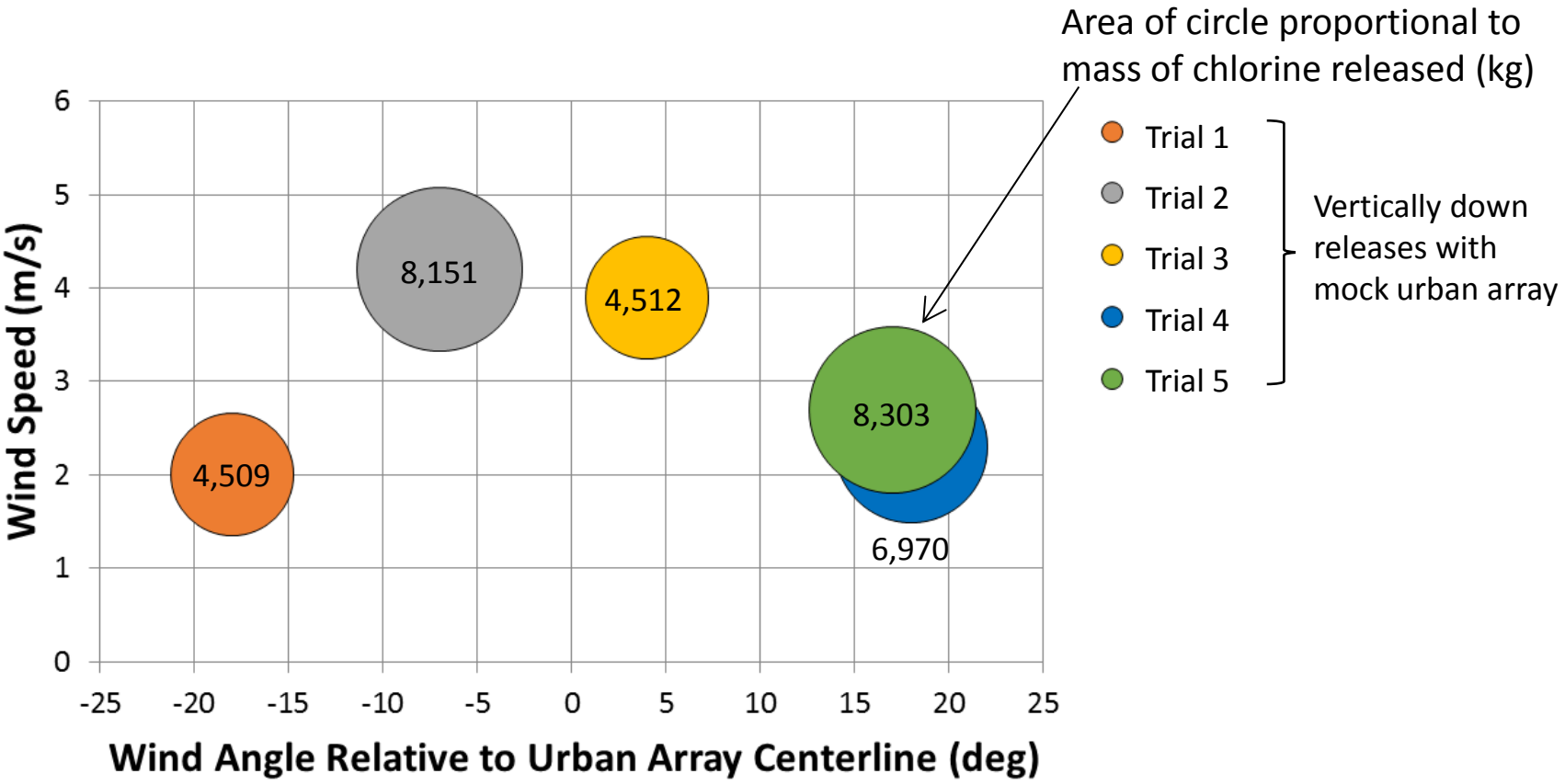
- Contribute modelling results and help support Jack Rabbit II project
- Validate HSE's regulatory dispersion model (DRIFT) against Jack Rabbit II data
- Assess capabilities of widely-used industry dispersion model (PHAST)
- Improve links with top international experts on: source terms, dispersion, deposition etc.

Jack Rabbit II (2015) Trials 1 – 5

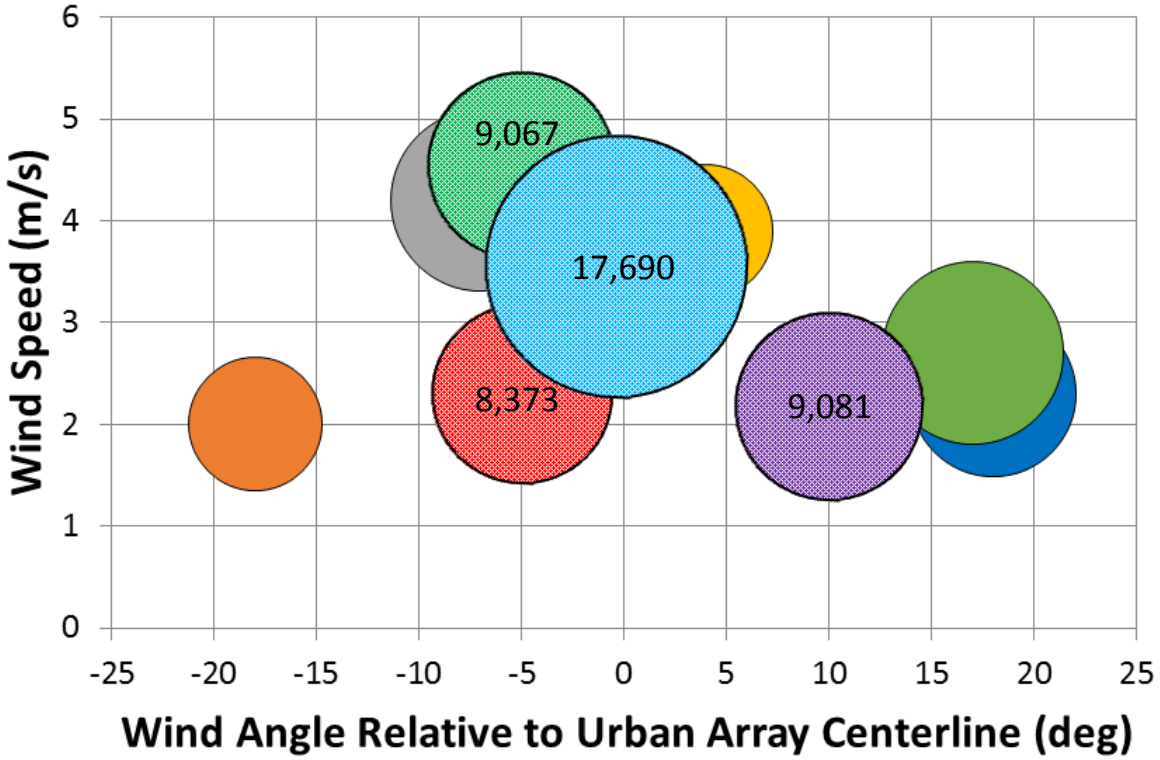


Jack Rabbit II (2016) Trials 6 – 9

JRII 2015 and 2016 Trial Summary



JRII 2015 and 2016 Trial Summary



- Trial 1
- Trial 2
- Trial 3
- Trial 4
- Trial 5

Vertically down releases with mock urban array

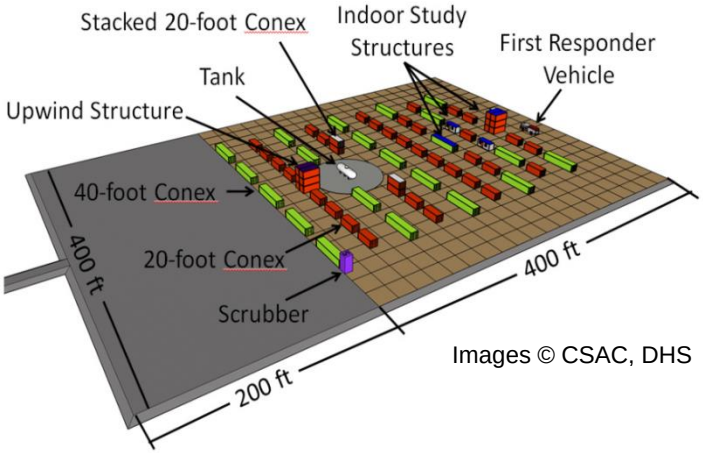
- Trial 6 : Vertically down
- Trial 7 : 45-deg down
- Trial 8 : Vertically up
- Trial 9 : Road tanker

Primary and later secondary releases of liquid heel

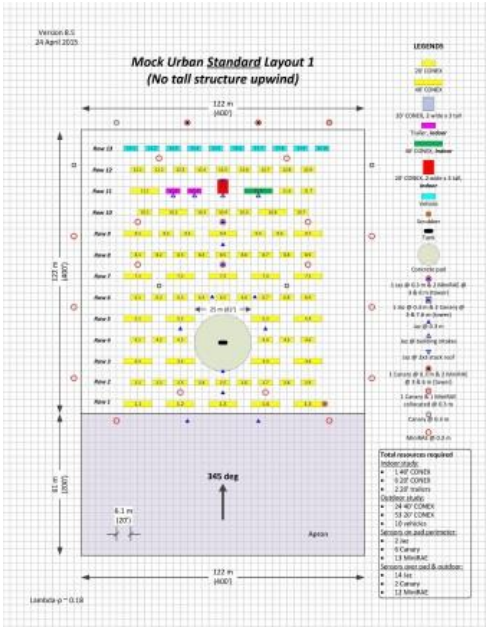
Concentration Sensor Array (2015)

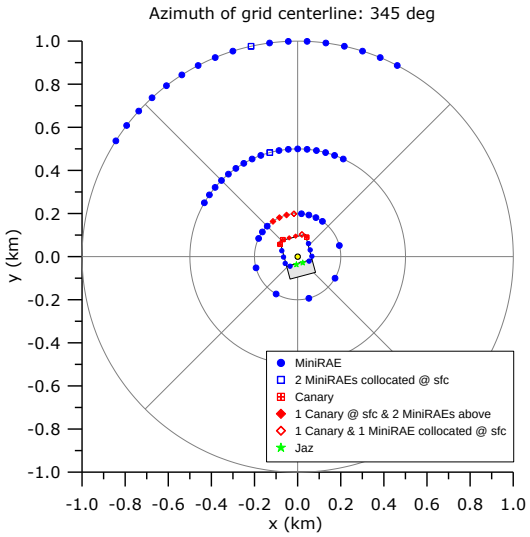
Concentration sensors (saturation levels)

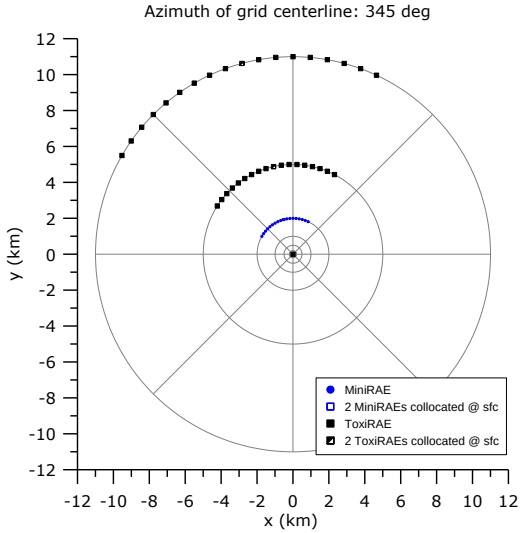
- 16 UV Jaz (100,000 ppmv)
- 28 Canary (10,000 ppmv)
- 128 MiniRAE (2,000 ppmv)
- 58 ToxiRAE (50 ppmv)
- 3 Scanning Lidars



