DRIFT Dispersion Model Predictions for the Jack Rabbit II Model Inter-Comparison Exercise

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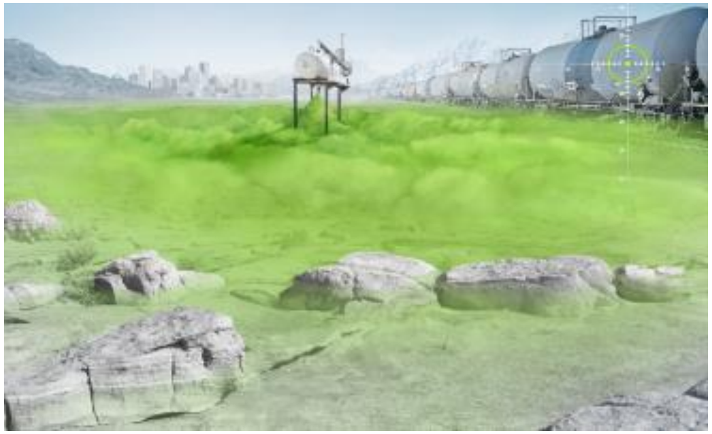
Outline

- Background
- Overview of DRIFT
  - Model capabilities
  - Configuration for JRII model inter-comparison exercise
- Results
- Summary and possible future work

Jack Rabbit II Trials (2015 – 2016)

Aims

- Conduct large-scale chlorine release experiments
- 10 – 20 ton chlorine releases (inc. road tanker)
- Mock urban array of obstacles
- Different release orientations
- Dispersion measurements to 11 km downwind
- Infiltration into buildings and vehicles
- Measure key source terms parameters
- Study effect of chlorine on emergency responders' equipment



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Impact

- Modelling – improve source term, dispersion, deposition, infiltration models
- Resiliency – inform planning, emergency response and policy
- Vulnerability and impact reduction – improve hazard and risk mitigation

Background

Aims of HSE's involvement in Jack Rabbit II

- Contribute modelling results and help support Jack Rabbit II project
- Validate HSE's regulatory dispersion model (DRIFT)
- Assess capabilities of other widely-used dispersion models
- Collaborate with experts in the Modelers Working Group and share findings

Benefits of model inter-comparison exercise

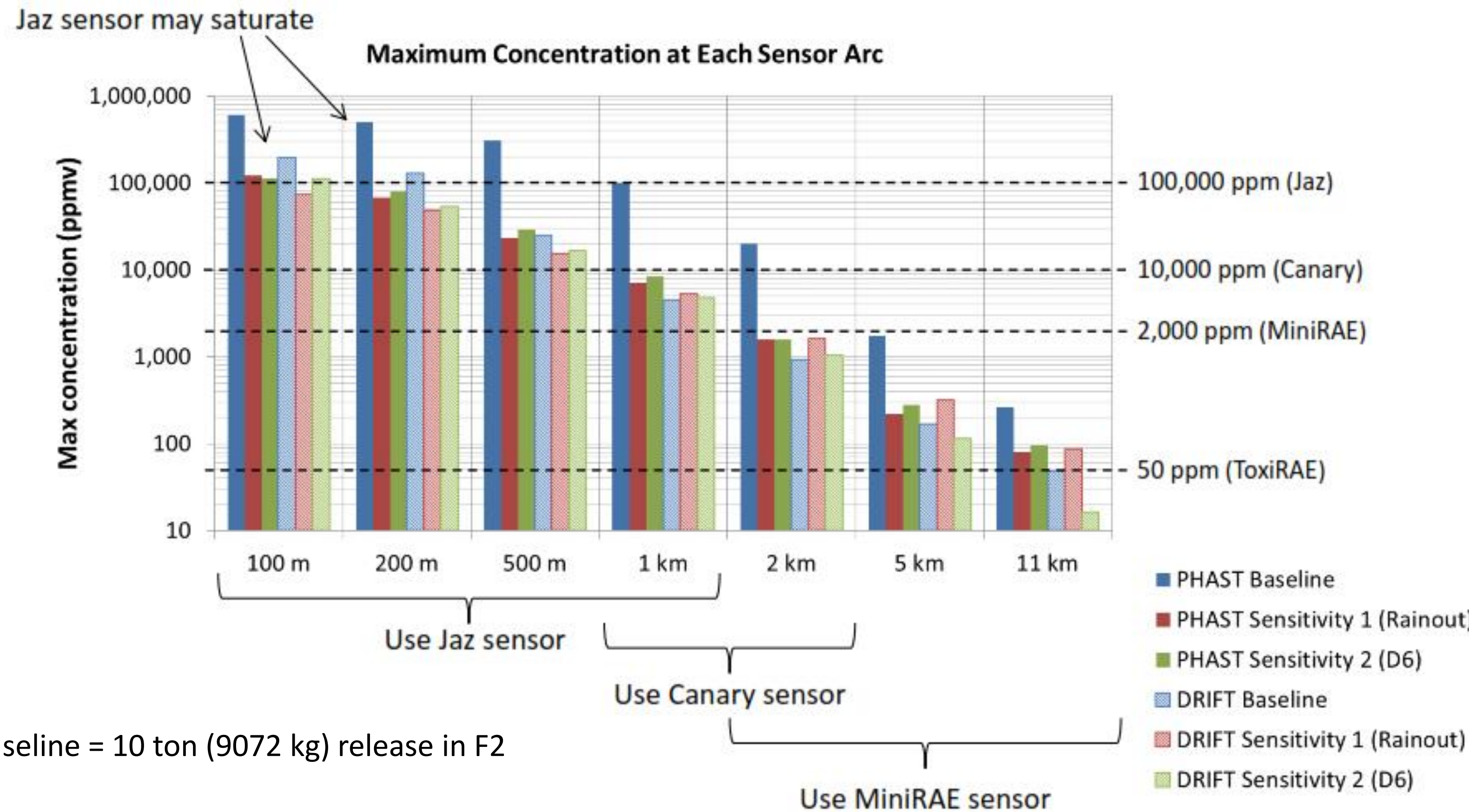
- Benchmark models to experimental data using standardized inputs and outputs
- Understand strengths/weaknesses of different modelling approaches
- Collaborate and ultimately help to develop improved models

Aims of this presentation

- Explain DRIFT configuration for model inter-comparison exercise
- Present short summary of results

Background

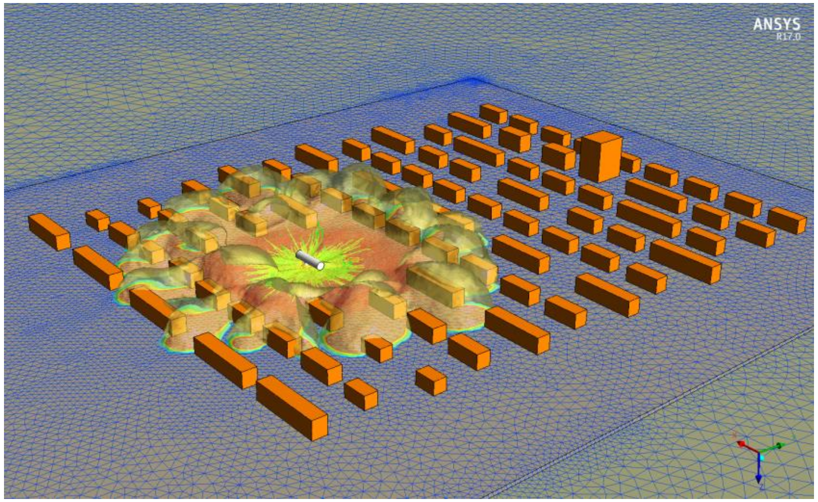
Previous work: HSL predictions prior to the 2015 trials to help the positioning of sensors

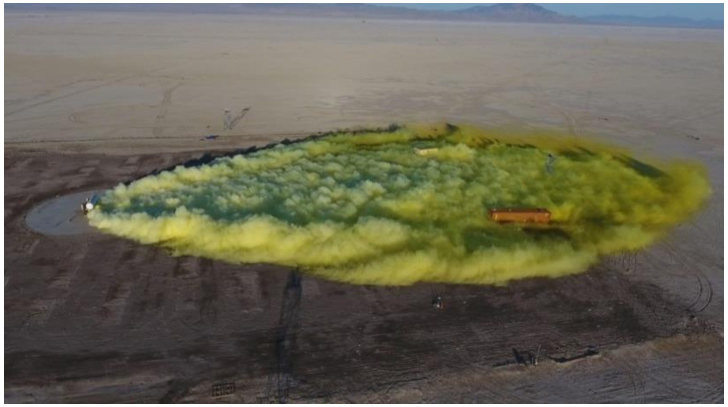


Baseline = 10 ton (9072 kg) release in F2

Background

Previous work: CFD simulations to help understand the near-field flow behaviour in the JRII 2015 and 2016 trials





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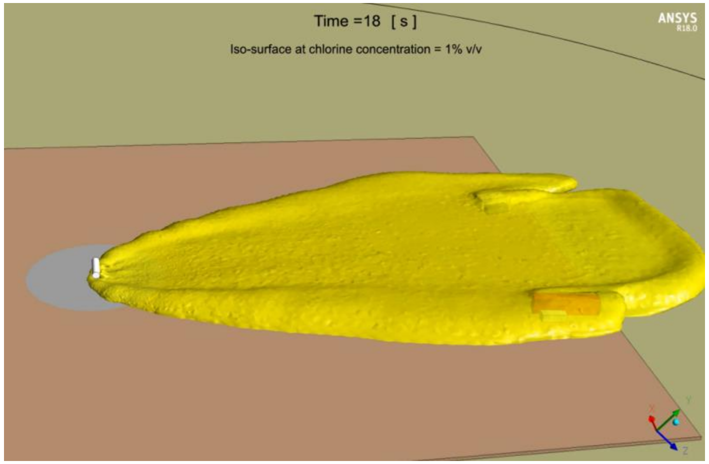
http://www.uvu.edu/esa/jackrabbit/



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DRIFT model: capabilities

DRIFT is an integral model

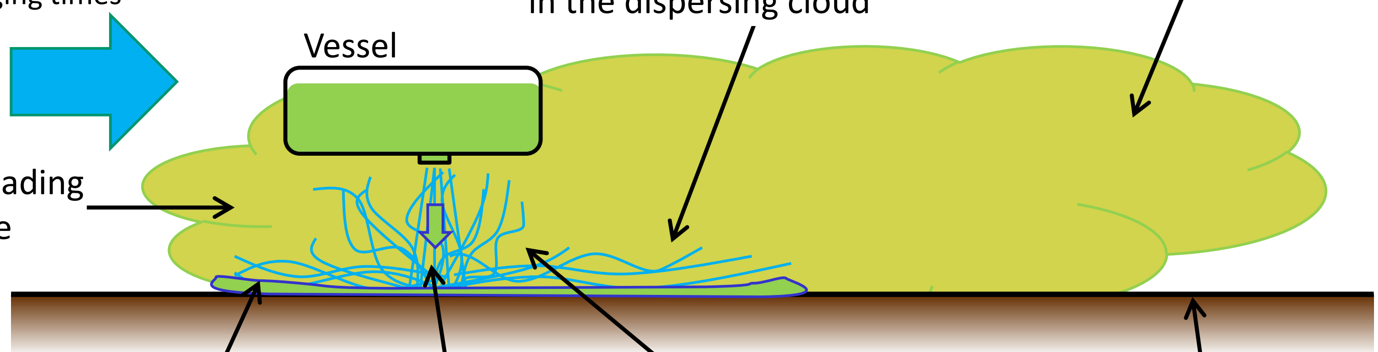
Constant mean wind speed and direction

Meander affects plume width for longer averaging times

Evaporating aerosol of chlorine droplets and condensed water vapour in the dispersing cloud

Along-wind diffusion and gravity spreading

Initial gravity spreading and dilution of the source



GASP pool spread and evaporation

Model accounts for heat transfer: conduction from ground (inc. ground cooling effects), air convection and thermal radiation

Two-phase jet

DRIFT does not account for additional turbulence and re-entrainment at impingement

Flat terrain with uniform aerodynamic roughness and specified dry deposition velocity

DRIFT may over-predict concentrations for short-duration releases in far-field due to its use of smaller Froude number for gravity spreading derived for continuous releases

DRIFT and GASP are hard-wired to use an atmospheric pressure of 101,325 Pa and cannot use the lower atmospheric pressure measured at Dugway Proving Ground in the Jack Rabbit II trials

JRII Model Inter-Comparison Exercise

Specified input conditions:

Version 0.4, 17 May 2018

Jack Rabbit II Coordinated Model Comparisons to Data
Initial Specification for Modelers

INTRODUCTION

PURPOSE AND OBJECTIVES

The aim of this information note is to specify the model inputs and outputs required to run an inter-model comparison exercise using the Jack Rabbit II data. This note concentrates on three of the nine JRII trials (Trials 1, 6 and 7). The reason for selecting these trials is that they involved different initial jet directions and/or the presence or absence of the mock-urban CONEX grid. Trial 1 involved a downwards-directed jet release within the mock-urban CONEX grid, Trial 6 involved the same release orientation but without the mock urban CONEX grid, and Trial 7 involved a release directed at 45 degrees downwards from the horizontal and azimuthally aligned with the prevailing winds and grid centerline, again without the mock-urban CONEX grid. These initial trials for comparison are further characterized under Release Parameters in Table 1. If there is sufficient interest in this first modeling exercise, other JRII trials may be selected for future model inter-comparisons.

