A decorative graphic on the left side of the slide consists of several overlapping, semi-transparent, dark red chevron shapes pointing to the right, creating a layered, arrow-like effect.

DRIFT Results for the Jack Rabbit II Coordinated Model Inter-Comparison Exercise

22st Annual George Mason University (GMU) Conference on
Atmospheric Transport and Dispersion Modeling

Fairfax, Virginia, USA, 19-21 June 2018

Simon Gant, Adrian Kelsey, Harvey Tucker and Mike
Wardman(HSE)

Graham Tickle (GT Science & Software)

Acknowledgements



DISCLAIMER:

- 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 contribution made to this paper by the HSE authors was funded solely by HSE. The contents, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy

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:

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

Outline

- Aims
- Overview of DRIFT model
 - Model capabilities
 - Configuration for model inter-comparison exercise
- Preliminary model results
 - Maximum arc-wise concentration versus downwind distance
 - Maximum concentration across the azimuth angle of the arcs
 - Contour plots
- Sensitivity analysis
 - Dry deposition velocity set to zero
 - Increased roughness for urban array in Trial 1
- Conclusions and Future Directions

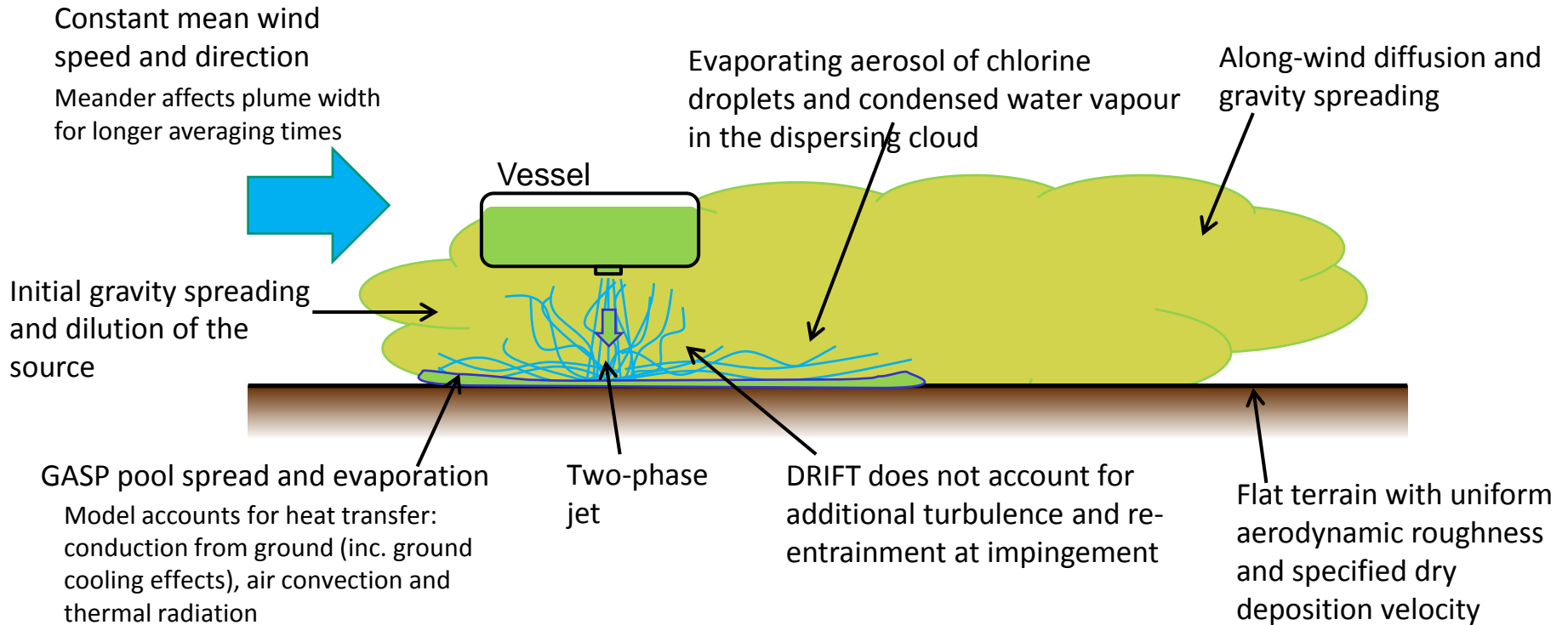
Aims

Aims of HSE's involvement in Jack Rabbit II:

- To contribute DRIFT model results to the model inter-comparison exercise
- To volunteer and provide help (if needed) to the coordinators:
 - Support Graham Tickle's source modelling efforts
 - Provide quality assurance checks on the experimental data
 - Volunteer to cross-plot other model results and compare to the data
- To work with DNV GL on the PHAST model results (later...)
- To collaborate with other experts in the Modelers' Working Group and share findings

DRIFT model: capabilities

DRIFT is an integral model



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

JRII Coordinated Model Inter-Comparison

Exercise: Source Conditions



Source conditions provided by Tom Spicer and Graham Tickle:

	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

JRII Coordinated Model Inter-Comparison

Exercise: Meteorological Conditions



Meteorological conditions provided by Steve Hanna:

	Trial 1	Trial 6	Trial 7
<i>Weather/Environment</i>			
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 , H_s , (K-m/s)	-0.012	-0.0034	-0.0160
<i>Vertical profiles of wind speed and direction and temperature⁴</i>			
Inverse Monin-Obukhov length (m^{-1})	0.124	0.056	0.0229
Pasquill Class ⁵	E/F	E	D/E

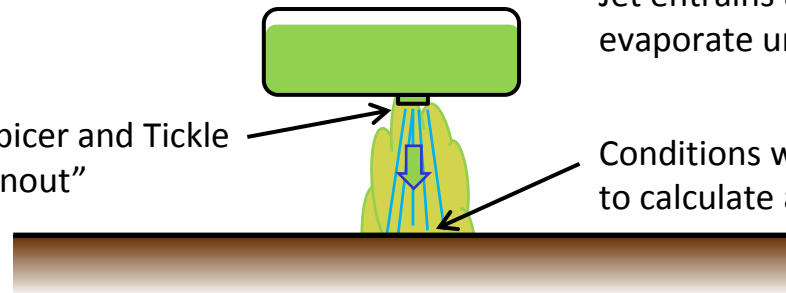
Dry deposition velocity, $v_d = 0.04$ cm/s

DRIFT model: setup for JRII simulations

Two-stage modelling process:

1.) Two-phase jet

Source conditions taken from: Spicer and Tickle
"Primary release modified for rainout"

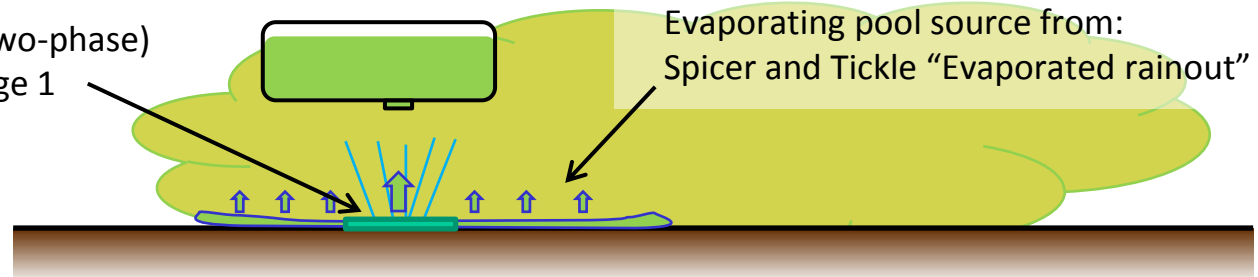


Jet entrains air and droplets
evaporate until it impinges

Conditions when jet hits ground used
to calculate area source for Stage 2

2.) Dispersion

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



Evaporating pool source from:
Spicer and Tickle "Evaporated rainout"

DRIFT model: setup for JRII simulations

Other DRIFT model inputs:

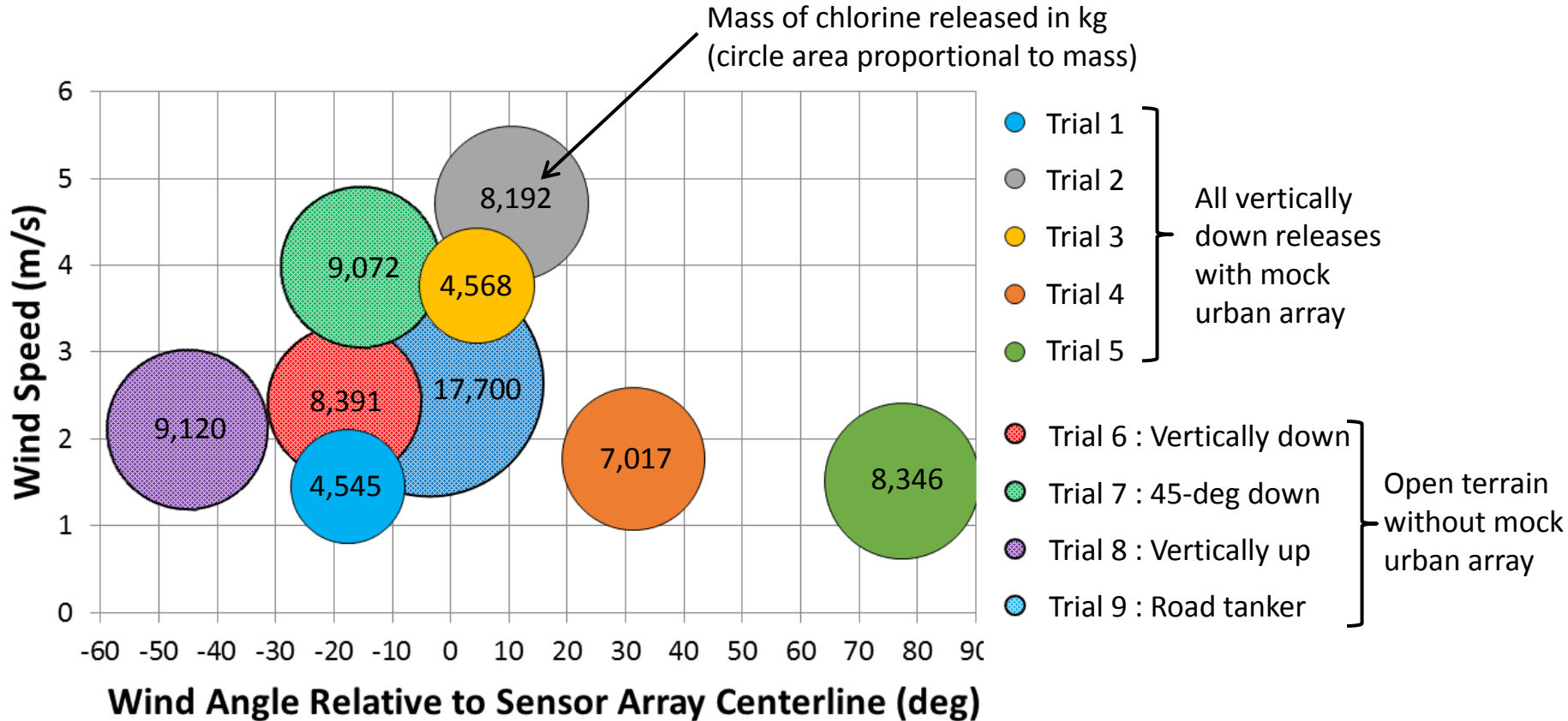
- Ground surface roughness, $z_0 = 0.5$ mm
 - No account taken of mock urban array in Trial 1
 - Sensitivity tests performed to investigate this matter
- Dry deposition velocity, $v_d = 0.04$ cm/s
 - Previous work has shown results are very sensitive to the deposition velocity, but this is a low value
 - Sensitivity tests performed with $v_d = 0$ cm/s
- Fixed wind speeds and atmospheric stability for the duration of each trial

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 - Maximum concentration across the azimuth angle of the arc
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- Sensitivity analysis
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JRII: Wind Conditions and Mass Released