Images © CSAC, DHS

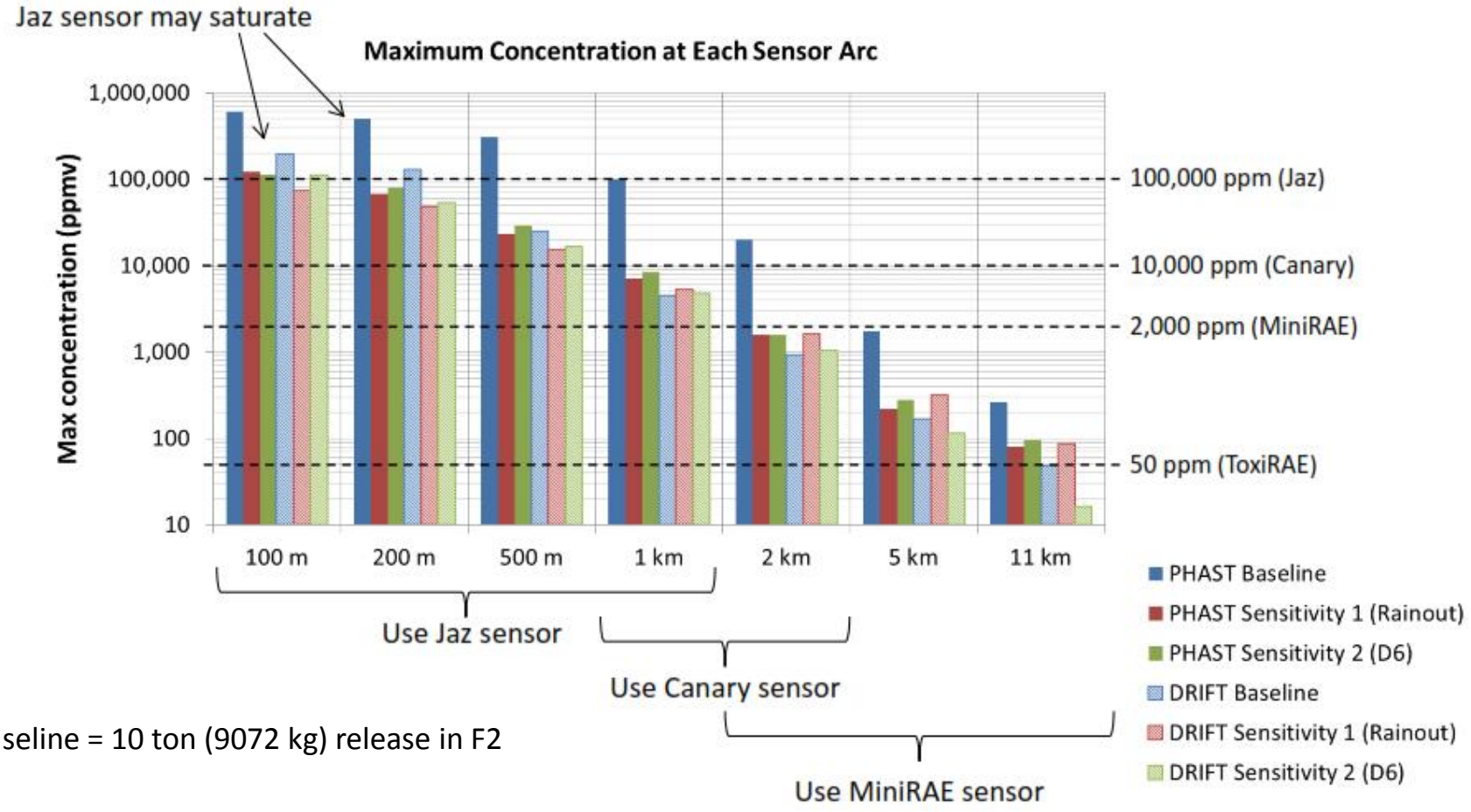






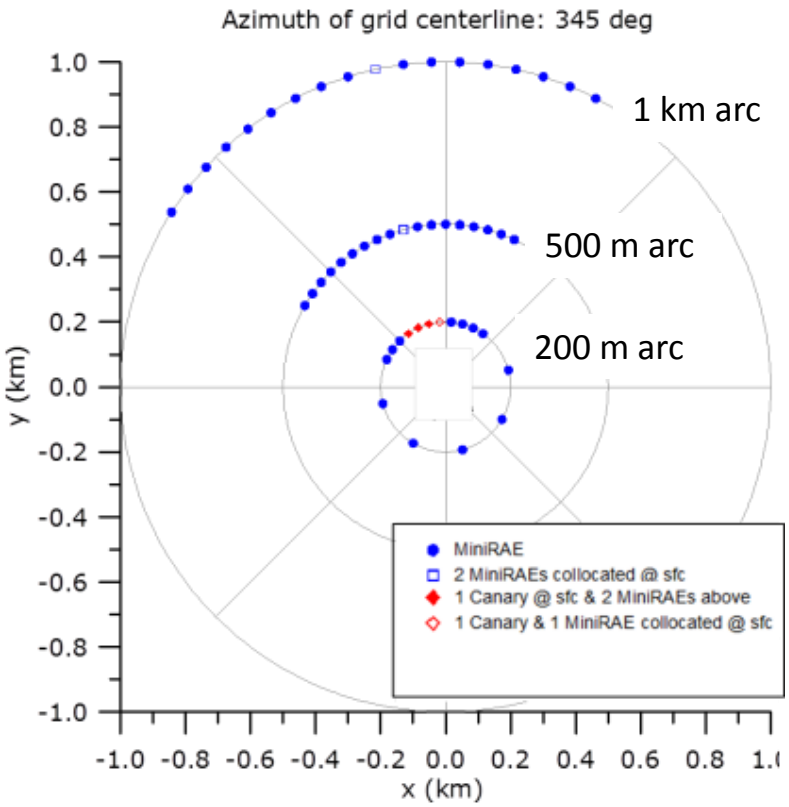
Jack Rabbit II Trials (2015)

HSE predictions prior to the 2015 trials for positioning of sensors

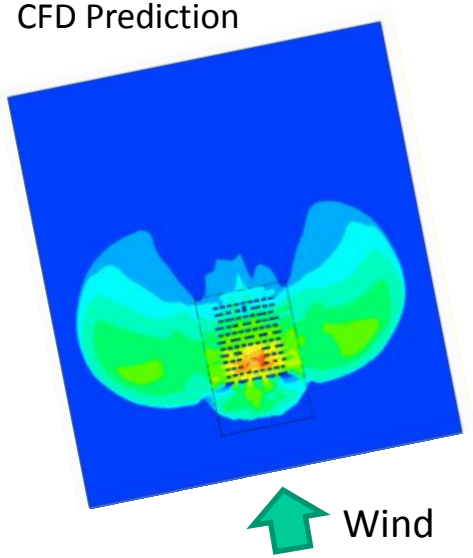


Baseline = 10 ton (9072 kg) release in F2

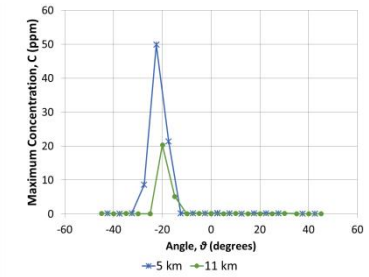
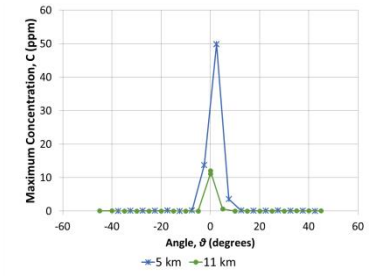
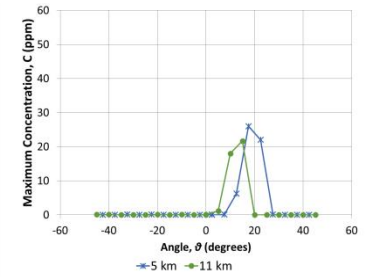
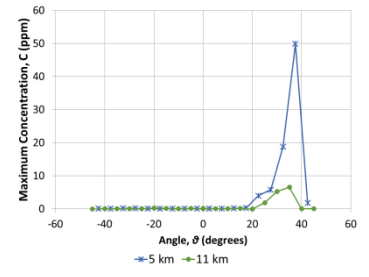
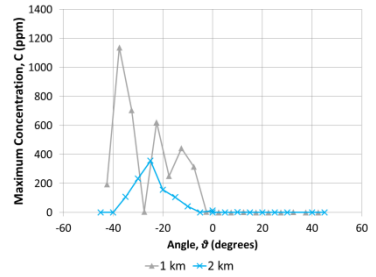
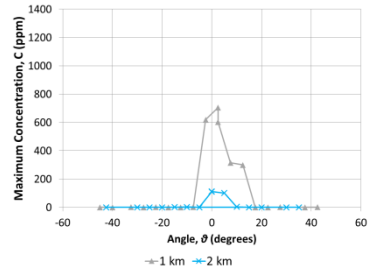
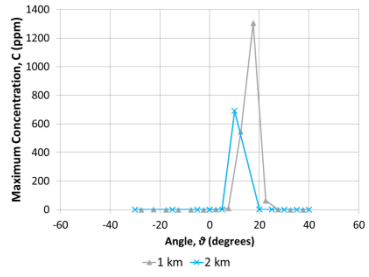
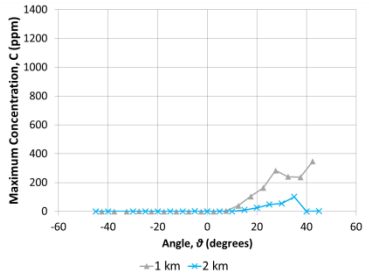
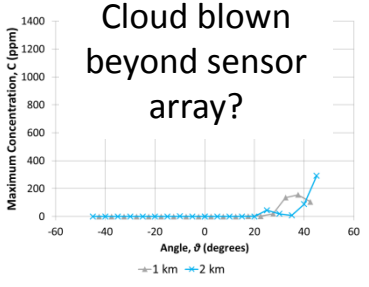
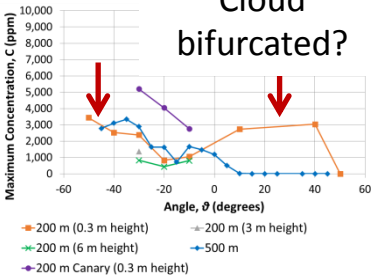
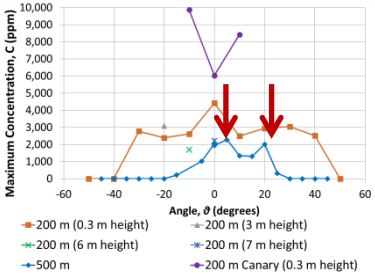
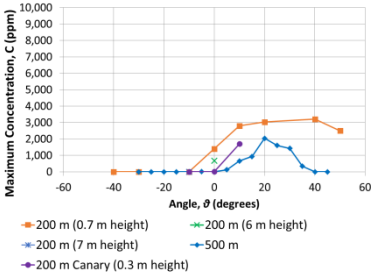
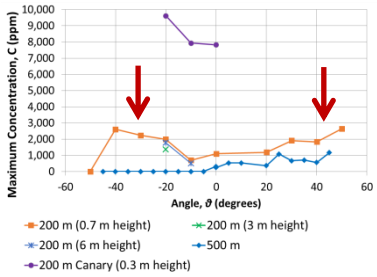
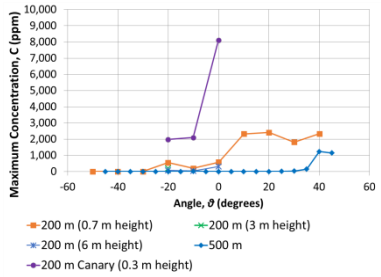
JR II 2015: Concentration Data



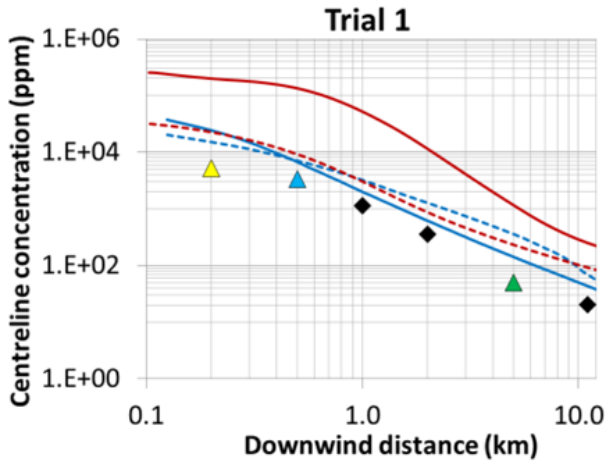
CFD Prediction

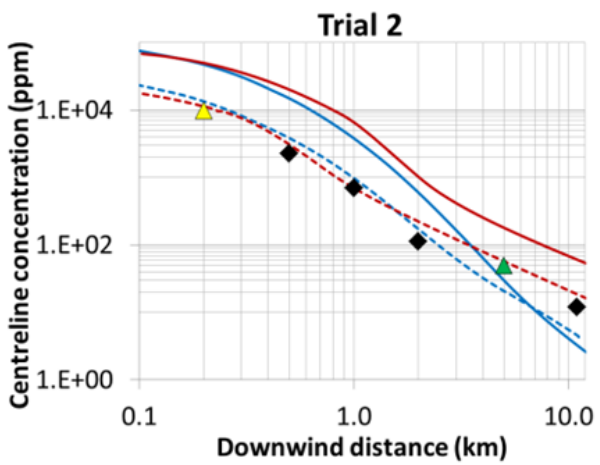


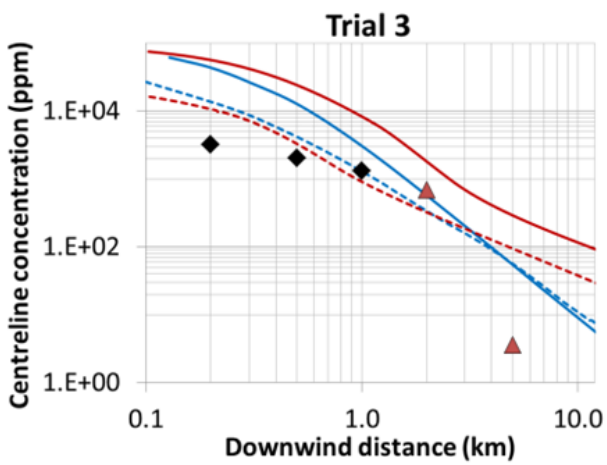
Is there any evidence of bifurcated cloud behavior at the 200 m and 500 m arcs?