The objectives of the intended inter-model comparison exercise are:

- More broadly disseminate a best understanding of the Jack Rabbit II data base
- Provide for a consistent comparison of models to data; as many models as possible; to inform the community and to provide a basis for model improvement where needed
- Provide a forum for technology transfer to the chlorine industry concerned with risk management
- Encourage collaboration among modelers, which should lead to improved models all-around.

File "JRII Model Comparison Specifications_REVISED 17May18b.docx"
in email from Tom Mazzola, 17 May 2018

Table 1. Complete set of inputs provided to modelers.

	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 C12)	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			
Weather conditions			
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
Vertical profiles of wind speed and direction and temperature[4]			
Inverse Monin-Obukhov length (m^{-1})	0.124	0.056	0.0229
Pasquill Class[5]	E/F	E	D/E

* - Trial 7 primary release shown. Secondary or "dump" release will be defined separately.
1 – The liquid in the tank should be considered at a saturated state and these experimental best numbers adjusted to assure that as needed by the analyst
2 – Initial wind is a 10 minute average at time of release initiation. More detail available in reference 7 and 8. Wind direction is the direction from which the wind blows in degrees clockwise from true North.
3 – Turbulent boundary layer parameters from 30 min average data at time of release. More detail available in reference 7.
4 – Vertical profiles of wind speed, wind direction and temperature are provided in reference 8.
5 – If the dispersion model has an option to use either Monin-Obukhov length or Pasquill Class to specify the atmospheric stability, please use the Monin-Obukhov length for consistency.

Table 2. Averaged source emission rates and parameters.

	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

DRIFT model: setup for JRII simulations

	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/m³)	18.3	18.2	18.1
Velocity (m/s)	50.8	44.2	44.2
Area (m²)	0.241	0.324	0.323
Primary release modified for rainout			
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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/m³)	3.16	3.15	3.14
Area (m²)	491	491	491

DRIFT uses -33.7 °C at standard atmospheric pressure of 101,325 Pa

Blue = DRIFT input

Red = DRIFT uses a different value

Green = Calculated internally by DRIFT (not prescribed)

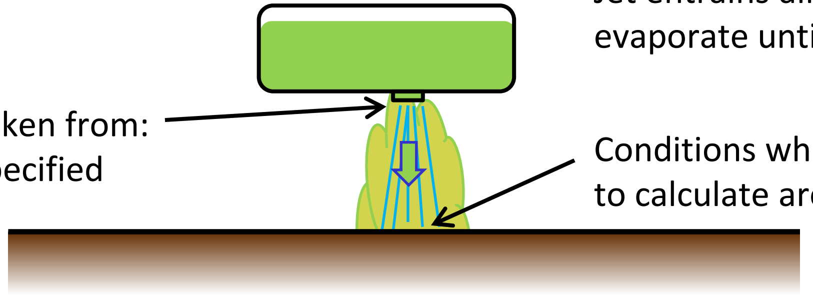
Black = Not used

From file: “JRII Model Comparison Specifications_REVISED 17May18b.docx “

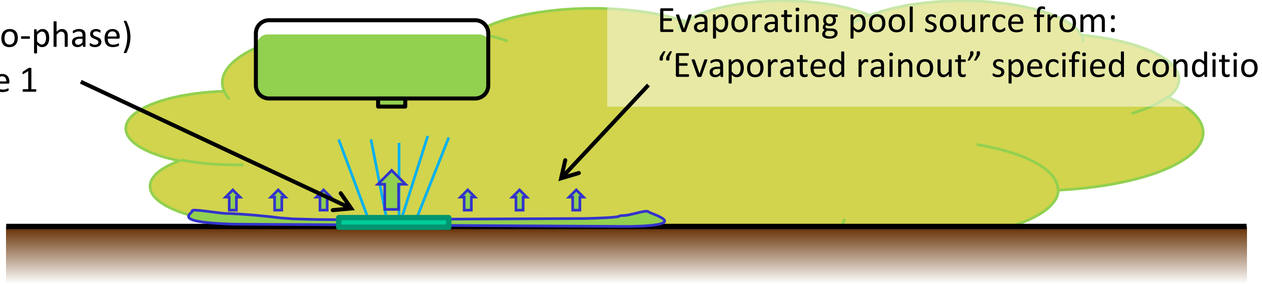
DRIFT model: setup for JRII simulations

Two-stage modelling process:

1.) Two-phase jet



2.) Dispersion

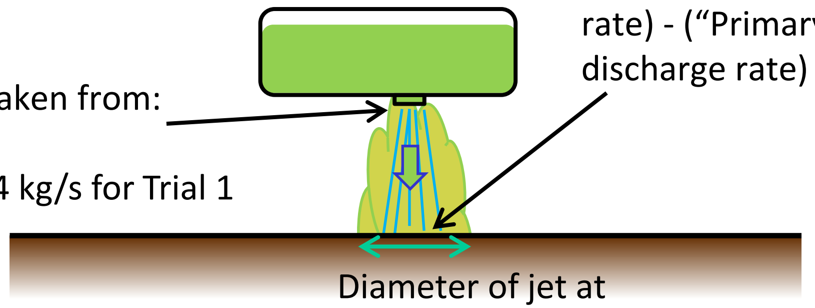


DRIFT model: setup for JRII simulations

Two-stage modelling process:

1.) Two-phase jet

Source conditions taken from:
"Primary release"
discharge rate = 224 kg/s for Trial 1



Rainout mass rate = ("Primary release" discharge rate) - ("Primary release modified for rainout" discharge rate) = 224 - 145 = 79 kg/s for Trial 1

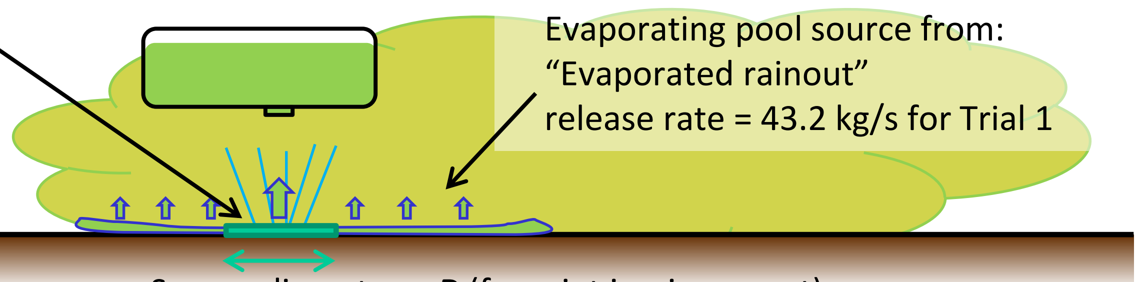
i.e. the rainout mass fraction = 79/224 = 35% for Trial 1

Diameter of jet at impingement, *D*

2.) Dispersion

Area source (two-phase) from jet in Stage 1

- Dispersed liquid droplet mass fraction accounts for rainout in impinging jet
- Condensed liquid water phase accounts for water lost in rainout
- Entrained air in impinging jet from Stage 1 is retained in area source for Stage 2



Evaporating pool source from:
"Evaporated rainout"
release rate = 43.2 kg/s for Trial 1

Source diameter = *D* (from jet impingement)

DRIFT grows this diameter *D* using its model for upwind spreading at the source (due to gravity spreading only)

DRIFT model: setup for JRII simulations

Meteorological conditions:

	Trial 1	Trial 6	Trial 7
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
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Vertical profiles of wind speed and direction and temperature[4]			
Inverse Monin-Obukhov length (m^{-1})	0.124	0.056	0.0229
Pasquill Class[5]	E/F	E	D/E

DRIFT standard atmospheric pressure of 101,325 Pa

See next slide

From file: “JRII Model Comparison Specifications_REVISED 17May18b.docx “

Blue = DRIFT input

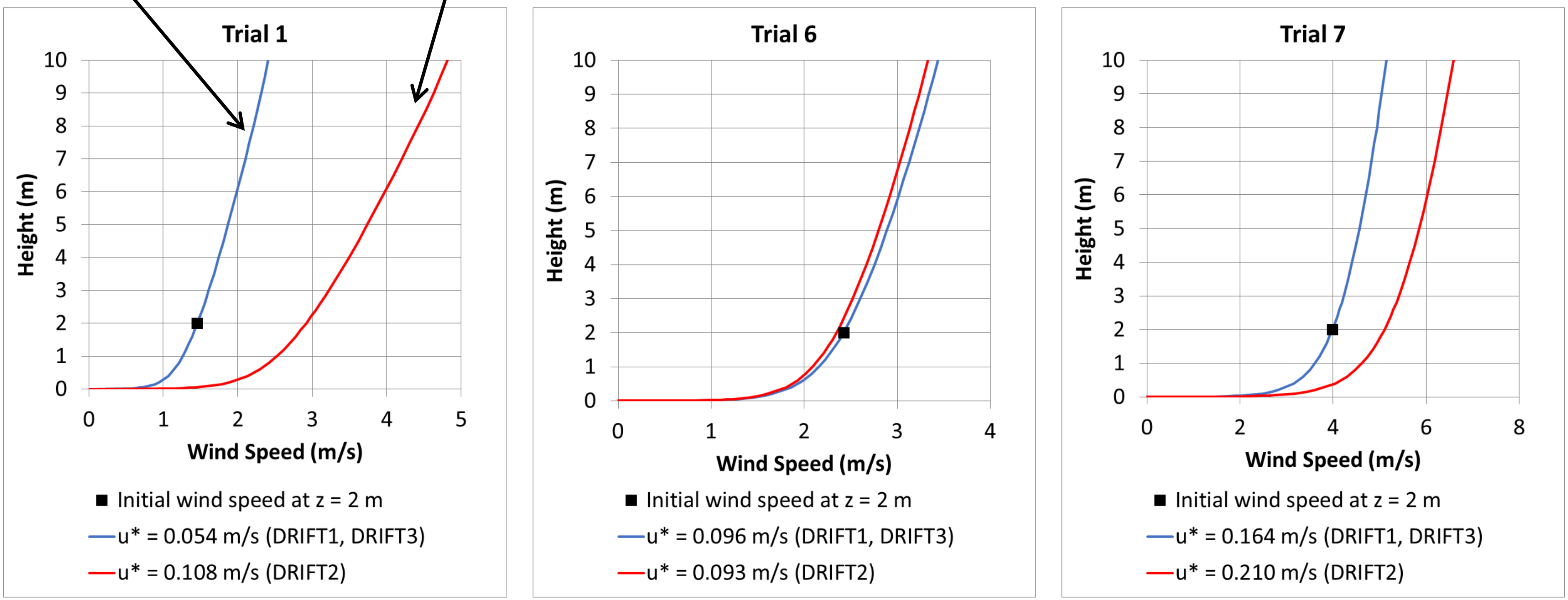
Red = DRIFT uses a different value

Black = Not used

DRIFT model: setup for JRII simulations

Wind speed profile defined using reference wind speed at 2 m height

Wind speed profile defined using specified friction velocity



DRIFT uses a standard log-law velocity profile with modifications for atmospheric stability in the surface layer from Businger (1973)

DRIFT model: setup for JRII simulations

Three sets of DRIFT results submitted to the model inter-comparison exercise:

1. **DRIFT1** = Baseline case: atmospheric wind profile based on the specified value of "**Initial wind speed at z = 2m**"

2. **DRIFT2** = Atmospheric wind profile based on the specified "**Friction velocity (u*)"**, instead of the initial wind speed at z = 2 m

3. **DRIFT3** = **Same as DRIFT1 baseline case but with dry deposition switched off**, by changing the deposition velocity from v_d = 0.04 cm/s (in DRIFT1 and DRIFT2) to v_d = 0.0 cm/s (in DRIFT3).