Analysis by Steve Hanna for meteorology and Tom Spicer for chlorine mass

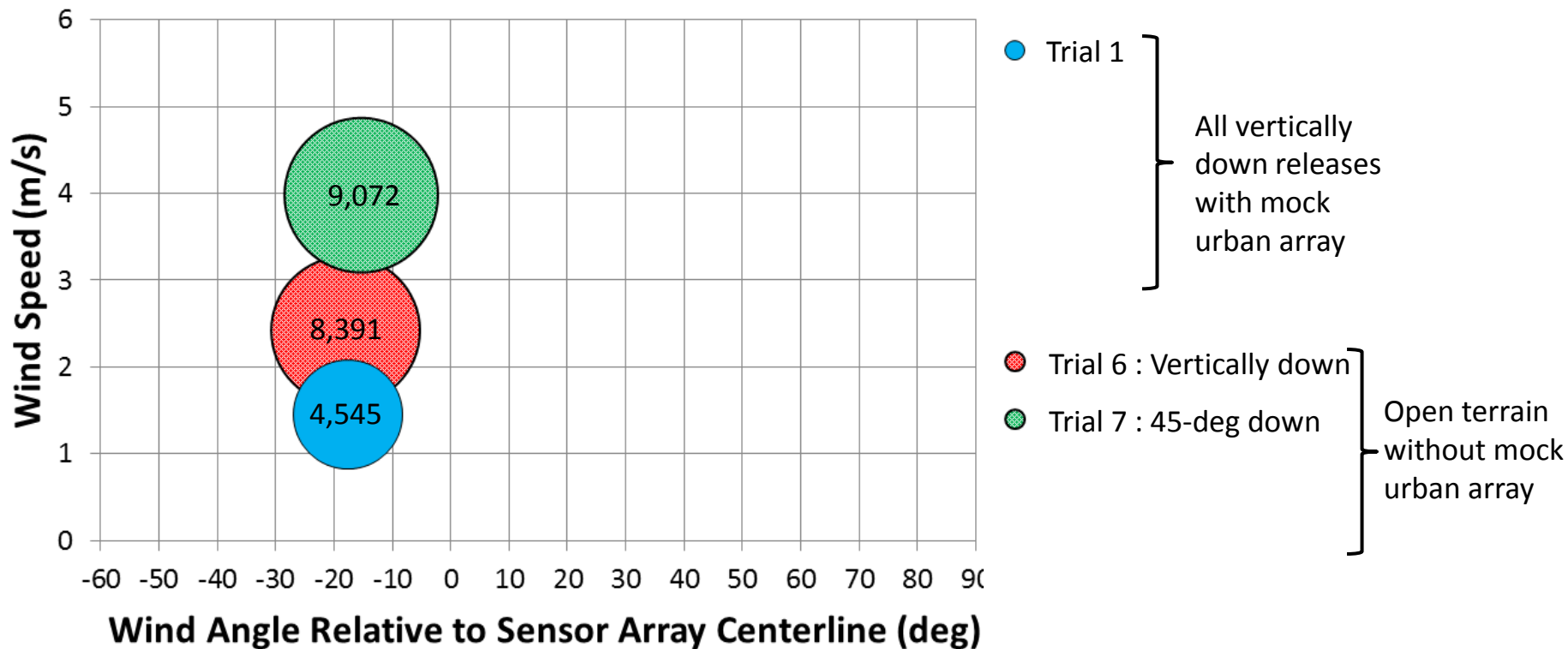


Data sources: "P190 JR II Recommended met for modelers 14 March 2018.xlsx" for meteorology

"GCPS-sp-2017-JR2-source+release-rate-PSP-final-JR2-rates-rev02.docx" for chlorine mass released

JRII: Selected trials for current exercise

Analysis by Steve Hanna for meteorology and Tom Spicer for chlorine mass



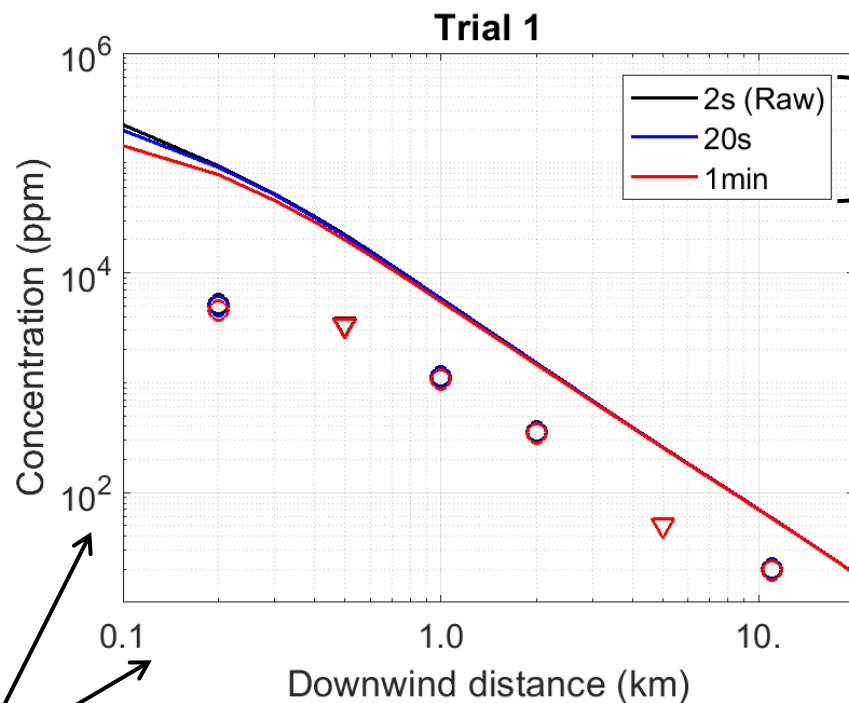
Data sources: "P190 JR II Recommended met for modelers 14 March 2018.xlsx" for meteorology

"GCPS-sp-2017-JR2-source+release-rate-PSP-final-JR2-rates-rev02.docx" for chlorine mass released

Max Arc-Wise Concentration vs. Distance

Key to plots shown on subsequent slides

Example plot:



Colors show three different averaging times

DRIFT used averaging time = 2 s, 20 s, 1 min
Sensor raw data was between 1 s and 3 s
Joe Chang sensor averages for 20 s and 1 min

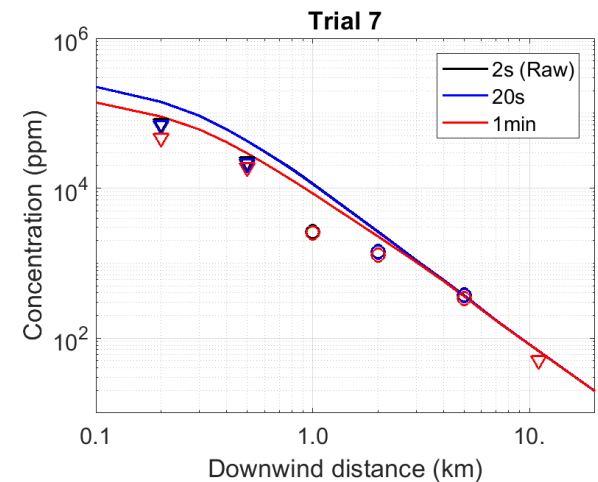
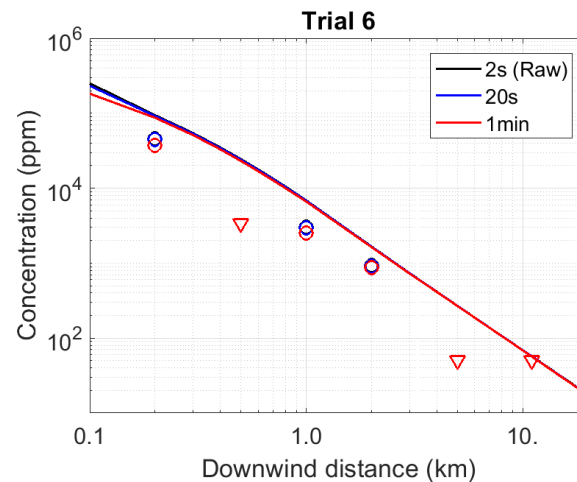
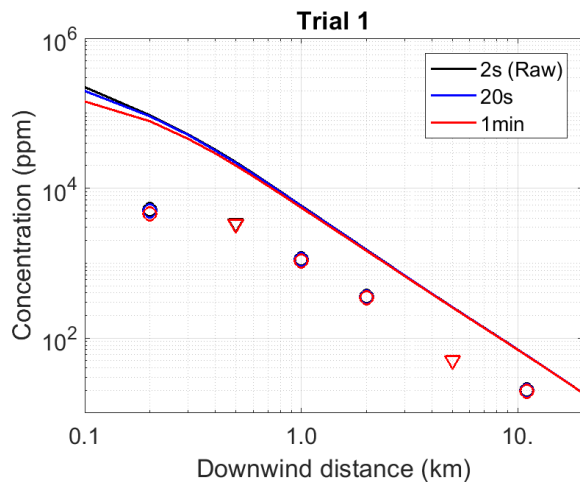
Lines show DRIFT base case results

Symbols show measurements:

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

Both x and y axes are log scales

Max Arc-Wise Concentration vs. Distance



Mock urban array

1.5 m/s
-18°

4,545 kg

Vertically down release

Open terrain

2.4 m/s
-18°

8,391 kg

Vertically down release

Open terrain

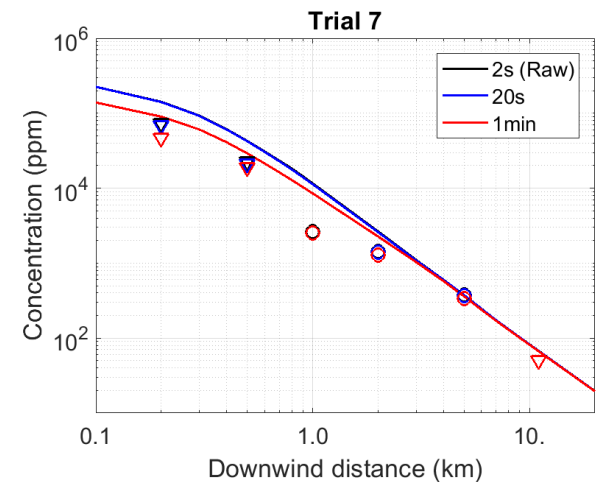
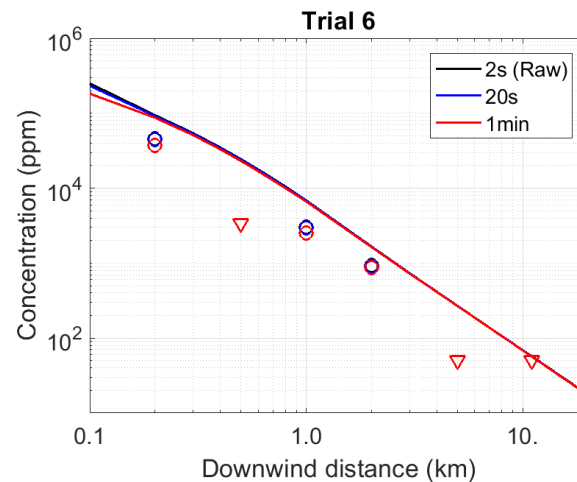
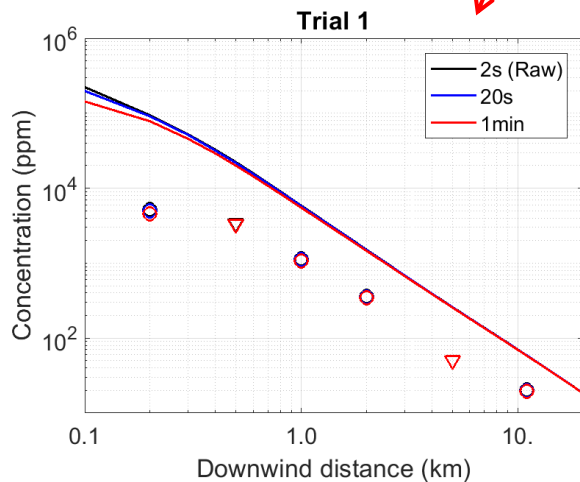
4.0 m/s
-15°

9,072 kg

45-deg down release

Max Arc-Wise Concentration vs. Distance

Does DRIFT over-predict concentration in Trial 1 because it does not account for the mock urban array? See later sensitivity tests...