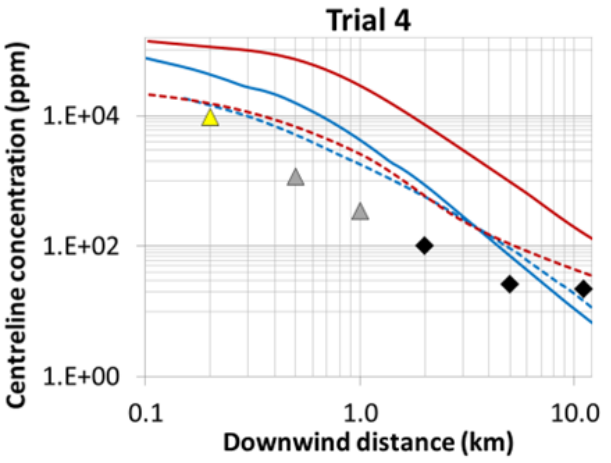
Trial 1	Trial 2	Trial 3	Trial 4	Trial 5
		Cloud passed in between sensors?		
				Cloud blown beyond sensor array? 
Cloud bifurcated? 				
2.0 m/s -18°	**4.2 m/s** -7°	**3.9 m/s** +4°	**2.3 m/s** +18°	**2.7 m/s** +17°
4509 kg	8151 kg	4512 kg	6970 kg	8303 kg

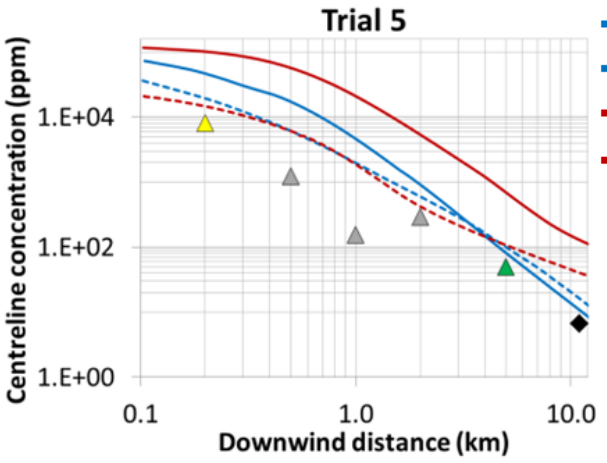
JR II 2015: Concentration Predictions

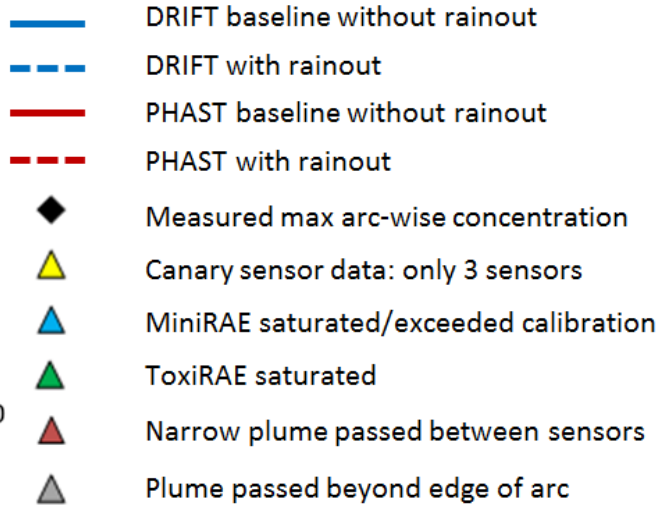




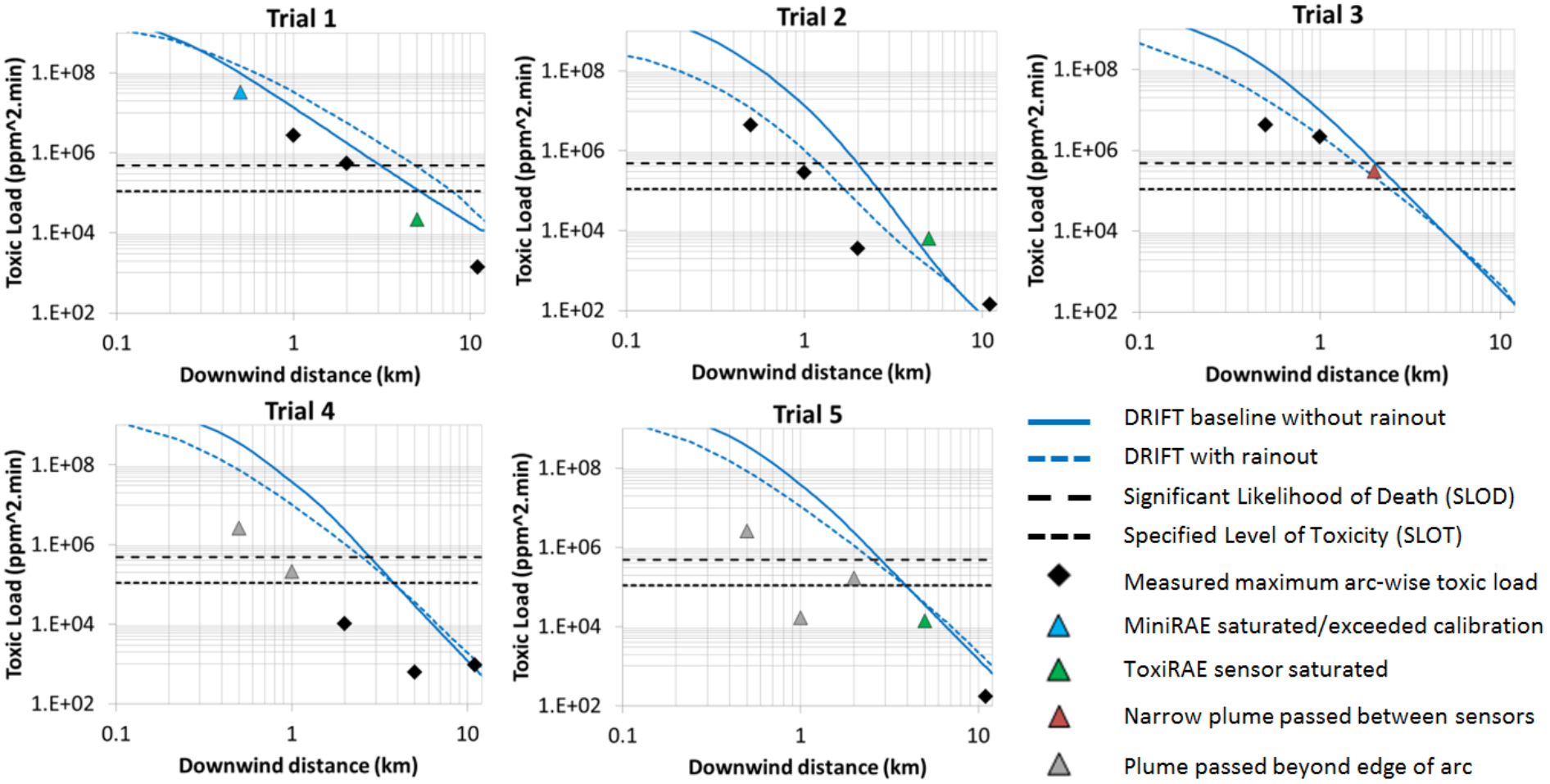




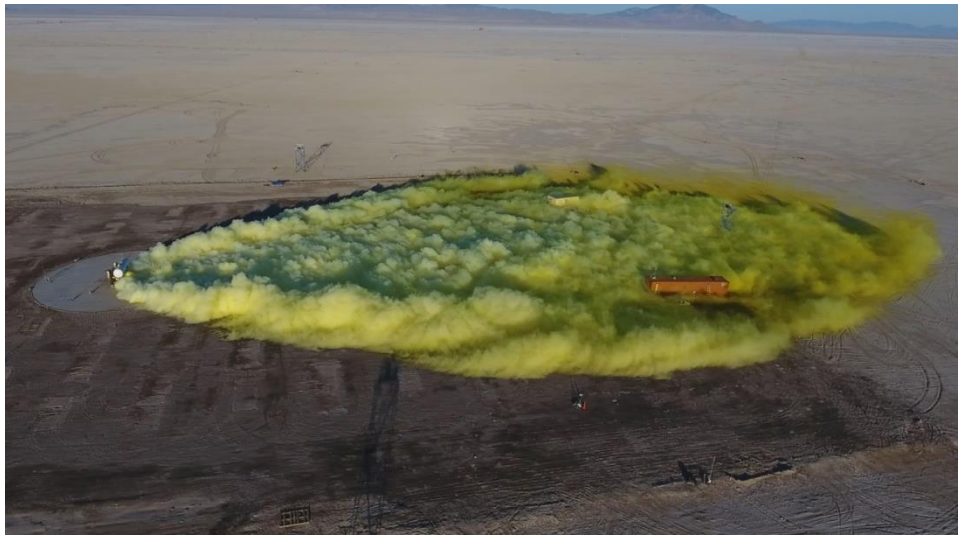




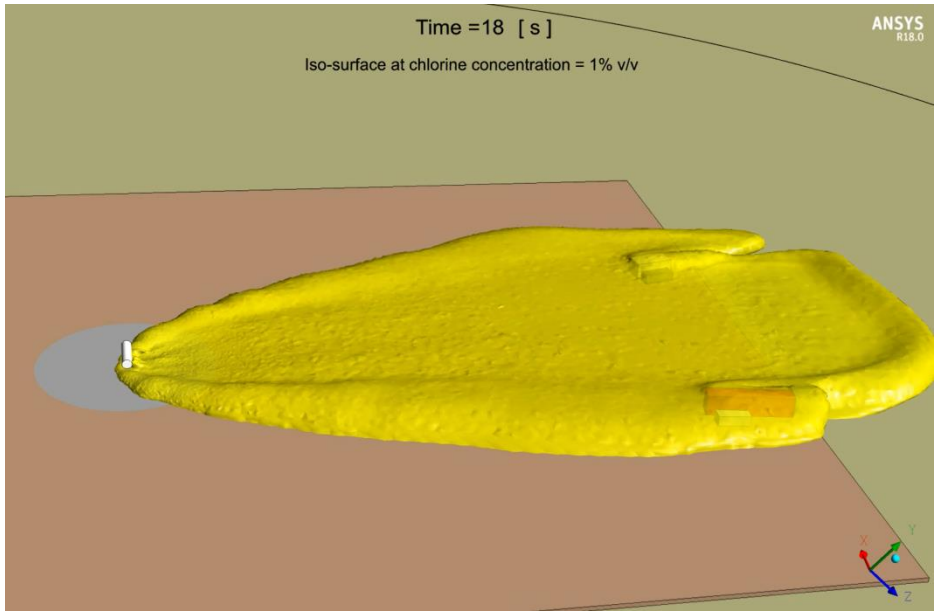
JR II 2015: Toxic Load Predictions



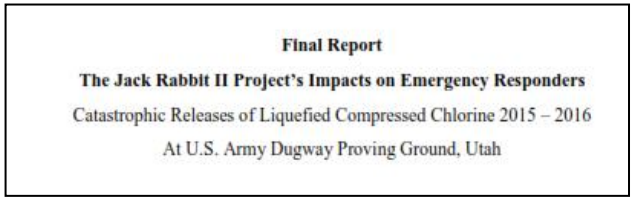
Jack Rabbit II Trial 7 (2016)



http://www.uvu.edu/esa/jackrabbit/



CFD modelling by HSE to understand near-field dispersion behavior



Final Report

The Jack Rabbit II Project's Impacts on Emergency Responders

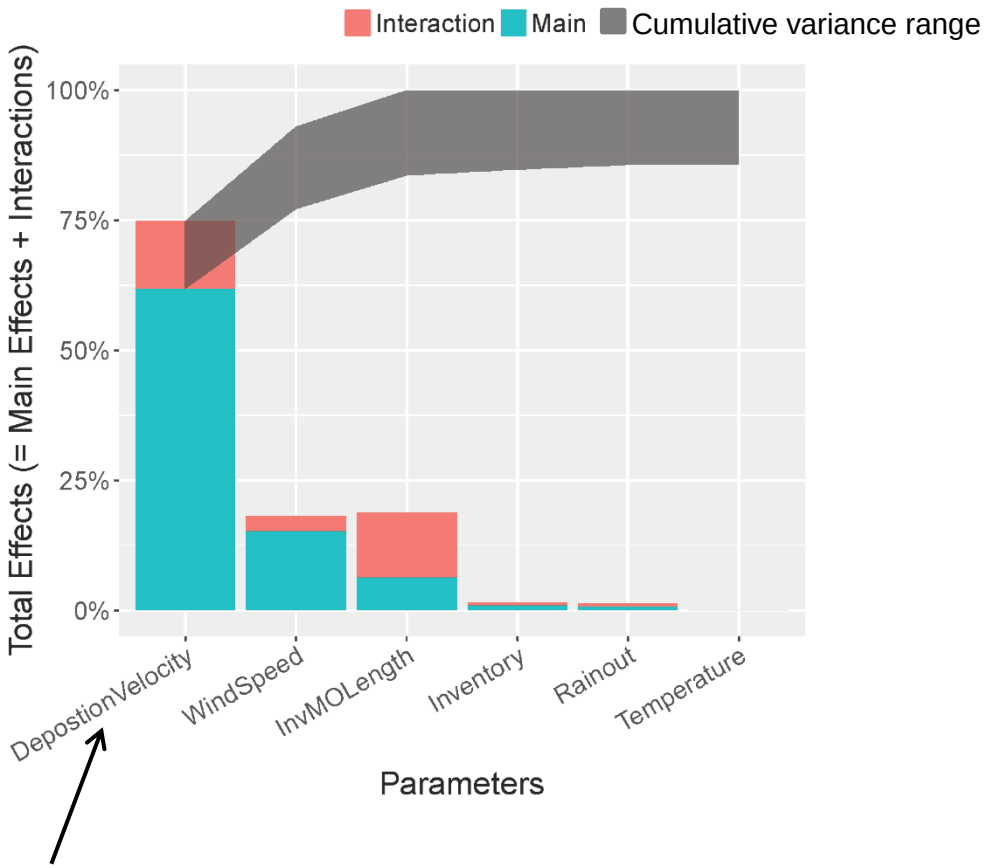
Catastrophic Releases of Liquefied Compressed Chlorine 2015 – 2016

At U.S. Army Dugway Proving Ground, Utah

← Useful report on Emergency Response available on UVU website

Global Sensitivity Analysis with DRIFT

Model Parameter	Min	Max
Chlorine amount	4 tonnes	9 tonnes
Rainout fraction	0	1
Wind speed	1.5 m/s	5 m/s
Temperature	15 °C	30 °C
Inverse M-O length	-0.12	0.08
Dry deposition velocity	0	5 cm/s