DRIFT model: setup for JRII simulations

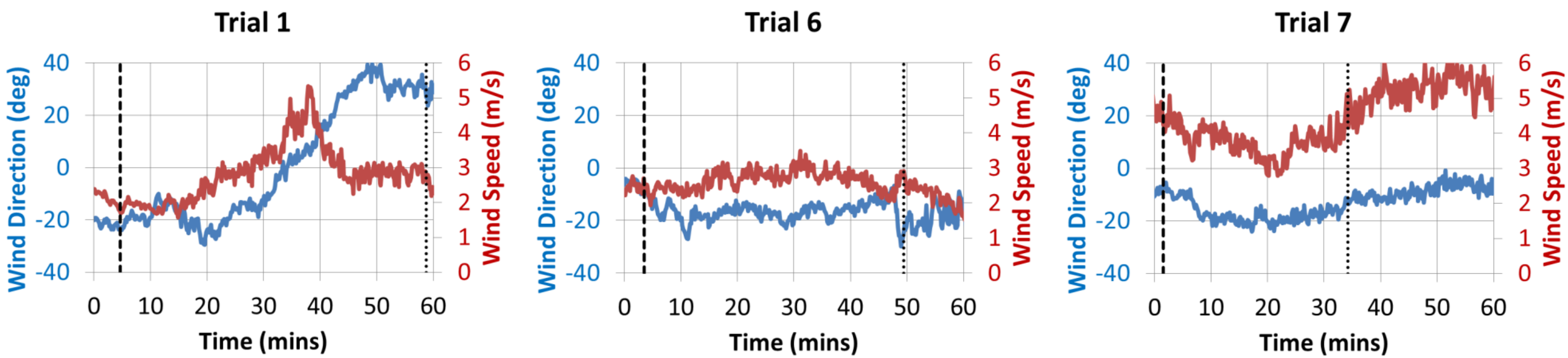
Other DRIFT model inputs:

- Ground surface roughness, z_0 = 0.5 mm
  - No account taken of mock urban array in Trial 1
  - Sensitivity tests could be performed to investigate this matter later
  - Previous DRIFT results presented at GMU conference and Harmo-18 used a high roughness length of z_0 = 0.4 m in first 100 m downwind of release point to account for presence of mock urban array (increased mixing and dilution)

- Fixed wind speeds and atmospheric stability for the duration of each trial, not changing over time like in the experiments

Measured wind speed and direction

Wind measurements taken by PWIDS 19, located 100 m upwind of release point



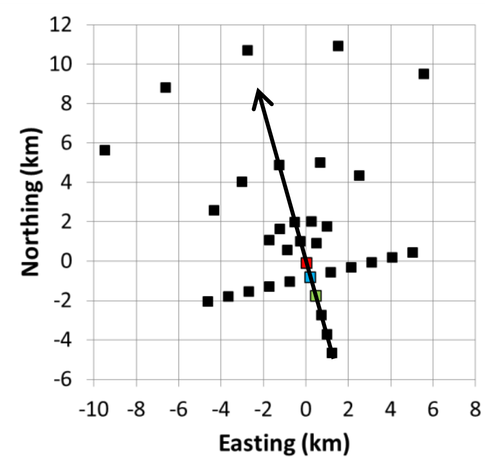
— Wind speed

— Wind direction

--- Arrival time of max concentration at 500 m arc

...... Arrival time of max concentration at 11 km arc

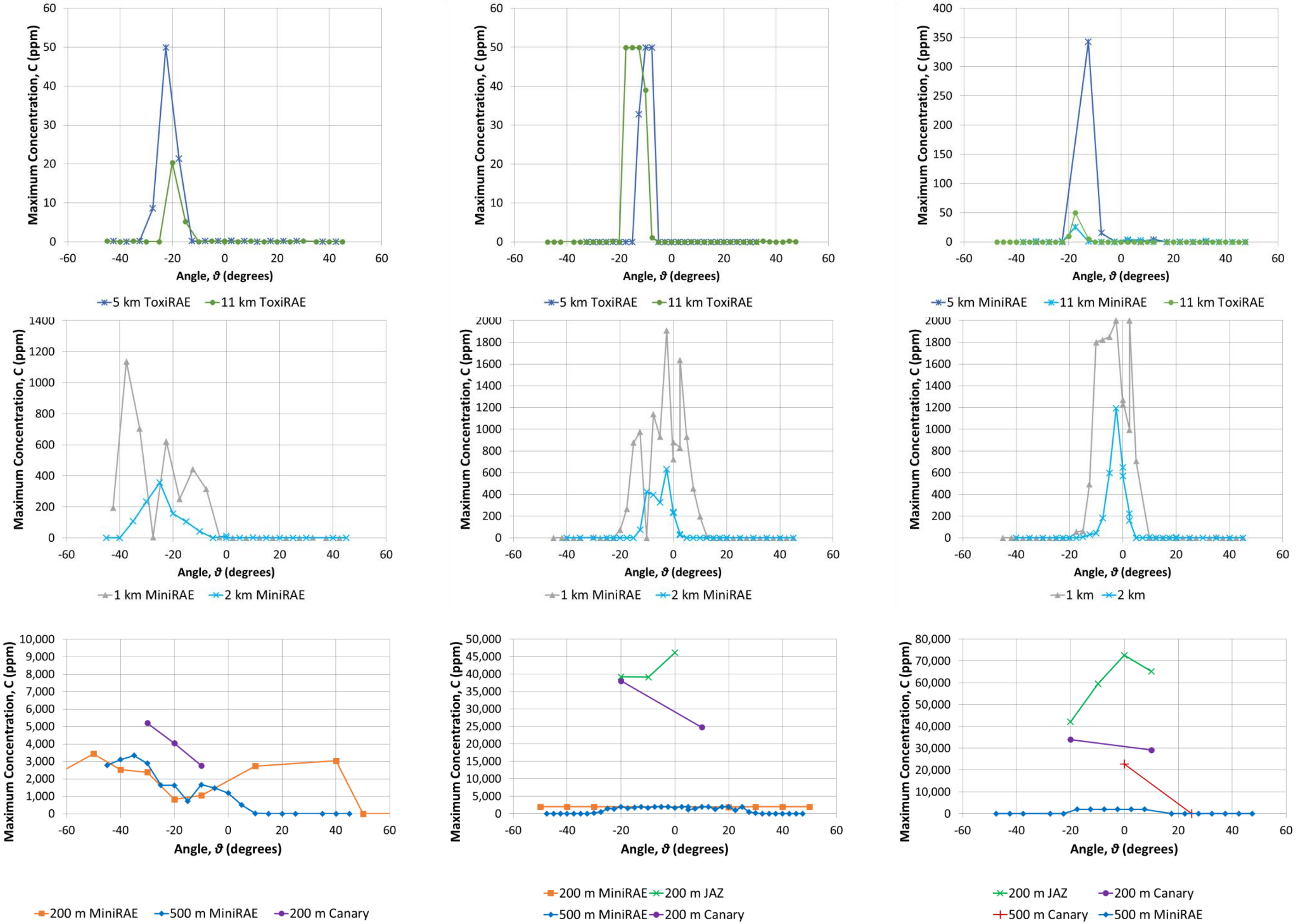
Wind direction is given relative to sensor axis of 345°
i.e. angle = 0° is along centerline of sensor array



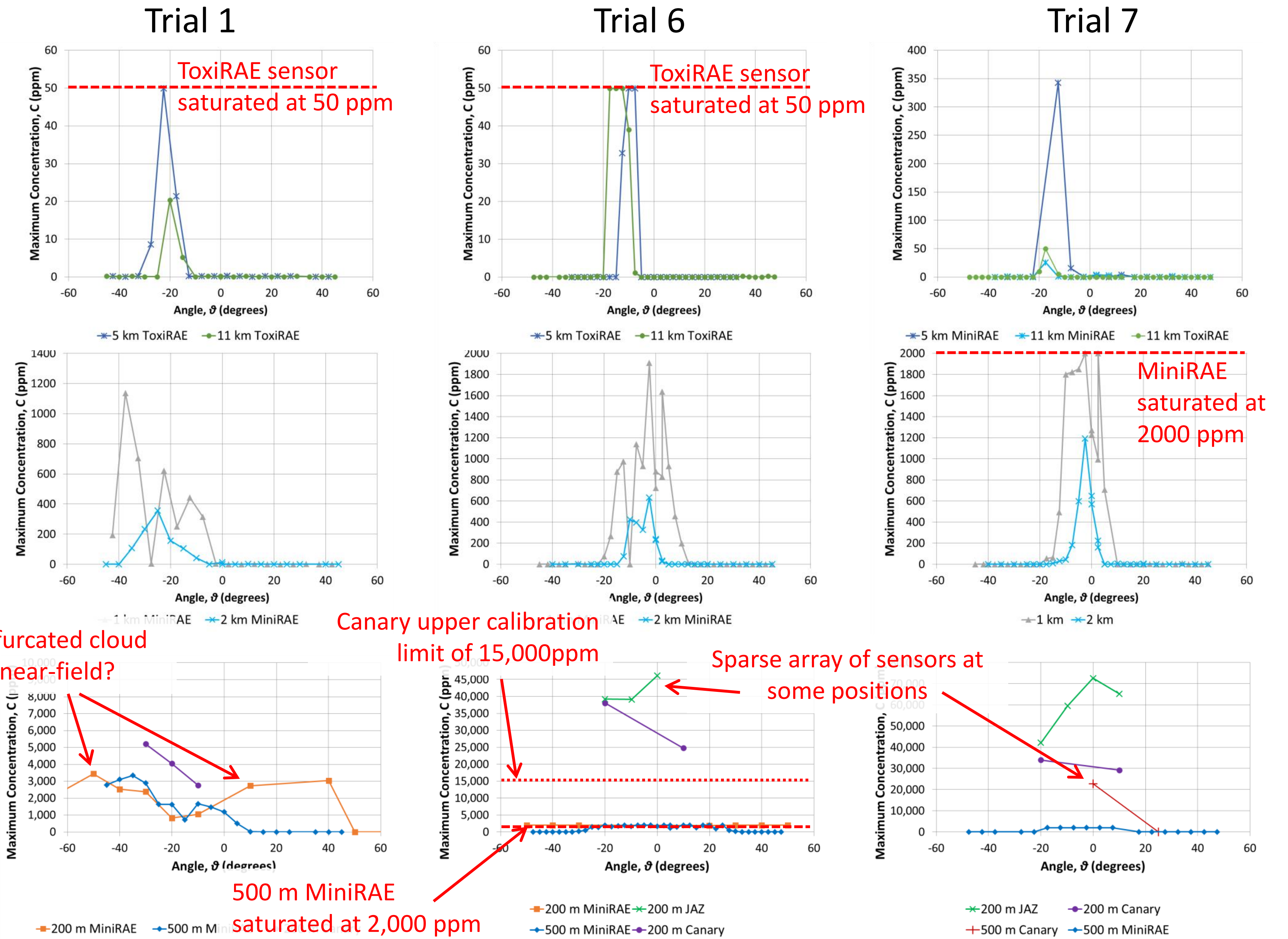
Outline

- Background
- Overview of DRIFT
  - Model capabilities
  - Configuration for JRII model inter-comparison exercise
- Results
  - Quick review of experimental data
  - Maximum arc-wise concentrations
  - Contour plots
- Summary and possible future work

Trial 1 | Trial 6 | Trial 7

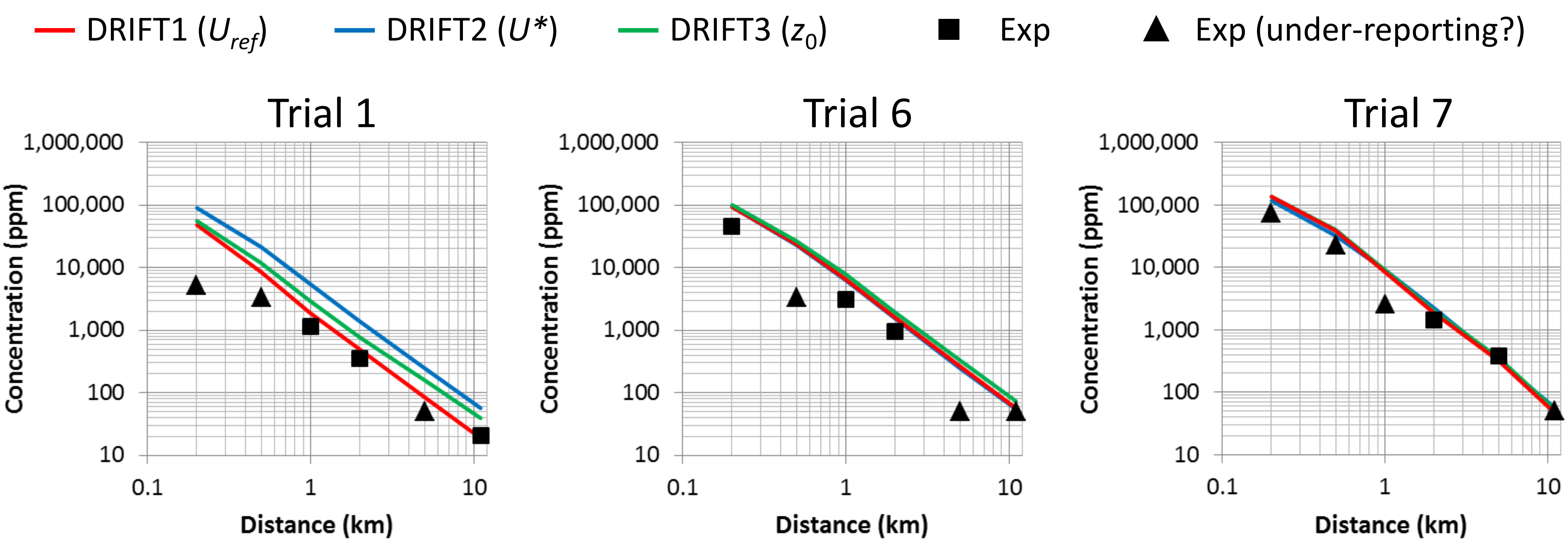


NB. Trial 6 and 7 MiniRAE data not scaled in response to pre/post calibration tests