Mock urban array

1.5 m/s
-18°

4,545 kg

Vertically down release

Open terrain

2.4 m/s
-18°

8,391 kg

Vertically down release

Open terrain

4.0 m/s
-15°

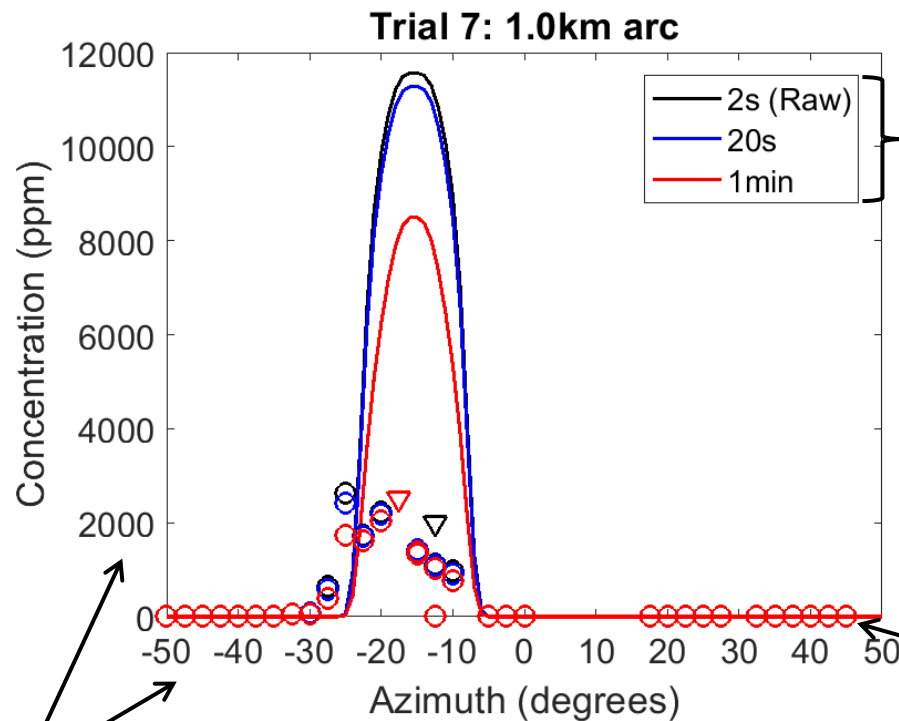
9,072 kg

45-deg down release

Max Concentration vs. Azimuth Angle

Key to plots shown on subsequent slides

Example plot:



Colors show three different averaging times

DRIFT used averaging time = 2 s, 20 s, 1 min
 Sensor raw data was between 1 s and 3 s
 Joe Chang sensor averages for 20 s and 1 min

Lines show DRIFT base case results

Symbols show measurements:

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

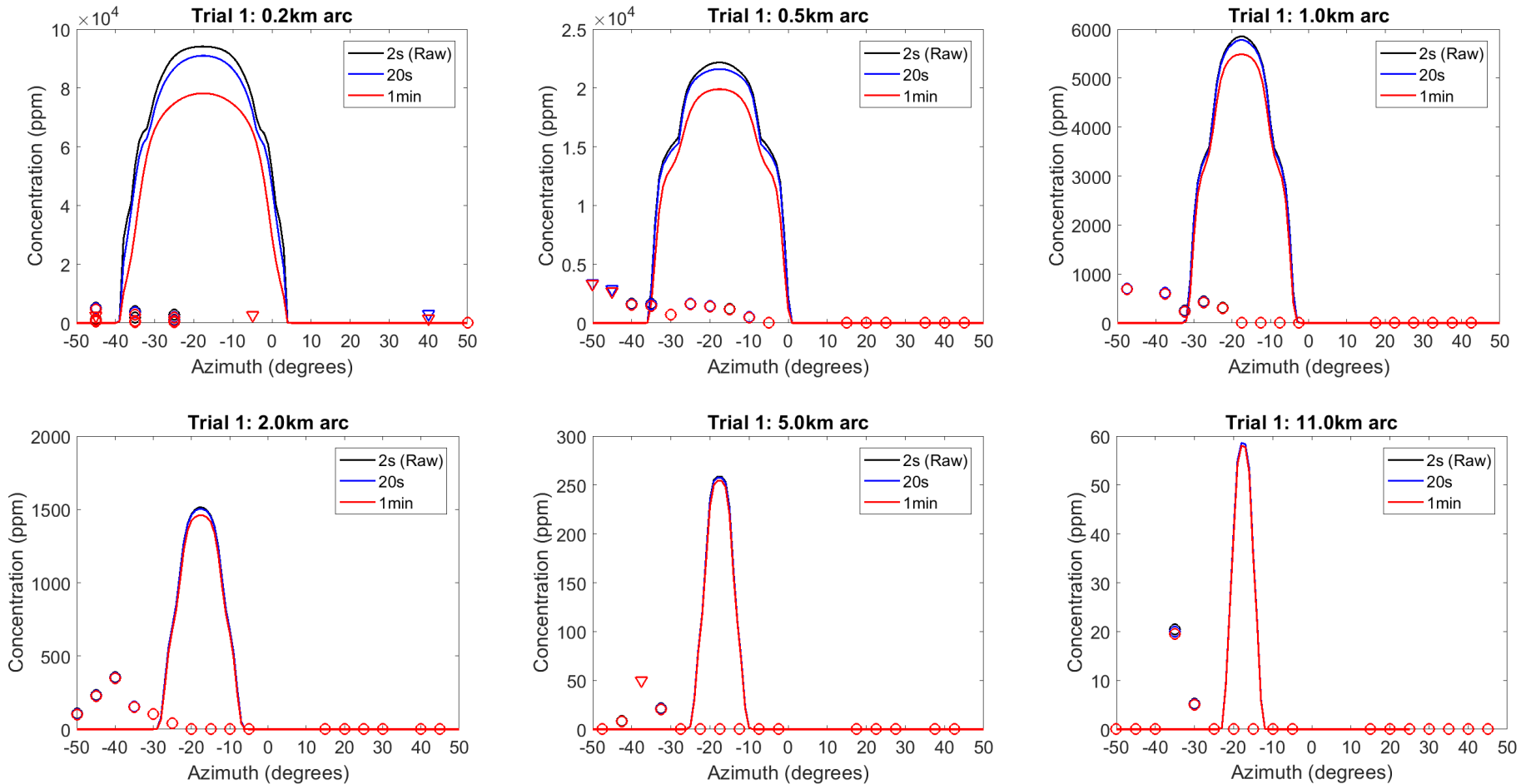
Any sensors that measured noise (not signal) have been set to zero concentration

Assessed by visual inspection of graphs of time-series concentration at each sensor

Both x and y axes are linear scales

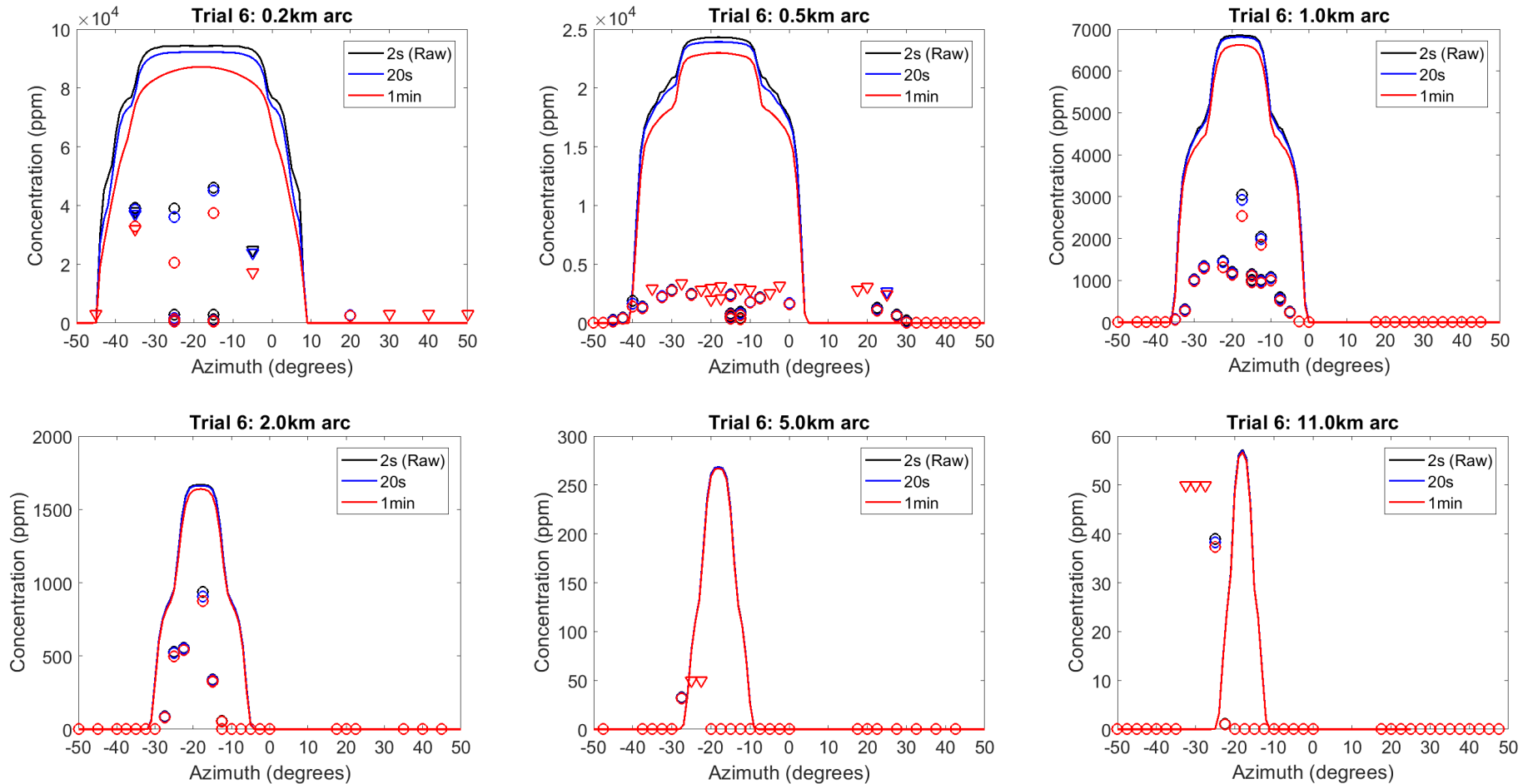
Max Concentration vs. Azimuth Angle

Trial 1: 4,545 kg vertically down release, mock urban array, wind speed 1.5 m/s



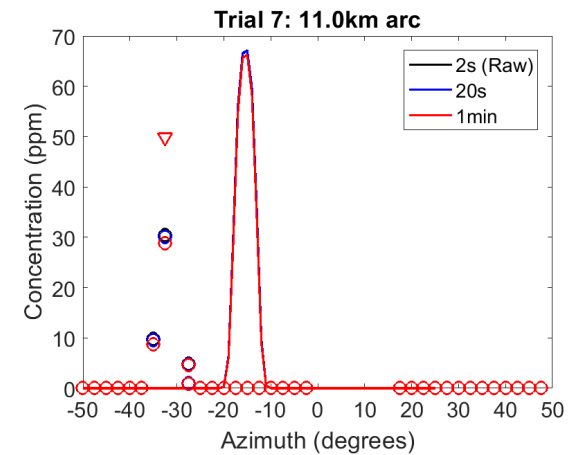
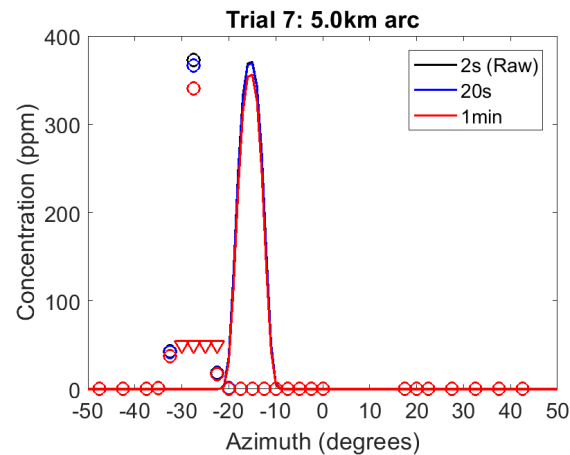
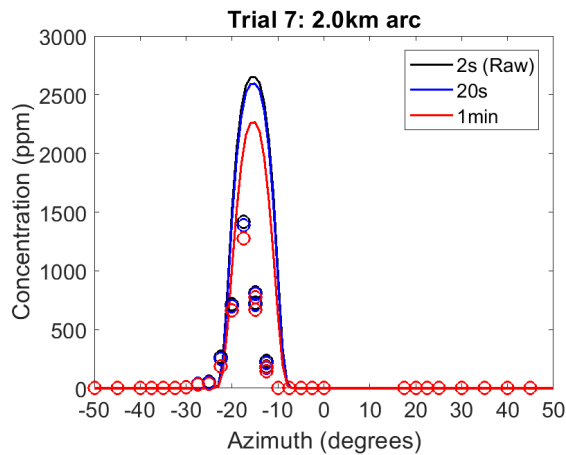
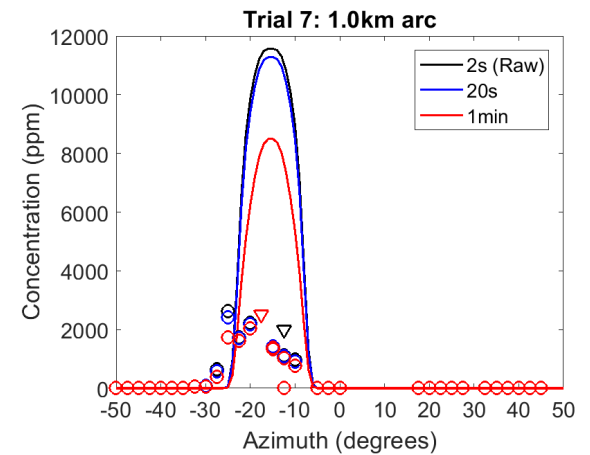
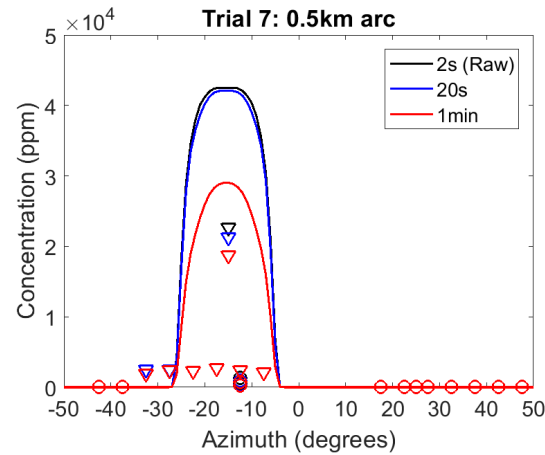
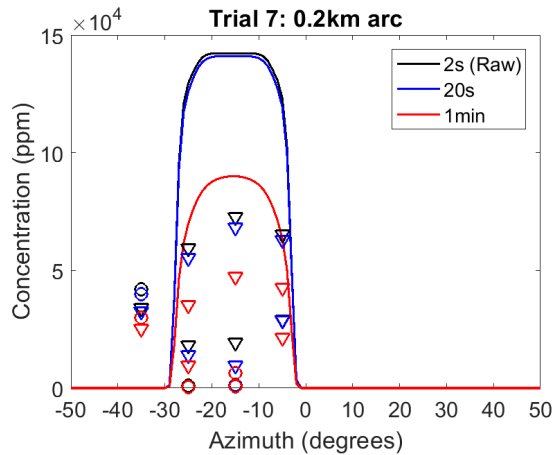
Max Concentration vs. Azimuth Angle