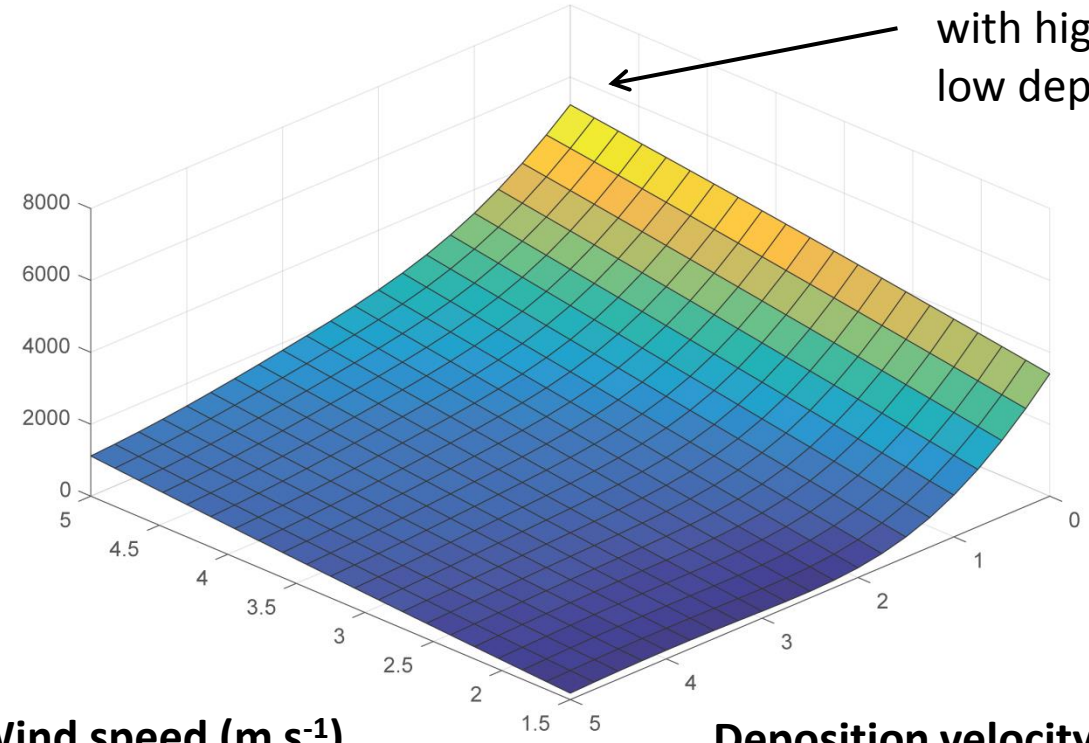


Deposition velocity has the strongest effect on the results
(when using wide range of deposition velocities)

Surface plot showing physical effects

Largest dispersion distance with high wind speed and low deposition velocity

Distance to 100 ppm concentration (m)



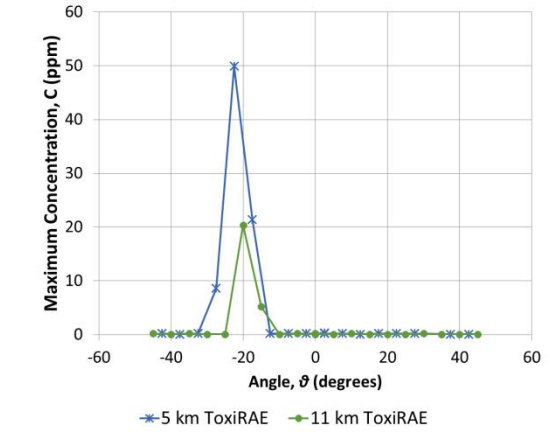
Wind speed (m s^{-1})

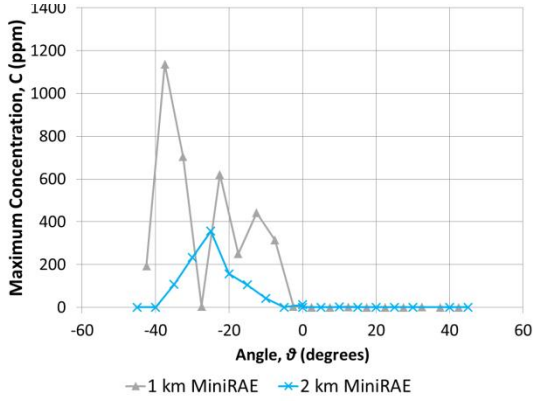
Deposition velocity (cm s^{-1})

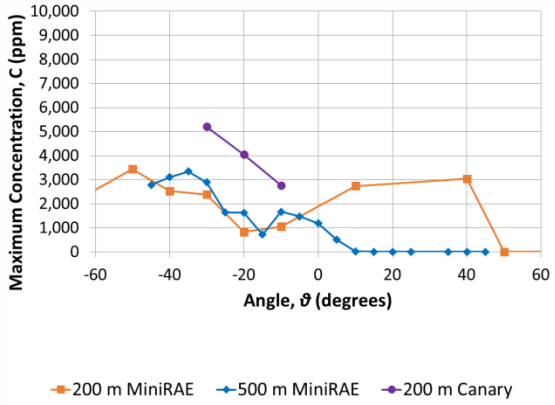
JRII model inter-comparison exercise

- Aims:
  - To compare models to measurements on equal basis (same inputs and standardized outputs)
  - To understand capabilities/limitations of different models
  - To share information and new understanding
- Kick-off telecon March 2018
- First stage comparison: Trials 1, 6 and 7
- Model inputs:
  - Atmospheric conditions defined by Steve Hanna
  - Source conditions defined by Tom Spicer and Graham Tickle

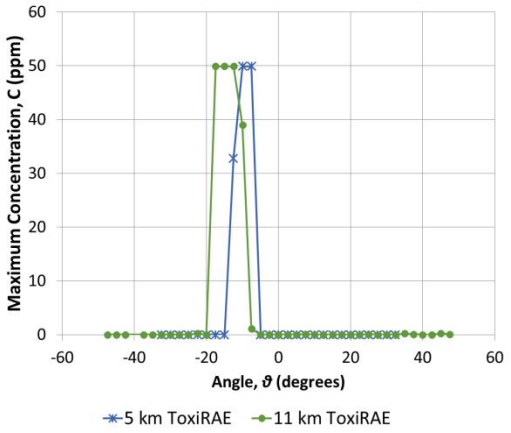
Trial 1

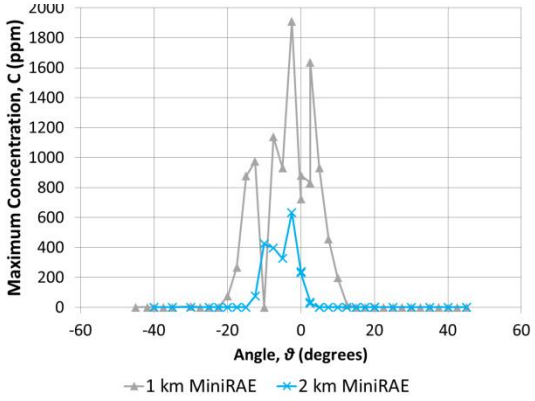


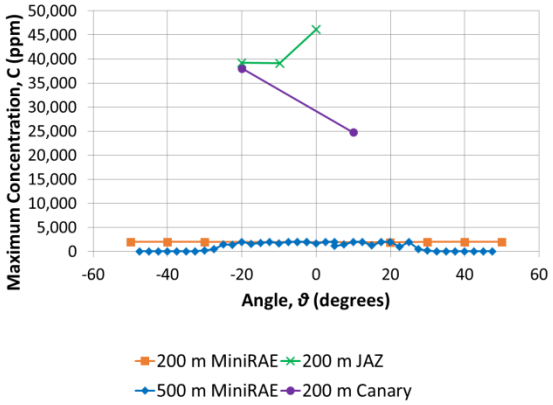




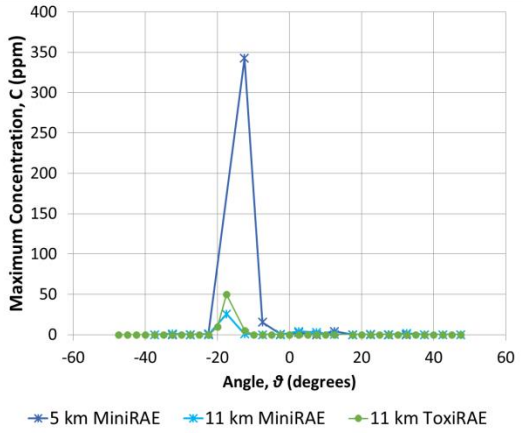
Trial 6

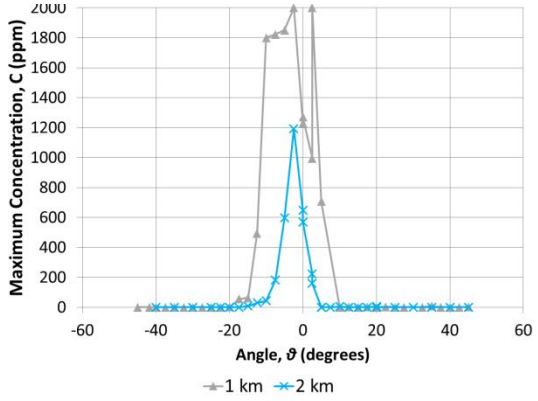


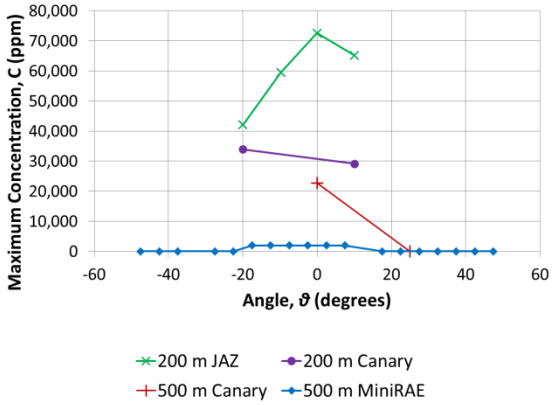




Trial 7

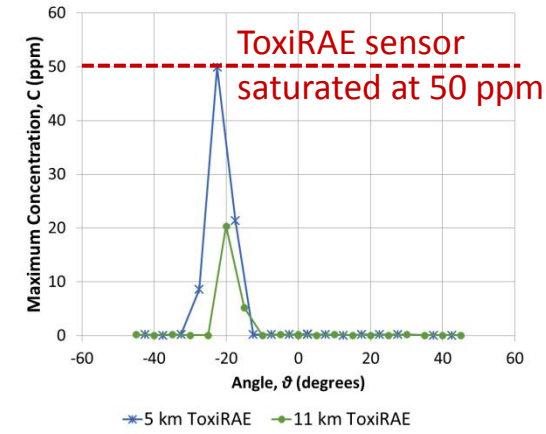


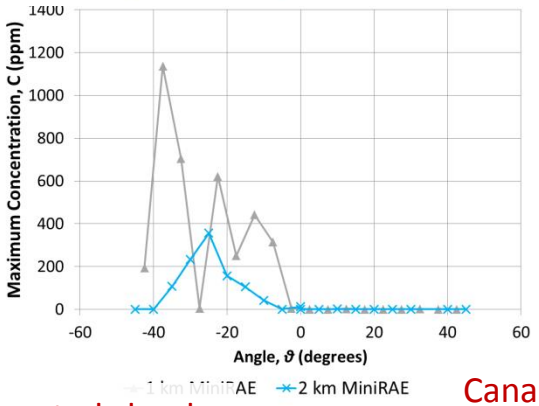




NB. Trial 6 and 7 MiniRAE data not scaled in response to pre/post calibration tests

Trial 1





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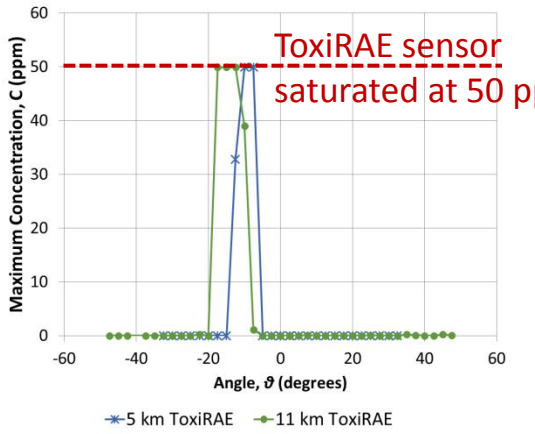
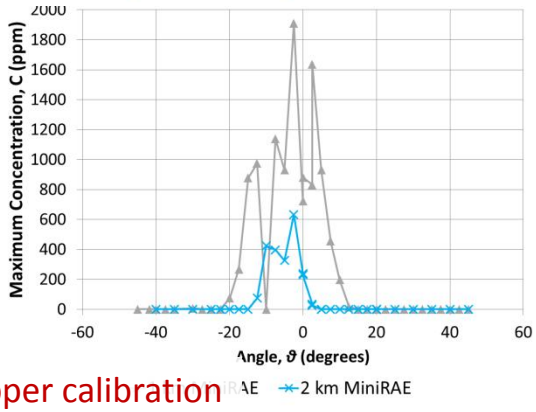
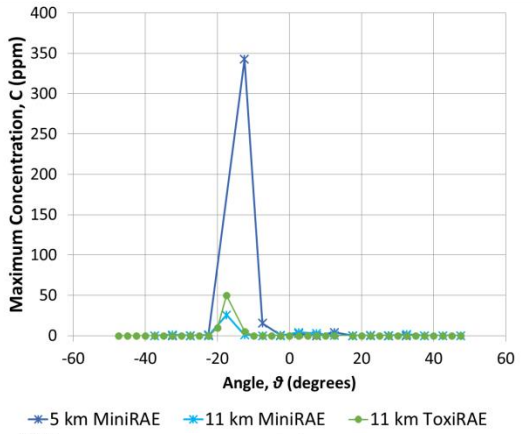
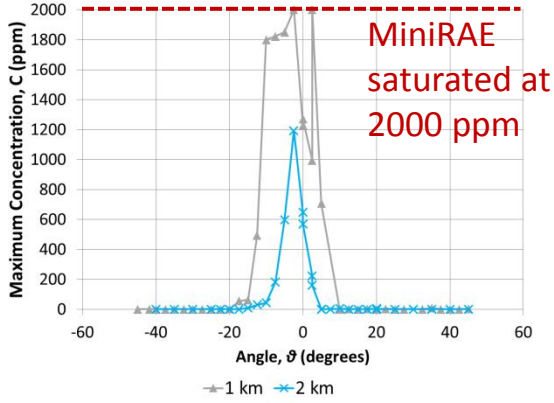