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

Maximum Arc-Wise Concentration



Wind speed and direction

1.5 m/s

2.4 m/s

4.0 m/s

Chlorine mass released

4.5 t

8.4 t

8.6 t

Mock urban array
Vertically-down release

Unobstructed
Vertically-down release

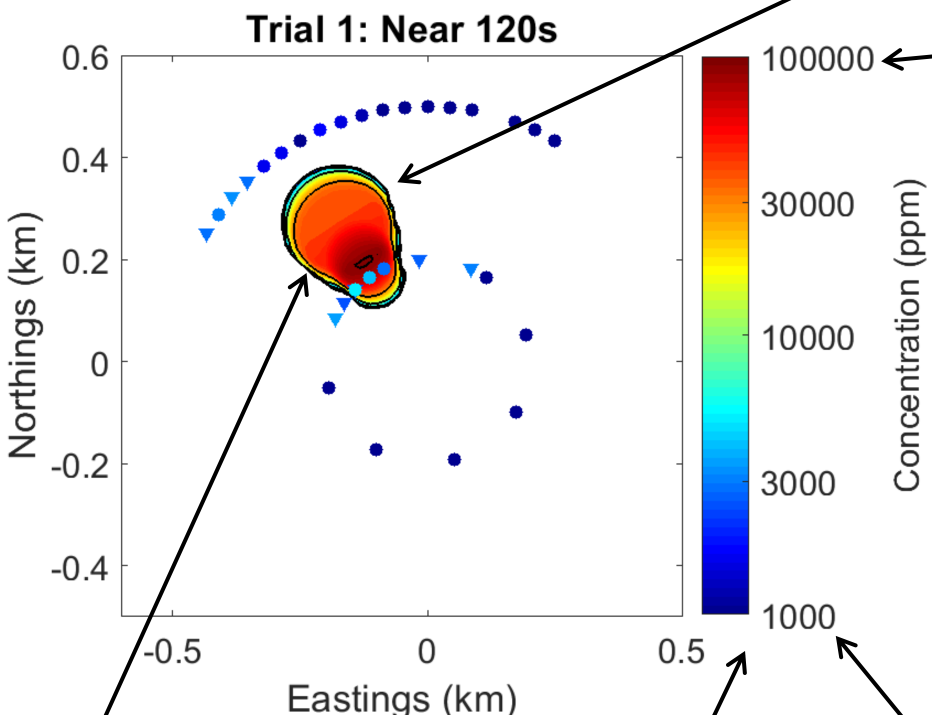
Unobstructed
45-deg down release

Concentration Contours

Key to plots shown on subsequent slides

Contours show predicted concentration at the specified time (t = 120 s in this case)

Example plot:



Predicted concentrations above upper scale limit (100,000 ppm here) are shown as red

Symbols show maximum measured concentration over all time at that location (not at the specified time). Symbol color scale matches the contours

- ▼ Triangles indicate sensor saturated (concentration may be higher than indicated)
- ● Circles indicate sensor did not saturate

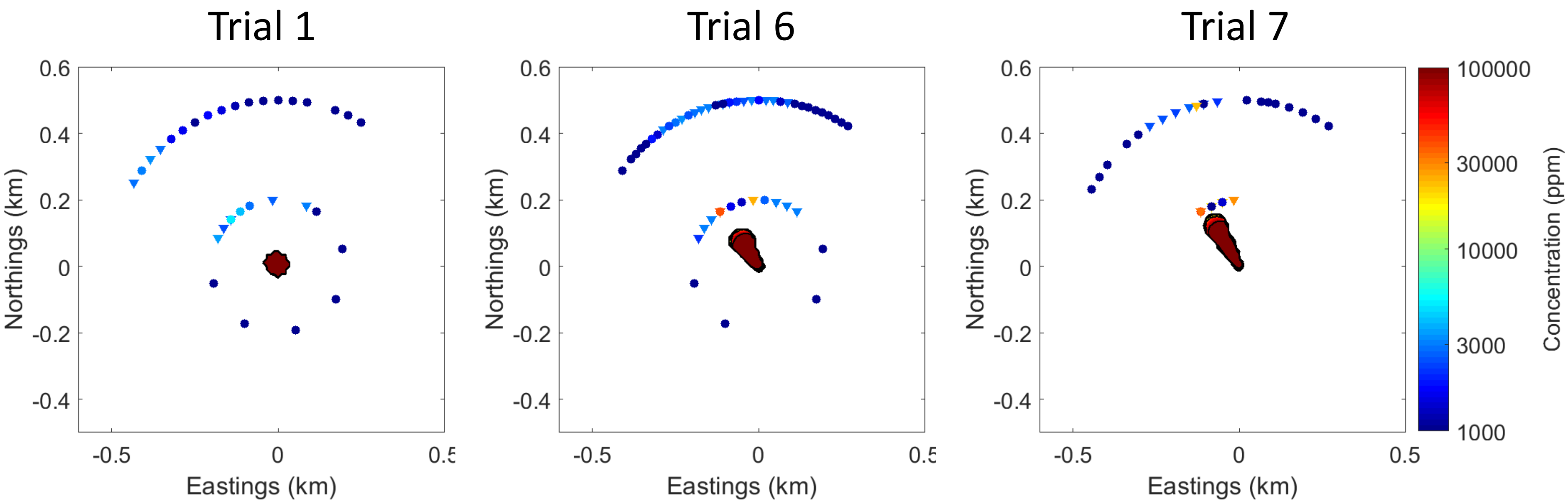
Any sensors that measured noise (not signal) have been set to zero concentration

Black contour lines highlight the 5 set levels: 1000, 3000, 10000 etc.

Color scale is logarithmic, not linear

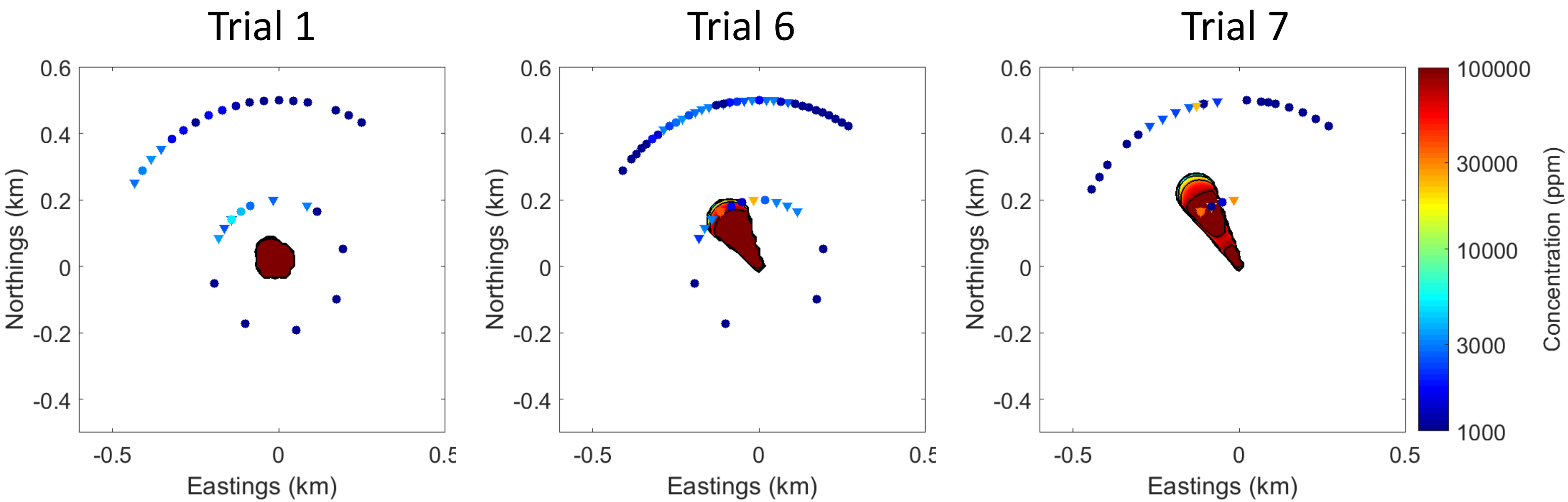
Predicted concentrations below lower scale limit (1,000 ppm here) are not shown, i.e. contour limits are clipped to this lower bound so that background appears white, not blue

Near-field: time = 30 s



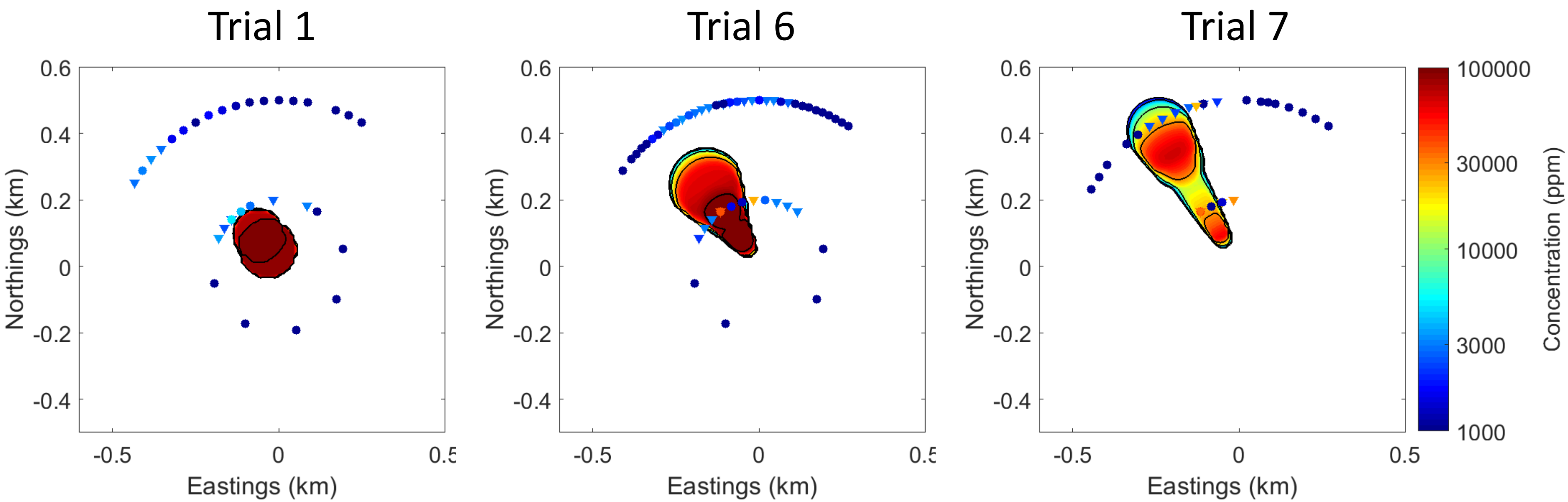
All results are for the DRIFT1 model using the specified reference velocity at 2 m height

Near-field: time = 60 s



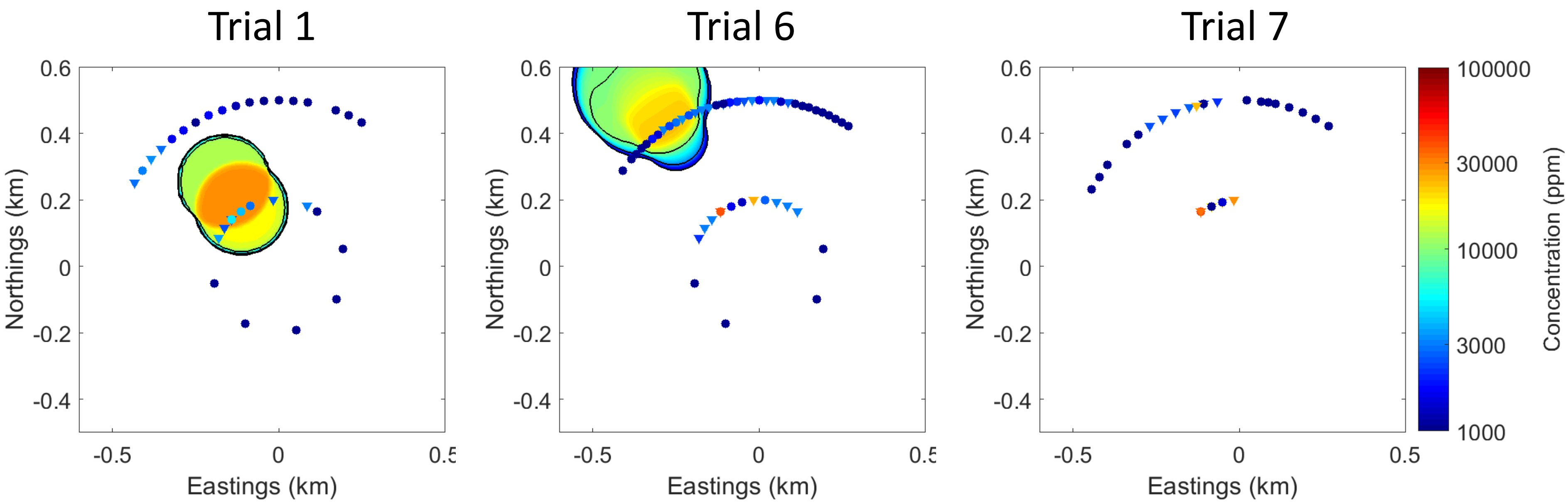
All results are for the DRIFT1 model using the specified reference velocity at 2 m height