Trial 6: 8,391 kg vertically down release, open terrain, wind speed 2.4 m/s



Max Concentration vs. Azimuth Angle

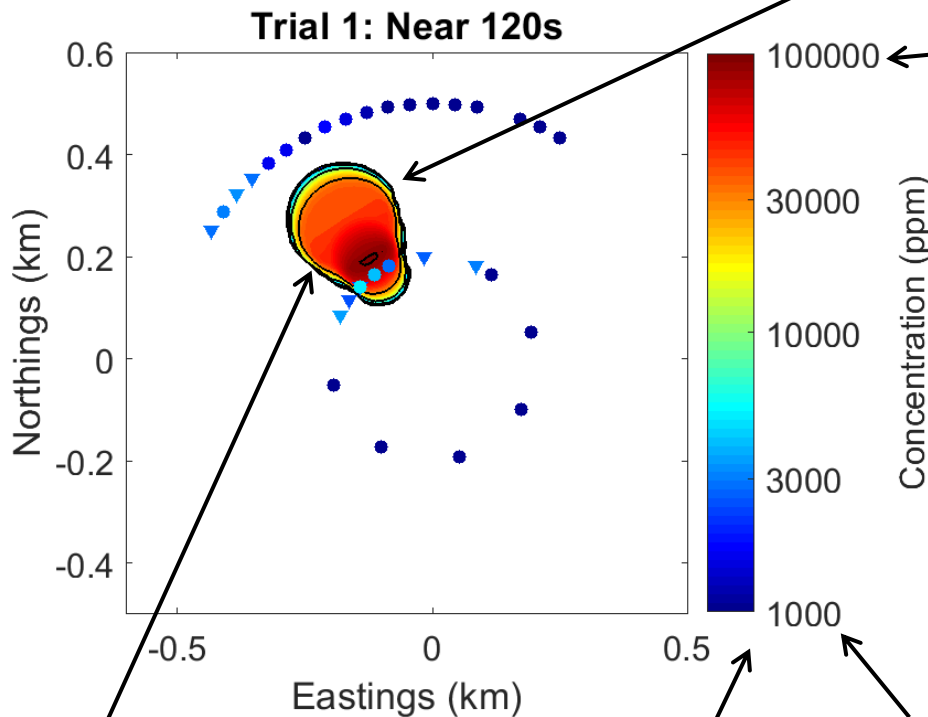
Trial 7: 9,072 kg 45-deg down release, open terrain, wind speed 4.0 m/s



Concentration Contours

Key to plots shown on subsequent slides

Example plot:



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

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

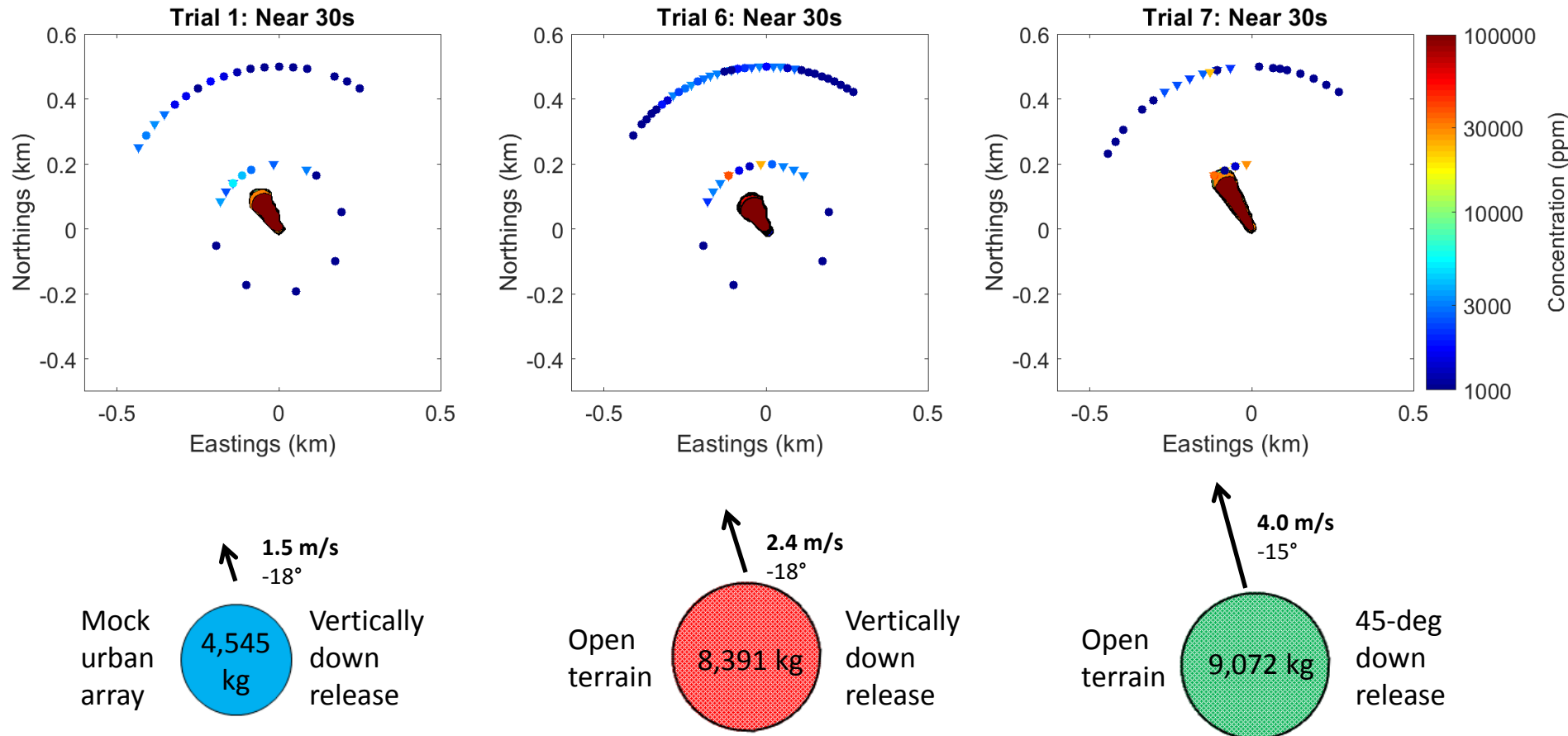
Any sensors that measured noise (not signal) have been set to zero concentration