Trial 7

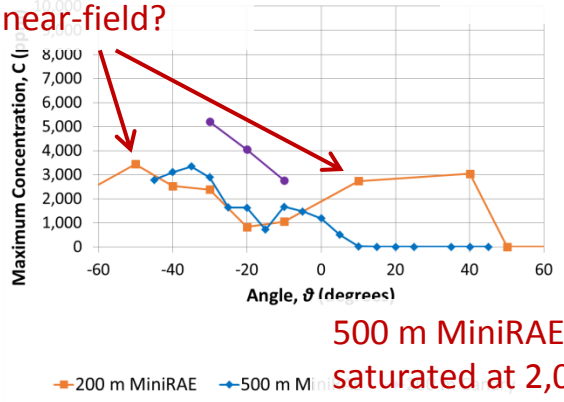


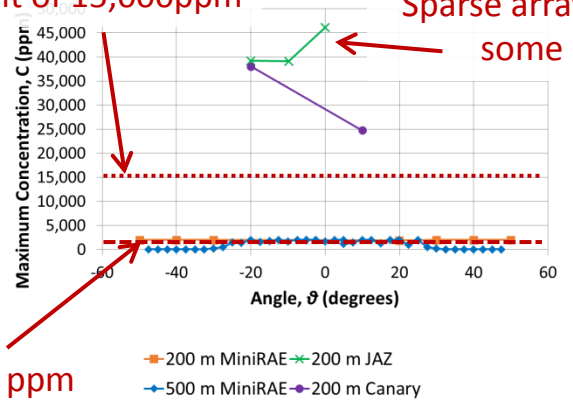


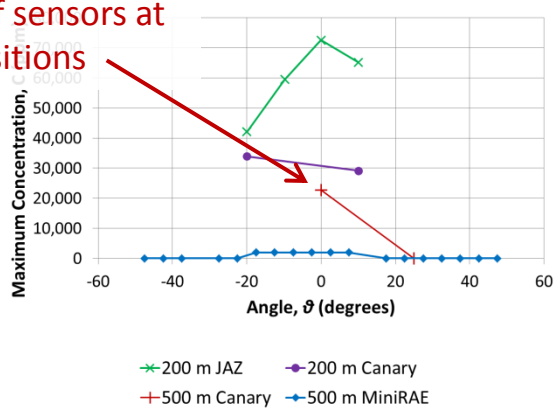
Bifurcated cloud in near-field?

Canary upper calibration limit of 15,000ppm

Sparse array of sensors at some positions







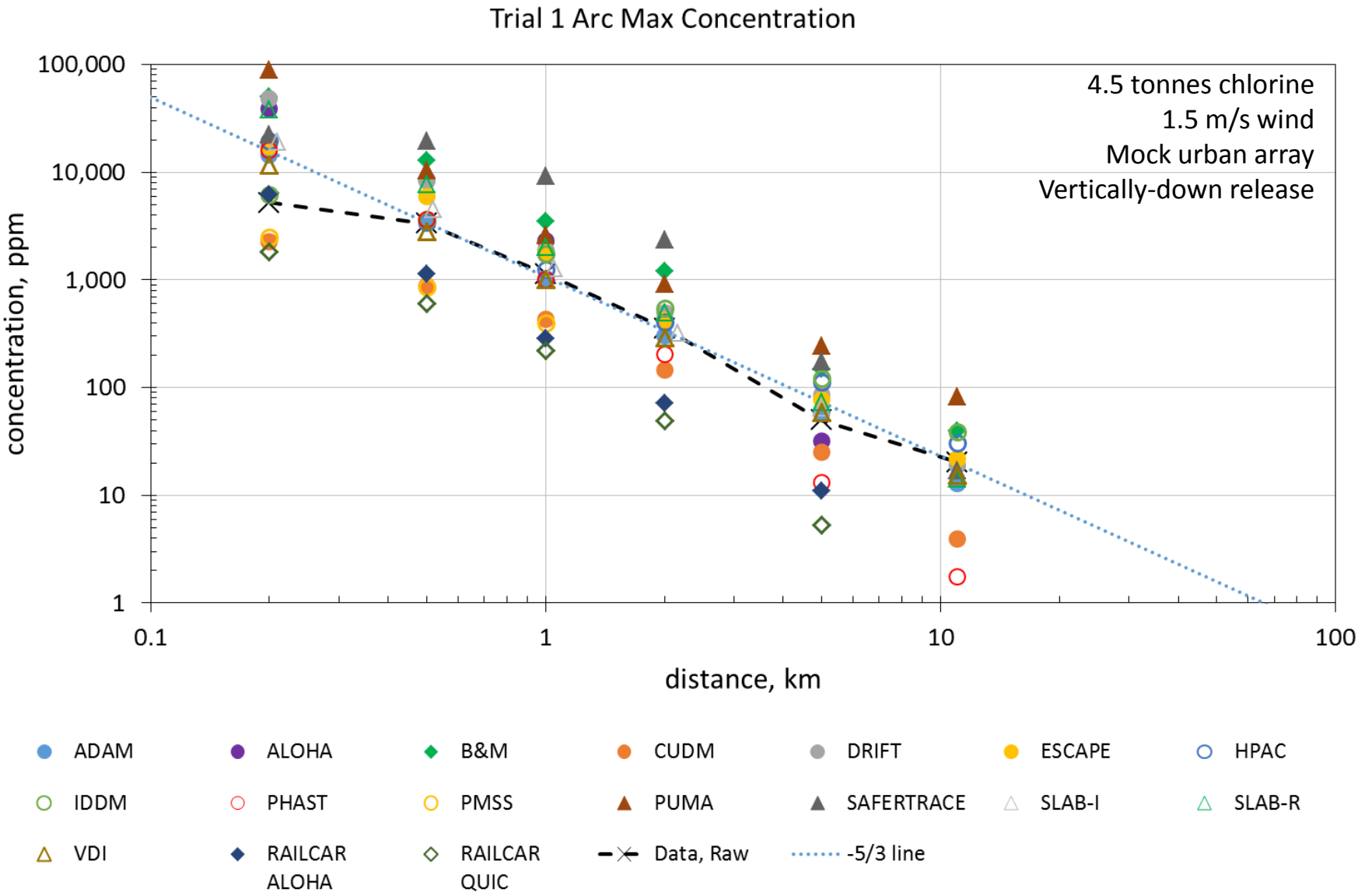
500 m MiniRAE saturated at 2,000 ppm

NB. Trial 6 and 7 MiniRAE data not scaled in response to pre/post calibration tests

JRII model inter-comparison exercise

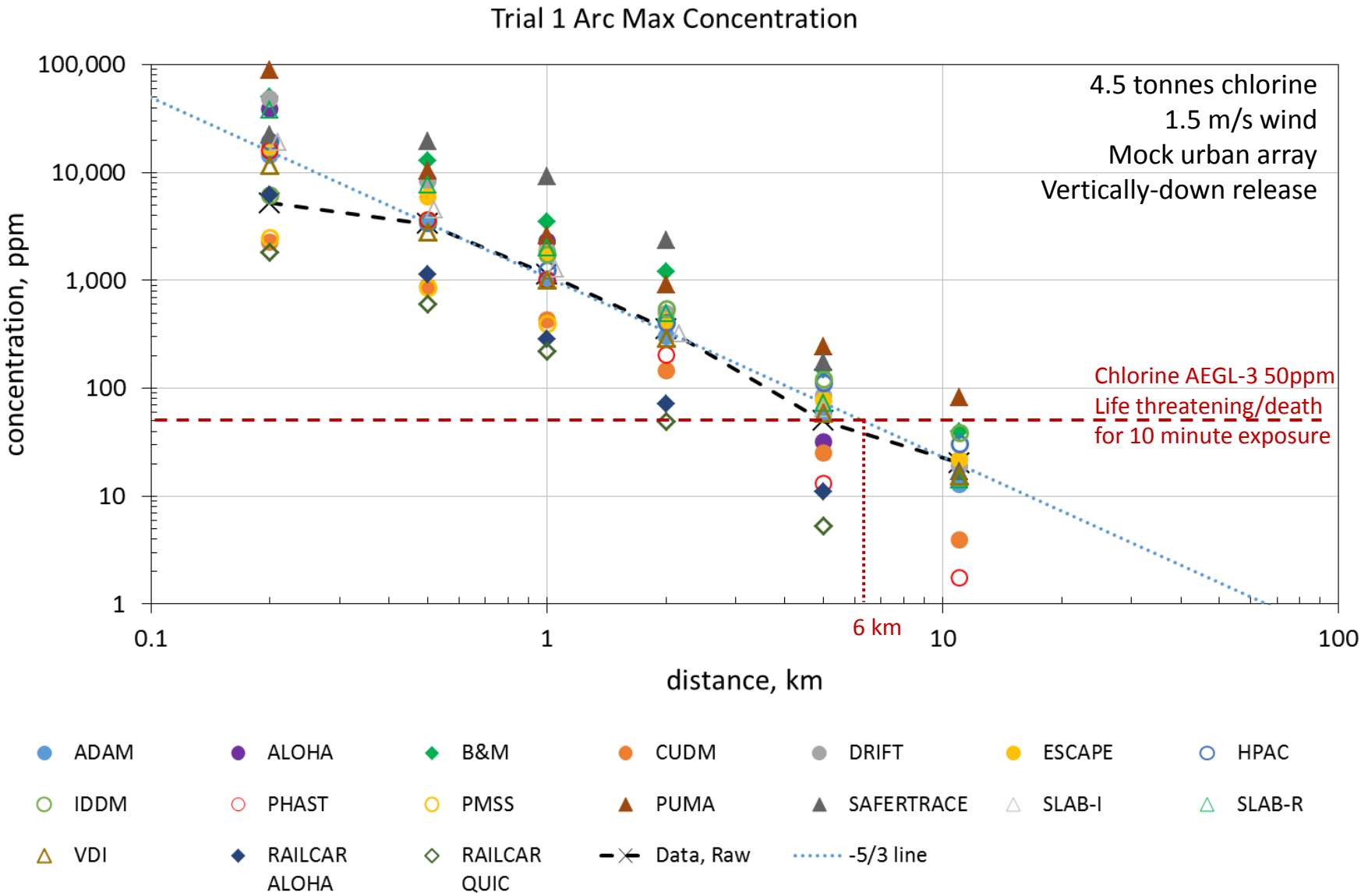
Country	Organization	Model(s) used
USA	DTRA Reachback	HPAC 6.5
USA	National Center for Atmospheric Research (NCAR)	Integral Dense-gas Dispersion Model (IDDM)
USA	RAND Corporation	ALOHA, SLAB-R
USA	Safer Systems	Trace
USA	Hanna Consultants	Britter & McQuaid Workbook (B&M)
Canada	Environment and Climate Change Canada	Canadian Urban Dispersion Modeling (CUDM)
UK	DNV GL	PHAST
UK	ESR Technology/GT Science and Software	DRIFT
UK	Health & Safety Executive (HSE)	DRIFT
France	Aria Technologies SA	Parallel-Micro-SWIFT-SPRAY (PMSS)
France	Atomic Energy Commission (CEA)	Parallel-Micro-SWIFT-SPRAY (PMSS)
France	INERIS	PHAST, SLAB, FDS
Germany	Federal Institute for Materials Research and Testing (BAM)	VDI 3783 Parts I & II
Sweden	Swedish Defence Research Agency (FOI)	PUMA
Finland	Finnish Meteorological Institute (FMI)	ESCAPE
EU	EU Joint Research Centre, Ispra	Accident Damage Analysis Module (ADAM)

JRII model inter-comparison exercise



From Hanna S., Chang J. and Mazzola T. (2019) Summary Findings of the Model Evaluation and Comparison: Jack Rabbit II Case Study, 19th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes (Harmo-19), Bruges, Belgium, 3 - 6 June 2019