Near-field: time = 120 s



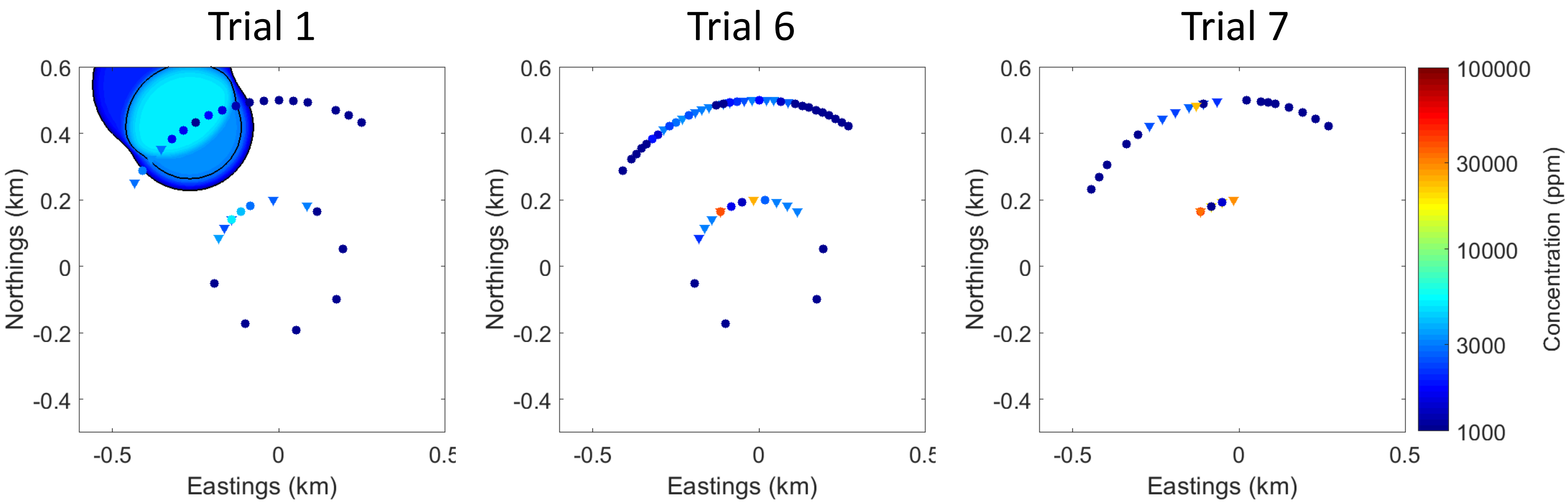
All results are for the DRIFT1 model using the specified reference velocity at 2 m height

Near-field: time = 300 s



All results are for the DRIFT1 model using the specified reference velocity at 2 m height

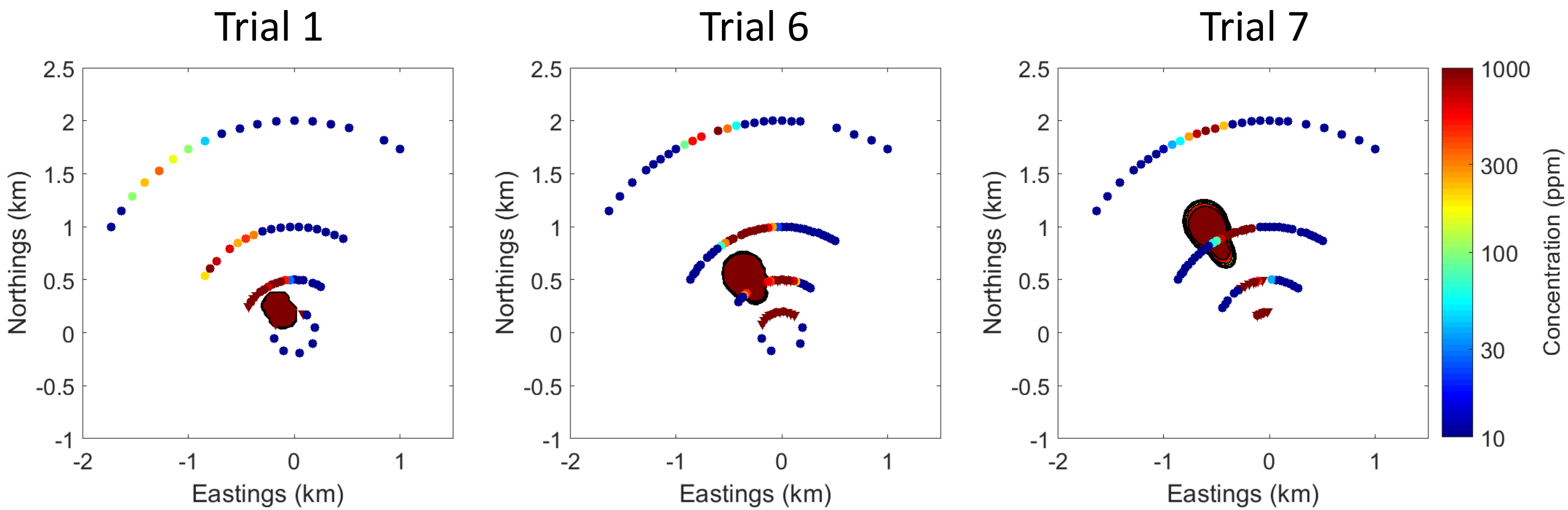
Near-field: time = 600 s



All results are for the DRIFT1 model using the specified reference velocity at 2 m height

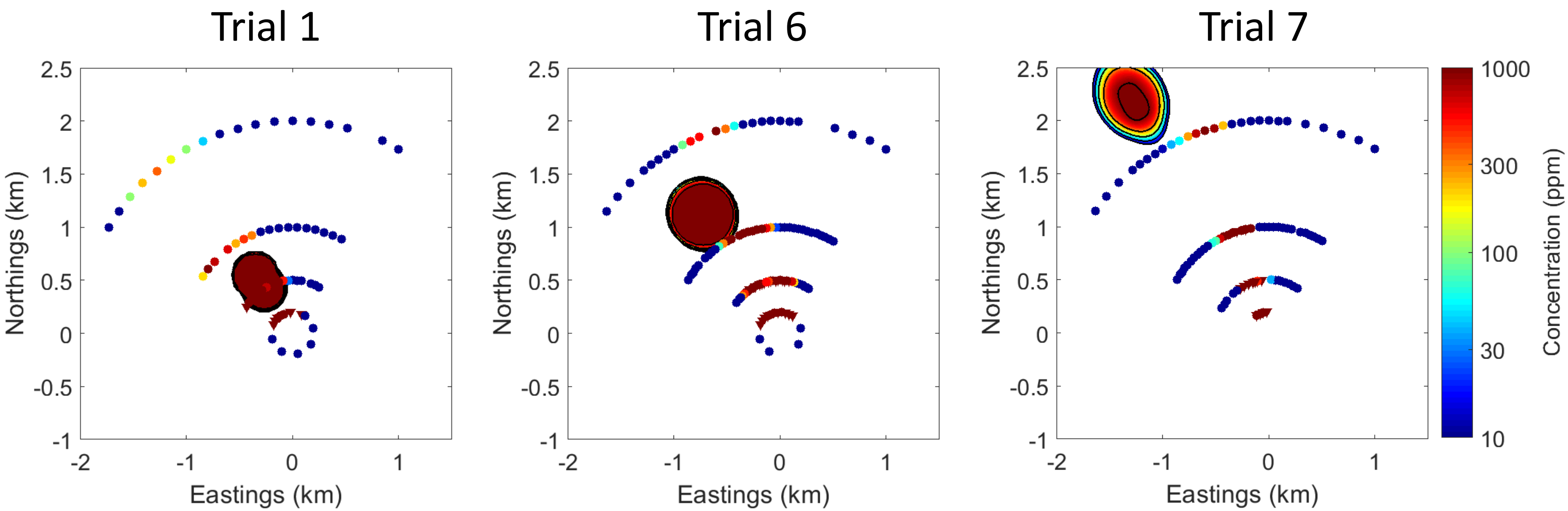
Mid-field

Mid-field: time = 300 s



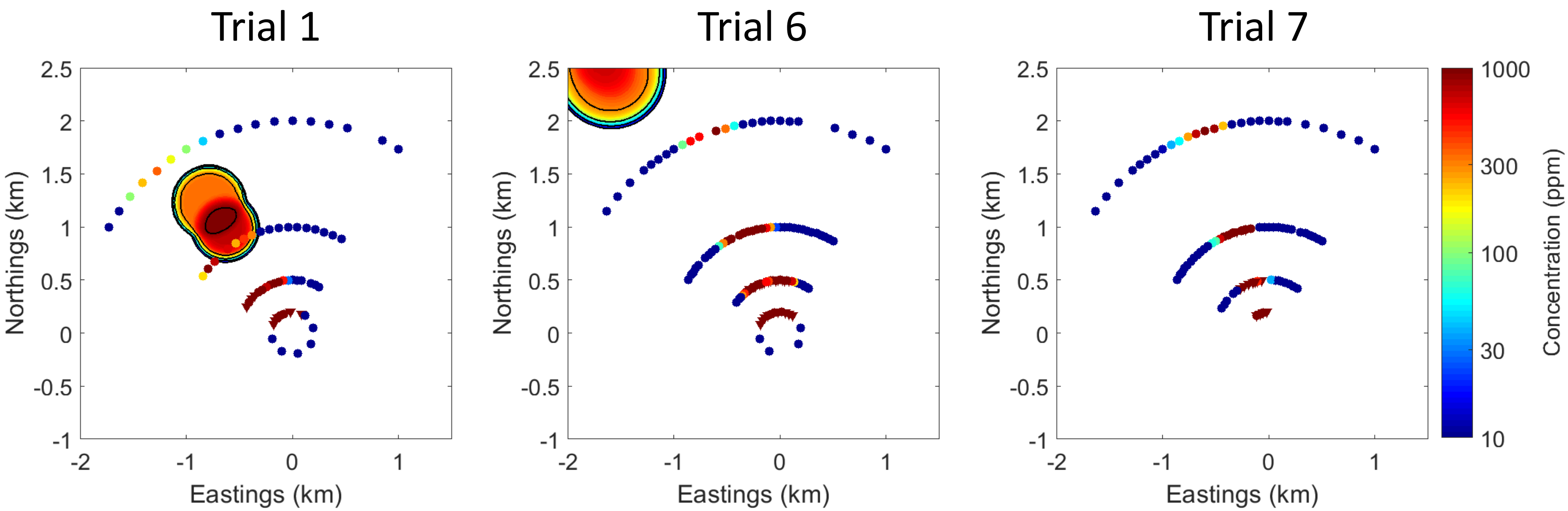
All results are for the DRIFT1 model using the specified reference velocity at 2 m height

Mid-field: time = 600 s



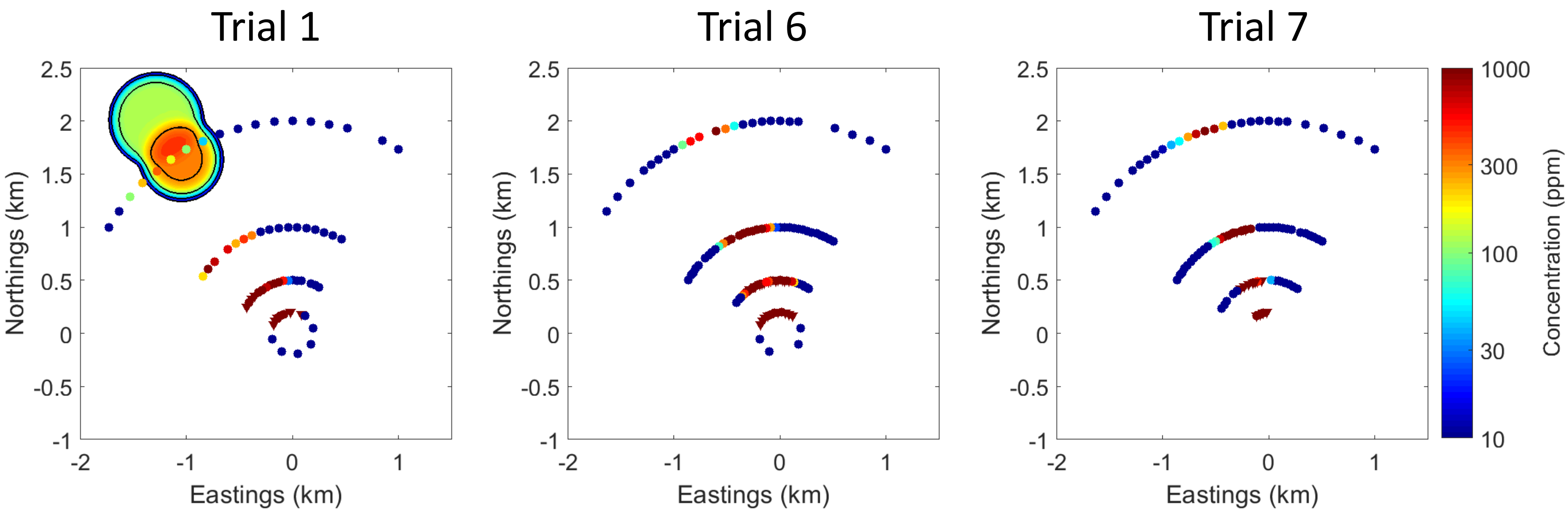
All results are for the DRIFT1 model using the specified reference velocity at 2 m height

Mid-field: time = 1200 s



All results are for the DRIFT1 model using the specified reference velocity at 2 m height