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

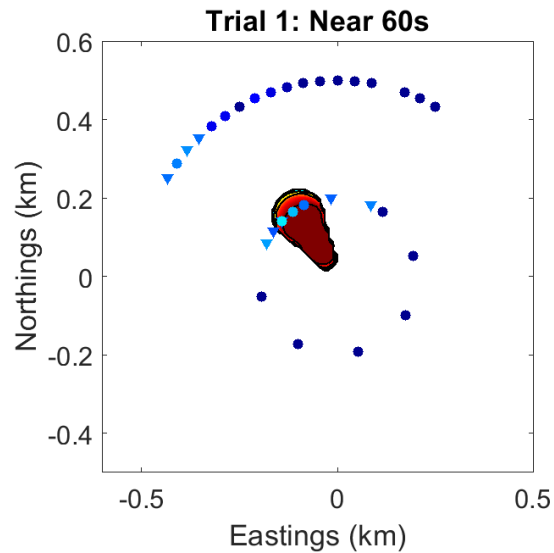
Color scale is logarithmic, not linear

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

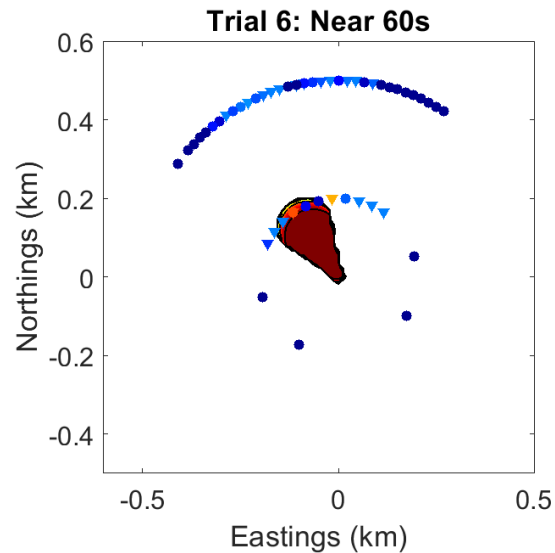
Concentration Contours



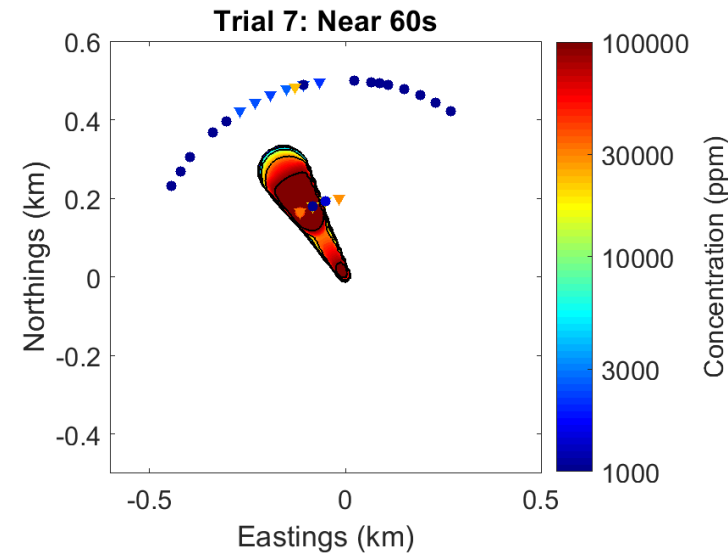
Concentration Contours



Mock urban array
 4,545 kg
 Vertically down release

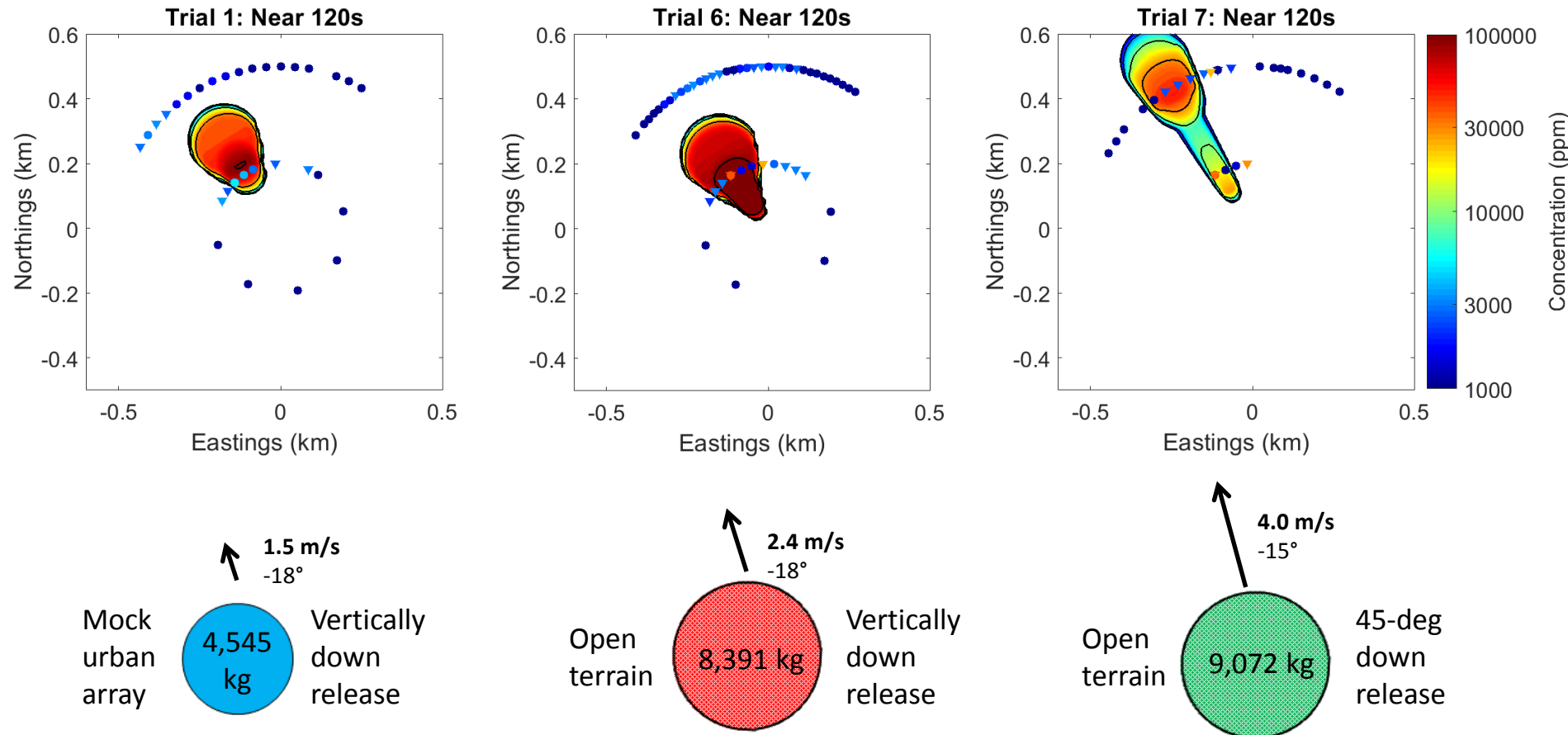


Open terrain
 8,391 kg
 Vertically down release

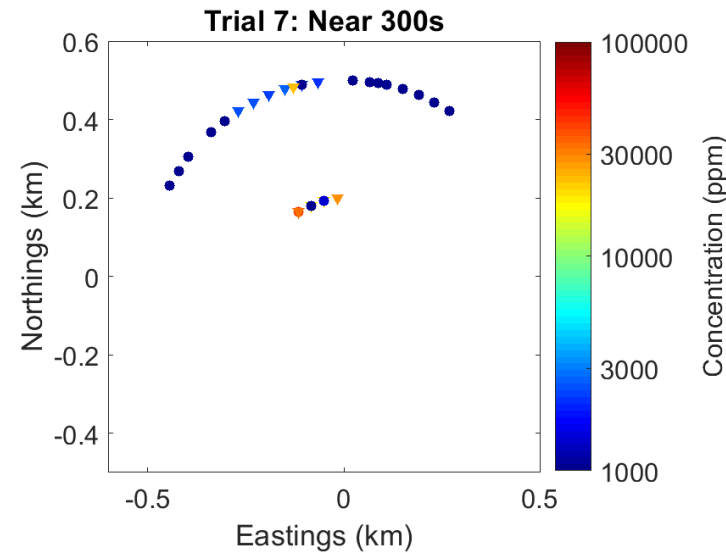
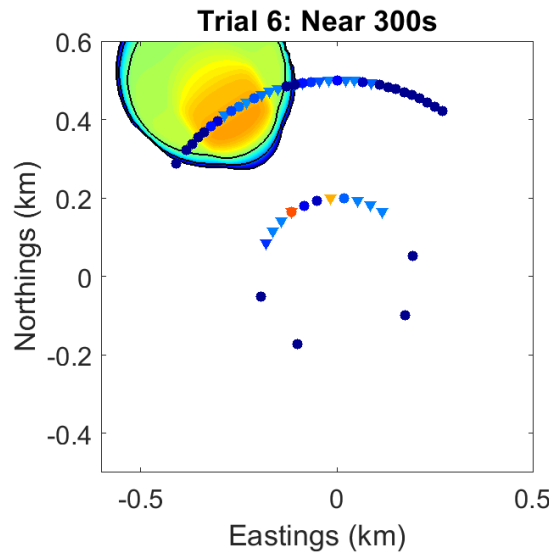
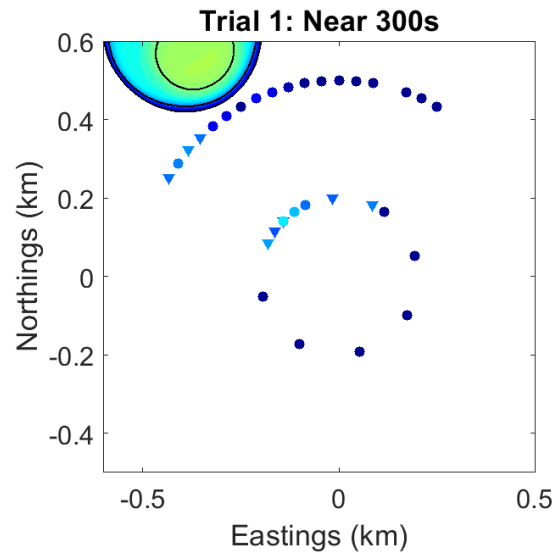


Open terrain
 9,072 kg
 45-deg down release

Concentration Contours



Concentration Contours

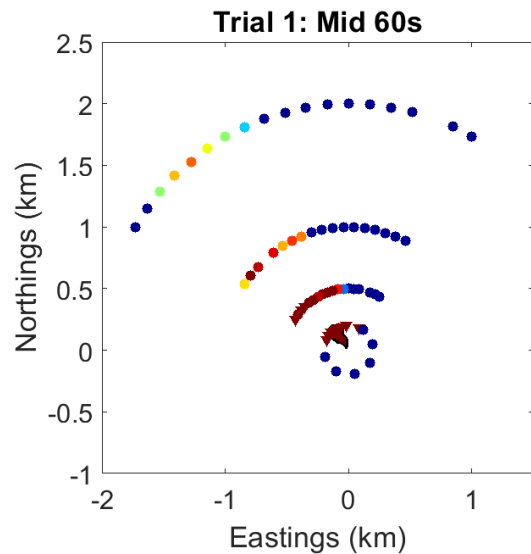


Mock urban array
 4,545 kg
 1.5 m/s
 -18°
 Vertically down release

Open terrain
 8,391 kg
 2.4 m/s
 -18°
 Vertically down release

Open terrain
 9,072 kg
 4.0 m/s
 -15°
 45-deg down release

Concentration Contours

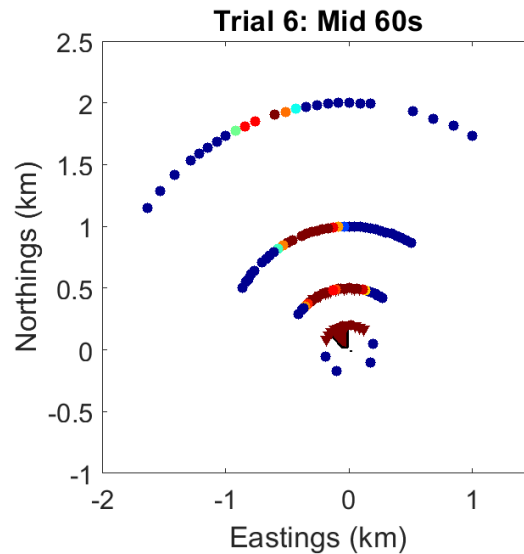


Mock urban array

1.5 m/s
-18°

4,545 kg

Vertically down release

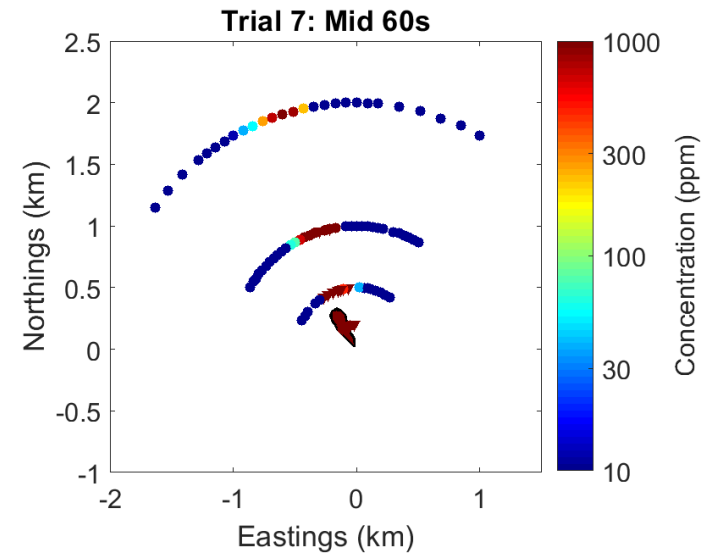


Open terrain

2.4 m/s
-18°

8,391 kg

Vertically down release



Open terrain

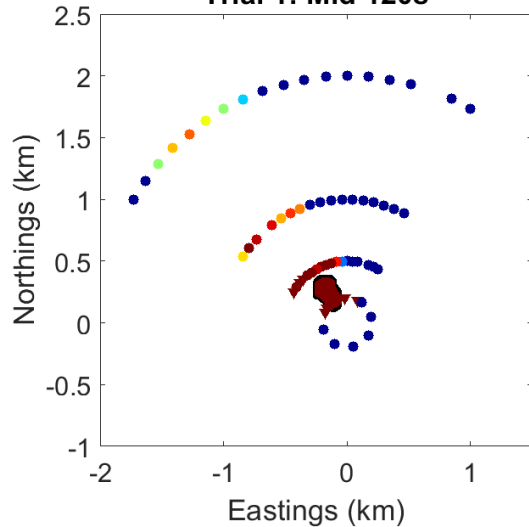
4.0 m/s
-15°

9,072 kg

45-deg down release

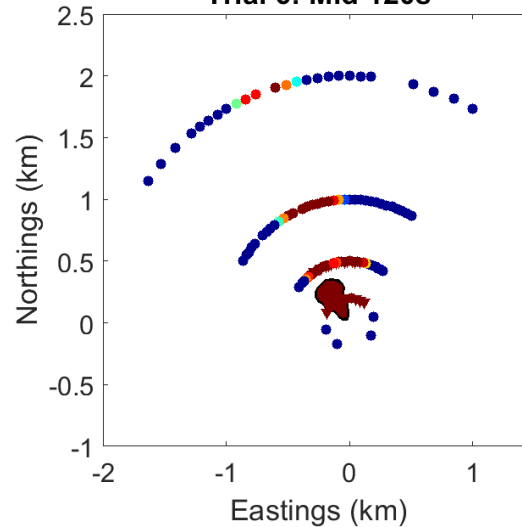
Concentration Contours

Trial 1: Mid 120s



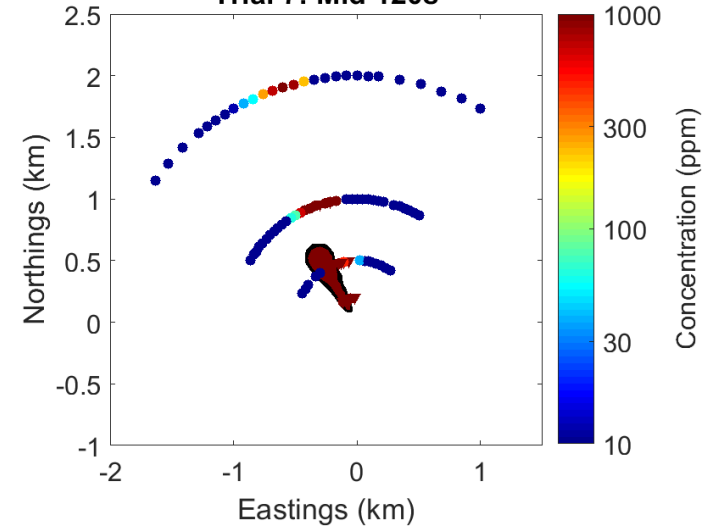
Mock urban array
 4,545 kg
 Vertically down release
 1.5 m/s
 -18°