JRII model inter-comparison exercise



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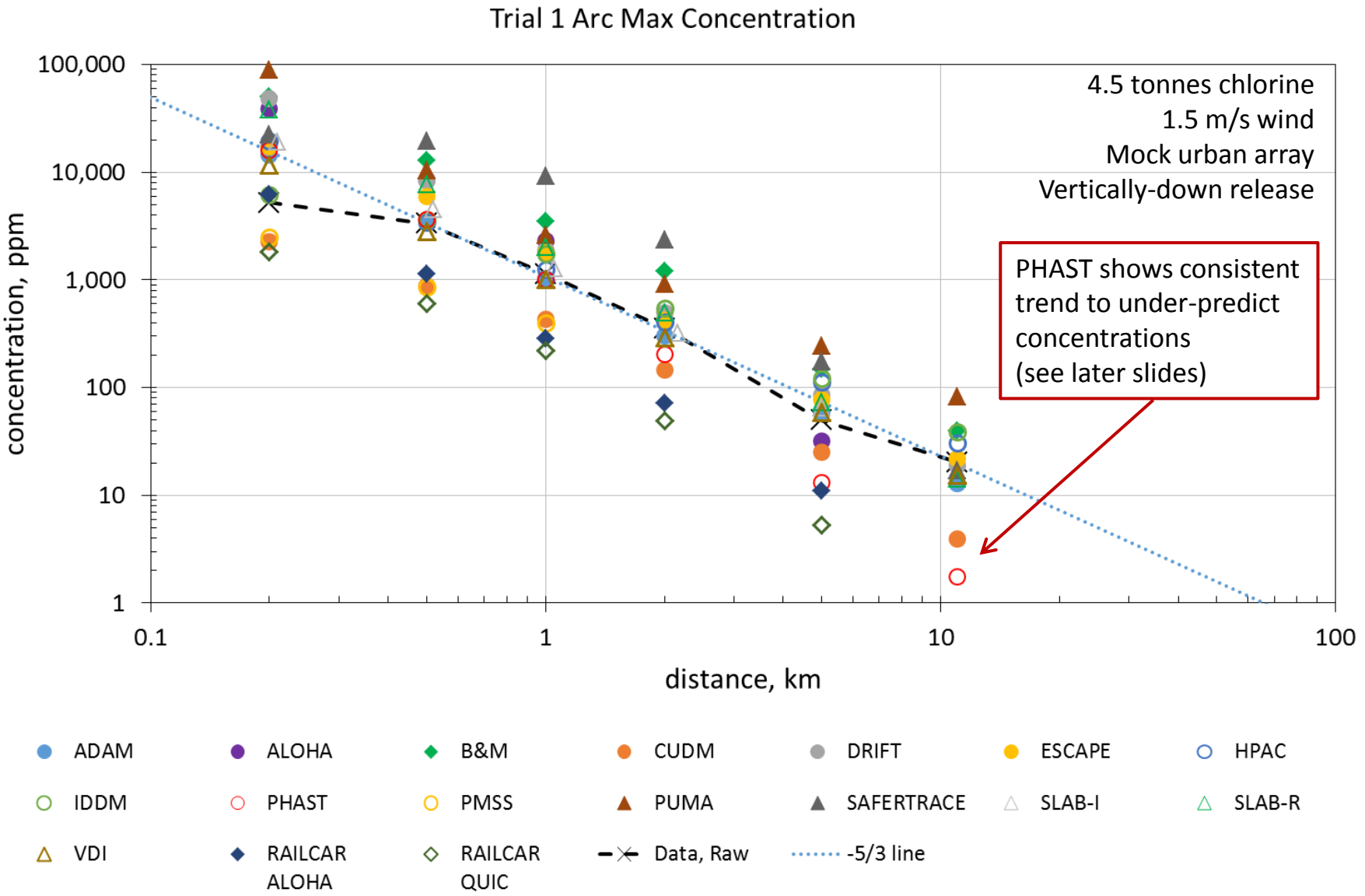

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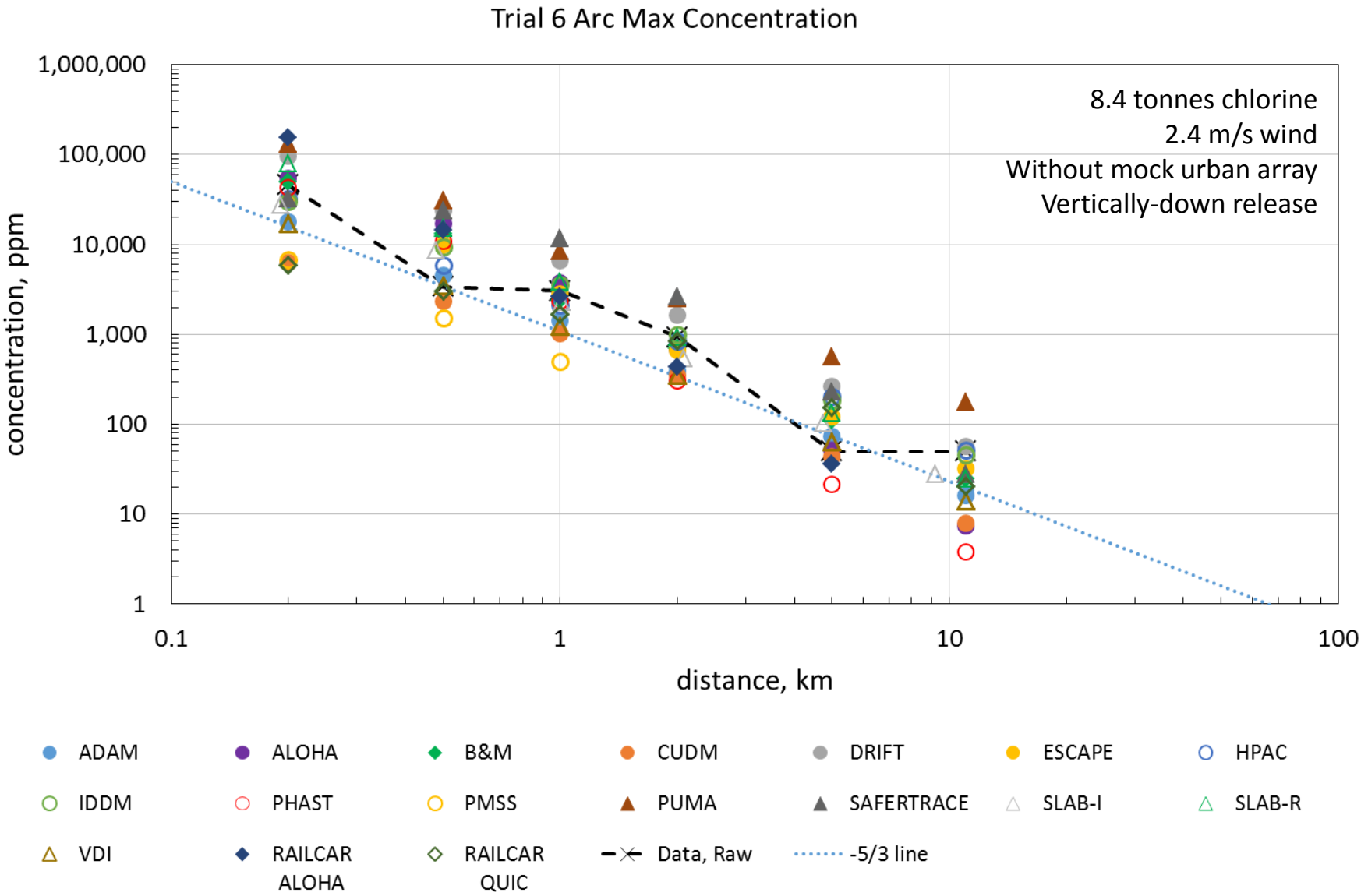

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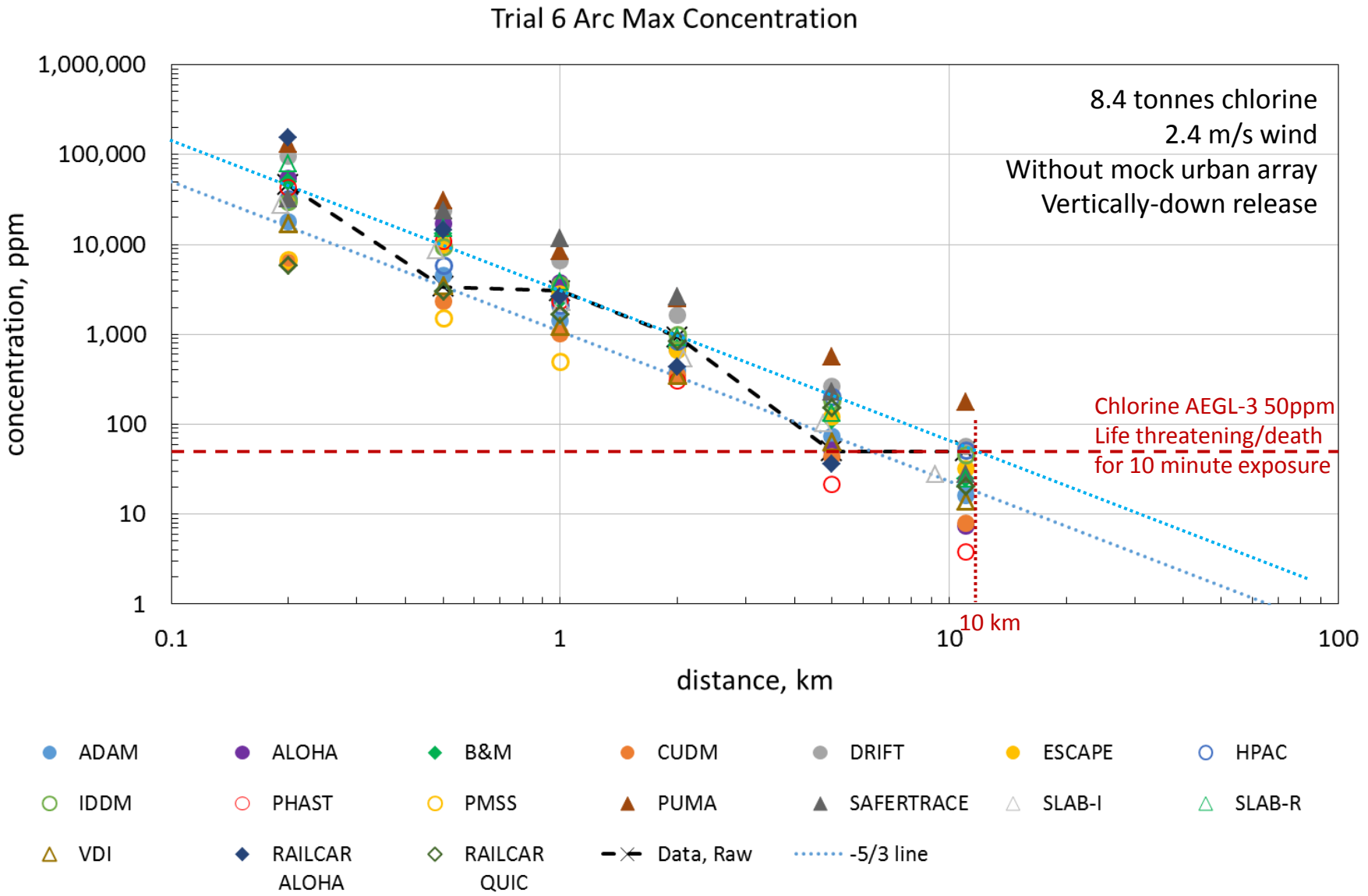

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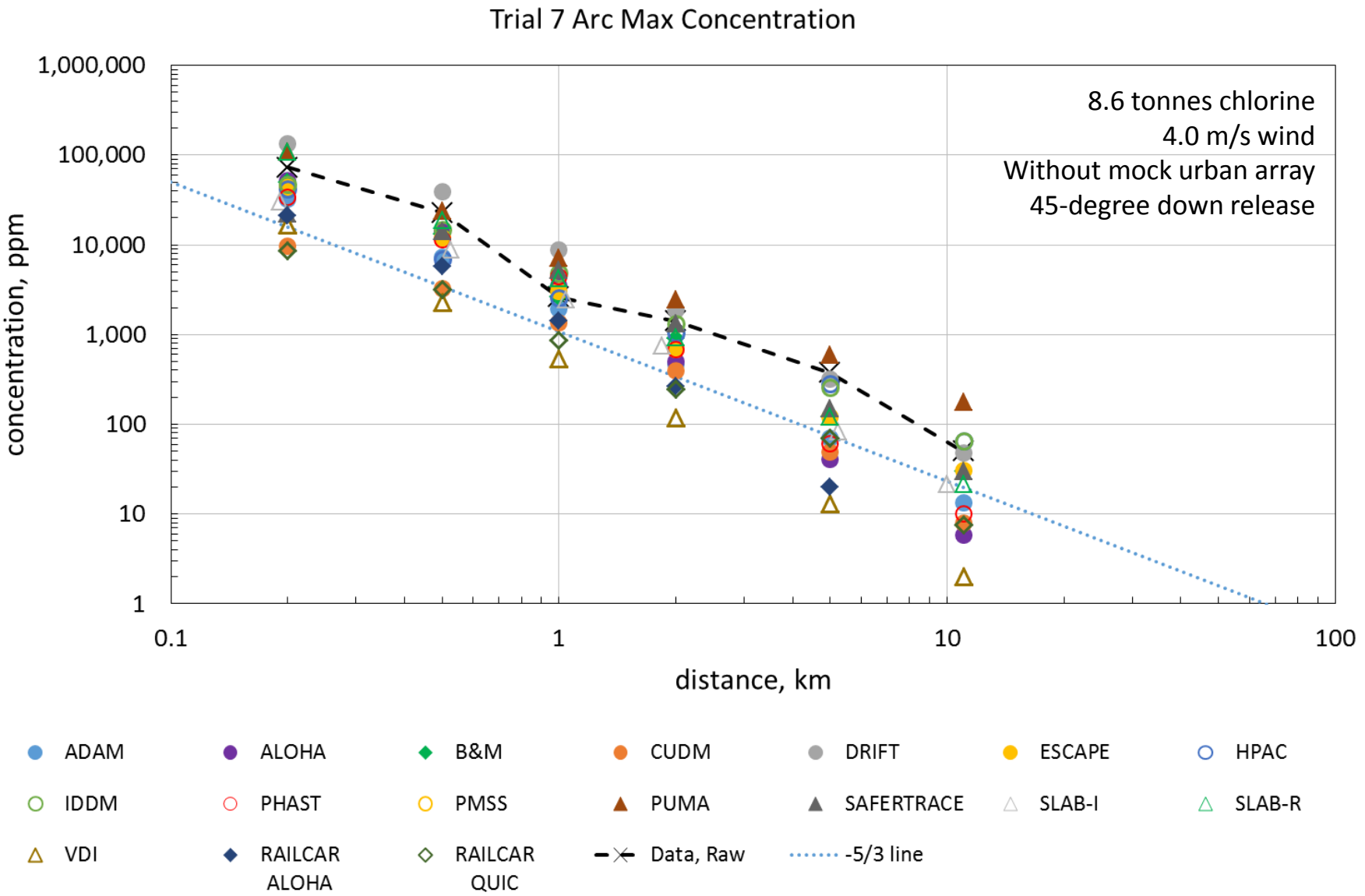