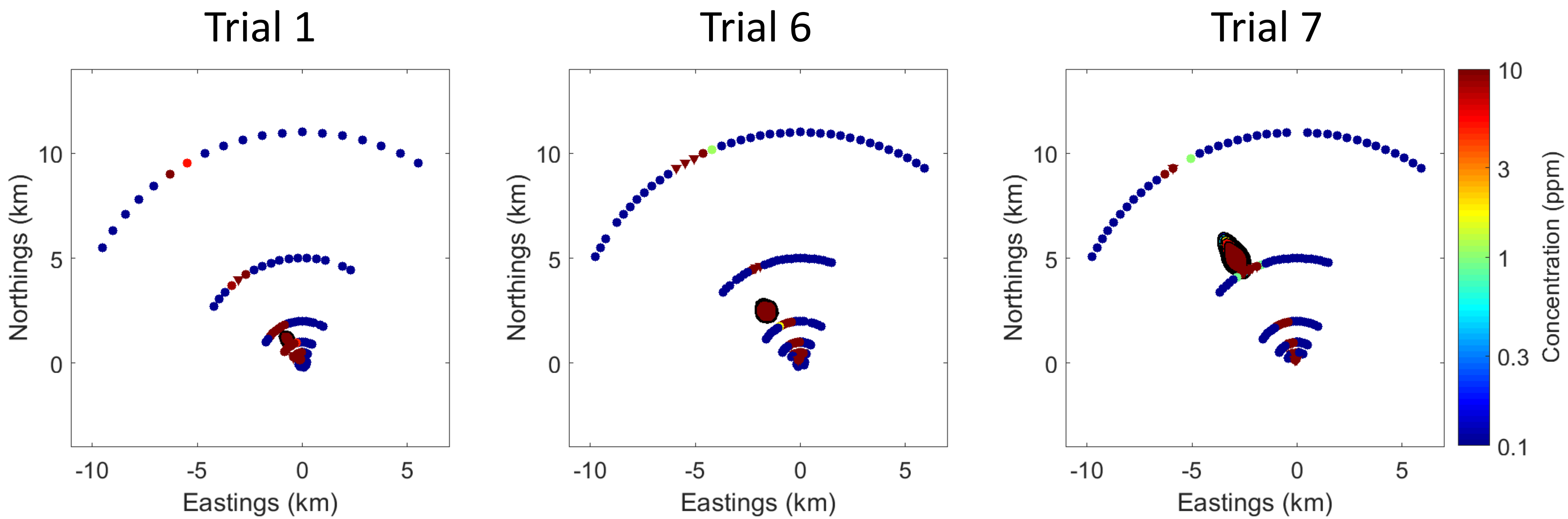
Mid-field: time = 1800 s



All results are for the DRIFT1 model using the specified reference velocity at 2 m height

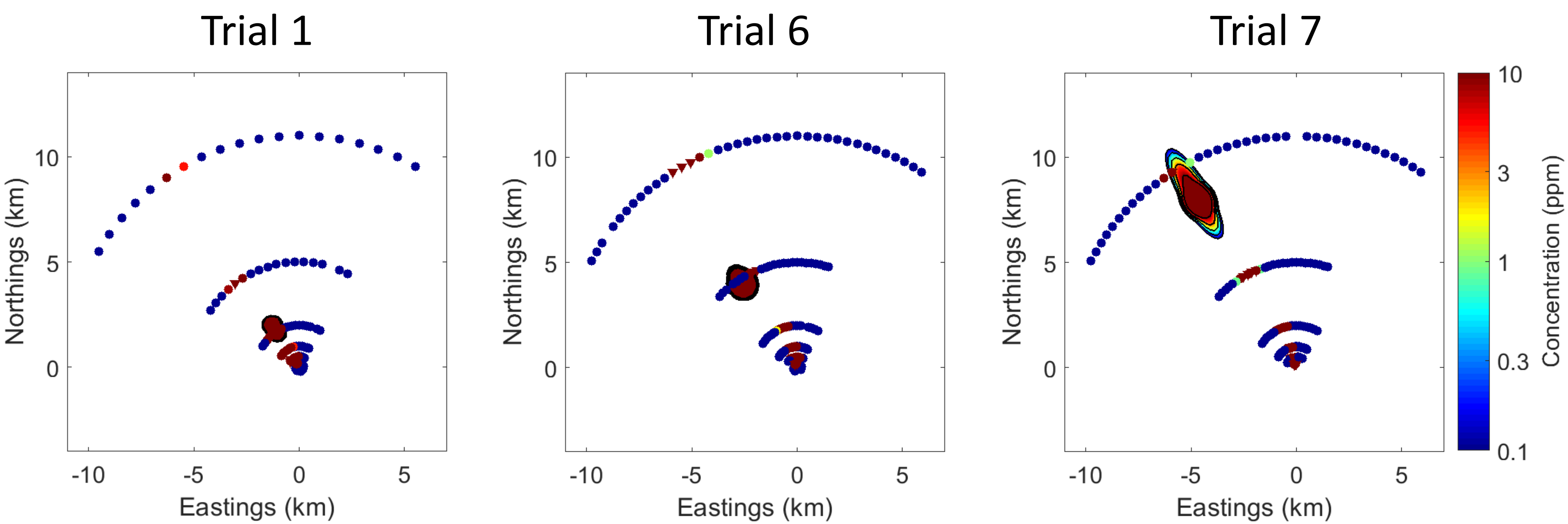
Far-field

Far-field: time = 1200 s



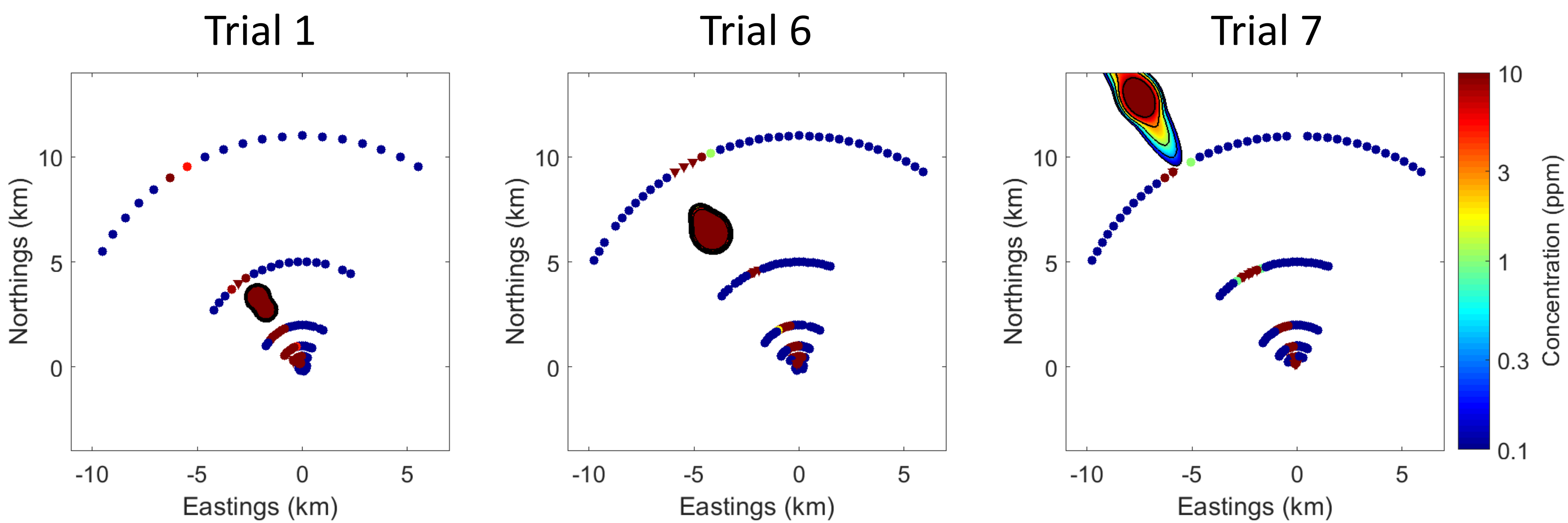
All results are for the DRIFT1 model using the specified reference velocity at 2 m height

Far-field: time = 1800 s



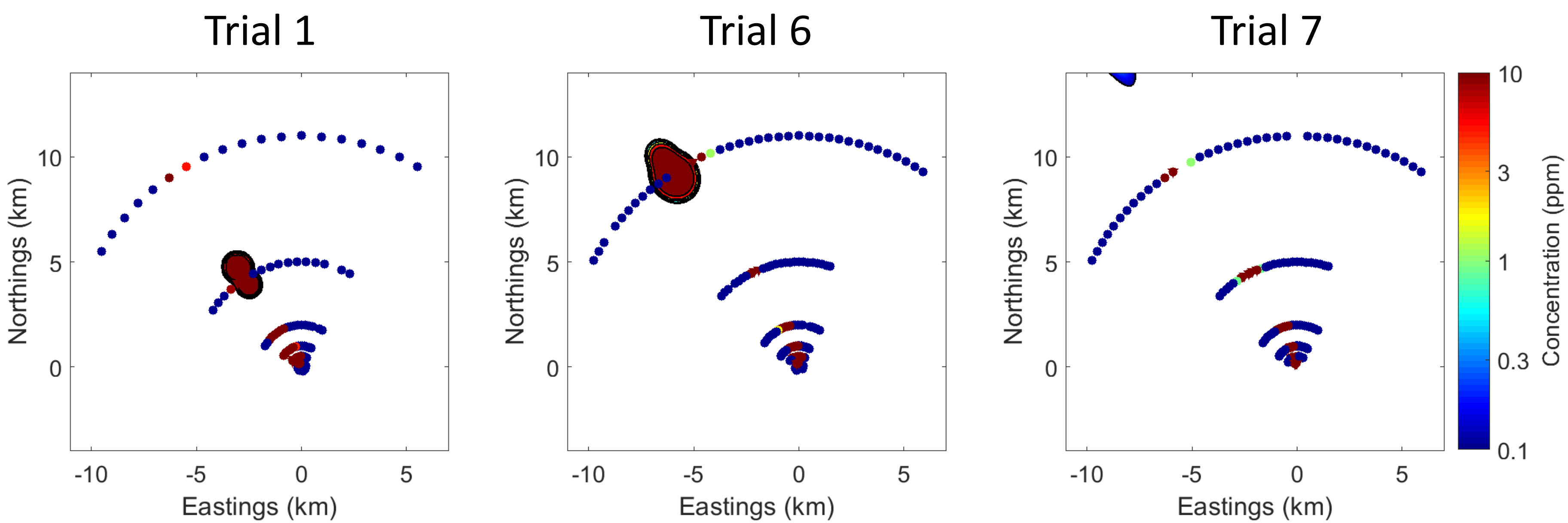
All results are for the DRIFT1 model using the specified reference velocity at 2 m height

Far-field: time = 2700 s



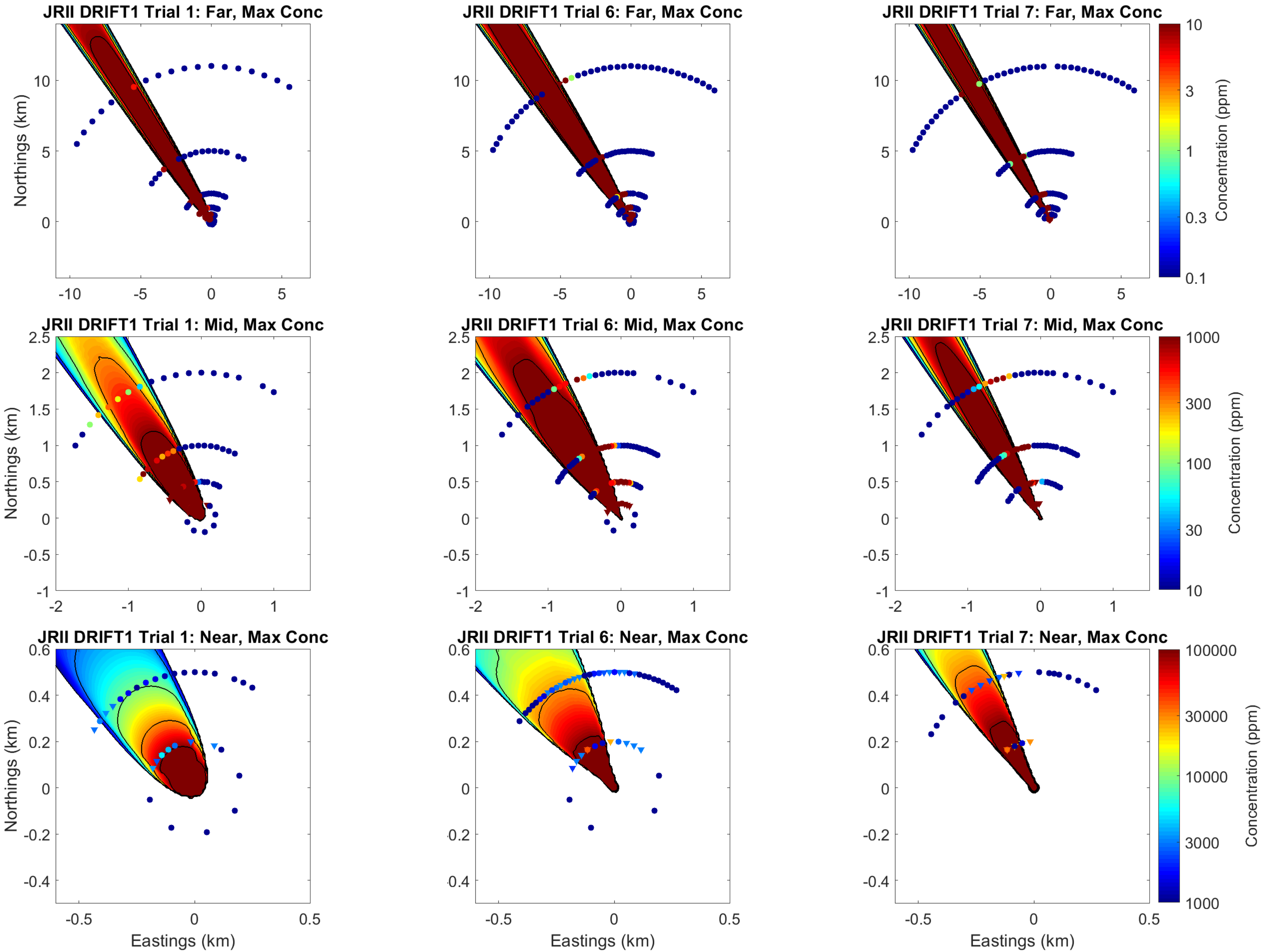
All results are for the DRIFT1 model using the specified reference velocity at 2 m height