Trial 6: Mid 120s



Open terrain
 8,391 kg
 Vertically down release
 2.4 m/s
 -18°

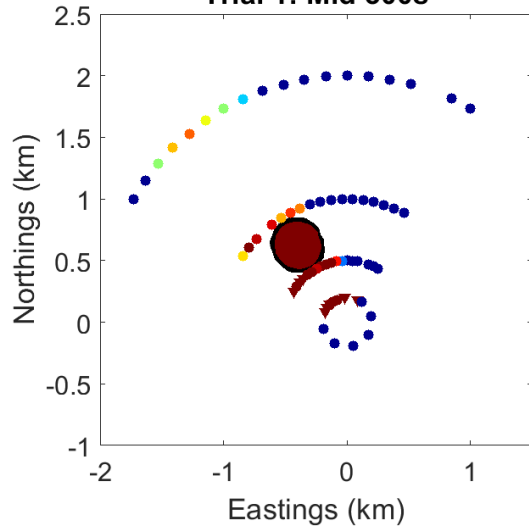
Trial 7: Mid 120s



Open terrain
 9,072 kg
 45-deg down release
 4.0 m/s
 -15°

Concentration Contours

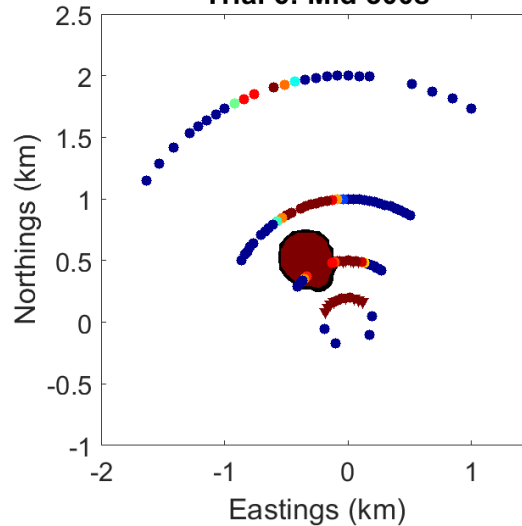
Trial 1: Mid 300s



Mock urban array
 4,545 kg
 Vertically down release

1.5 m/s
 -18°

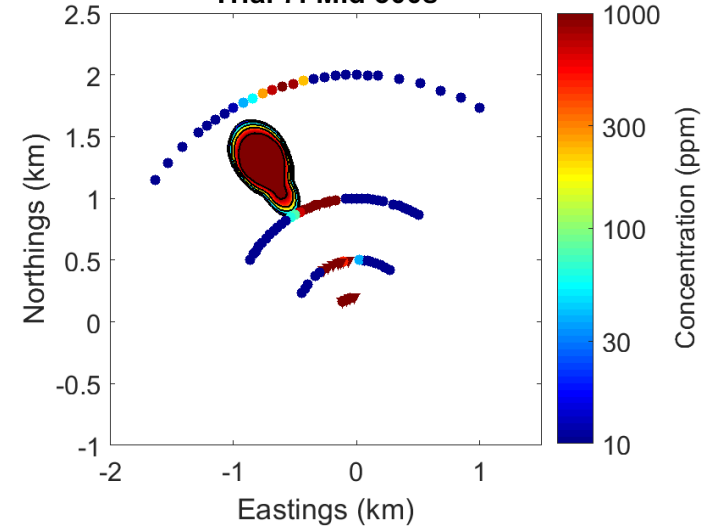
Trial 6: Mid 300s



Open terrain
 8,391 kg
 Vertically down release

2.4 m/s
 -18°

Trial 7: Mid 300s

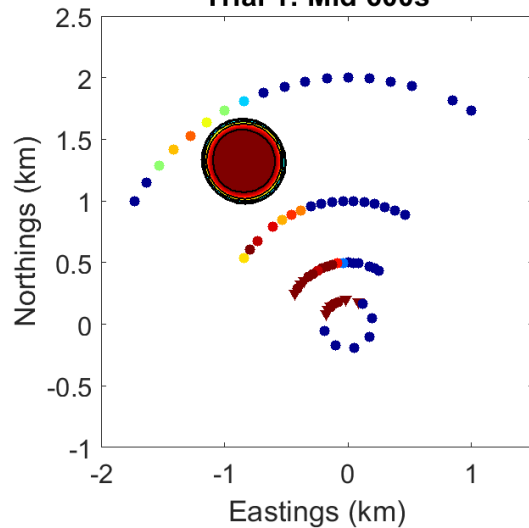


Open terrain
 9,072 kg
 45-deg down release

4.0 m/s
 -15°

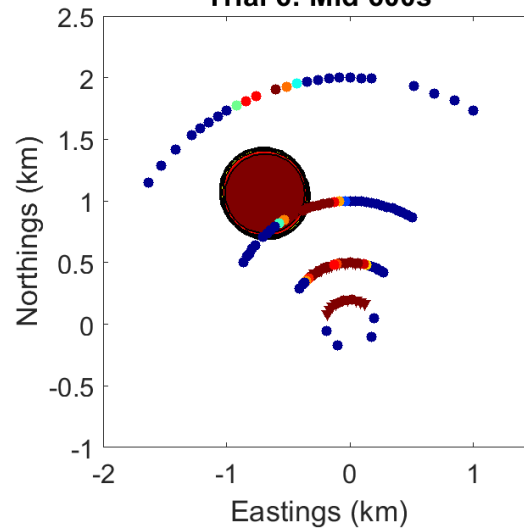
Concentration Contours

Trial 1: Mid 600s



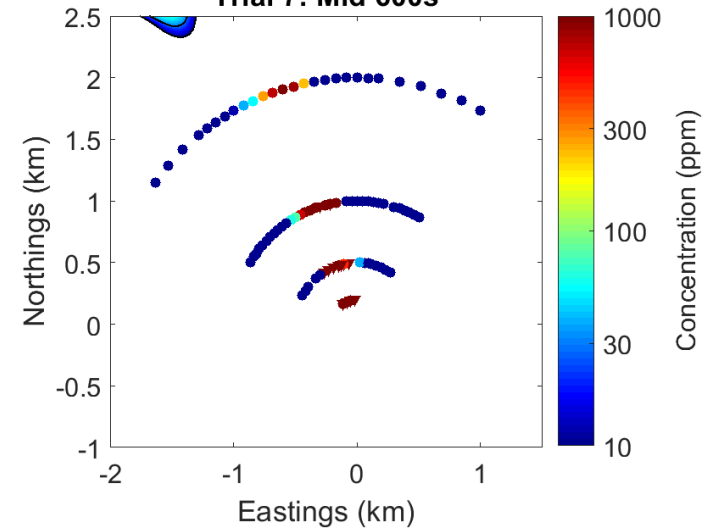
Mock urban array
 4,545 kg
 Vertically down release
 1.5 m/s
 -18°

Trial 6: Mid 600s



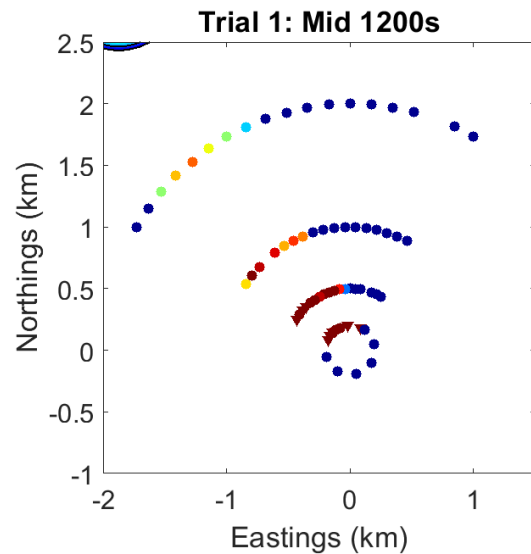
Open terrain
 8,391 kg
 Vertically down release
 2.4 m/s
 -18°

Trial 7: Mid 600s



Open terrain
 9,072 kg
 45-deg down release
 4.0 m/s
 -15°

Concentration Contours

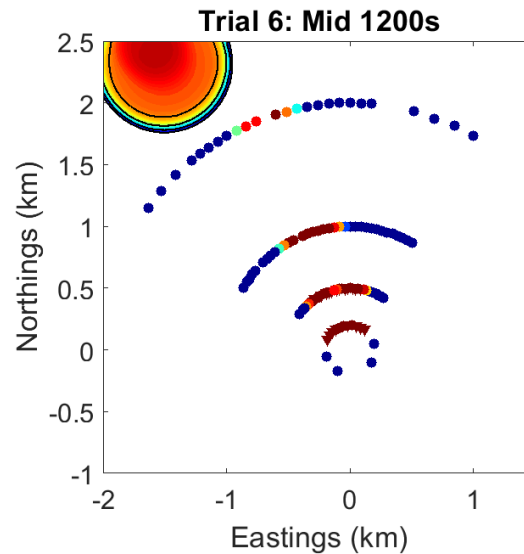


Mock urban array

1.5 m/s
-18°

4,545 kg

Vertically down release

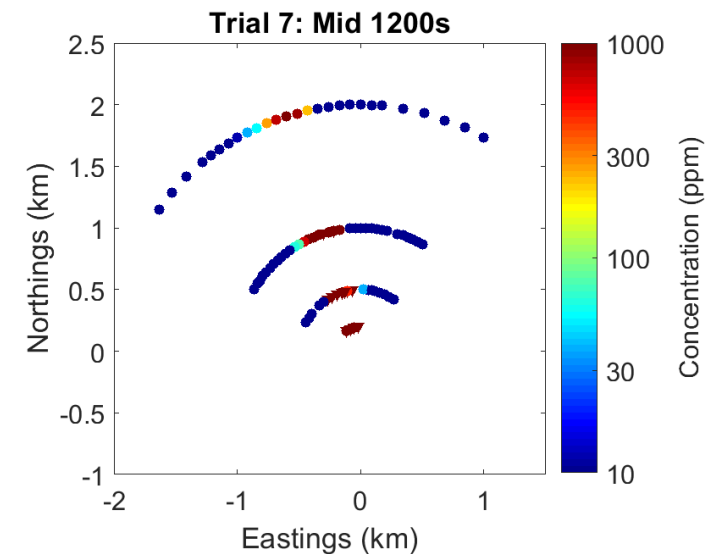


Open terrain

2.4 m/s
-18°

8,391 kg

Vertically down release



Open terrain

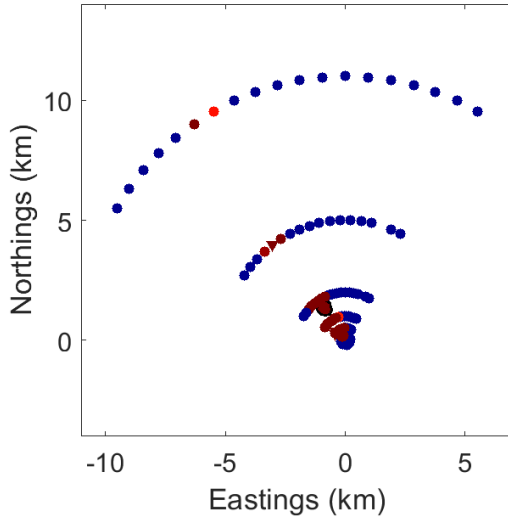
4.0 m/s
-15°

9,072 kg

45-deg down release

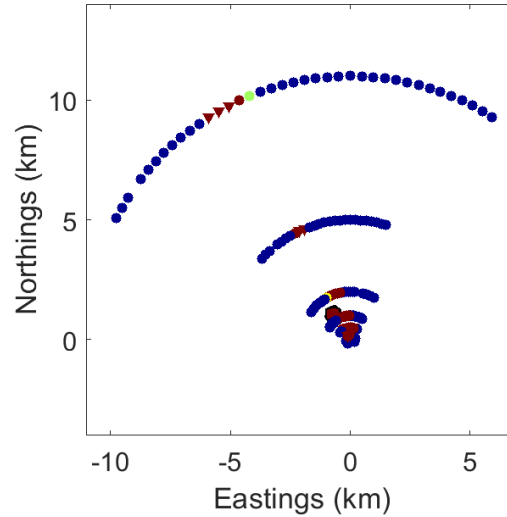
Concentration Contours

Trial 1: Far 600s



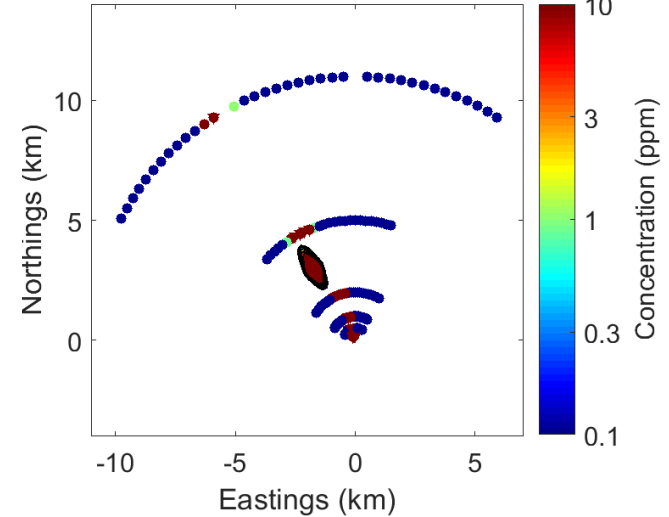
Mock urban array
 4,545 kg
 Vertically down release
 1.5 m/s
 -18°

Trial 6: Far 600s



Open terrain
 8,391 kg
 Vertically down release
 2.4 m/s
 -18°

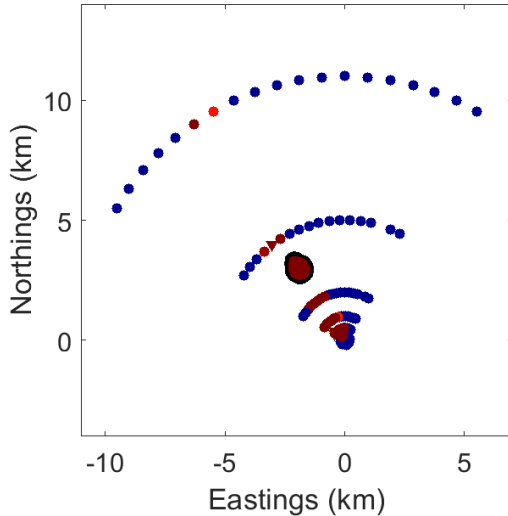
Trial 7: Far 600s



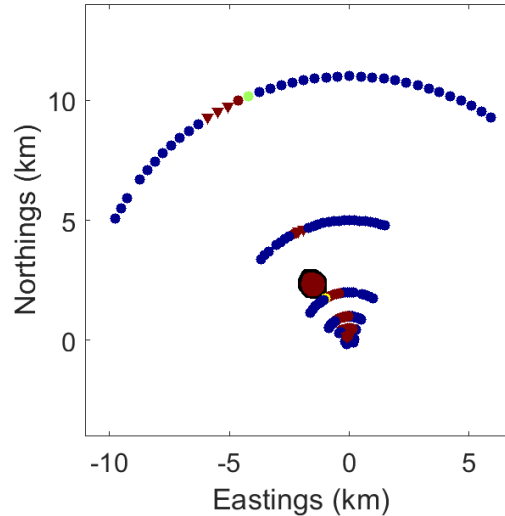
Open terrain
 9,072 kg
 45-deg down release
 4.0 m/s
 -15°

Concentration Contours

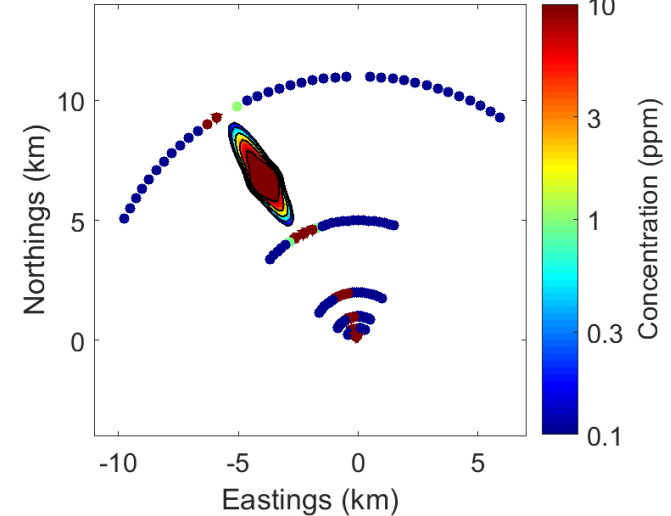
Trial 1: Far 1200s



Trial 6: Far 1200s



Trial 7: Far 1200s



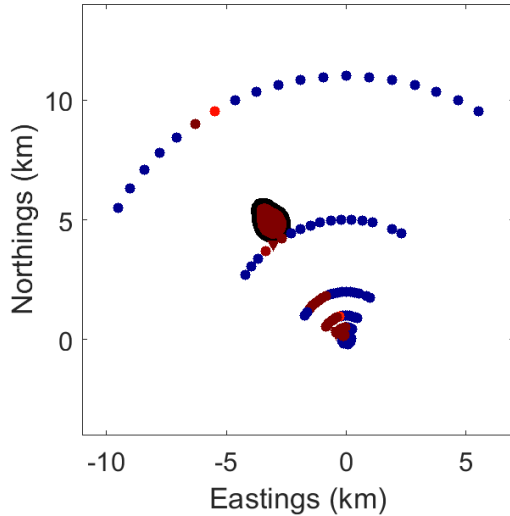
Mock urban array
 4,545 kg
 Vertically down release
 1.5 m/s
 -18°

Open terrain
 8,391 kg
 Vertically down release
 2.4 m/s
 -18°

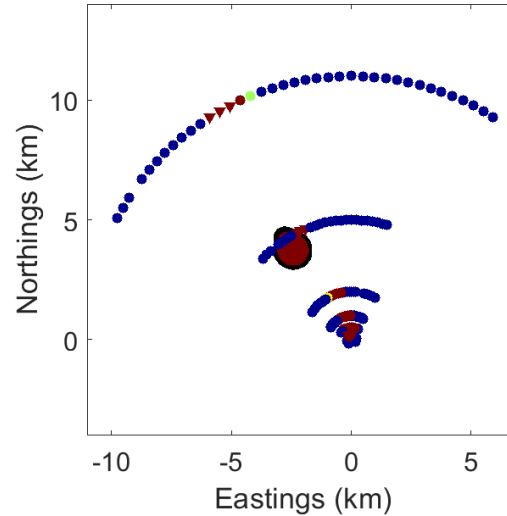
Open terrain
 9,072 kg
 45-deg down release
 4.0 m/s
 -15°

Concentration Contours

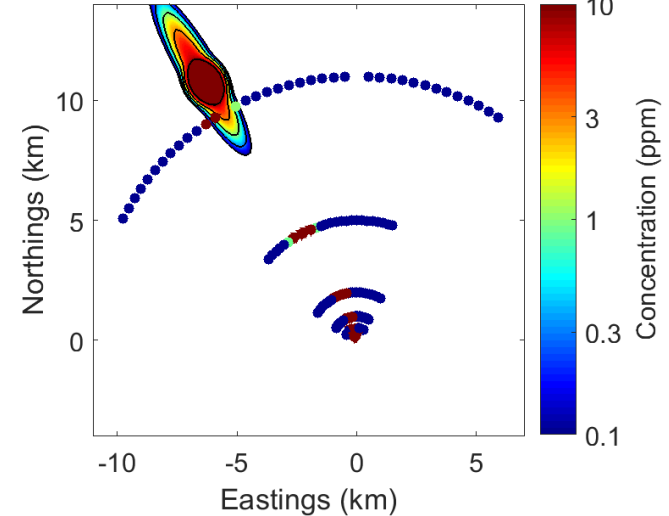
Trial 1: Far 1800s





Trial 6: Far 1800s




Trial 7: Far 1800s



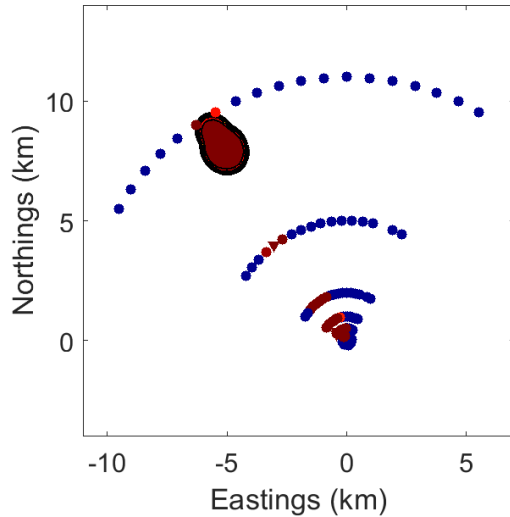
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 45-deg down release

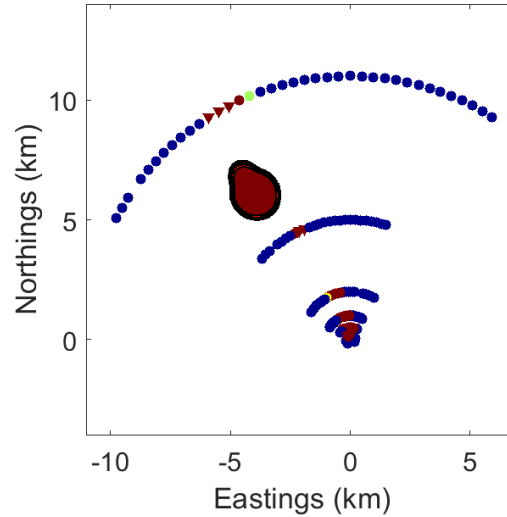
Concentration Contours

Trial 1: Far 2700s



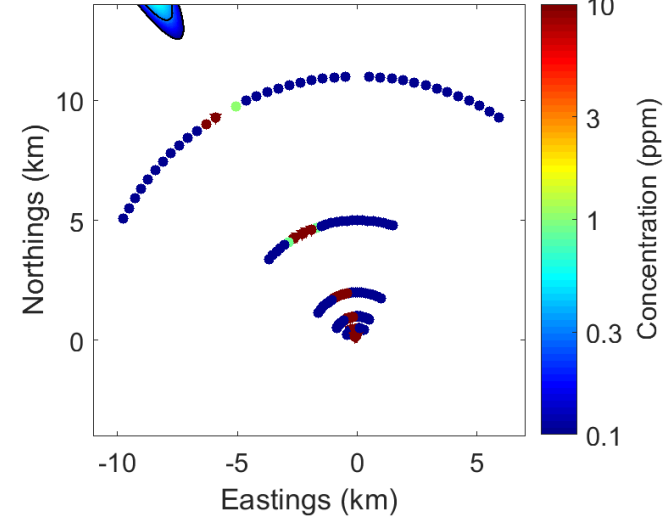
Mock urban array
 4,545 kg
 Vertically down release
 1.5 m/s
 -18°

Trial 6: Far 2700s



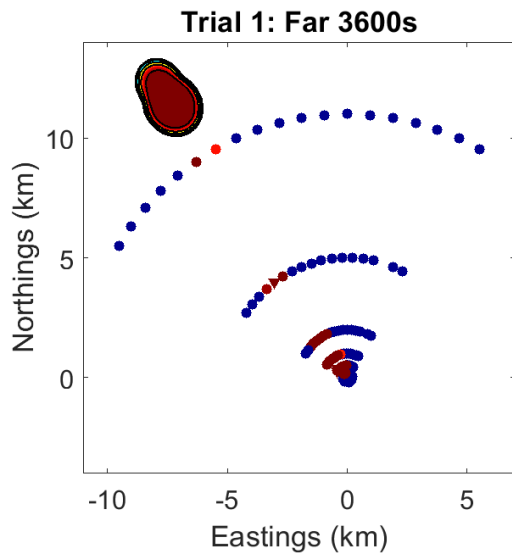
Open terrain
 8,391 kg
 Vertically down release
 2.4 m/s
 -18°

Trial 7: Far 2700s

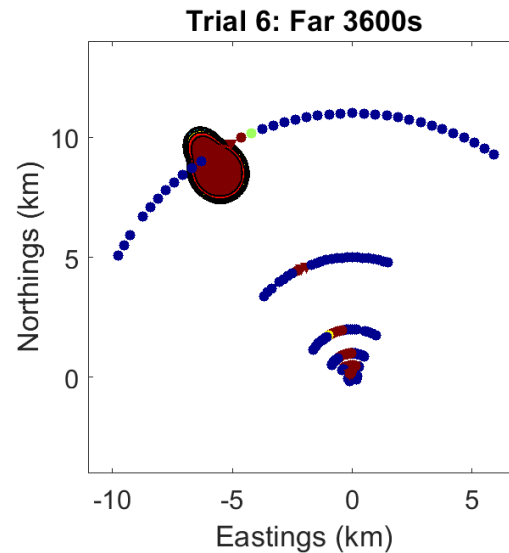


Open terrain
 9,072 kg
 45-deg down release
 4.0 m/s
 -15°

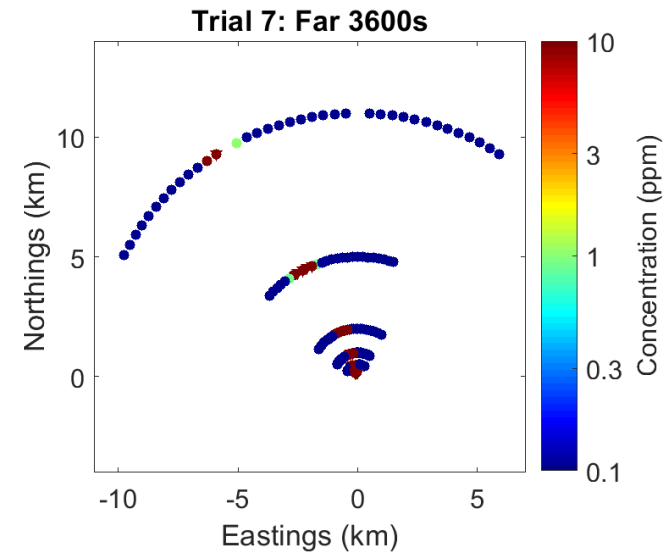
Concentration Contours



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 Vertically down release
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Open terrain
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 Vertically down release
 2.4 m/s
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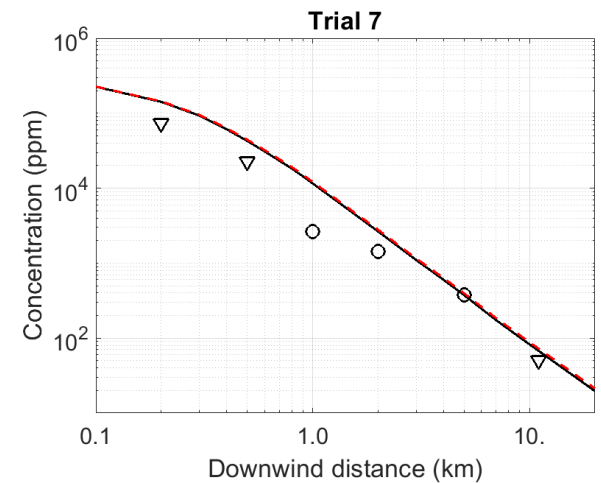
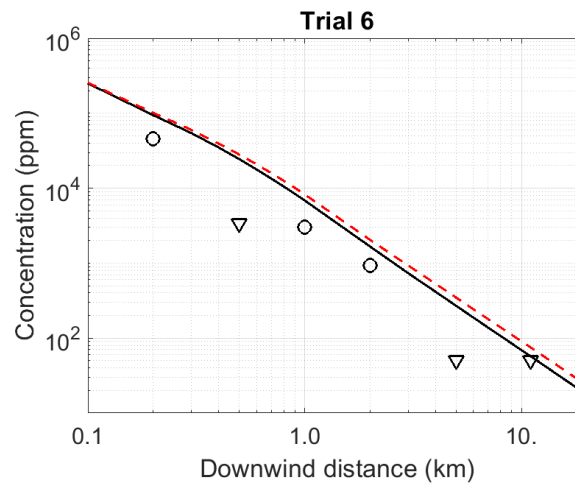
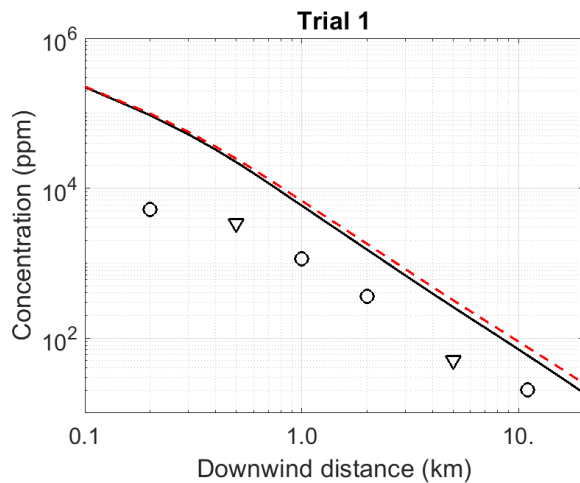
Open terrain
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Outline

- Aims
- Overview of DRIFT model
 - Model capabilities
 - Configuration for model inter-comparison exercise
- Preliminary model results
 - Maximum arc-wise concentration versus downwind distance
 - Maximum concentration across the azimuth angle of the arcs
 - Contour plots
- Sensitivity analysis
 - Dry deposition velocity set to zero
 - Increased roughness for urban array in Trial 1
- Conclusions and Future Directions

Dry Deposition Sensitivity Test

- Base case with dry deposition velocity $v_d = 0.04$ cm/s
- - - Dry deposition velocity set to zero (no deposition)



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 -18°
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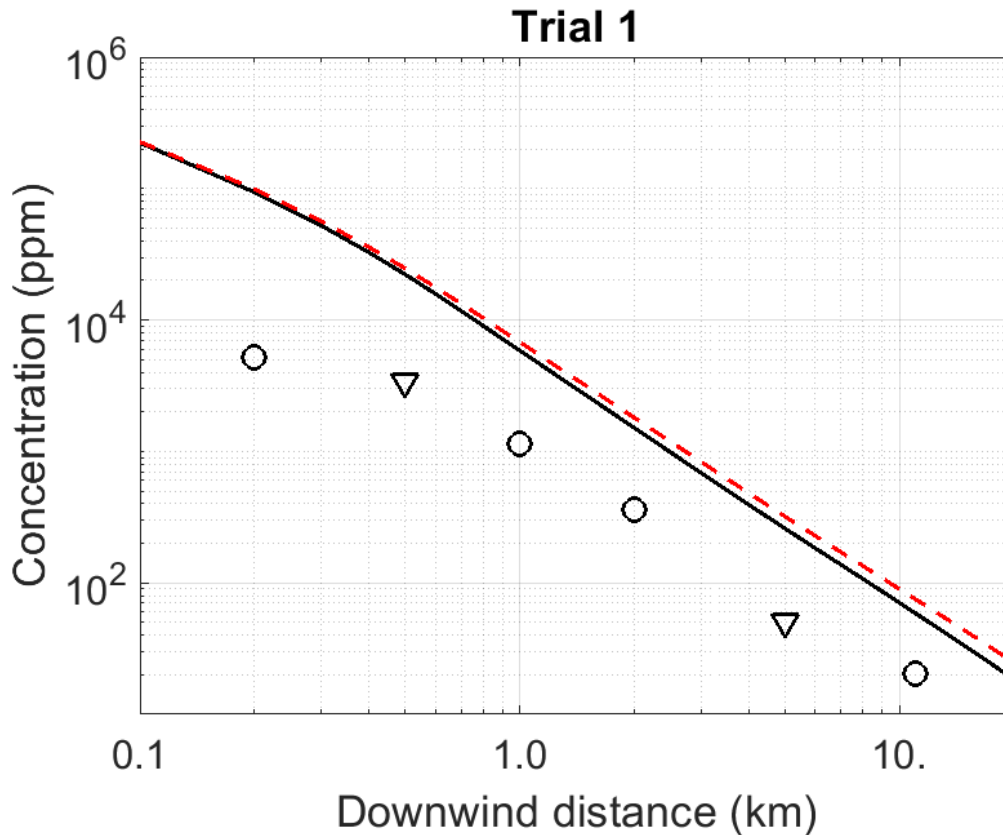
Open terrain
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 -15°
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All results are for 2 s (raw) averaging times

Dry Deposition Sensitivity Test

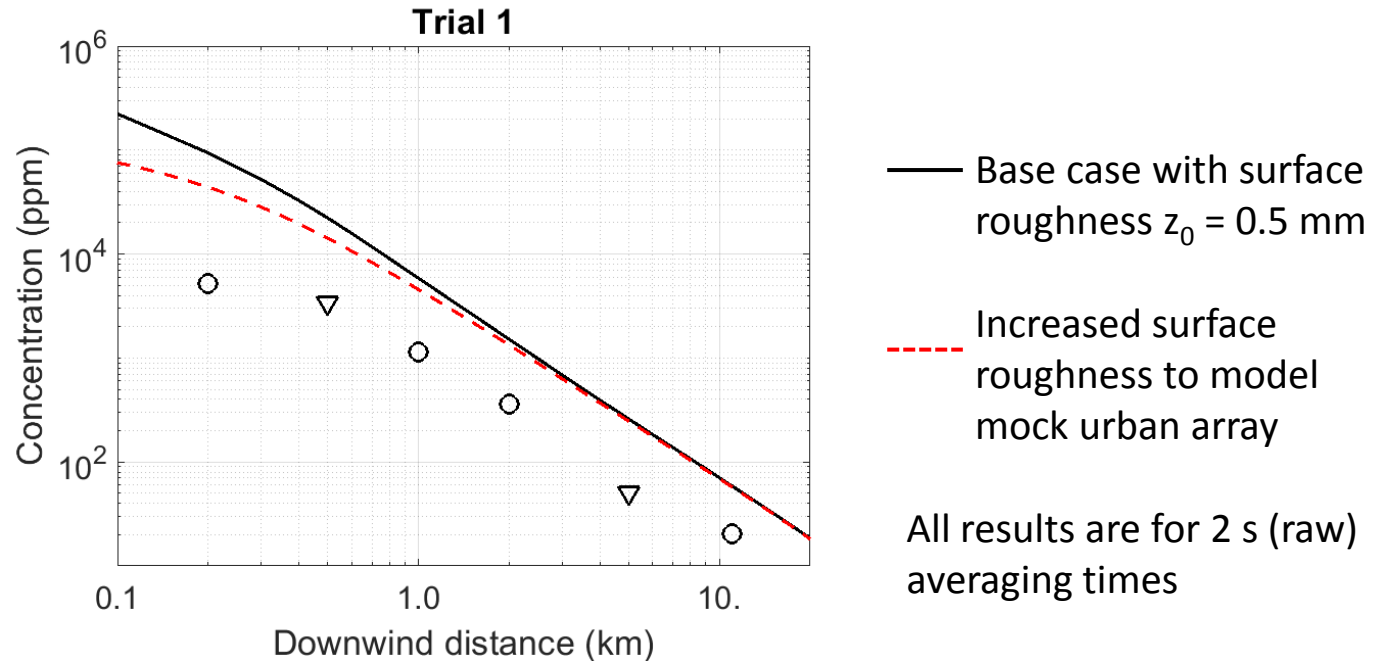
- Base case with dry deposition velocity $v_d = 0.04$ cm/s
- - - Dry deposition velocity set to zero (no deposition)



Enlarged image for Trial 1

Logarithmic scale:
the difference is roughly 20 ppm
versus 30 ppm at 11 km

Mock Urban Array Sensitivity Test



- There is no obstacle-resolving model in DRIFT, only a uniform surface roughness can be used
- Approach: run two simulations with different roughness lengths: a.) $z_0 = 0.4$ m, b.) $z_0 = 0.5$ mm
- Blend the two simulations together at the downwind edge of the mock urban array (approx. 100 m)
- Displace the centerline concentration profile of the $z_0 = 0.5$ mm result to match the $z_0 = 0.4$ m result
- This approach was taken in HSL's previous DRIFT and PHAST simulations for JR11 at GMU last year

Conclusions and Future Directions

- DRIFT results for model inter-comparison exercise
 - Reasonably good predictions for Trials 6 and 7
 - Over-prediction in Trial 1: Effect of mock urban array? Wind speed profile?
 - Dry deposition velocity of 0.04 cm/s has a small effect (e.g. 20 ppm to 30 ppm at 11 km)
- Effect of averaging times
 - Small difference in using raw, 20 s or 1 minute averaging times
- Future DRIFT work
 - Investigate further the cloud speed in Trials 1 and 6, and over-prediction in Trial 1
 - Toxic load: calculate from time-varying concentrations and compare to IDA data
 - Source terms: sensitivity test using standard risk assessment approach for modelling Trials 1, 6 and 7 using DRIFT source models
 - Sensitivity tests to investigate other uncertainties: e.g. changing meteorology and dry deposition

Conclusions and Future Directions

- Future work on model inter-comparison exercise
 - Work with DNV GL on PHAST simulations
 - Help to cross-plot results from other models
- Chlorine incident analysis
 - Re-examine model predictions for three chlorine incidents (Festus, Macdona, Graniteville) using PHAST and DRIFT
 - Do we understand yet why the six models over-predicted the number of casualties in the original Hanna *et al.* (2008) study?

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

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AICHE

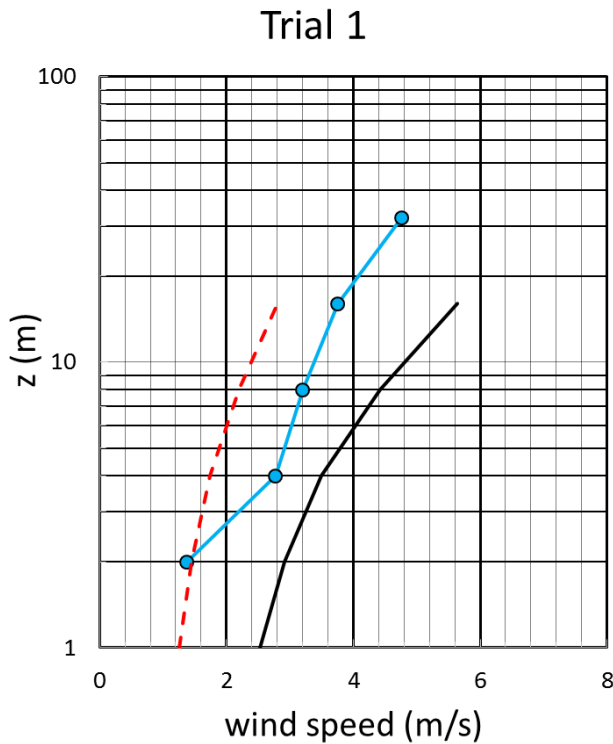
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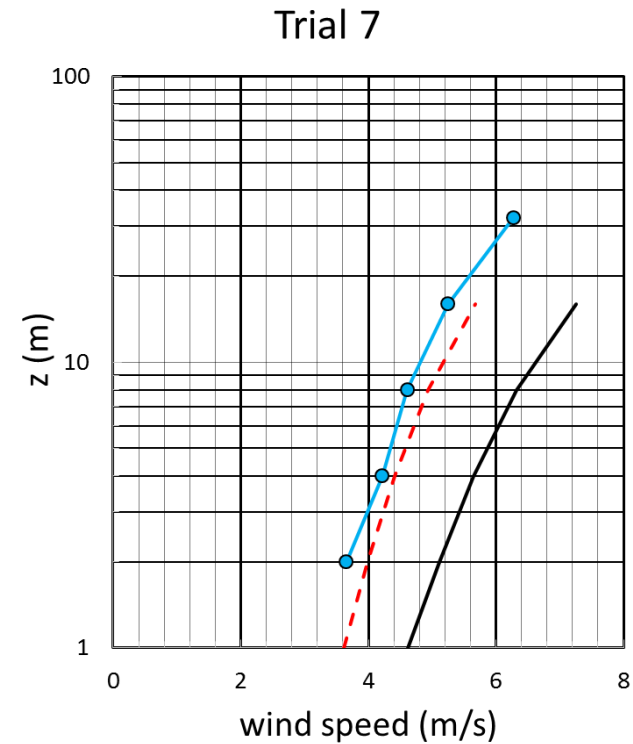
Thank you

Questions?

Modified u^* to match reference wind speed



- T3 PWIDS avg 1340 and 1350
- DRIFT $u^* = 0.108 \text{ m/s}$; $1/L = 0.124 \text{ /m}$; $z_0 = 0.5 \text{ mm}$
- - - DRIFT $u^* = 0.0537 \text{ m/s}$; $1/L = 0.124 \text{ /m}$; $z_0 = 0.5 \text{ mm}$



- T3 PWIDS avg 1400 and 1410
- DRIFT $u^* = 0.21 \text{ m/s}$; $1/L = 0.0229 \text{ /m}$; $z_0 = 0.5 \text{ mm}$
- - - DRIFT $u^* = 0.164 \text{ m/s}$; $1/L = 0.0229 \text{ /m}$; $z_0 = 0.5 \text{ mm}$

Modified u^* to match reference wind speed