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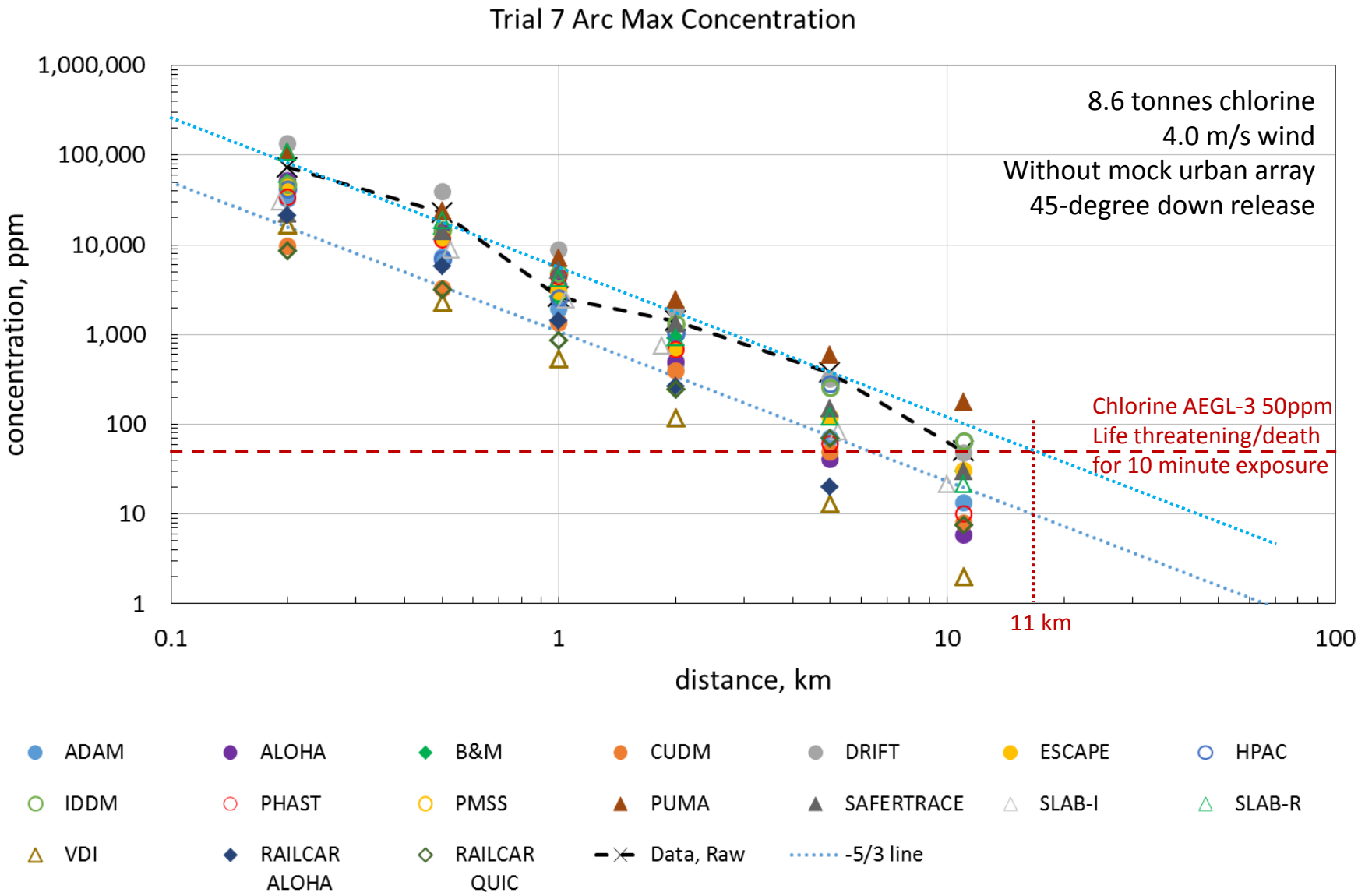

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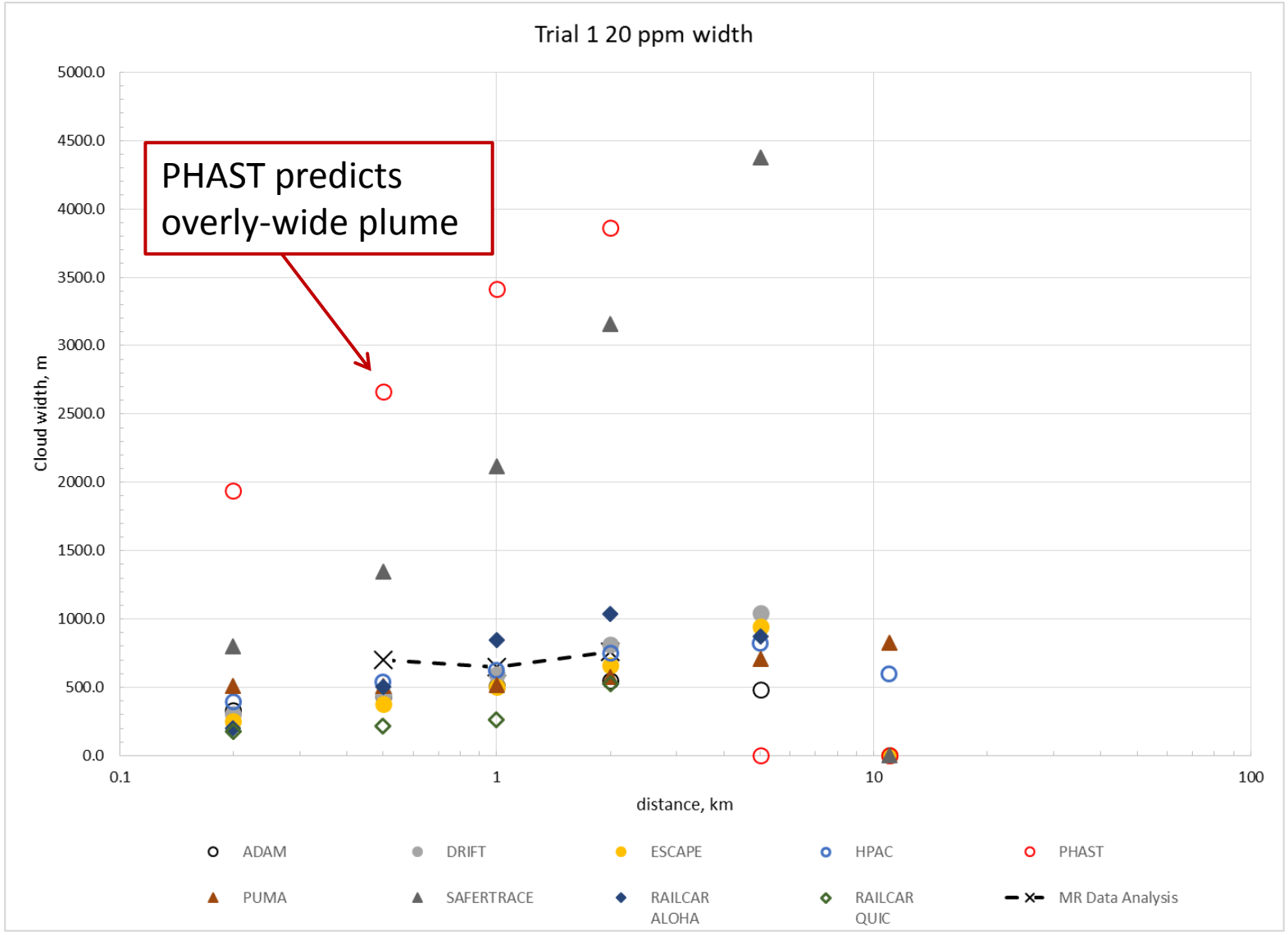
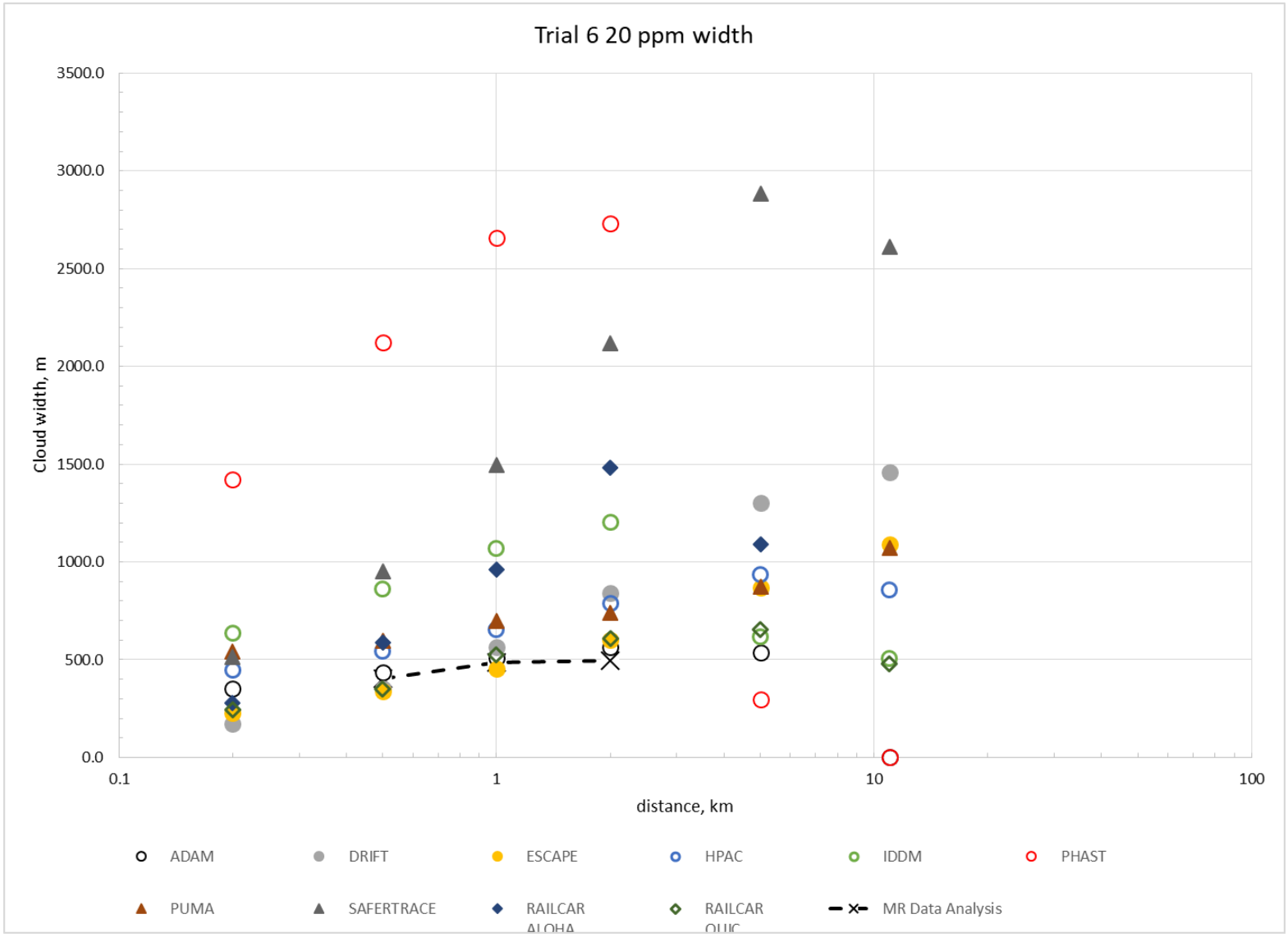


From Mazzola, T. (2019) Jack Rabbit II Analysis of Cloud Dimensions and Inter-model Comparisons, GMU Atmospheric Transport & Dispersion Conference, Fairfax, Virginia, USA, 18 - 20 June 2019