Far-field: time = 3600 s



All results are for the DRIFT1 model using the specified reference velocity at 2 m height

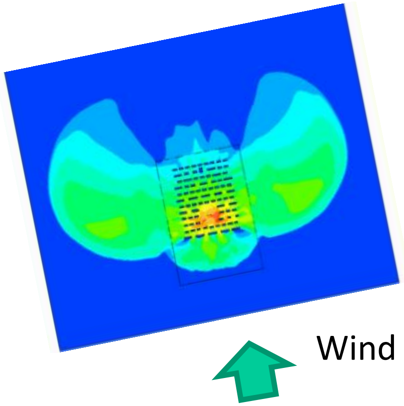
Maximum concentrations over all time



JRII DRIFT1 Trial 1: Far, Max Conc
JRII DRIFT1 Trial 6: Far, Max Conc
JRII DRIFT1 Trial 7: Far, Max Conc
JRII DRIFT1 Trial 1: Mid, Max Conc
JRII DRIFT1 Trial 6: Mid, Max Conc
JRII DRIFT1 Trial 7: Mid, Max Conc
JRII DRIFT1 Trial 1: Near, Max Conc
JRII DRIFT1 Trial 6: Near, Max Conc
JRII DRIFT1 Trial 7: Near, Max Conc
Northings (km)
Eastings (km)
Concentration (ppm)
10
3
1
0.3
0.1
1000
300
100
30
10
100000
30000
10000
3000
1000

Summary

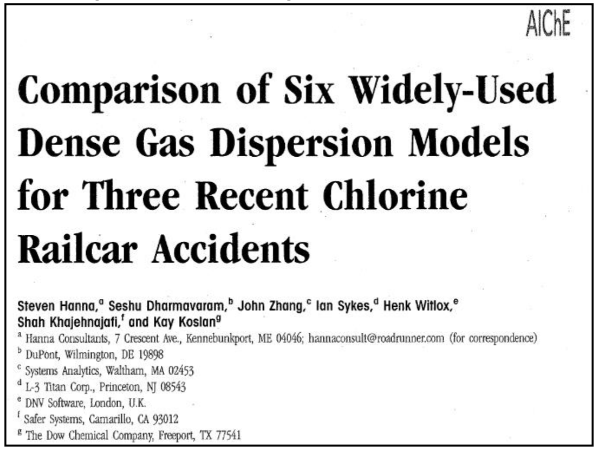
- Details have been provided of the DRIFT model configuration
- Baseline DRIFT1 using reference wind speed predicted:
  - Around 60% of the maximum arc-wise concentrations within a factor of two of the measurements
  - Trend to over-prediction, but several measurements may have under-reported the actual concentrations
- Sensitivity tests
  - DRIFT2: using U^* instead of U_{ref} affects Trial 1 results
  - DRIFT3: Switching deposition off had minor effect in Trial 1
- Need to be careful not to over-interpret DRIFT results in Trial 1 due to presence of mock urban array



CFD prediction for Trial 1

Possible Future Work

- Further analysis of Jack Rabbit II Trial 1, 6 and 7
  - Comparisons of cloud width and height
  - Time-varying concentrations and toxic load
  - Statistical Performance Measures (SPMs): FAC2, VG, MG etc.
- Assess impact of sensors saturating or cloud missing sensors
  - Calculate second set of SPMs using subset of data unaffected by these issues?
- Examine the other Jack Rabbit II trials?
- Validate pool evaporation models with Trial 7 and 8 liquid dump data
- Update HSE model evaluation protocol for DRIFT
- Revisit simulations from 2008 of chlorine railcar incidents (Graniteville, Festus and Macdona) using learning gained from Jack Rabbit II


AIChE

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

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Co-authors:

- Graham Tickle (GT Science and Software)
- Adrian Kelsey and Harvey Tucker (HSE)

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Extra material

DRIFT model: setup for JRII simulations

Summary of differences between runs DRIFT1, DRIFT2 and DRIFT3

	Trial 1			Trial 6			Trial 7		
	DRIFT1	DRIFT2	DRIFT3	DRIFT1	DRIFT2	DRIFT3	DRIFT1	DRIFT2	DRIFT3
Initial wind speed (m/s) at z = 2 m	1.45	2.92	1.45	2.42	2.34	2.42	3.98	5.11	3.98
Friction velocity, u* (m/s)	0.054	0.108	0.054	0.096	0.093	0.096	0.164	0.210	0.164
Deposition velocity, v_d (cm/s)	0.04	0.04	0.0	0.04	0.04	0.0	0.04	0.04	0.0

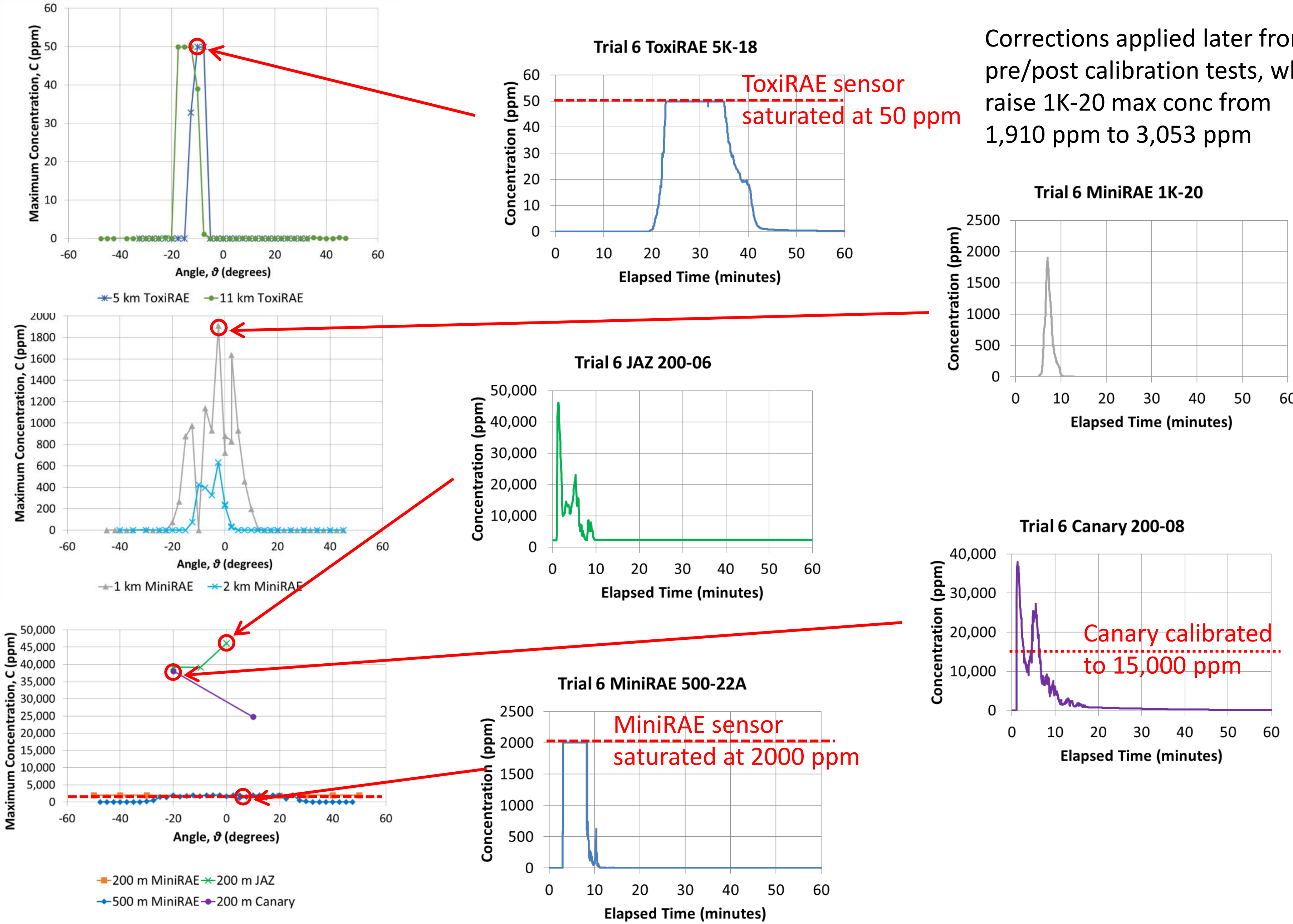
Further plots of the JRII experimental data

- To show behaviour of some ToxiRAE and MiniRAE sensors that saturated and recorded a plateau in the recorded concentration over time
- Time-varying concentrations for Canary sensors to show that they recorded useful data even when above their calibration limit

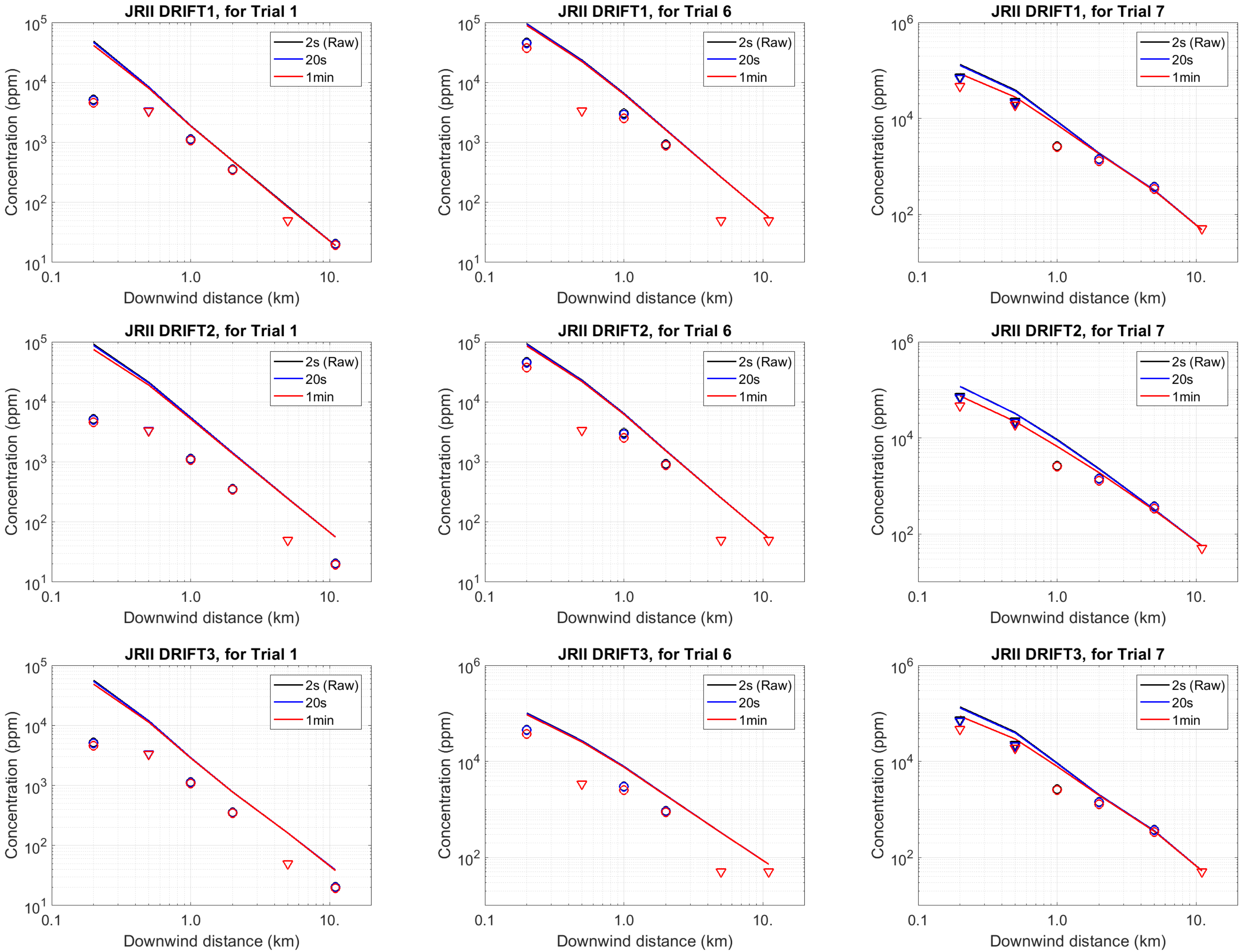
Trial 6

Time-Series Concentrations at Selected Sensors

Corrections applied later from pre/post calibration tests, which raise 1K-20 max conc from 1,910 ppm to 3,053 ppm



Extra slide with plots of the maximum arc-wise concentrations for different averaging times, showing that it has relatively little effect on the data


JRII DRIFT1, for Trial 1
JRII DRIFT1, for Trial 6
JRII DRIFT1, for Trial 7
JRII DRIFT2, for Trial 1
JRII DRIFT2, for Trial 6
JRII DRIFT2, for Trial 7
JRII DRIFT3, for Trial 1
JRII DRIFT3, for Trial 6
JRII DRIFT3, for Trial 7
2s (Raw)
20s
1min
Concentration (ppm)
Downwind distance (km)
0.1
1.0
10.
10^1
10^2
10^3
10^4
10^5
10^6

Extra slides taken from Harmo-18 presentation H18-134:

"Jack Rabbit II 2015 chlorine release experiments: simulations of the trials using DRIFT and PHAST"
by Bryan McKenna, Maria Garcia, Simon Gant, Adrian Kelsey, Alison McGillivray, James Stewart, Rachel Batt, Mike Wardman, Harvey Tucker, Graham Tickle and Henk Witlox

To demonstrate that dispersion model predictions can be very sensitive to the deposition rate – it can have a greater effect than wind speed or atmospheric stability in some cases

Range of model inputs and outputs

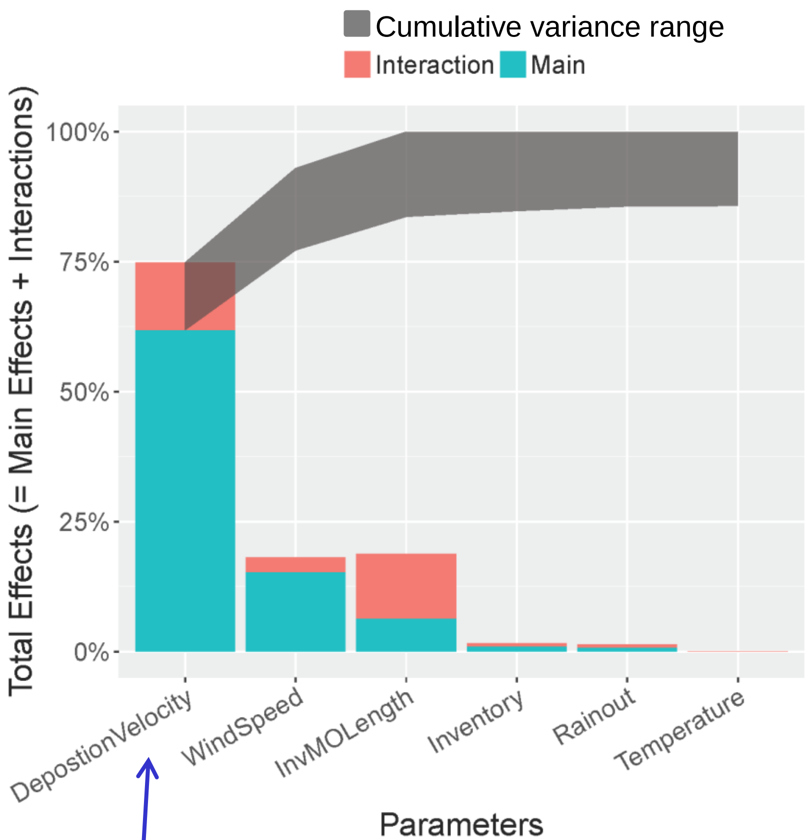
- Model inputs:
  - Chosen based on Jack Rabbit II experimental ranges and uncertainties:

Inventory (kg)	DRIFT Rainout Fraction	Wind Speed at 2m reference height (m s^{-1})	Temperature (K)	1/Monin-Obukhov Length (m^{-1})	Vapour Deposition Velocity (cm s^{-1})
4000	0	1.5	288	-0.12	0
9000	1	5	303	0.08	5

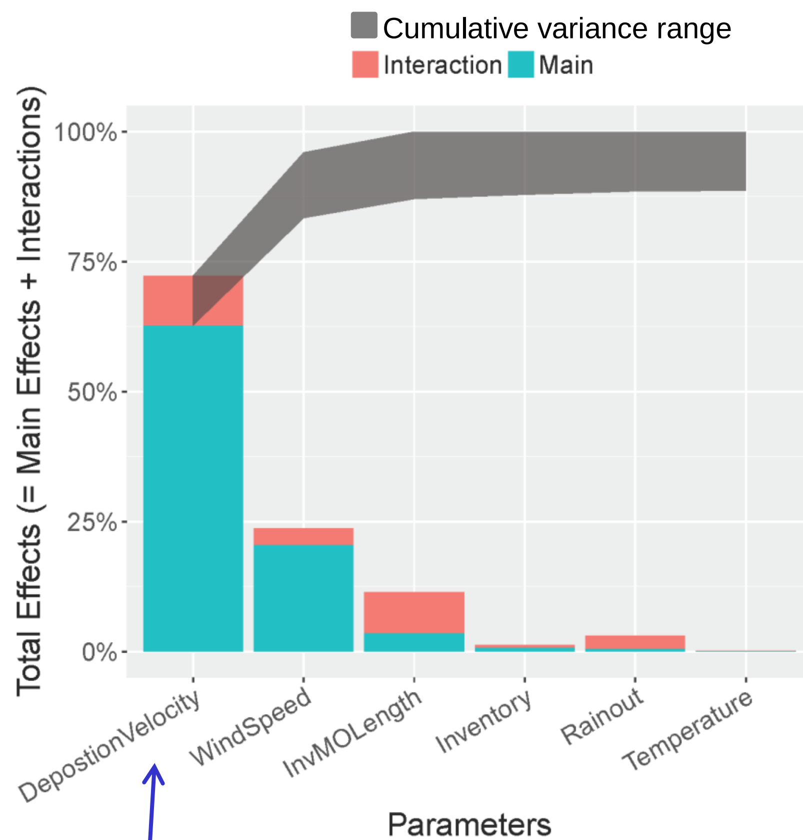
5 cm s^{-1} chosen as highest value of deposition rate found in the literature (upper bounding case)
Not representative of Dugway salt playa

  - Flashing or metastable release
- Model output: Distance to 100 ppm concentration

Main and total effects on Lowry Plot



Metastable



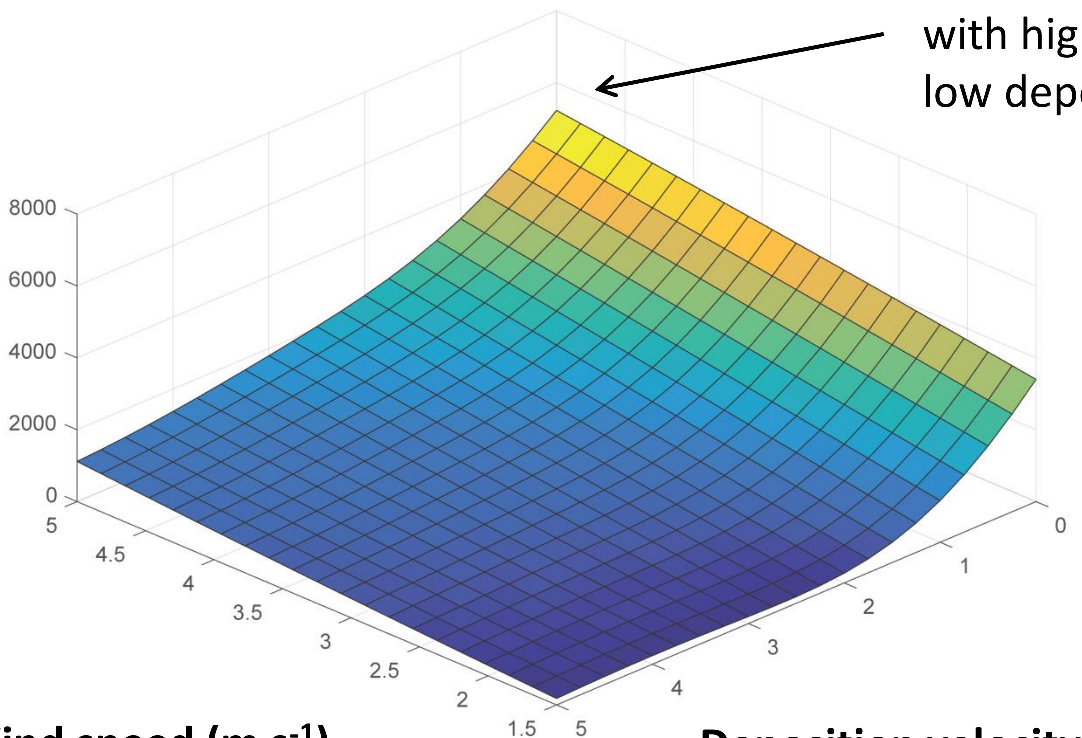
Flashing

Deposition velocity has the strongest effect on the results

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 ($cm\ s^{-1}$)

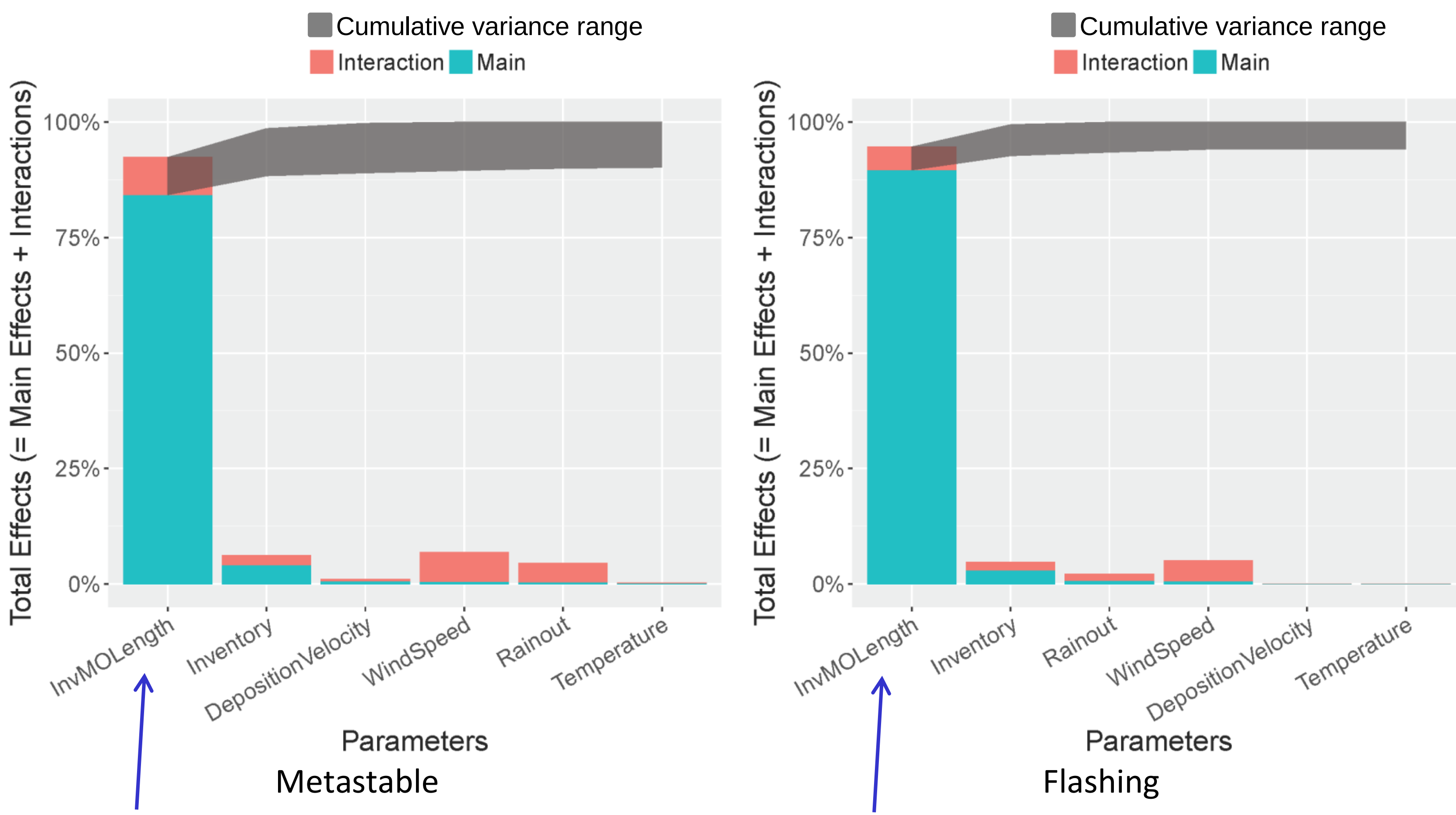
Range of model inputs and outputs

- Model inputs:
  - Chosen based on Jack Rabbit II experimental ranges and uncertainties:

Inventory (kg)	DRIFT Rainout Fraction	Wind Speed at 2m reference height ($m\ s^{-1}$)	Temperature (K)	1/Monin-Obukhov Length (m^{-1})	Vapour Deposition Velocity ($cm\ s^{-1}$)
4000	0	1.5	288	-0.12	0
9000	1	5	303	0.08	~~5~~ 0.05

  - Flashing or metastable release
- Model output: Distance to 100 ppm concentration

Deposition velocity range: 0 – 0.05 cm s^{-1}



Atmospheric stability has the strongest effect on the results