JRII model inter-comparison exercise



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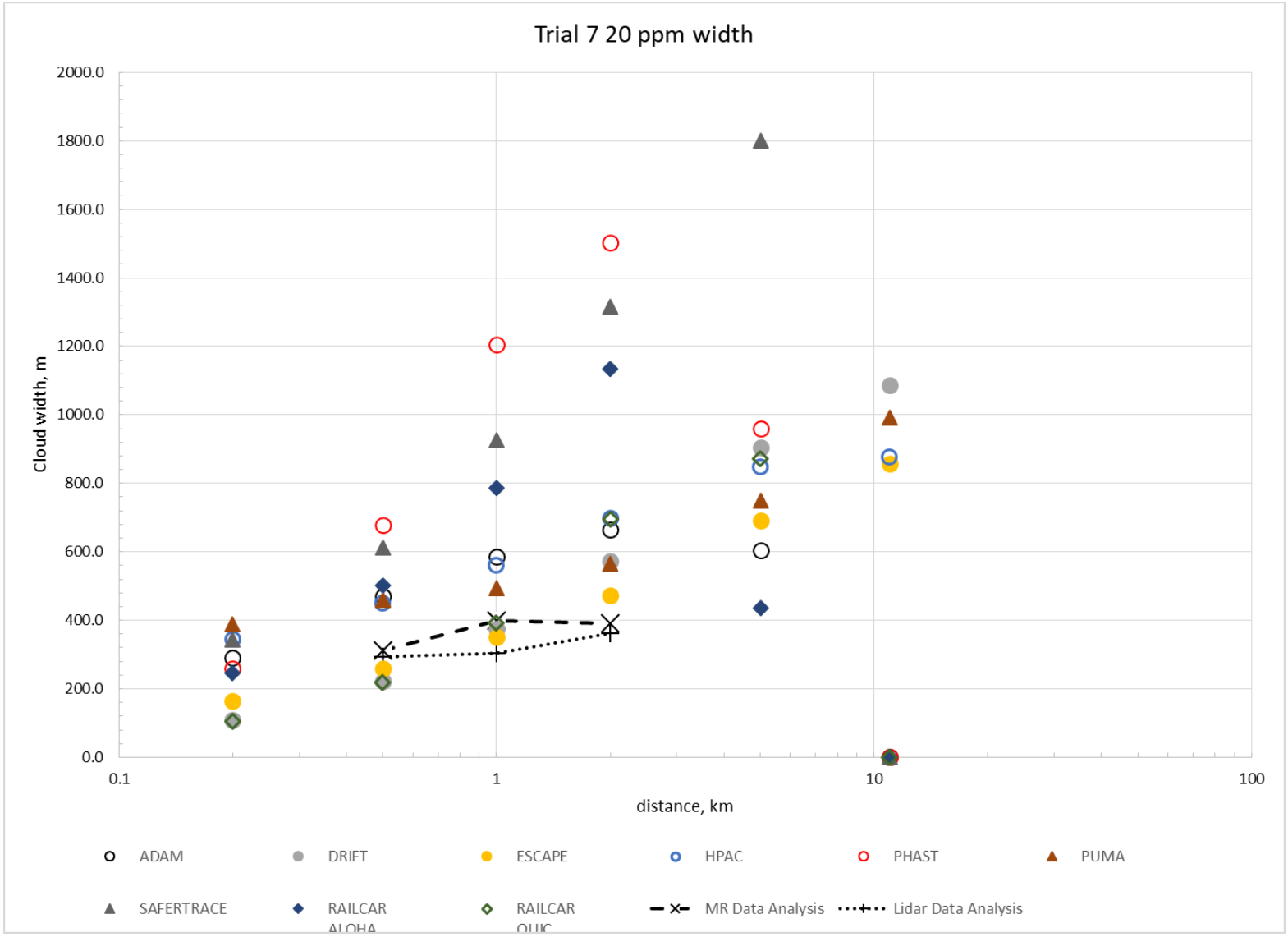
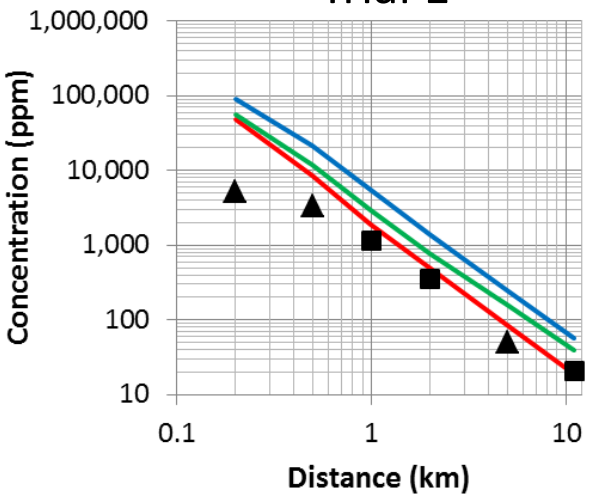


From Mazzola, T. (2019) Jack Rabbit II Analysis of Cloud Dimensions and Inter-model Comparisons, GMU Atmospheric Transport & Dispersion Conference, Fairfax, Virginia, USA, 18 - 20 June 2019

Sensitivity Tests

DRIFT1 (U_{ref}) DRIFT2 (U^*) DRIFT3 (No Deposition) Exp Exp (under-reporting?)

Trial 1

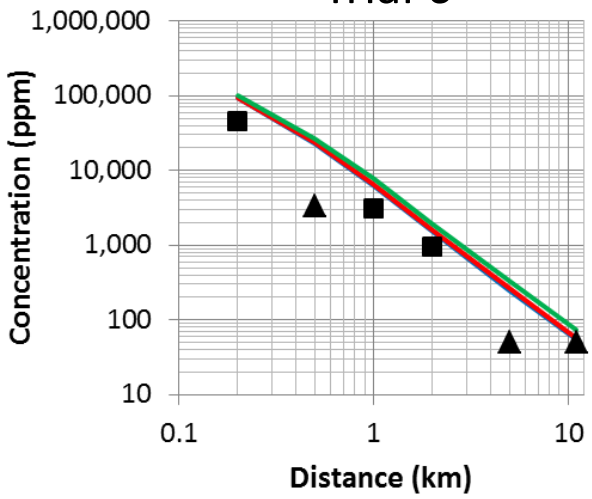


Wind speed and direction: 1.5 m/s

Chlorine mass released: 4.5 t

Mock urban array
Vertically-down release

Trial 6

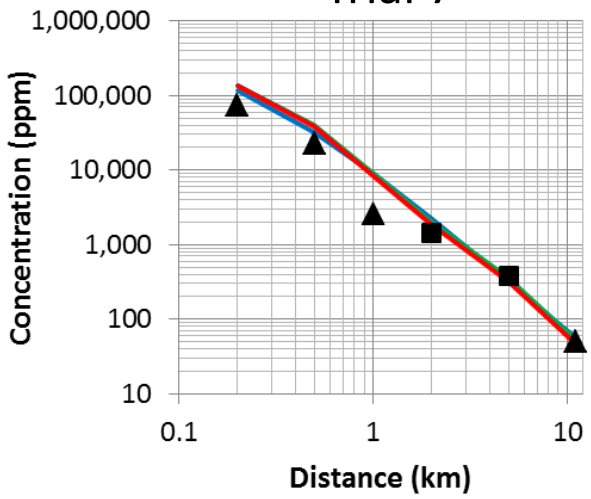


2.4 m/s

8.4 t

Unobstructed
Vertically-down release

Trial 7

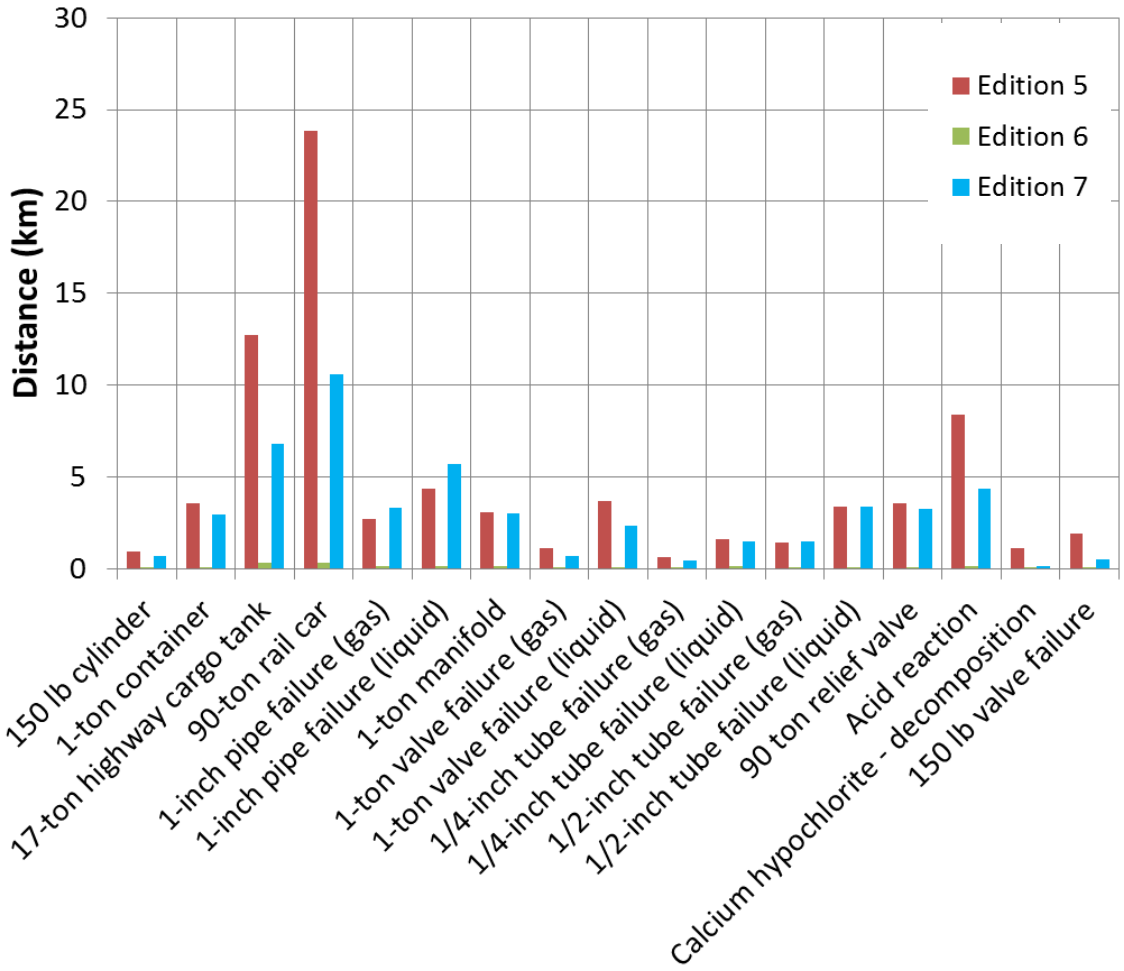


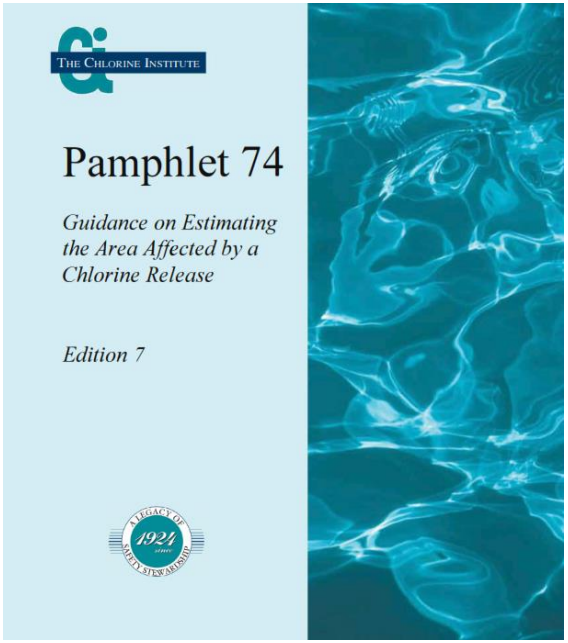
4.0 m/s

8.6 t

Unobstructed
45-deg down release

Chlorine Institute - Pamphlet 74





Comparison shown for worst case (Pasquill Class F) atmospheric stability

FLACS error with chlorine probit

Email received Tuesday 3 December 2019

View this email in your browser

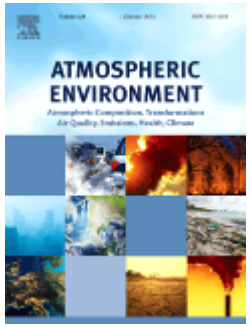
GEXCON SOFTWARE

FLACS v11.0 release information, chlorine issue and new FLACS product manager

Dear FLACS user,

We also need to inform you that we have discovered a **critical issue in the Chlorine Probit values** used in all version of FLACS v9.x and v10.x, which can result in an under-prediction of the TDose, Probit and Lethality output for built in toxic chlorine component. More information about this issue can be found below.

Ongoing Work



- Special JRII issue of Atmospheric Environment journal
  - 15 papers by different groups (deadline 1 Feb 2020)
  - Guest Editors: Steve Hanna and Simon Gant
- Chlorine deposition experiments in a new closed-circuit wind tunnel at Arkansas University
  - Work sponsored by Dept. Homeland Security
  - Contact point: Prof Tom Spicer (tos@uark.edu)

Images © Arkansas University

Future Work?

- Calculate statistical model performance measures
  - Both with/without data-points where sensors under-reported concentrations?
- Model comparisons in terms of toxic dose?
  - Comparison to SLOT/SLOD
- Inter-model comparison for Trials 2, 3, 4, 8, 9?
  - Source conditions and meteorology already defined
  - Uncertainties in Trial 9 as no load cells (road tanker)
- Re-analysis of chlorine railcar incidents?
  - Based on new findings resulting from JRII
- Jack Rabbit III?

Acknowledgements

Sincere thanks to the organisations responsible for funding and managing the Jack Rabbit II trials and the Jack Rabbit II Modeler's Working Group coordinators and participants, in particular:

- Shannon Fox (DHS)
- Ronald Meris (DTRA)
- Thomas Mazzola, John Magerko (Engility/SAIC)
- Steven Hanna (Hanna Consultants)
- Joseph Chang (RAND)
- Andy Byrnes (UVU)
- Thomas Spicer (Arkansas University)
- Richard Babarsky (US Army)
- Nathan Platt, Jeffry Urban and Kevin Luong (IDA)
- Jeffrey Weil (NCAR)
- Luca delle Monache (NCAR/UCSD)
- John Boyd (ARA)
- Steven Herring and Joel Howard (DSTL)

HSE Team

- Graham Tickle (GT Science and Software)
- Harvey Tucker, Adrian Kelsey, Maria Garcia, Bryan McKenna (SEPA), James Stewart, Alison McGillivray, Rachel Batt, Mike Wardman

GT Science & Software contributed towards the work on DRIFT, but the DRIFT simulations presented in this paper were performed by HSE and have not been independently checked by the software developer. The work presented here was funded by HSE. The contents, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy.