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.

Integral model predictions of the Jack Rabbit II 2015 experiments using DRIFT and PHAST

21st Annual George Mason University (GMU) Conference on
Atmospheric Transport and Dispersion Modeling

Fairfax, Virginia, USA, 13-15 June 2017

Simon Gant, Bryan McKenna, Maria Mallafrè Garcia, James
Stewart, Alison McGillivray, Mike Wardman, Harvey Tucker (HSE)

Graham Tickle (GT Science & Software)

Henk Witlox (DNV GL)

Outline

- Aims
- Overview of DRIFT and PHAST models
- Brief review of JR11 2015 data
- Model validation
 - Discharge
 - Maximum concentrations
 - Toxic load
- Preliminary results from sensitivity analysis
- Conclusions and Future Directions

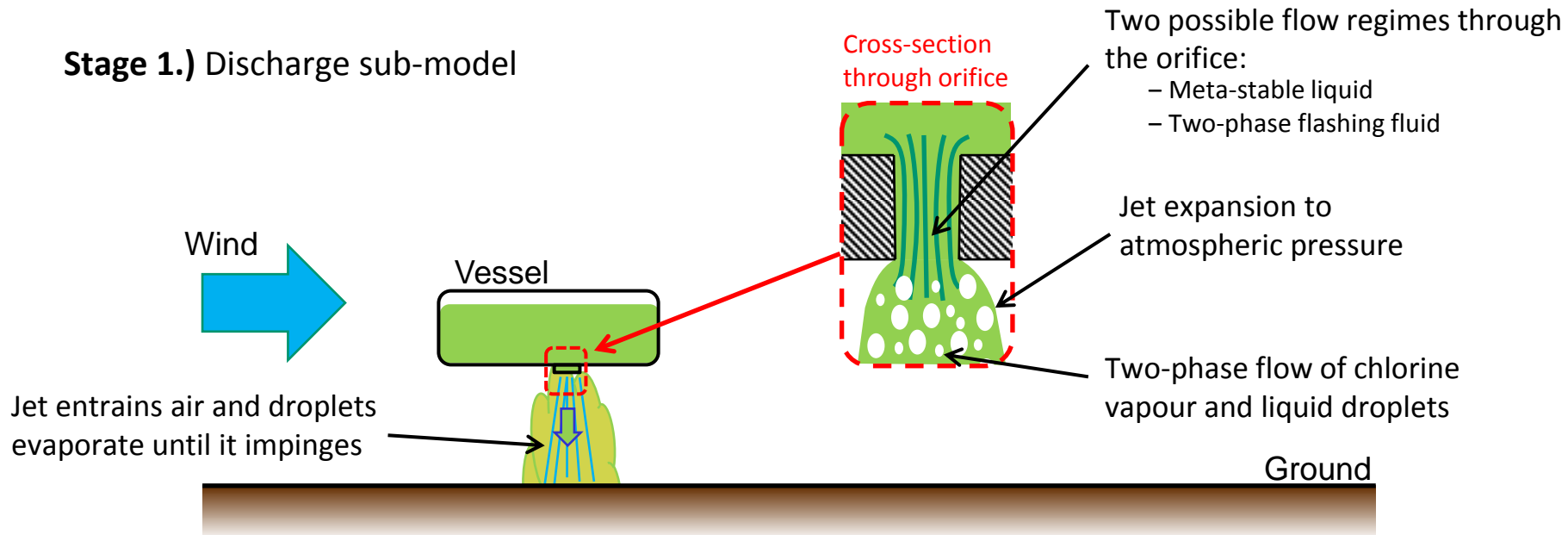
Aims

Aims of our involvement in Jack Rabbit II:

- Before the experiments
 - To help setup the experiments by providing dispersion model predictions for positioning of sensors
- After the experiments
 - To help interpret measurement data
 - To validate DRIFT and PHAST models
 - To use CFD to investigate the near-field dispersion behaviour
- To collaborate with other experts in the Modelers' Working Group and share findings

Overview of DRIFT and PHAST models

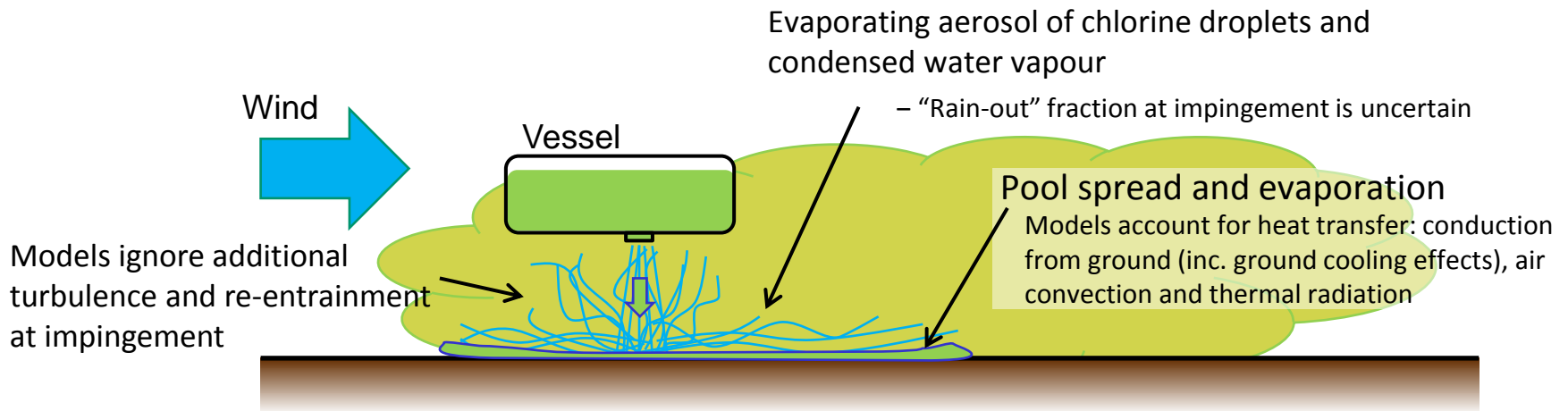
Stage 1.) Discharge sub-model



Model sensitivity tests performed to assess the impact of the flow regime through the orifice

Overview of DRIFT and PHAST models

Stage 2.) Modelling interaction of the two-phase jet with the ground

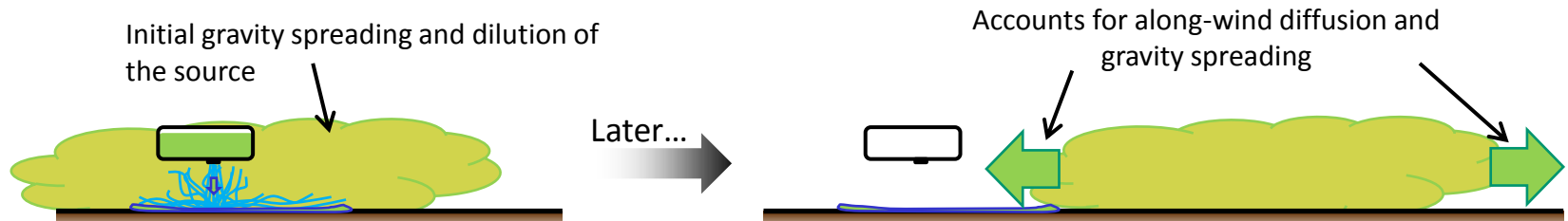


Model sensitivity tests performed to assess impact of liquid rain-out and pool formation

Overview of DRIFT and PHAST models

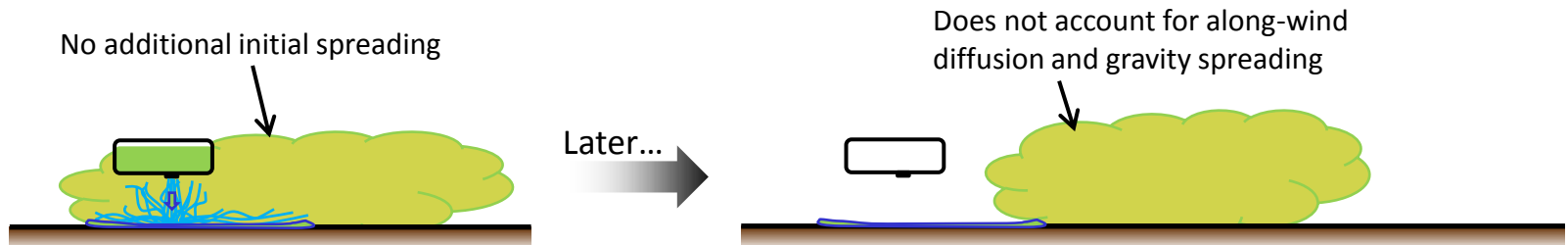
Stage 3.) Modelling dispersion of cloud

DRIFT



- 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

PHAST



- PHAST can produce clouds that spread laterally more than along-wind, and over-predict concentrations in near-field
- Found to under-predict extent of cloud in stable conditions
- New PHAST version 8.0 (not used here, released in late 2017) accounts for along-wind diffusion and gravity spreading

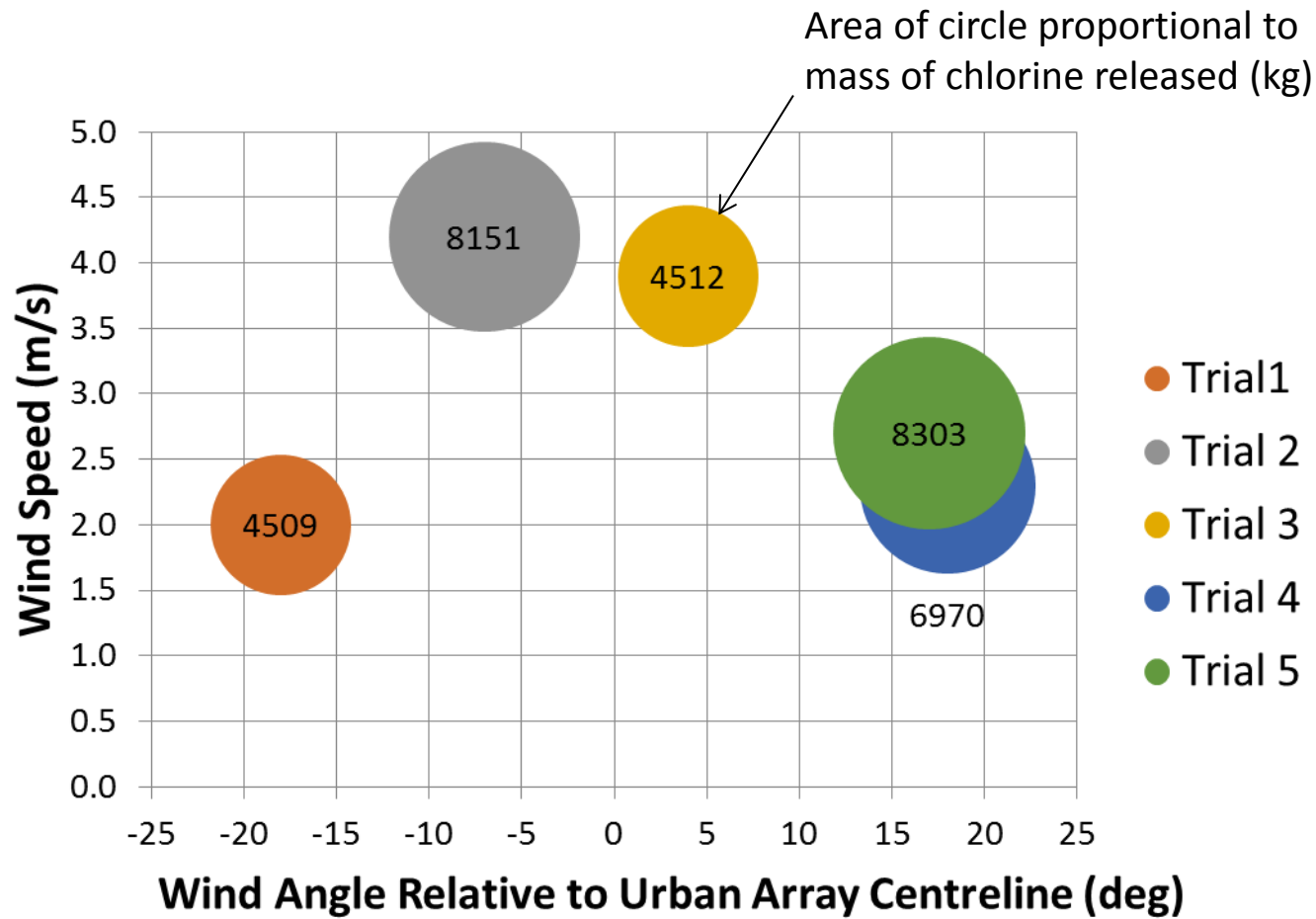
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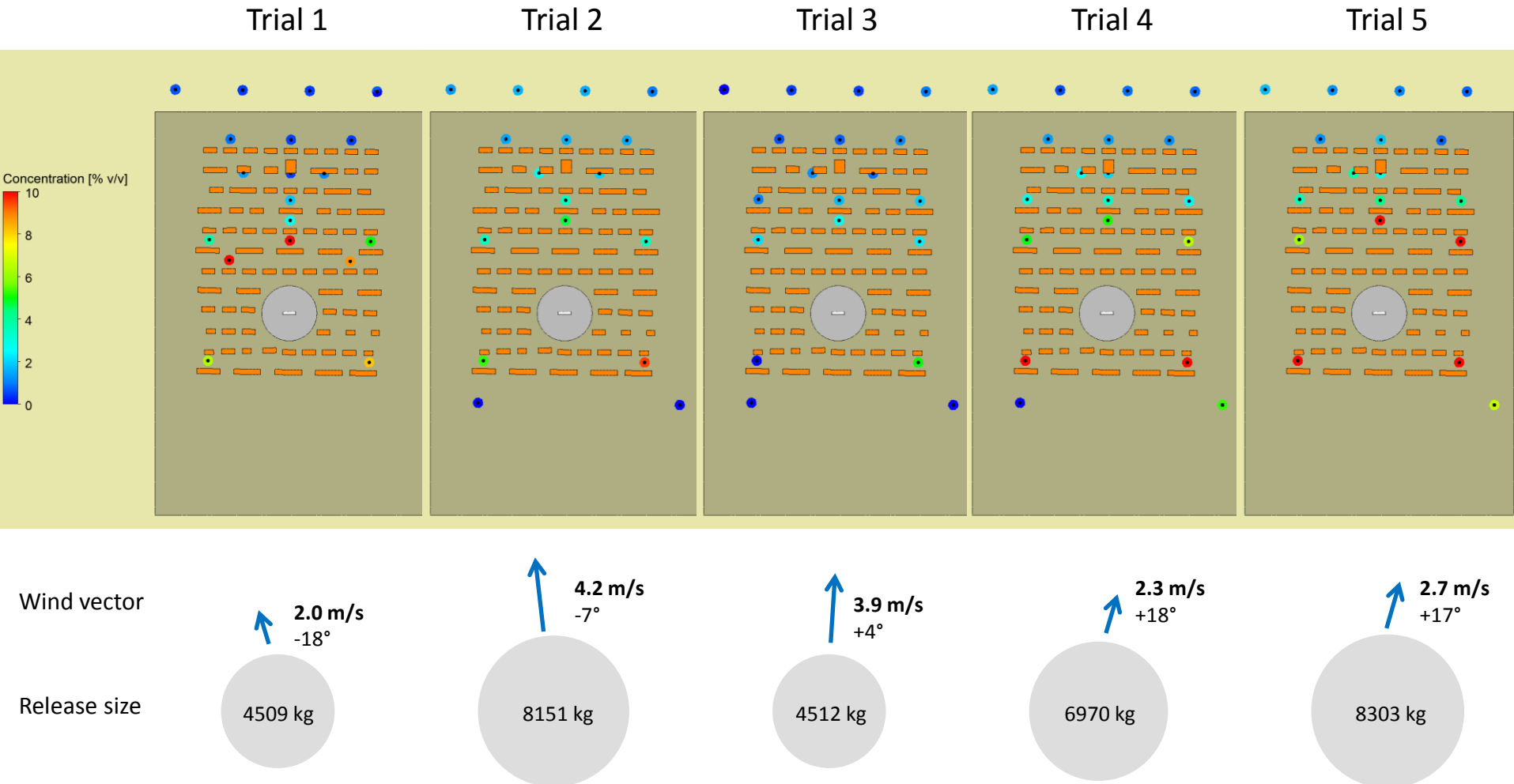
Brief Review of JRII 2015 data

Trial	Chemical Amount (kg)	Initial Tank Pressure (barg)	Wind direction offset to urban array (deg)	Wind Speed (m/s)	Atmospheric Temperature (°C)	Relative Humidity (%)	Atmospheric Pressure (Pa)	Pasquill Stability Class
1	4509	6.50	-18	2.0	17.7	39.2	87,350	F
2	8151	6.06	-7	4.2	22.7	33.6	87,512	C → B
3	4512	5.71	+4	3.9	22.5	30.3	87,097	D
4	6970	5.16	+18	2.3	22.5	26.9	86,926	C-D → B
5	8303	5.87	+17	2.7	22.2	26.5	86,653	D ?

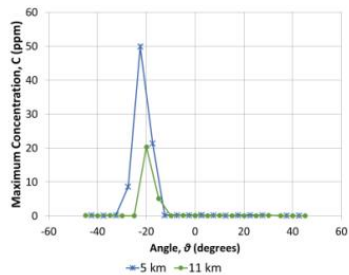
Brief Review of JRII 2015 data



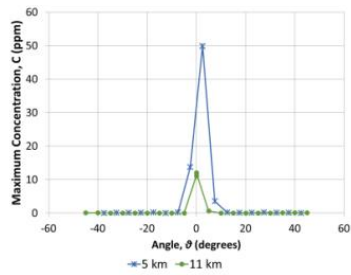
Brief Review of JRII 2015 data



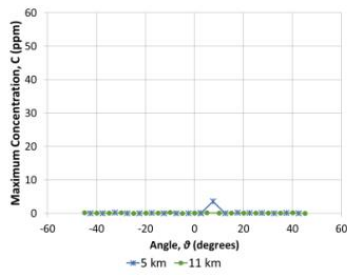
Trial 1



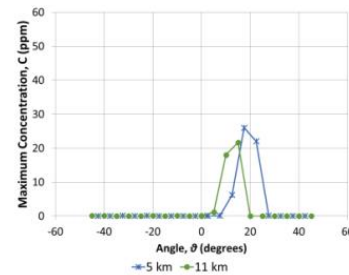
Trial 2



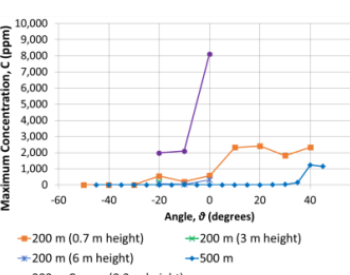
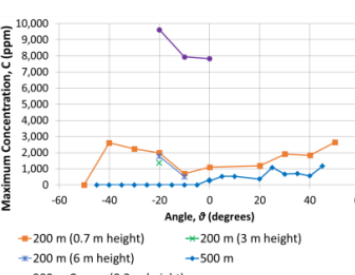
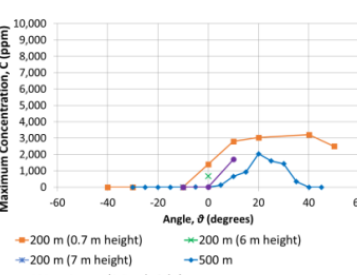
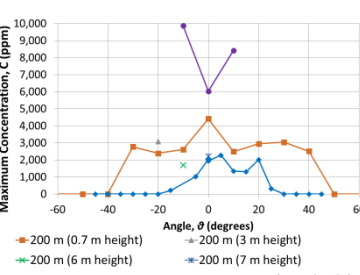
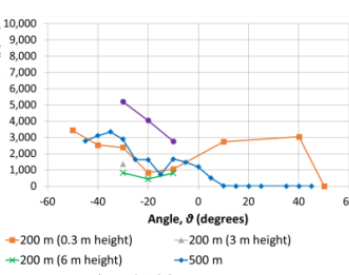
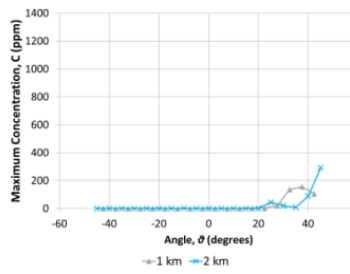
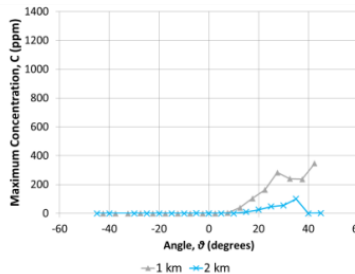
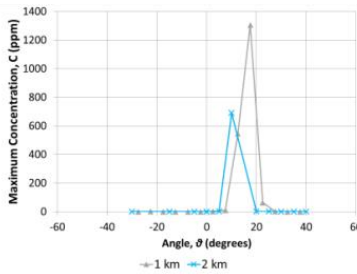
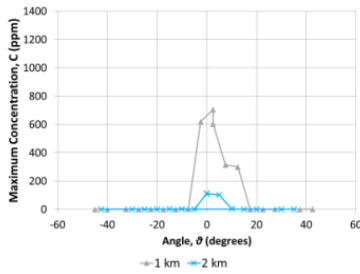
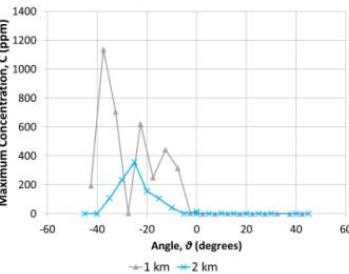
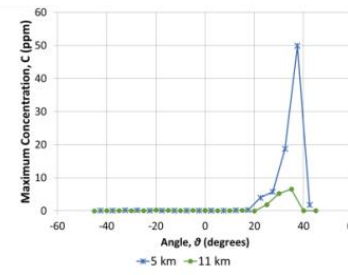
Trial 3



Trial 4



Trial 5



4509 kg
2.0 m/s
-18°

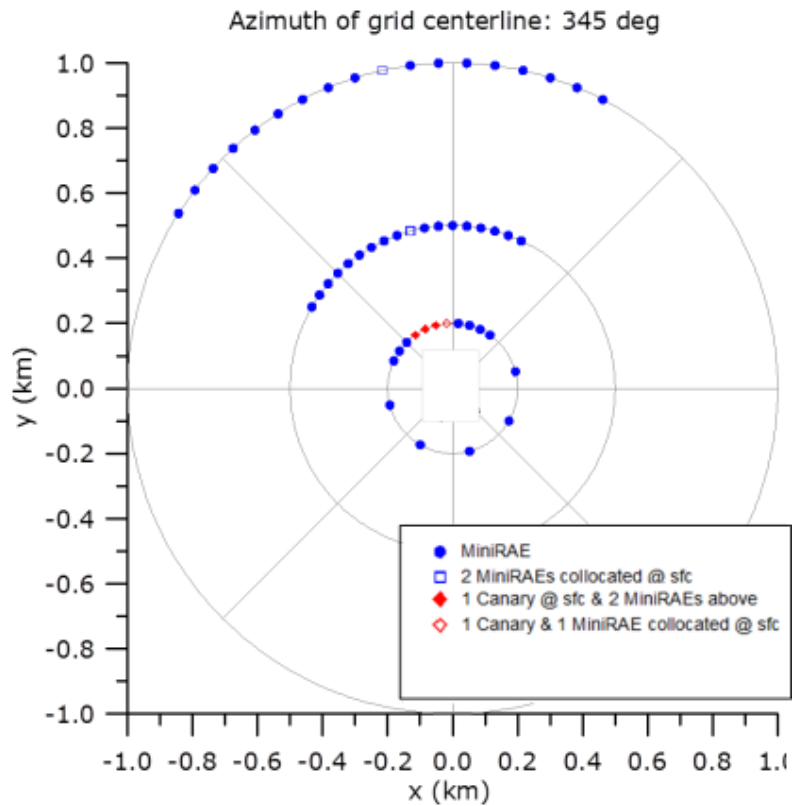
8151 kg
4.2 m/s
-7°

4512 kg
3.9 m/s
+4°

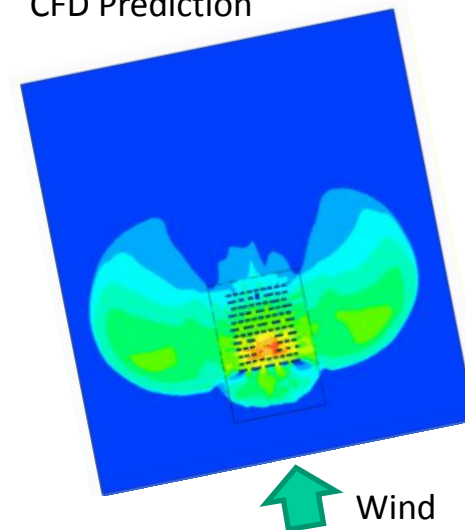
6970 kg
2.3 m/s
+18°

8303 kg
2.7 m/s
+17°

Brief Review of JRII 2015 data

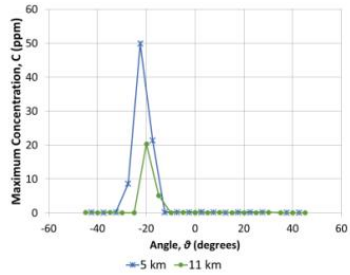


CFD Prediction

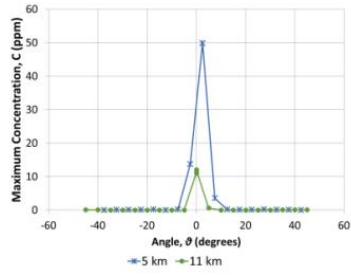


Is there any evidence of bifurcated cloud behavior at the 200 m and 500 m arcs?

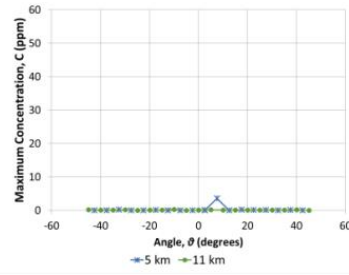
Trial 1



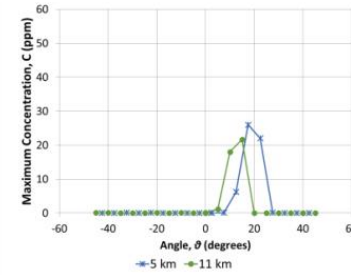
Trial 2



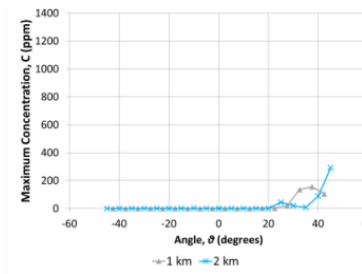
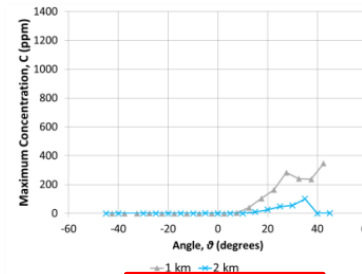
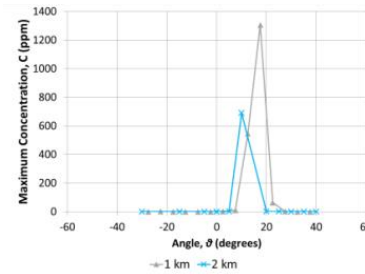
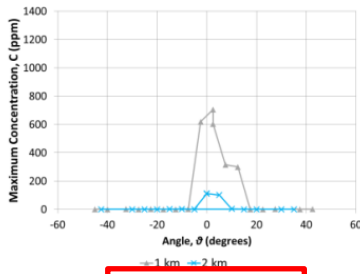
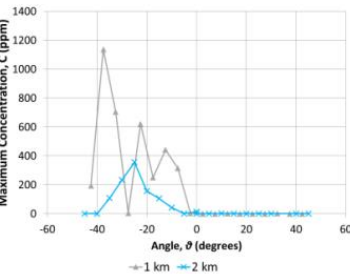
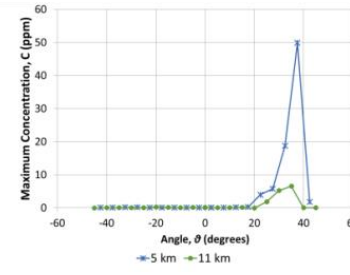
Trial 3



Trial 4



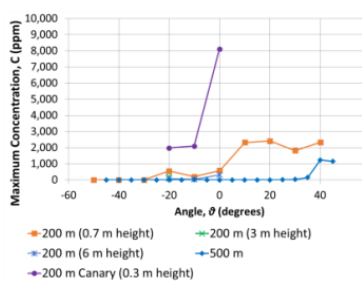
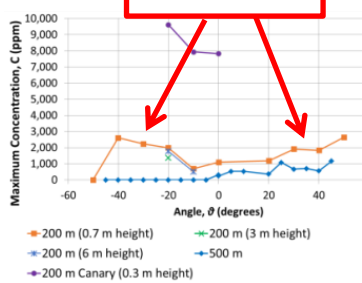
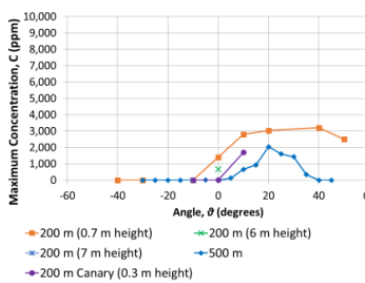
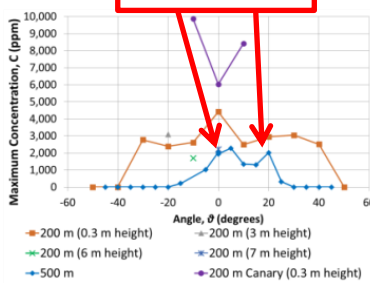
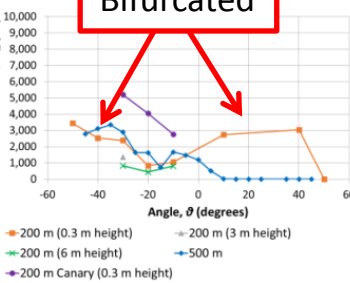
Trial 5



Bifurcated

Bifurcated

Bifurcated



2.0 m/s
-18°
4509 kg

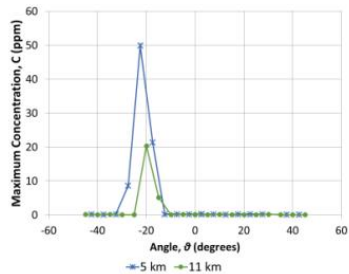
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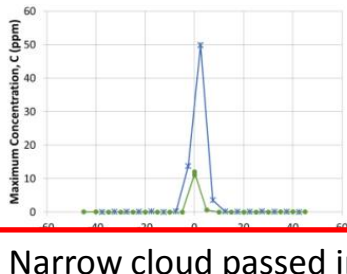
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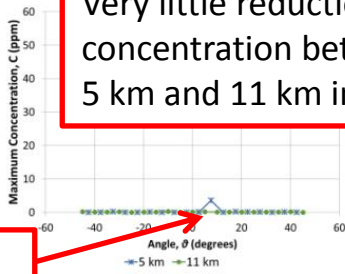
Trial 1



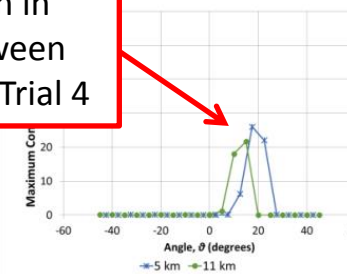
Trial 2



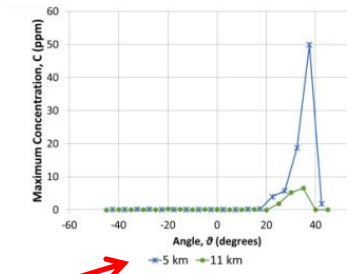
Trial 3



Trial 4



Trial 5

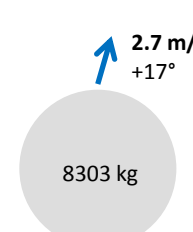
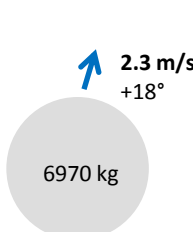
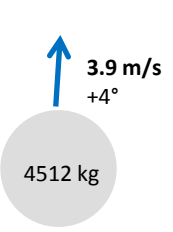
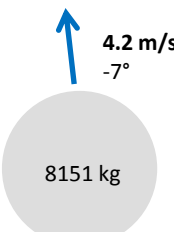
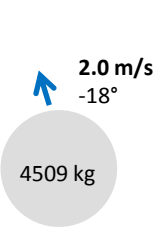
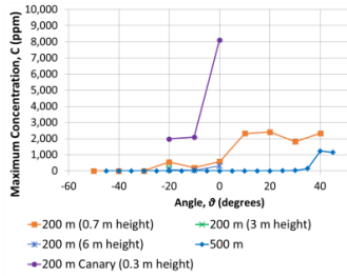
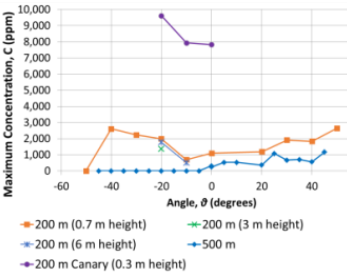
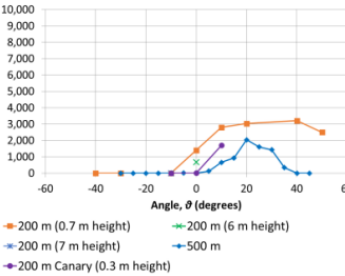
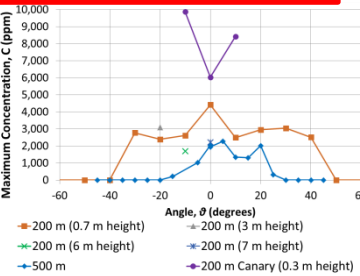
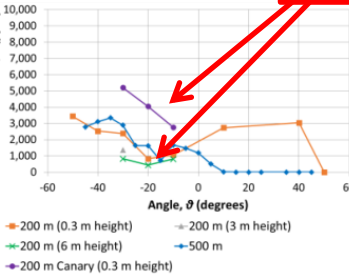
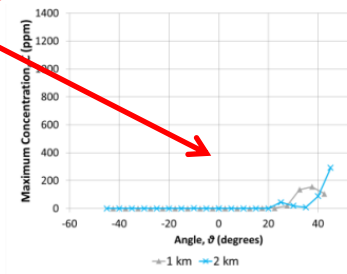
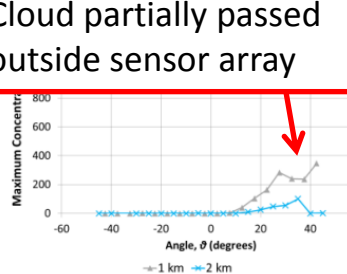
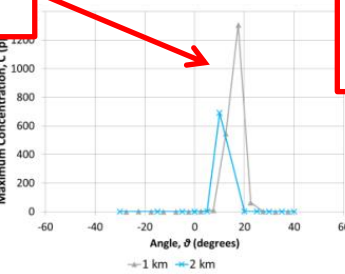
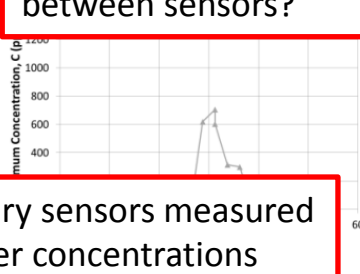
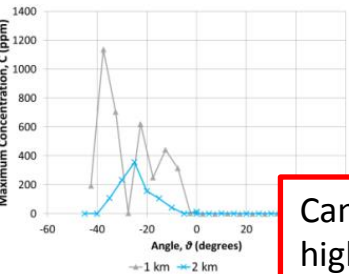


Very little reduction in concentration between 5 km and 11 km in Trial 4

Narrow cloud passed in between sensors?

Cloud partially passed outside sensor array

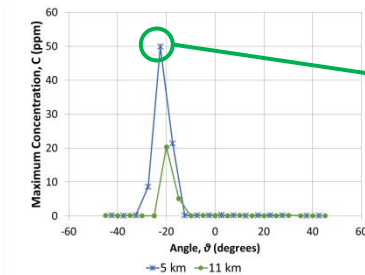
Canary sensors measured higher concentrations than MiniRAE at 200 m



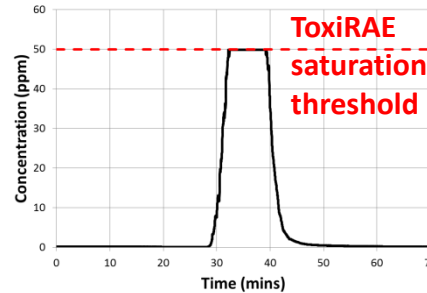
Brief Review of JRII 2015 data

Measured time-varying concentrations at each sensor

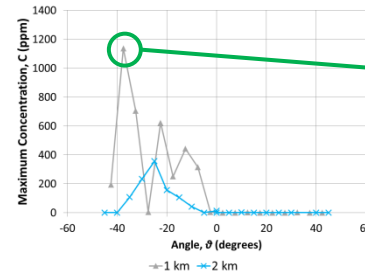
Trial 1



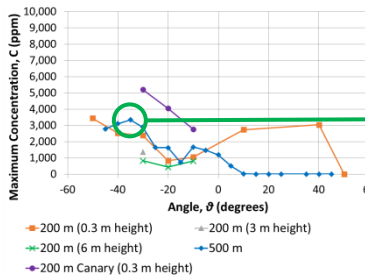
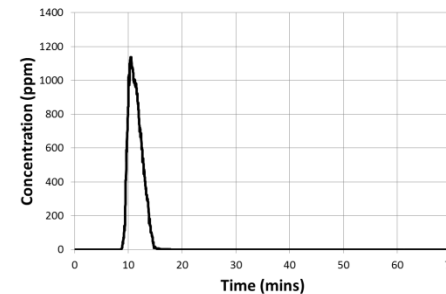
5 km



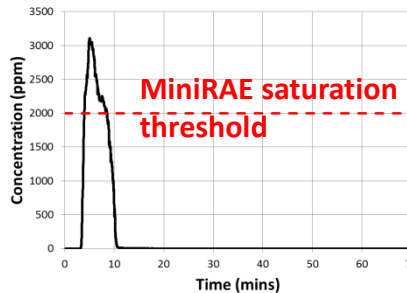
“Actual” concentration higher than measured



1 km



500 m



MiniRAE values corrected using the pre- and post-experiment calibration tests, so the maximum sometimes exceeded the saturation threshold

16

Trial 1

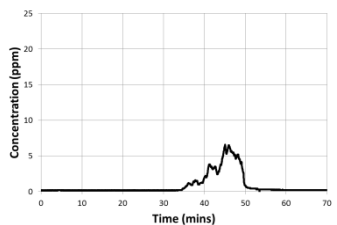
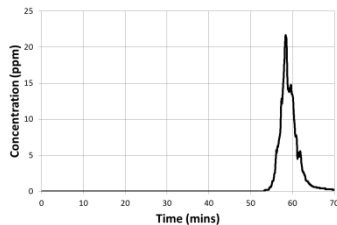
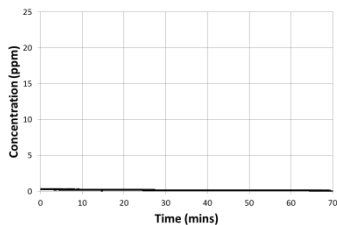
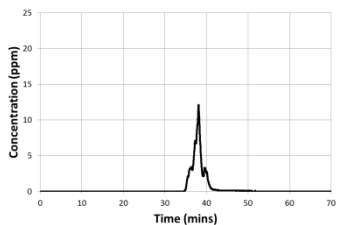
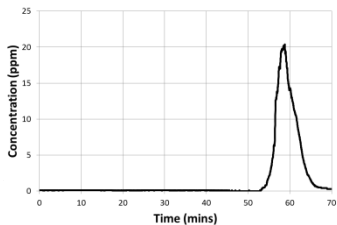
Trial 2

Trial 3

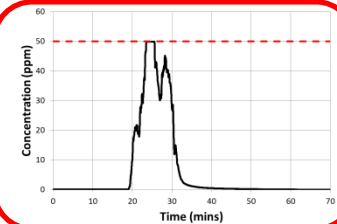
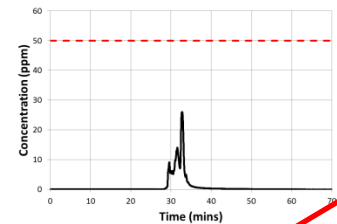
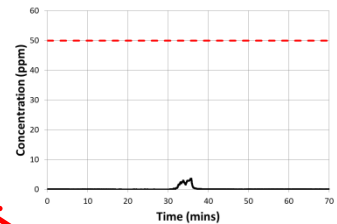
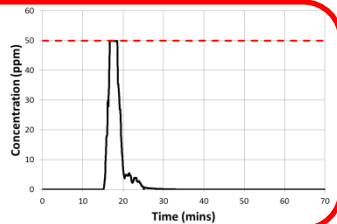
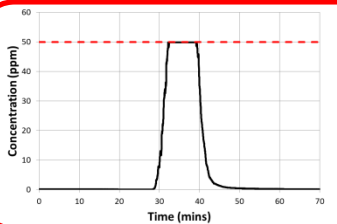
Trial 4

Trial 5

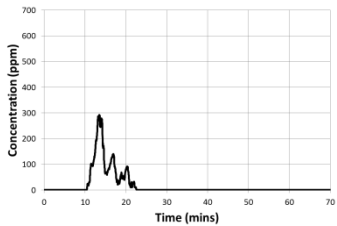
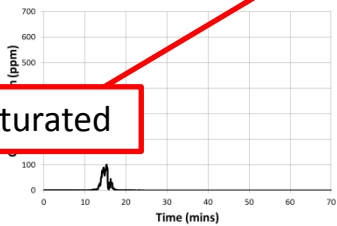
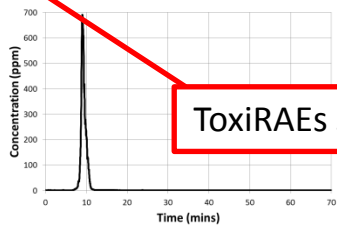
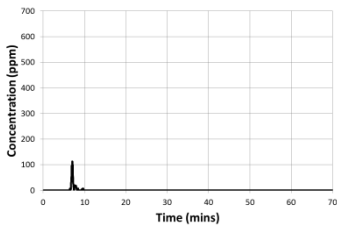
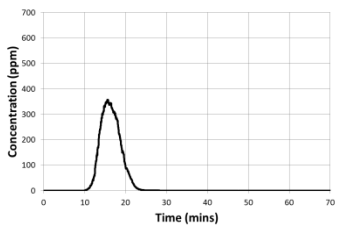
11 km



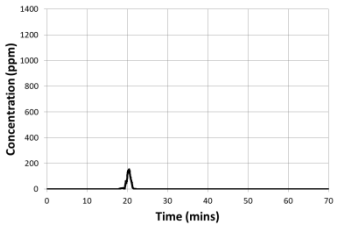
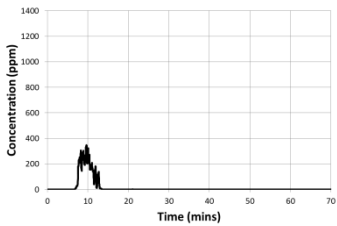
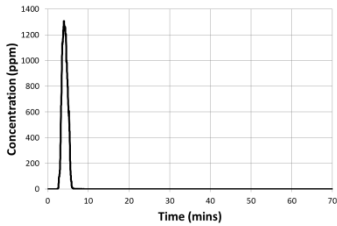
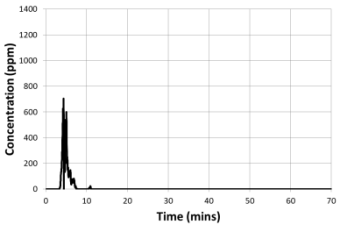
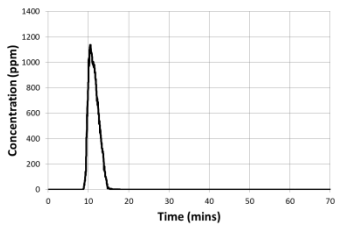
5 km



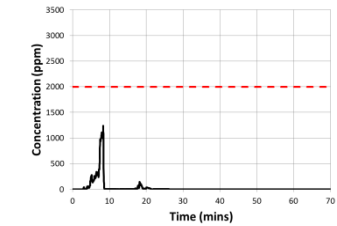
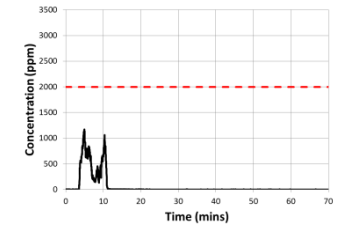
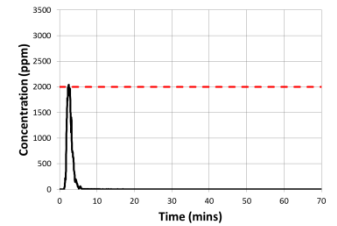
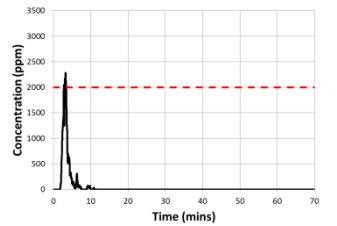
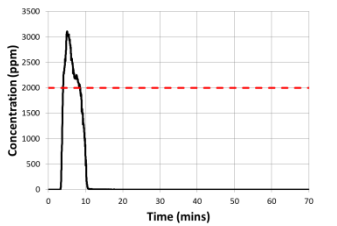
2 km



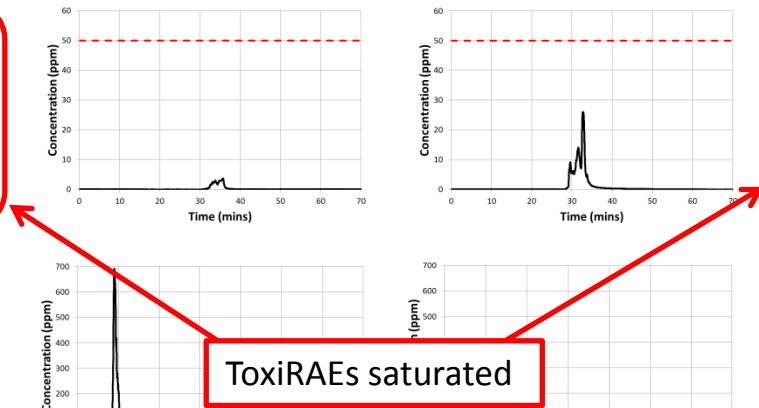
1 km



500 m








ToxiRAEs saturated



Brief Review of JRII 2015 data

Maximum arc-wise concentrations (ppm)

Distance (km)	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5
0.2	5,204	9,869	3,210	9,624	8,110
0.5	3,348	2,282	2,041	1,173	1,235
1	1,137	705	1,307	347	155
2	357	112	691	101	292
5	50	50	3.6	26	50
11	20	12	0	22	7

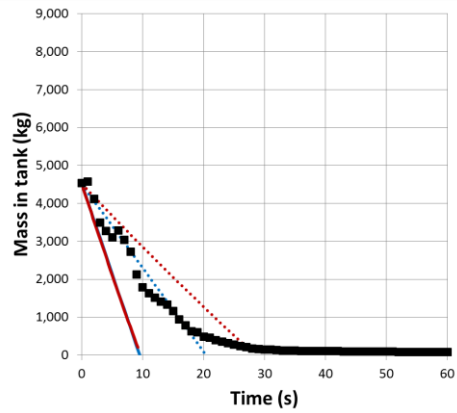
-  Canary sensor data: only 3 sensors, may have missed plume maximum
-  MiniRAE sensor saturated or significantly exceeded nominal calibration limits (2000 ppm)
-  ToxiRAE sensor saturated (50 ppm)
-  Narrow plume passed between sensors: plume maximum may have been missed
-  Plume passed beyond edge of arc: plume maximum may have been missed

Outline

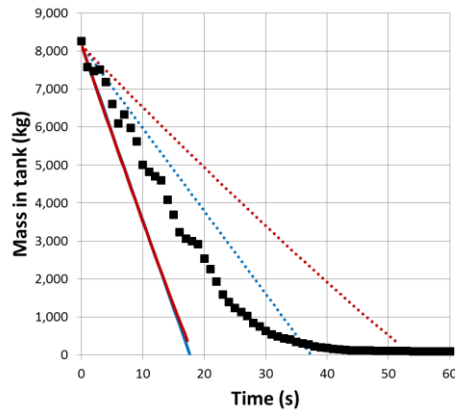
- Aims
- Overview of DRIFT and PHAST models
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 - Discharge
 - Maximum concentrations
 - Toxic load
- Preliminary results from sensitivity analysis
- Conclusions and Future Directions

Model Validation: JRII 2015 Discharge

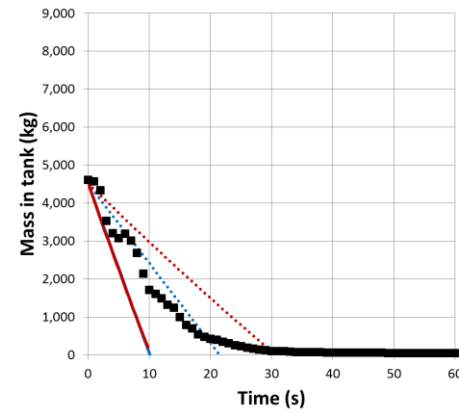
Trial 1



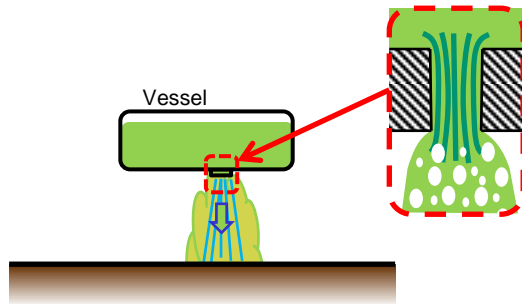
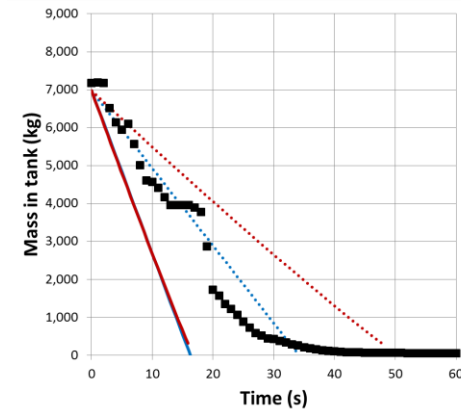
Trial 2



Trial 3

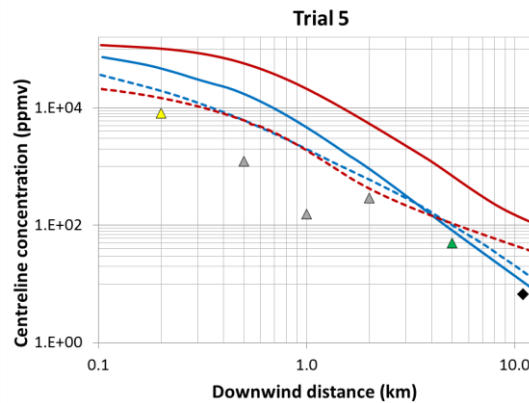
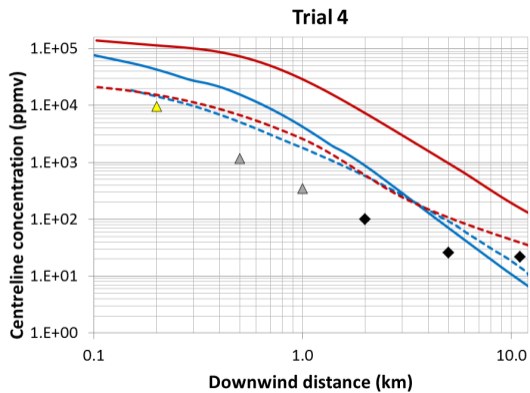
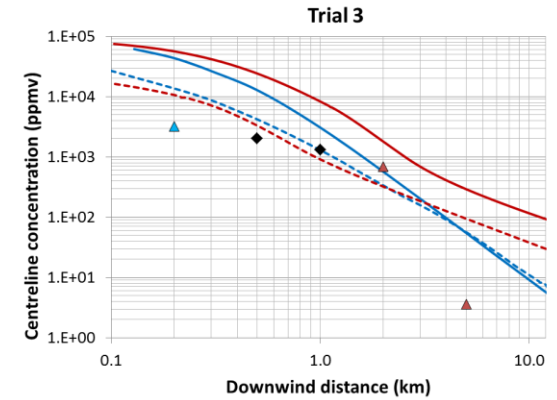
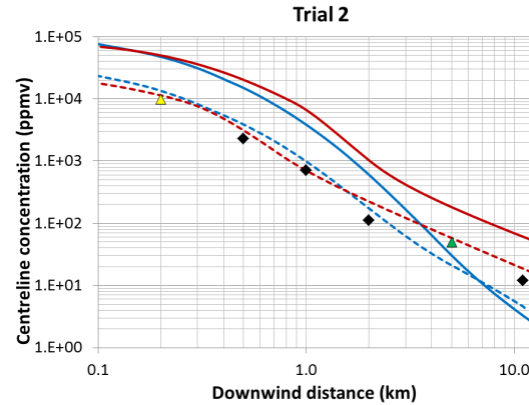
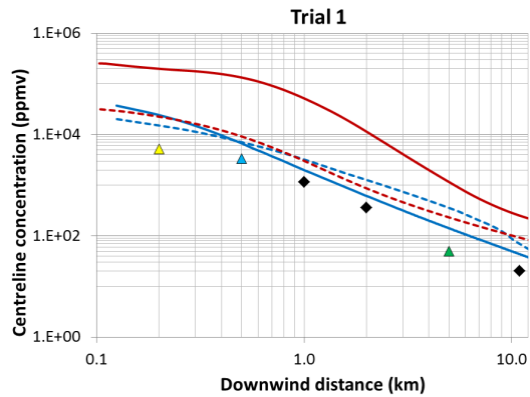


Trial 4



- DRIFT metastable liquid
 - DRIFT flashing in orifice
 - PHAST metastable liquid
 - PHAST flashing in orifice
 - Measurements from load cell data
- } Results from HSE's STREAM outflow model

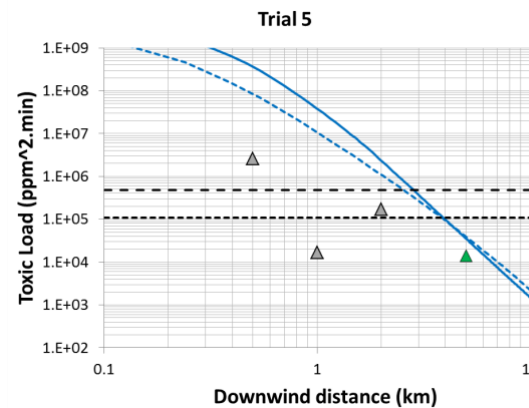
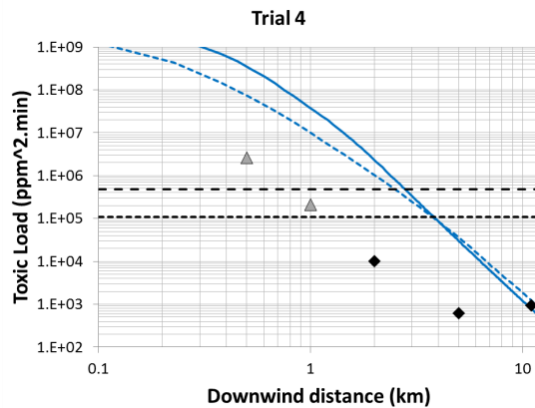
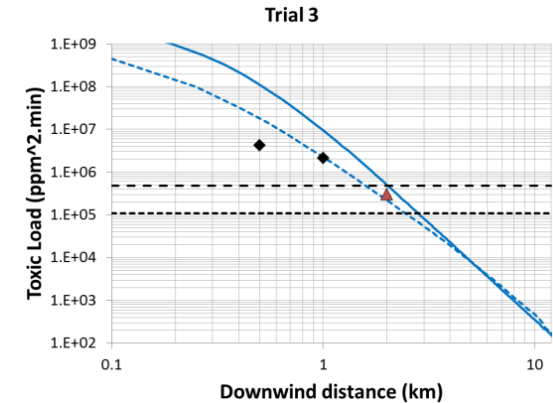
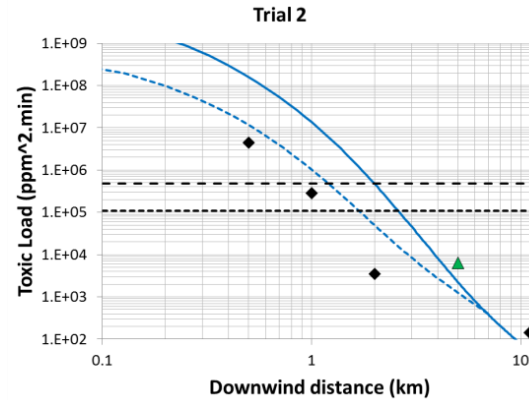
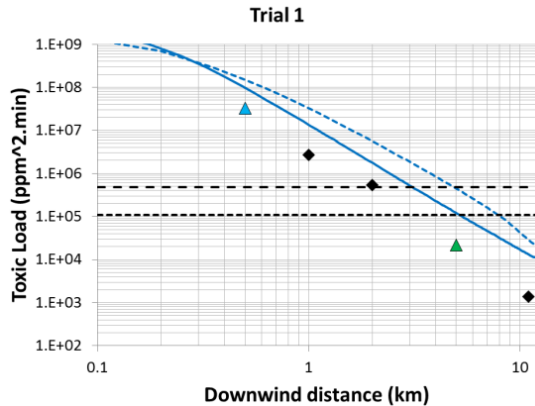
Model Validation: JRII 2015 Concentration



- DRIFT without droplet rainout
- - - DRIFT with droplet rainout
- PHAST without droplet rainout
- - - PHAST with droplet rainout
- ◆ Measured maximum arc-wise concentration
- ▲ Canary sensor data: only 3 sensors, may have missed plume maximum
- ▲ MiniRAE sensor saturated or exceeded calibration
- ▲ ToxiRAE sensor saturated
- ▲ Narrow plume passed between sensors: plume maximum may have been missed
- ▲ Plume passed beyond edge of arc: plume maximum may have been missed

Both PHAST and DRIFT models assumed metastable liquid discharge from the vessel

Model Validation: JRII 2015 Toxic Load



- DRIFT without droplet rainout
- - - DRIFT with droplet rainout
- - - Specified Level of Toxicity (SLOT)
- - - Significant Likelihood of Death (SLOD)
- ◆ Measured maximum arc-wise concentration
- ▲ Canary sensor data: only 3 sensors, may have missed plume maximum
- ▲ MiniRAE sensor saturated or exceeded calibration
- ▲ ToxiRAE sensor saturated
- ▲ Narrow plume passed between sensors: plume maximum may have been missed
- ▲ Plume passed beyond edge of arc: plume maximum may have been missed

$$\text{Toxic Load} = \int C^n dt$$

Results presented here using UK HSE value $n = 2.0$
(USA value is $n = 2.75$), data points provided by IDA

Outline

- Aims
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- Preliminary results from sensitivity analysis
- Conclusions and Future Directions

Sensitivity Analysis

- Global sensitivity analysis on DRIFT covering ranges of seven input variables relevant to JR11 2015 experiments

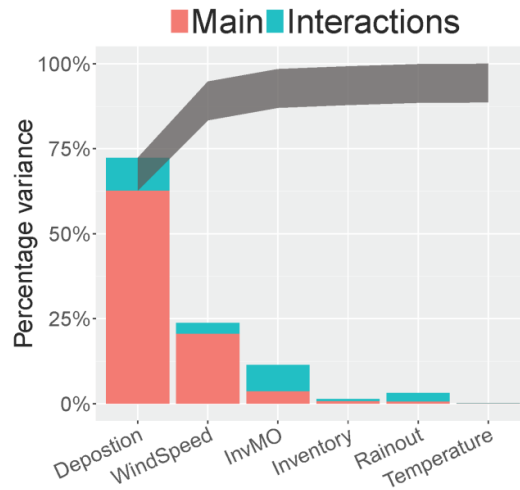
	Chlorine Inventory (kg)	DRIFT rainout fraction	Wind speed (m/s)	Temperature (K)	Inverse Monin-Obukhov length (m ⁻¹)	Vapour Deposition Velocity (m/s)	Discharge model
Minimum	4000	0	1.5	288.15	-0.12	0	Metastable liquid
Maximum	9000	1	5	303.15	0.08	0.05	Flashing

- 127 DRIFT simulations performed using Sobol' sequence sampling method
 - 64 metastable liquid discharge model
 - 63 flashing discharge model
- Model output of interest: distance to 10 and 100 ppm concentrations
- Variance based sensitivity analysis performed using Gaussian emulators
- Only preliminary results, work ongoing...

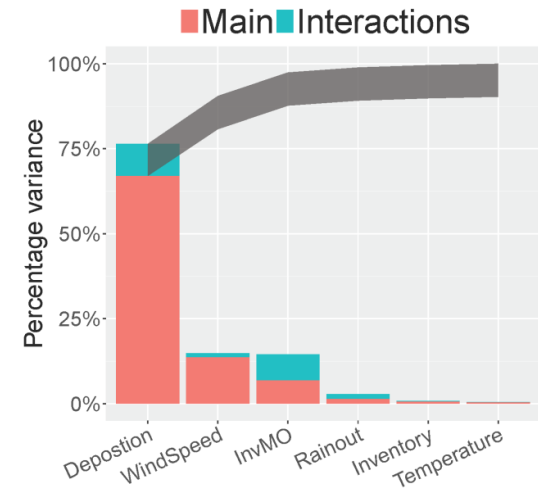
Sensitivity Analysis

Flashing

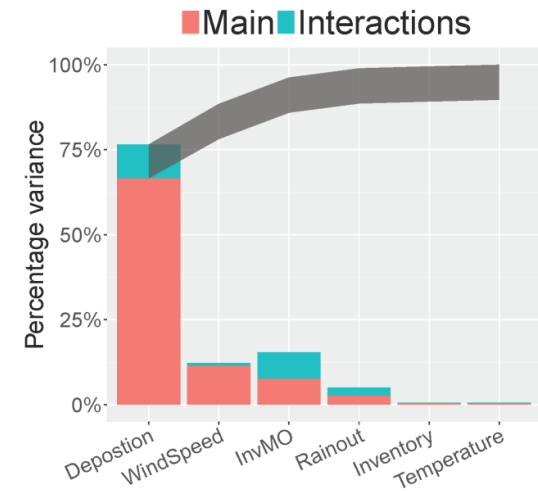
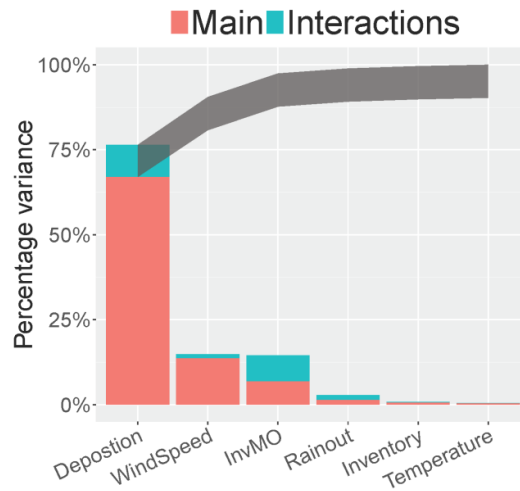
Distance to 100 ppm



Distance to 10 ppm



Metastable liquid



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Conclusions and Future Directions

- Model validation
 - Preliminary results for Jack Rabbit II 2015 show that DRIFT and PHAST provide reasonably good predictions of concentration when the models account for rainout
 - Concentrations are generally over-predicted slightly, but sometimes under-predicted
 - When models assume no rainout, concentrations are over-predicted (significantly for PHAST)
- Effect of averaging time on JR11 2015 measured maximum concentrations data has been investigated
 - No significant difference in using either no averaging or using 20 s or 30 s averaging times
- Wind speed, wind direction and atmospheric stability conditions in JR11 2015 tests
 - Further analysis of weather data is required
 - Conditions changed during the experiments (the cloud typically took 1 hour to reach 11 km), whereas models assumed constant conditions
 - Sensitivity tests are currently ongoing

Conclusions and Future Directions

- Dry deposition
 - Models did not explicitly include deposition effects
 - Ongoing model sensitivity tests and analysis
- Future work
 - Analysis of data from the Jack Rabbit II 2016 trials
 - Re-examination of 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 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 Khajehnejati,^f and Kay Koslan^g

Acknowledgements



DISCLAIMER:

- GT Science & Software contributed towards the work on DRIFT, and DNV GL Software contributed towards the work on PHAST, but the DRIFT and PHAST simulations presented in this paper were performed by HSE and have not been independently checked by the software developers
- 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:

- Shannon Fox (DHS)
- Thomas Mazzola and John Magerko (Engility)
- Ronald Meris (DTRA)
- 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 (NCAR)
- John Boyd (ARA)
- Steven Herring (DSTL)
- Andy Byrnes (UVU)

Additional Slides...

Averaging Times

Concept

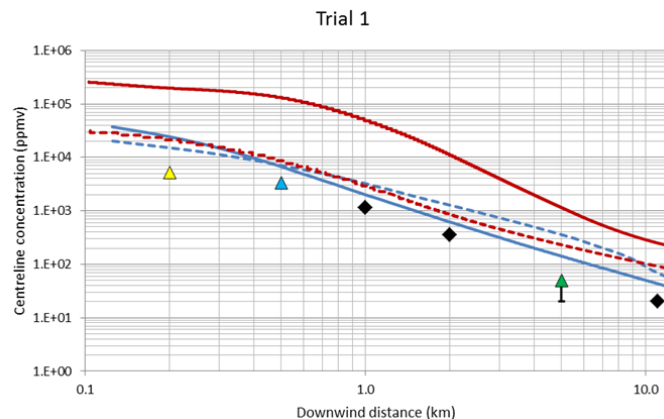
- Aim to compare models to measurements on like-for-like basis, using the same averaging times

Issues

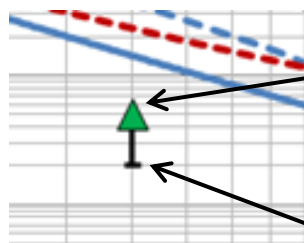
- Averaging times used by integral models and RANS CFD models are not clearly defined
- For the experimental data, JR11 max concentration measurements shown previously used a short time-average of approx. 1 second
- Joe Chang has also produced a summary of max concentrations based on 10 s, 20 s, 30 s, 1 min, 2 min, 5 min, 10 min, 20 min and 30 min averaged concentrations
- IDA produced toxic load data from measurements by integrating time-varying concentration using 0.1 and 1.0 min running time-average

Averaging Times

Aim: To assess the potential significance of averaging times, present the JRII 2015 measured maximum arc-wise concentrations using no time average, and using 20 s and 30 s time averages. Compare the results to PHAST and DRIFT



- Results presented in this format: graph of max arc-wise concentration, using error bars to show the range in values
- Data taken from Joe Chang spreadsheet: "Condensed_Scan_InSitu_2015JR_AllAvg_120716.xlsx"



Max concentration (no time averaging)

Error bar shows range in values of 20 s and 30 s time-averaged concentrations

PHAST Averaging Time

- PHAST uses a 18.75 s averaging time for instantaneous concentrations (commonly used for assessing flammable gas hazards)

- Originates from:

$$\frac{\sigma_{y1}}{\sigma_{y2}} = \left(\frac{t_{av1}}{t_{av2}} \right)^{0.2}$$

where

σ_y = Horizontal dispersion parameter

t_{av} = Averaging time

- Dispersion parameter σ_y for non-averaged instantaneous concentrations is approx. half the value for a 10 minute average (TNO Yellow Book, CCPS Guidelines)
- Since $(18.75 / 600)^{0.2} = 0.5$, the instantaneous concentrations equate to an averaging time of 18.75 s
- $t_{av} = 18.75$ s is not an actual averaging time, but its use is consistent with extrapolating the dispersion parameter from long time-averaged to instantaneous concentrations

DRIFT Averaging Time

Dilution predicted by DRIFT depends upon two factors:

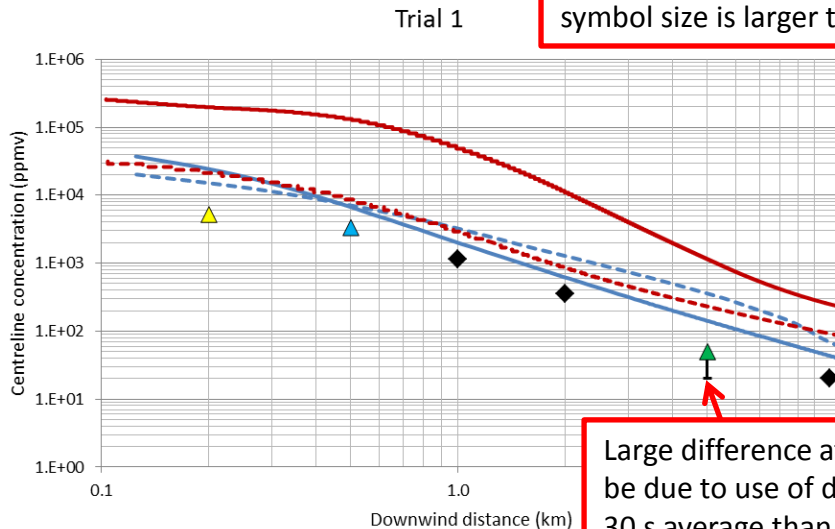
1. Empirically determined entrainment coefficients
 - Different coefficients for dispersion regimes (e.g. momentum dominated, dense, buoyant or passive)
 - Coefficients are based on averaging values across experimental datasets
 - In most cases, values determined without wind meandering effects

2. Additional spreading due to meander of the plume in the wind
 - Approach in DRIFT is based on wind-induced meander model of Nielsen *et al.* 2002 (Risoe-R-1329(EN))
 - Model is based upon the passive (ambient turbulent) part of the cloud spread only and depends upon the cloud travel time and the averaging time (or release duration if that is shorter)
 - For short averaging times (e.g. a few tens of seconds for JRII releases), the effect of meander averaging time on centreline concentration is predicted to be small – with dilution mainly determined by the model entrainment coefficients



Averaging Times: JRII 2015 Trial 1

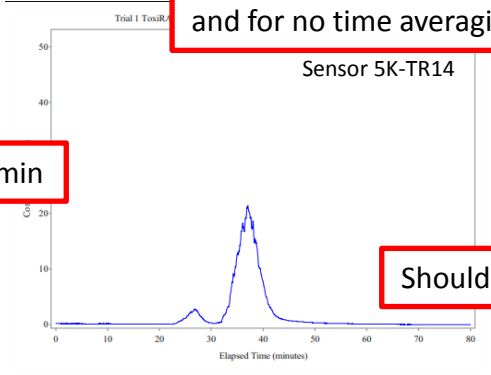
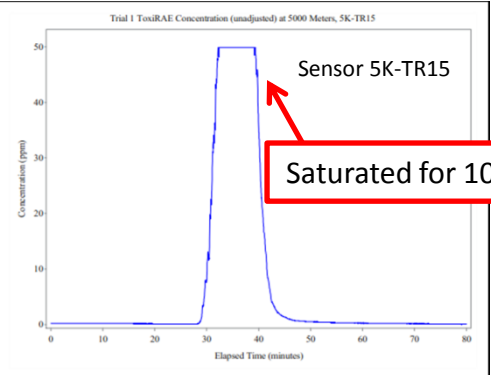
Concentrations are slightly different for max, 20 s and 30 s averaging times but error bars do not show up in graph in most cases, since the symbol size is larger than the width of the error bars



Distance (m)	Trial 1					
	Max.	Sensor	20 s	Sensor	30 s	Sensor
200	5202.8	200M-C08	4993.8	200M-C08	4856.3	200M-C08
500	3348.0	500M-MR18	3169.5	500M-MR18	3047.6	500M-MR19
1000	1137.1	1K-MR18	1117.1	1K-MR18	1068.6	1K-MR18
2000	356.6	2K-MR16	350.7	2K-MR16	348.8	2K-MR16
5000	49.9	5K-TR15	48.0	5K-TR15	20.5	5K-TR14
11000	20.4	11K-TR15	19.8	11K-TR15	19.7	11K-TR15

Large difference at 5 km appears to be due to use of different sensor for 30 s average than for 20 s average and for no time averaging

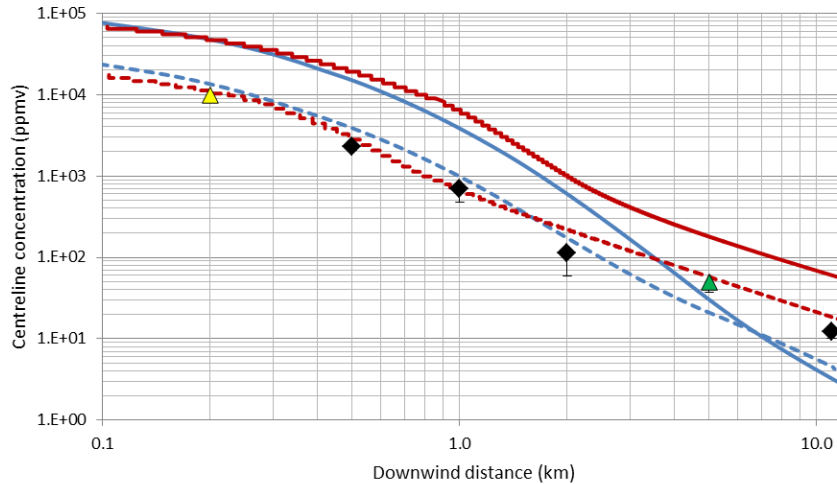
- DRIFT without droplet rainout
- - - DRIFT with droplet rainout
- PHAST without droplet rainout
- - - PHAST with droplet rainout
- ◆ Measured maximum arc-wise concentration
- ▲ Canary sensor data: only 3 sensors, may have missed plume maximum
- ▲ MiniRAE sensor saturated or exceeded calibration
- ▲ ToxiRAE sensor saturated
- ▲ Narrow plume passed between sensors: plume maximum may have been missed
- ▲ Plume passed beyond edge of arc: plume maximum may have been missed



Trial	Sensor	Group	Location	r (km)	az_pad (deg)	Ht (m)	Raw Cmax (ppm)	Raw CmaxTime (min)	Raw Cmin (ppm)	Tavg= 10s Hi1 (ppm)	Tavg= 10s Hi1Time (min)	Tavg= 10s Hi2 (ppm)	Tavg= 10s Hi2Time (min)	Tavg= 20s Hi1 (ppm)	Tavg= 20s Hi1Time (min)	Tavg= 20s Hi2 (ppm)	Tavg= 20s Hi2Time (min)	Tavg= 30s Hi1 (ppm)	Tavg= 30s Hi2 (ppm)	
1	ToxiRAE	5km	5K-TR14	5	327.5	0.3	21.4	37.067	-999.9	21.1	36.985	20.9	36.84	20.8	36.996	20.2	36.663	20.5		
1	ToxiRAE	5km	5K-TR15	5	322.5	0.3	49.9	32.183	-999.9	999999	32.154	49	39.151	48	31.997	47.2	39.325	999999		

Averaging Times: JRII 2015 Trial 2

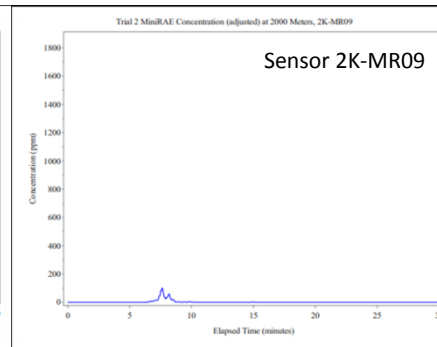
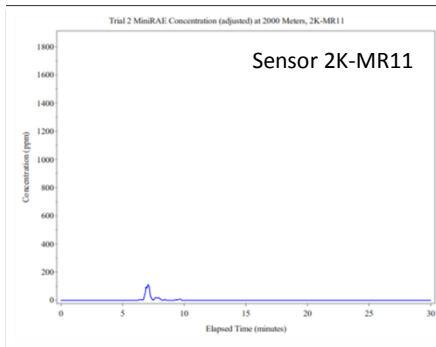
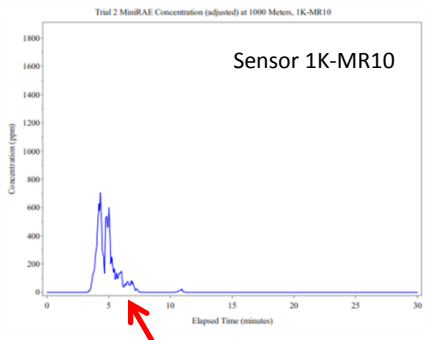
Trial 2



Distance (m)	Trial 2					
	Max.	Sensor	20 s	Sensor	30 s	Sensor
200	9867.3	200M-C06	8099.6	200M-C06	8322.4	200M-C06
500	2281.7	500M-MR09	2113.9	500M-MR09	2063.8	500M-MR09
1000	705.2	1K-MR10	506.4	1K-MR10	479.9	1K-MR10
2000	112.4	2K-MR11	76.8	2K-MR11	59.1	2K-MR09
5000	49.9	5K-TR09	38.1	5K-TR09	37.4	5K-TR10
11000	12.1	11K-TR10	11.1	11K-TR10	10.0	11K-TR10

- DRIFT without droplet rainout
- - - DRIFT with droplet rainout
- PHAST without droplet rainout
- - - PHAST with droplet rainout

- ◆ Measured maximum arc-wise concentration
- ▲ Canary sensor data: only 3 sensors, may have missed plume maximum
- ▲ MiniRAE sensor saturated or exceeded calibration
- ▲ ToxiRAE sensor saturated
- ▲ Narrow plume passed between sensors: plume maximum may have been missed
- ▲ Plume passed beyond edge of arc: plume maximum may have been missed

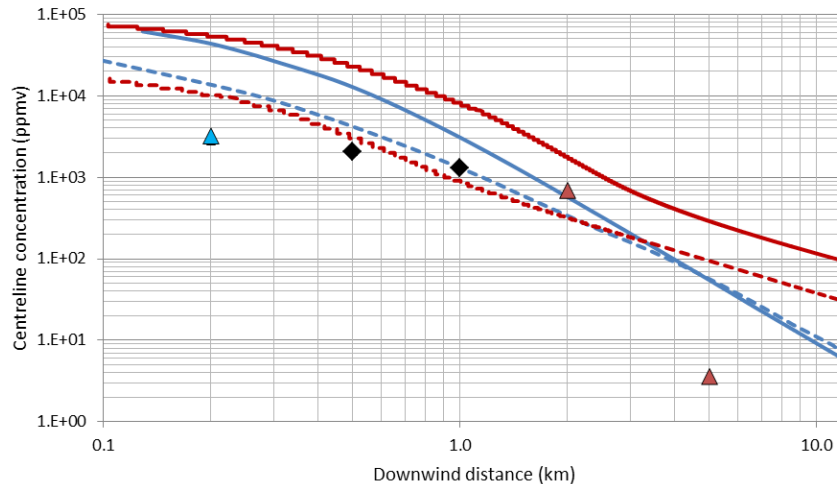


Twin peak causes differences in averaging times

Two different sensors used at 2 km depending on averaging times

Averaging Times: JRII 2015 Trial 3

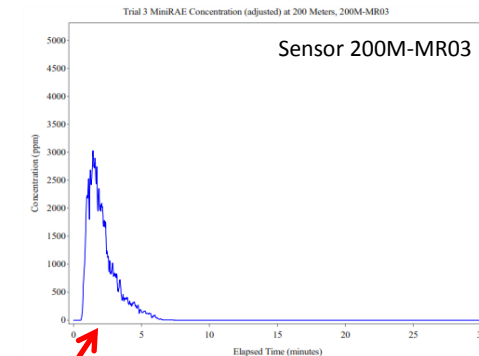
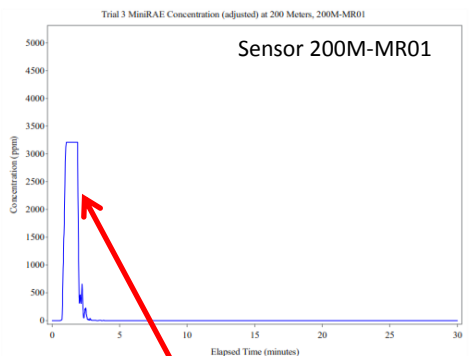
Trial 3



Distance (m)	Trial 3					
	Max.	Sensor	20 s	Sensor	30 s	Sensor
200	3210.3	200M-MR01	2776.7	200M-MR03	2484.3	200M-MR03
500	2041.3	500M-MR06	1941.5	500M-MR06	1866.7	500M-MR06
1000	1306.8	1K-MR06	1263.6	1K-MR06	1244.6	1K-MR06
2000	691.4	2K-MR08	648.3	2K-MR08	580.5	2K-MR08
5000	3.6	5K-TR08	3.3	500M-MR11	3.1	5K-TR08
11000	0.3	11K-TR13	0.3	11K-TR13	0.3	11K-TR13

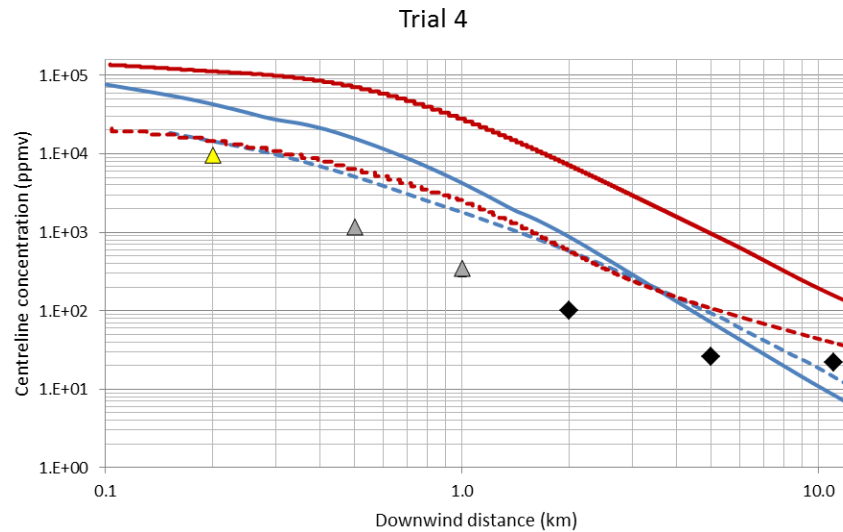
- DRIFT without droplet rainout
- - - DRIFT with droplet rainout
- PHAST without droplet rainout
- - - PHAST with droplet rainout

- ◆ Measured maximum arc-wise concentration
- ▲ Canary sensor data: only 3 sensors, may have missed plume maximum
- ▲ MiniRAE sensor saturated or exceeded calibration
- ▲ ToxiRAE sensor saturated
- ▲ Narrow plume passed between sensors: plume maximum may have been missed
- ▲ Plume passed beyond edge of arc: plume maximum may have been missed



Sensor 200M-MR01 saturated at 200 m so Sensor 200M-MR03 used instead for 20 s and 30 s averages, but the use of data from a different sensor has little effect on the max concentrations

Averaging Times: JRII 2015 Trial 4



Distance (m)	Trial 4					
	Max.	Sensor	20 s	Sensor	30 s	Sensor
200	9622.6	200M-C07	8734.3	200M-C07	8581.2	200M-C07
500	1173.2	500M-MR01	1094.4	500M-MR01	1017.1	500M-MR01
1000	347.4	1K-MR01	299.9	1K-MR01	272.1	1K-MR01
2000	100.8	2K-MR03	89.6	2K-MR03	88.7	2K-MR03
5000	26	5K-TR06	25.4	5K-TR06	24.5	5K-TR06
11000	21.7	11K-TR07	21	11K-TR07	20.2	11K-TR07

— DRIFT without droplet rainout

- - - DRIFT with droplet rainout

— PHAST without droplet rainout

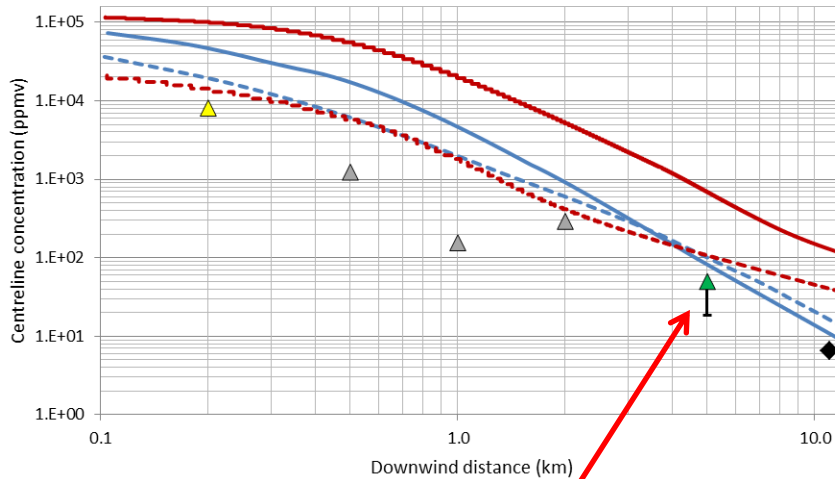
- - - PHAST with droplet rainout

- ◆ Measured maximum arc-wise concentration
- ▲ Canary sensor data: only 3 sensors, may have missed plume maximum
- ▲ MiniRAE sensor saturated or exceeded calibration
- ▲ ToxiRAE sensor saturated
- ▲ Narrow plume passed between sensors: plume maximum may have been missed
- ▲ Plume passed beyond edge of arc: plume maximum may have been missed



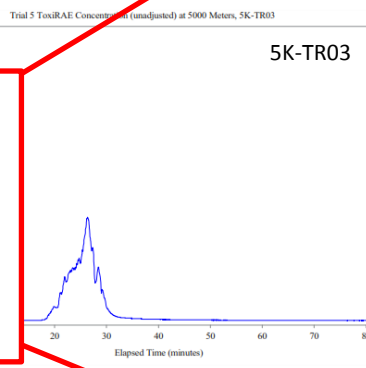
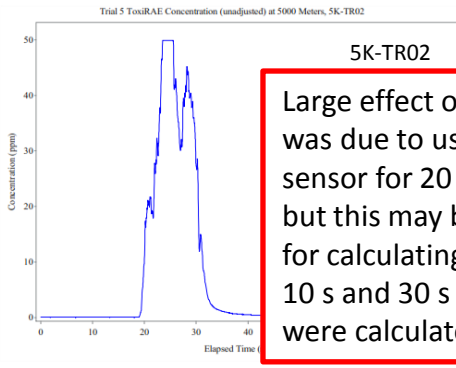
Averaging Times: JRII 2015 Trial 5

Trial 5



Distance (m)	Trial 5					
	Max.	Sensor	20 s	Sensor	30 s	Sensor
200	8108.4	200M-C05	7465.3	200M-C05	6899	200M-C05
500	1235.1	500M-MR02	1067.8	500M-MR02	1013.1	500M-MR02
1000	155.4	1K-MR02	142	1K-MR02	137.1	1K-MR02
2000	292	2K-MR01	277	2K-MR01	273.9	2K-MR01
5000	49.9	5K-TR02	18.3	5K-TR03	44.1	5K-TR02
11000	6.6	11K-TR03	6.3	11K-TR03	6.1	11K-TR03

- DRIFT without droplet rainout
- - - DRIFT with droplet rainout
- PHAST without droplet rainout
- - - PHAST with droplet rainout
- ◆ Measured maximum arc-wise concentration
- ▲ Canary sensor data: only 3 sensors, may have missed plume maximum
- ▲ MiniRAE sensor saturated or exceeded calibration
- ▲ ToxiRAE sensor saturated
- ▲ Narrow plume passed between sensors: plume maximum may have been missed
- ▲ Plume passed beyond edge of arc: plume maximum may have been missed



Large effect of averaging time at 5 km was due to use of data from different sensor for 20 s averaged concentration, but this may be an artefact of the rules for calculating time averages, since both 10 s and 30 s averaged concentrations were calculated at sensor 5K-TR02

Trial	Sensor	Group	Location	r (km)	az_pad (deg)	Ht (m)	Raw Cmax (ppmv)	Raw CmaxTime (min)	Raw Cmin (ppmv)	Tavg= 10s Hi1 (ppmv)	Tavg= 10s Hi1Time (min)	Tavg= 10s Hi2 (ppmv)	Tavg= 10s Hi2Time (min)	Tavg= 20s Hi1 (ppmv)	Tavg= 20s Hi1Time (min)	Tavg= 20s Hi2 (ppmv)	Tavg= 20s Hi2Time (min)	Tavg= 30s Hi1 (ppmv)	Tavg= 30s Hi1Time (min)
5	ToxiRAE	5km	5K-TR02	5	22.5	0.3	49.9	23.533	-999.9	49.1	25.49	47	23.524	999999	23.331	43.2	27.997	44.1	25.5
5	ToxiRAE	5km	5K-TR03	5	17.5	0.3	18.8	26.35	-999.9	18.6	26.323	18.5	26.156	18.3	26.331	18	25.997	18.2	26

Averaging Times

Joe Chang rules for calculating time averages:

1. Consider only concentration between 0 and 240 min after the release, assuming the information on elapsed time is correct.
2. Do not perform time averaging when >20% of the measurements in an averaging period are saturated, in which case the average for that time period is set to 999999.
3. Saturated concentrations are not used in calculating time averages (when >80% of the measurements in an averaging period are not saturated).
4. Do not perform time averaging when >50% of the measurements in an averaging period are missing, in which case the average for that time period is set to 0.
5. Consider non-overlapping averages.
6. All negative concentrations are set to zero. (Jaz and Canary often show background in negative concentrations.)
7. The time interval between successive measurements doesn't have to be regular.
8. Time for an averaging period refers to time beginning.

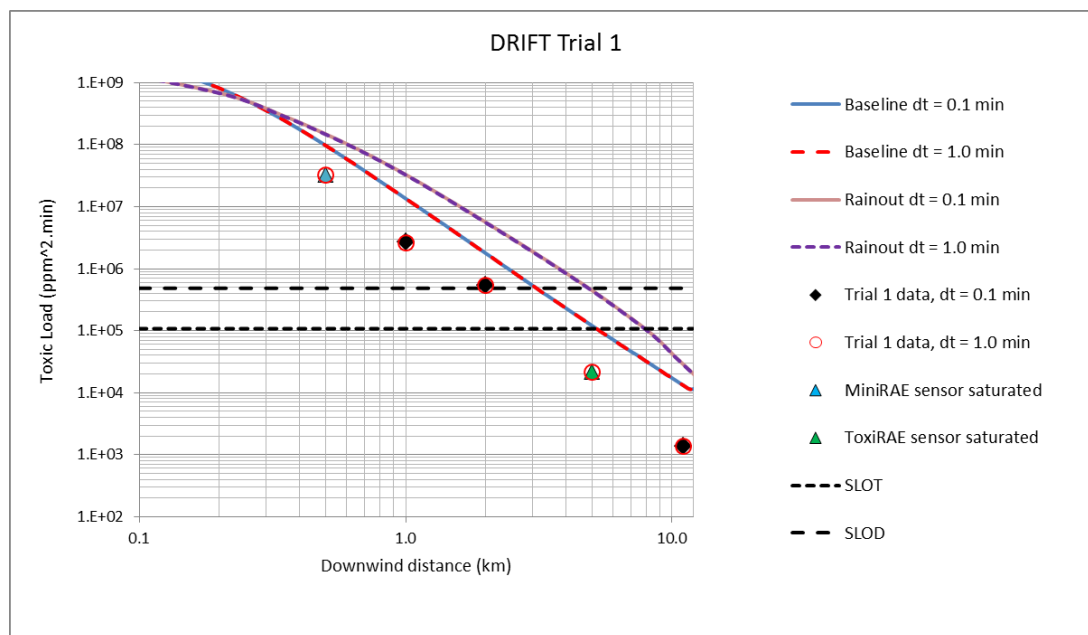
Averaging Times

Conclusions

- Difficult to define the averaging time used by integral models or RANS CFD models when they are nominally predicting “instantaneous” concentrations (ensemble-averaged instantaneous concentrations)
- Sensitivity tests with JR11 2015 experimental data shows that there is little difference in using maximum concentrations calculated from either no time averaging, or from time averages of 20 s or 30 s

Toxic Load: Averaging Times

- IDA provided toxic loads calculated by integrating over time the measured concentrations that were smoothed using a 0.1 minute or 1.0 minute running average
- Results were compared to DRIFT simulations using a lateral meander averaging time of 0.1 minute and 1.0 minute

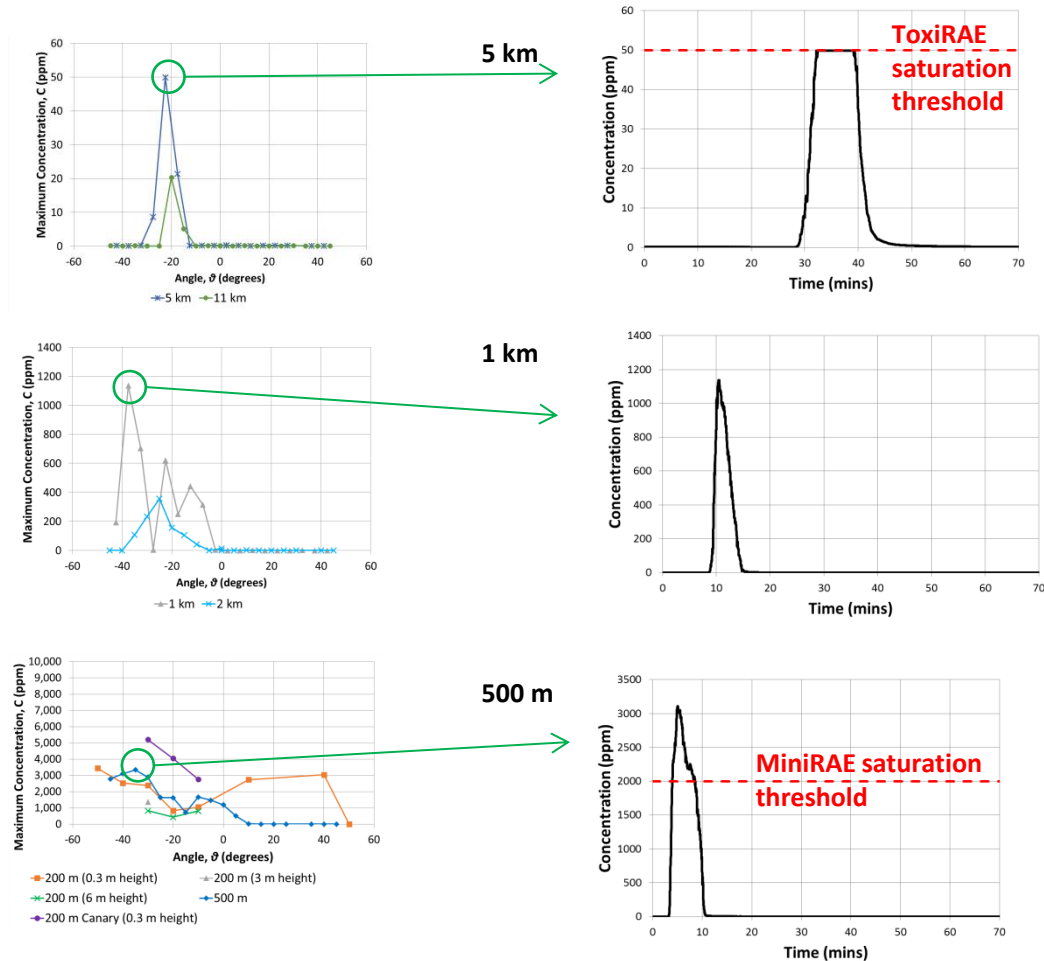


Conclusion

- Choice of 0.1 minute or 1.0 minute averaging time has no significant effect on the results

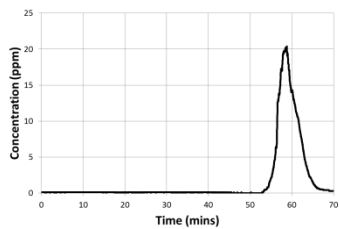
Time-Varying Concentration Data

The next slide presents data for the time-varying concentrations at sensors that recorded the highest concentration on each arc like this:

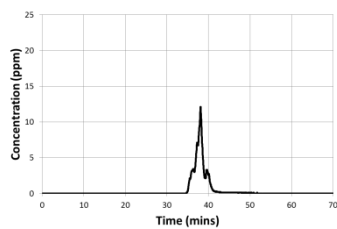


MiniRAE values corrected using the pre- and post-experiment calibration tests, so the maximum sometimes exceeds the saturation threshold

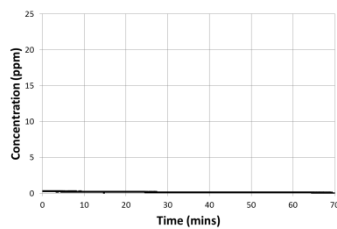
Trial 1



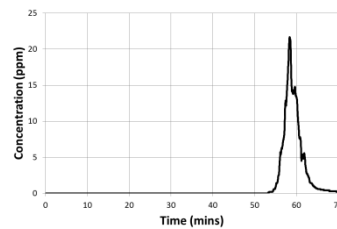
Trial 2



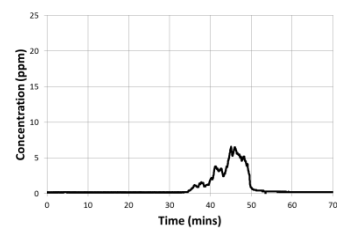
Trial 3



Trial 4

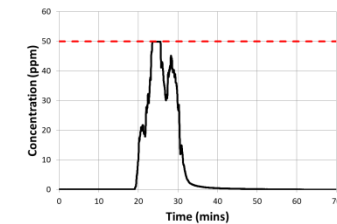
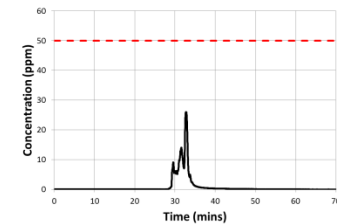
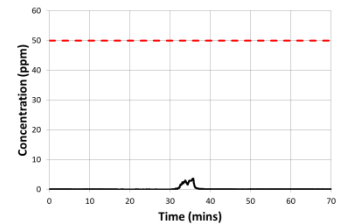
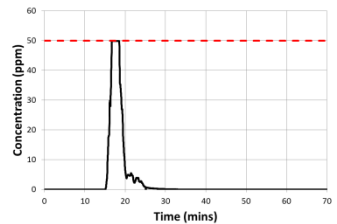
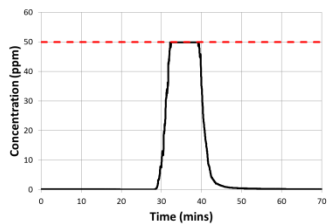


Trial 5

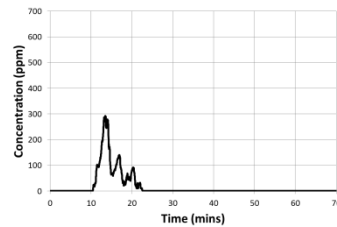
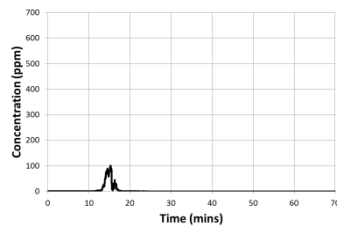
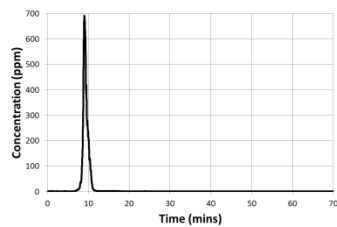
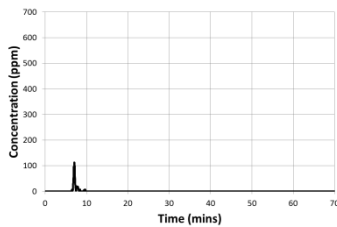
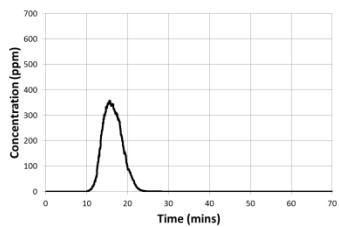


11 km

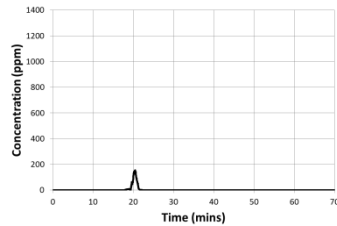
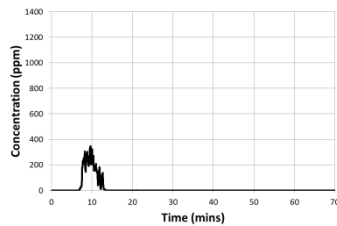
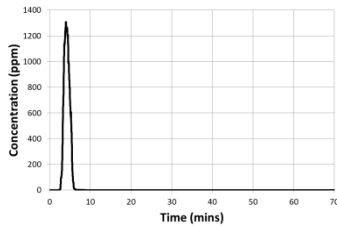
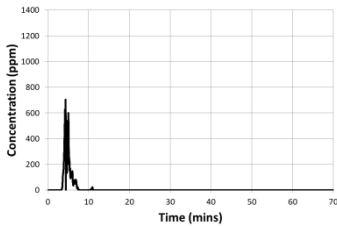
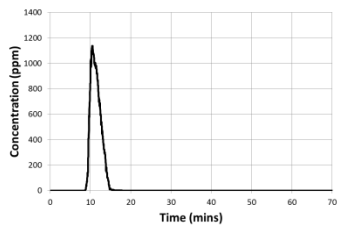
5 km



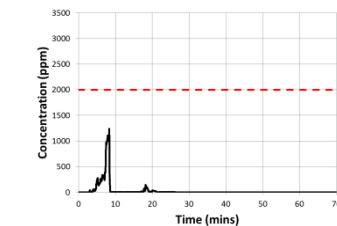
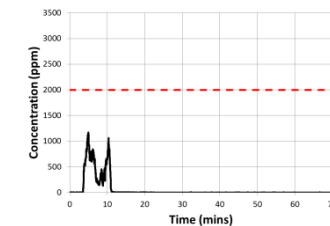
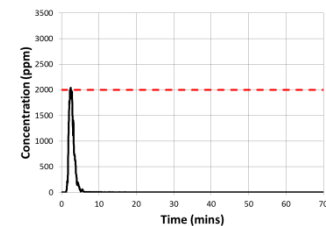
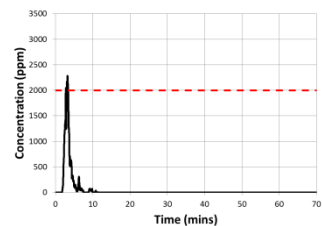
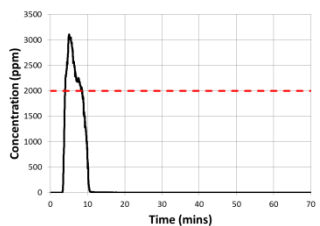
2 km



1 km



500 m



Trial 1

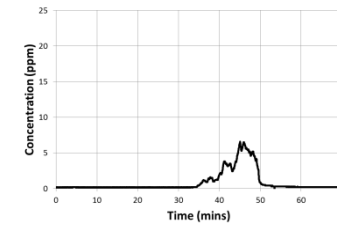
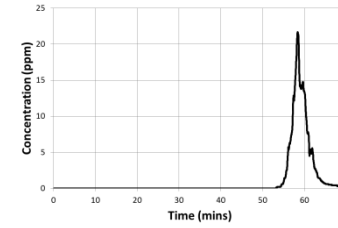
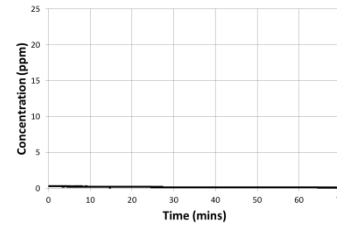
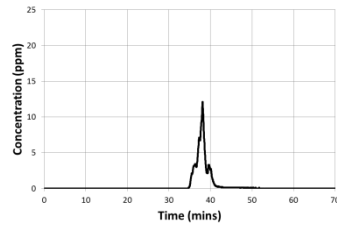
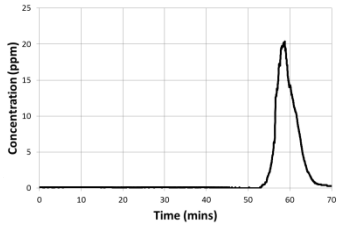
Trial 2

Trial 3

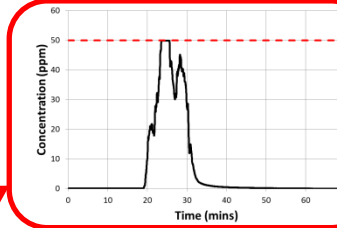
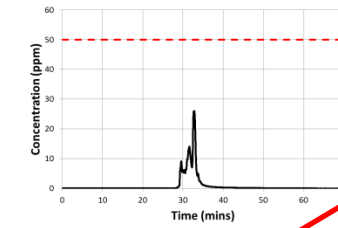
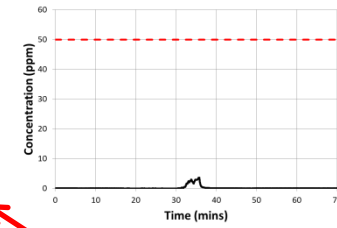
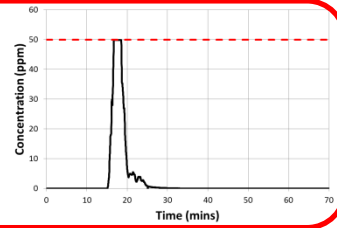
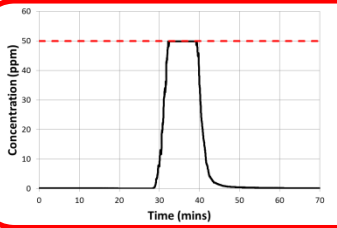
Trial 4

Trial 5

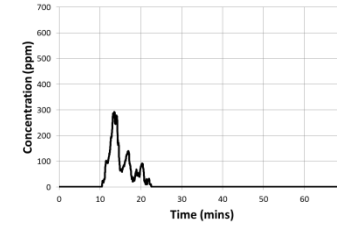
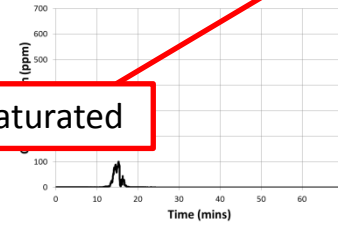
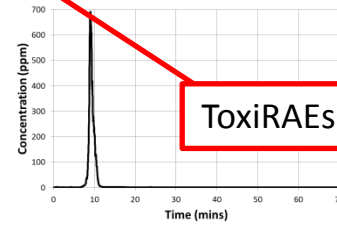
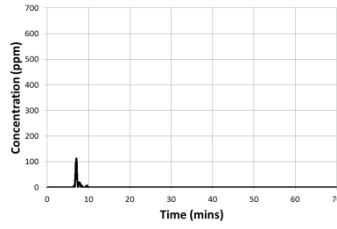
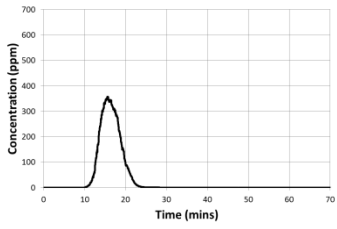
11 km



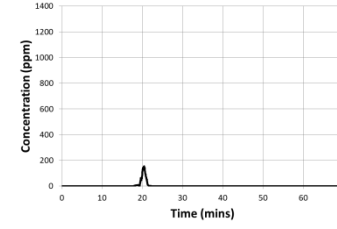
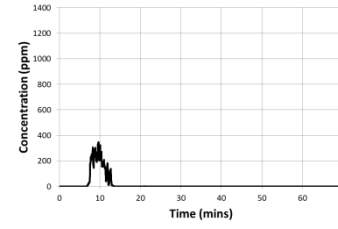
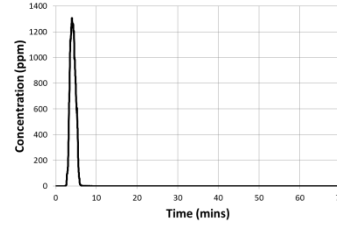
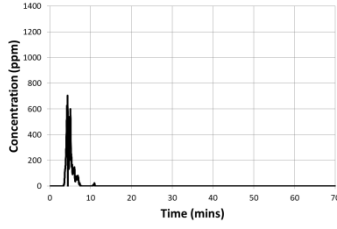
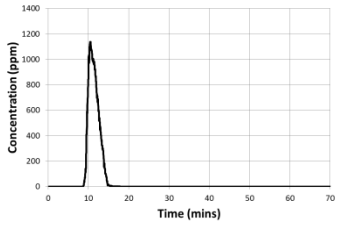
5 km



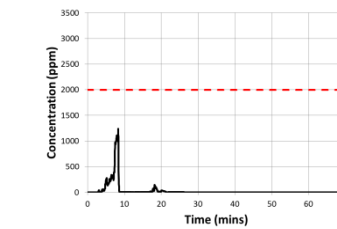
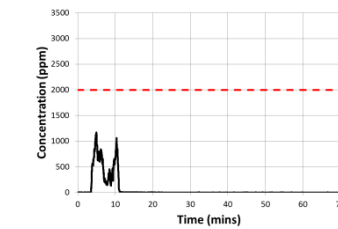
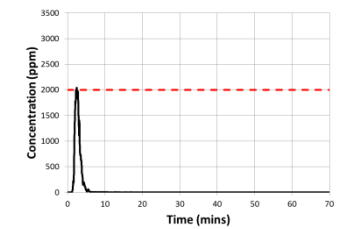
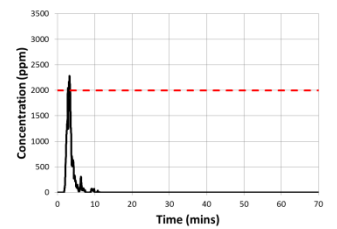
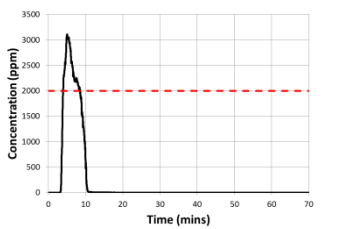
2 km



1 km

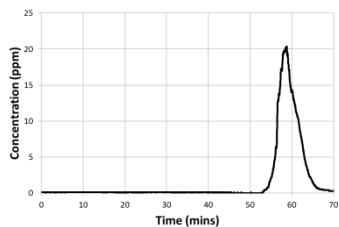


500 m

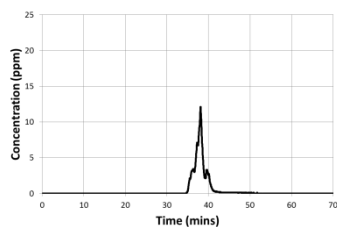


ToxiRAEs saturated

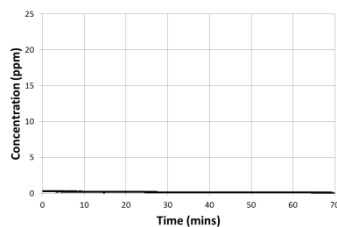
Trial 1



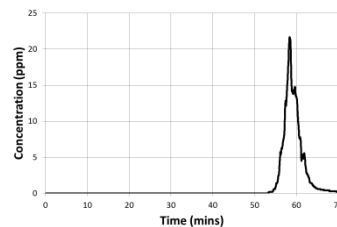
Trial 2



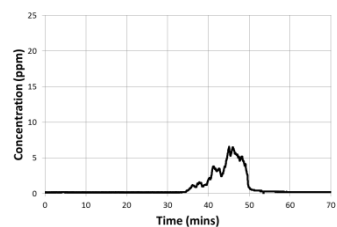
Trial 3



Trial 4

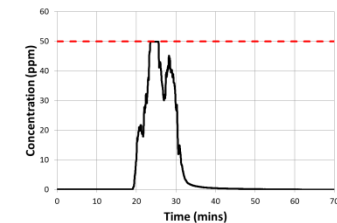
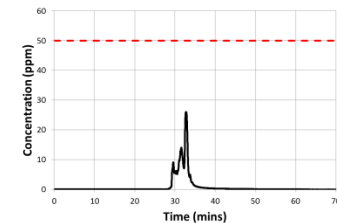
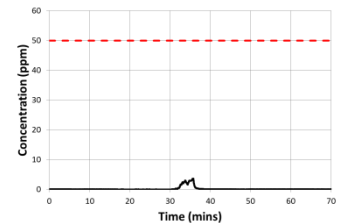
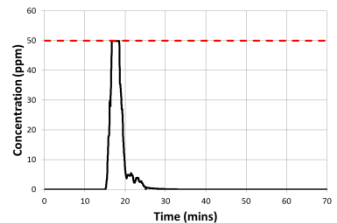
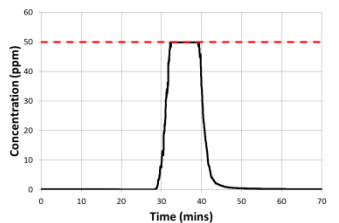


Trial 5

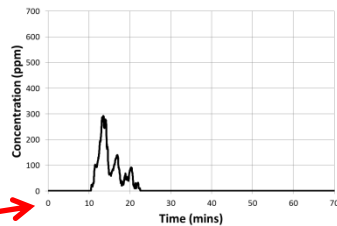
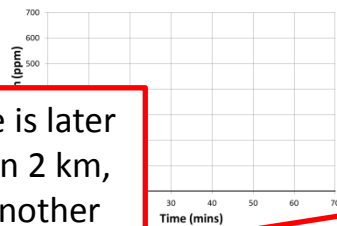
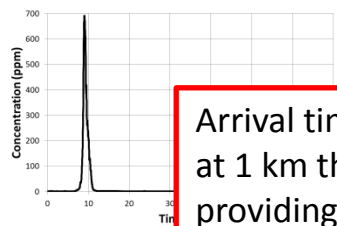
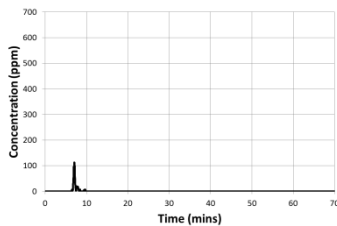
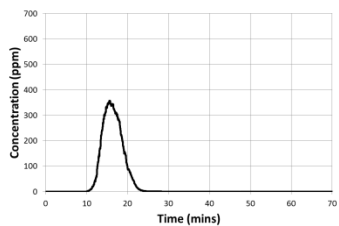


11 km

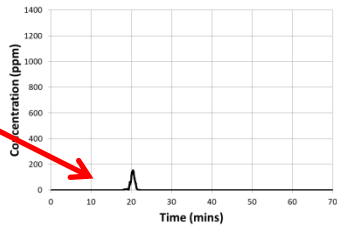
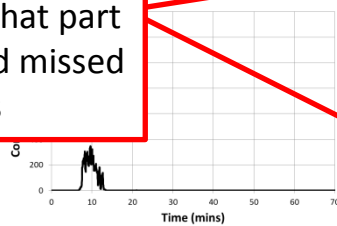
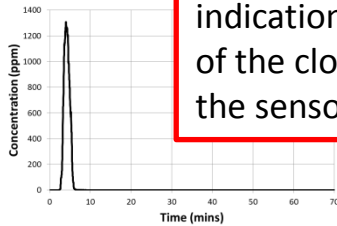
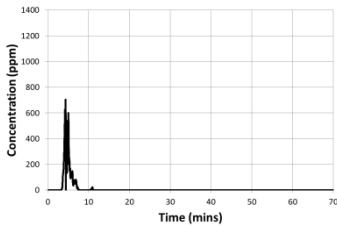
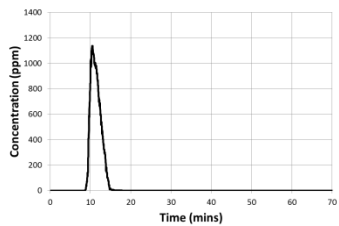
5 km



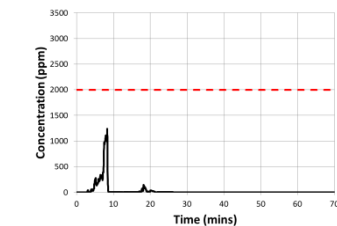
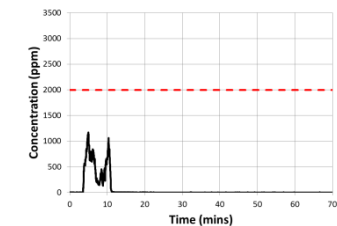
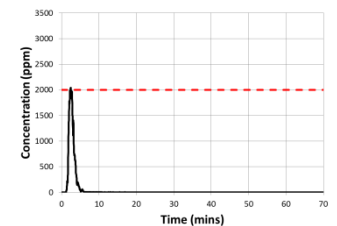
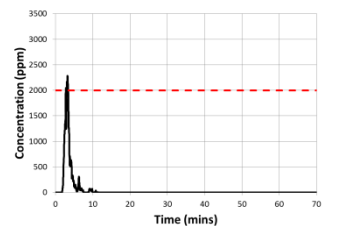
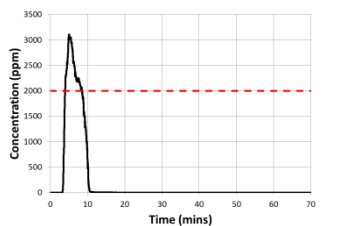
2 km



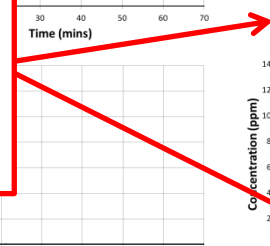
1 km



500 m



Arrival time is later
at 1 km than 2 km,
providing another
indication that part
of the cloud missed
the sensors



Trial 1

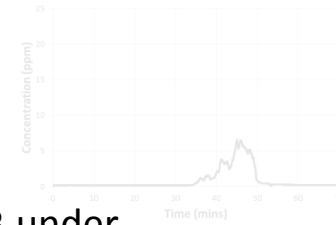
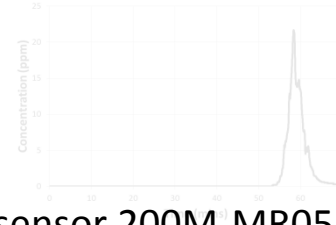
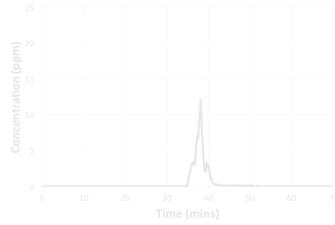
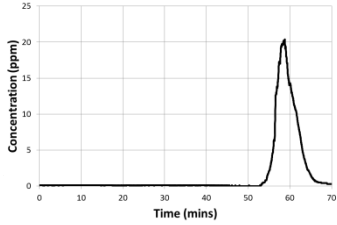
Trial 2

Trial 3

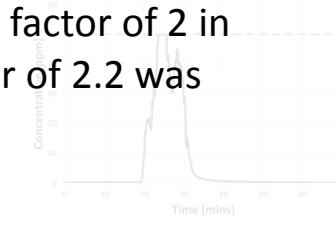
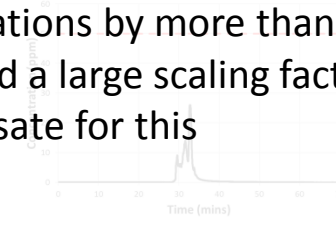
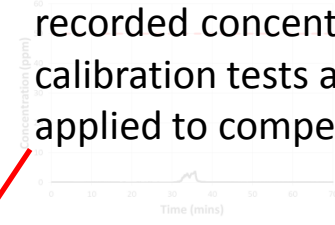
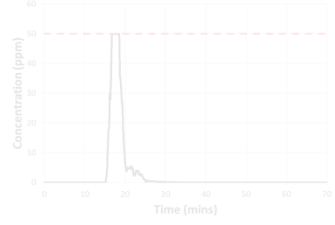
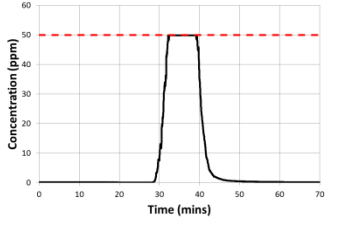
Trial 4

Trial 5

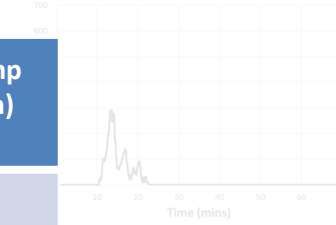
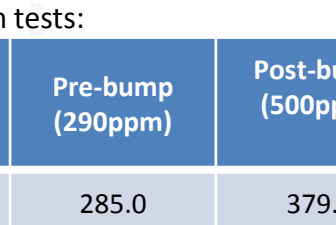
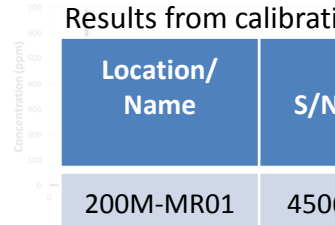
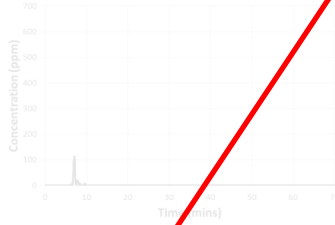
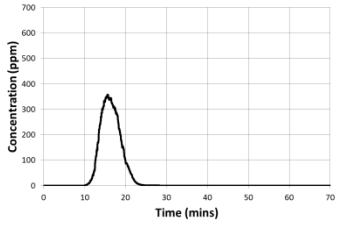
11 km



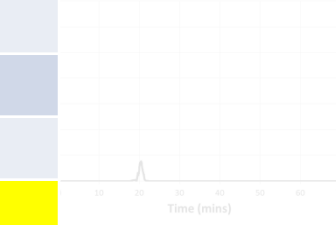
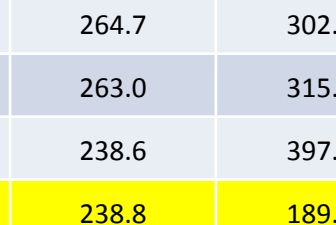
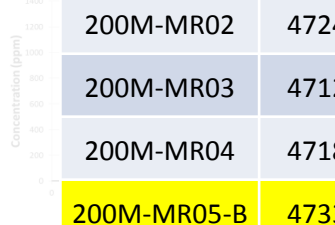
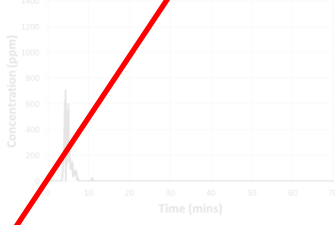
5 km



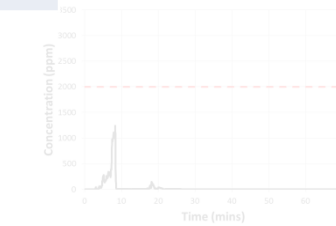
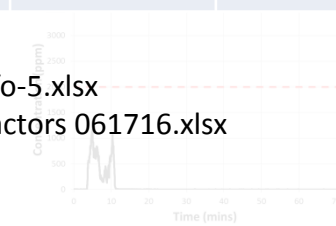
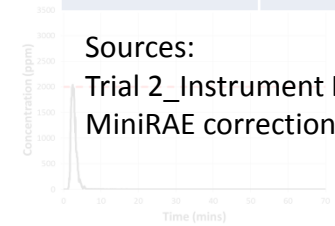
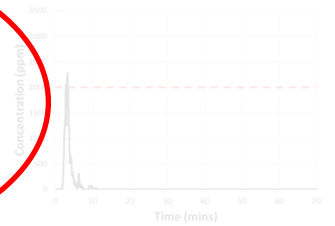
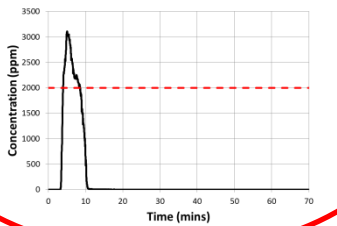
2 km



1 km



500 m



In Trial 1, MiniRAE sensor 200M-MR05-B under-recorded concentrations by more than a factor of 2 in calibration tests and a large scaling factor of 2.2 was applied to compensate for this

Results from calibration tests:

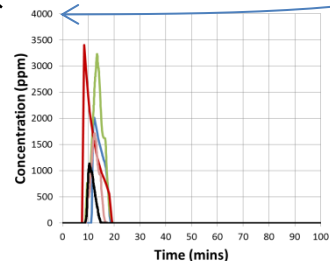
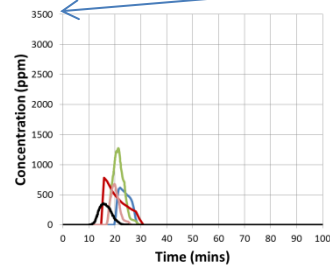
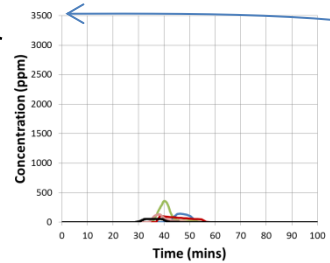
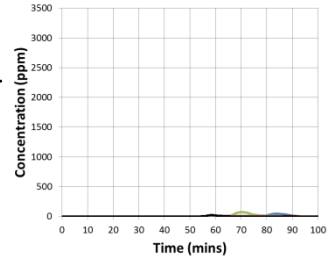
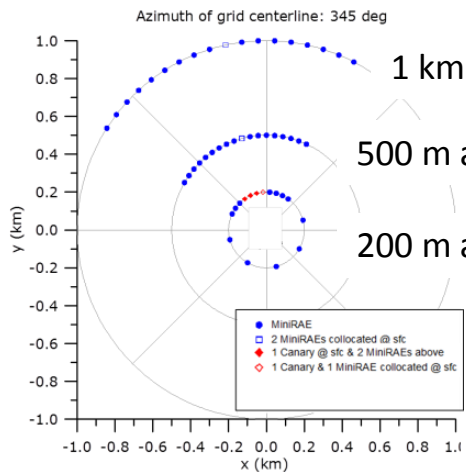
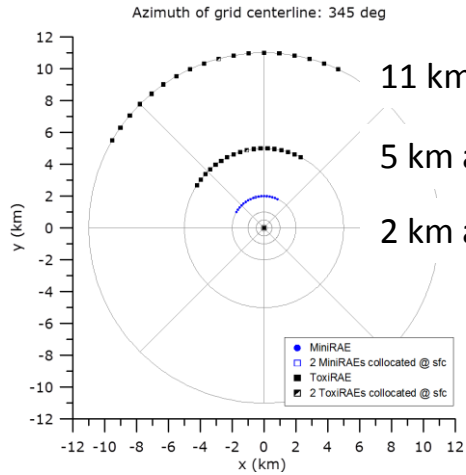
Location/ Name	S/N	Pre-bump (290ppm)	Post-bump (500ppm)
200M-MR01	4506	285.0	379.0
200M-MR02	4724	264.7	302.3
200M-MR03	4712	263.0	315.5
200M-MR04	4718	238.6	397.7
200M-MR05-B	4733	238.8	189.3
200M-MR05-T	1048	284.0	443.9

Sources:

Trial 2_Instrument Info-5.xlsx

MiniRAE correction factors 061716.xlsx

Time-Varying Concentration Predictions



Drift predicted maximum concentrations for different sub-models

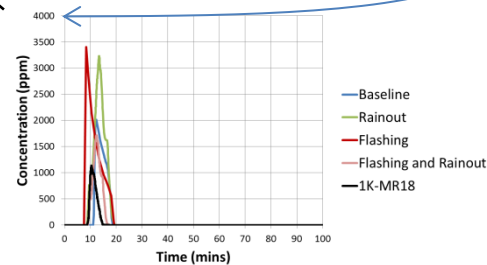
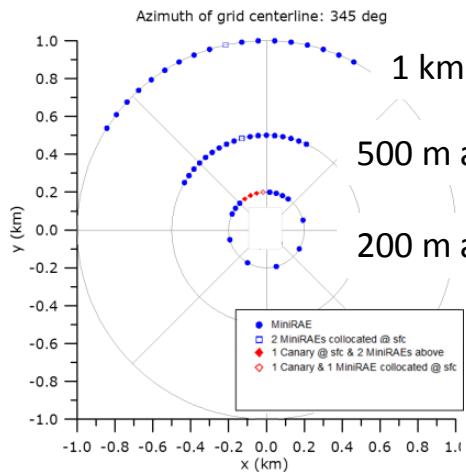
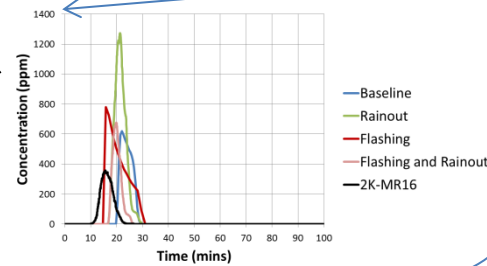
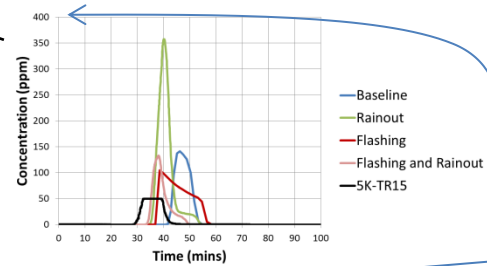
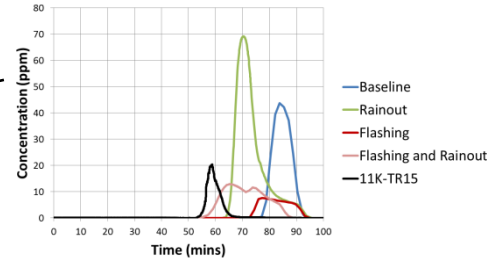
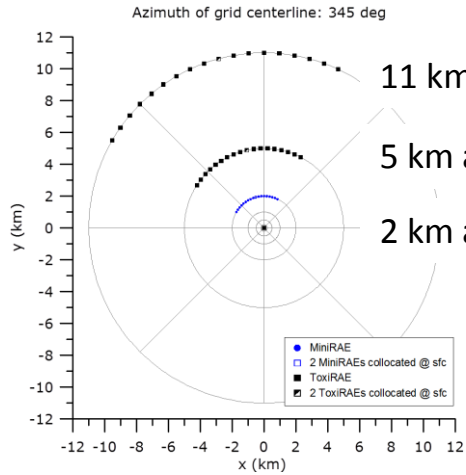
Measured concentration at sensor that recorded the highest concentration on that arc

Note: concentration scales on vertical axes the same in each graph

“Baseline” Drift model involves:

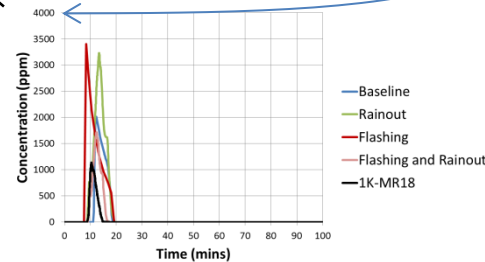
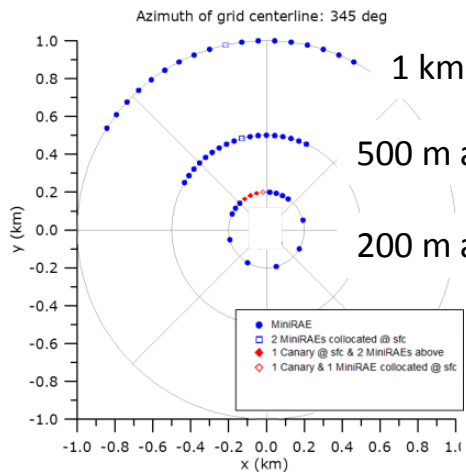
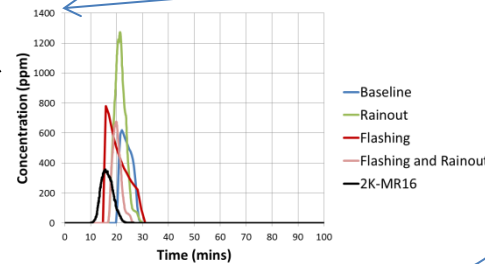
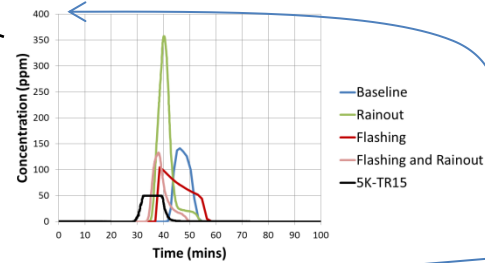
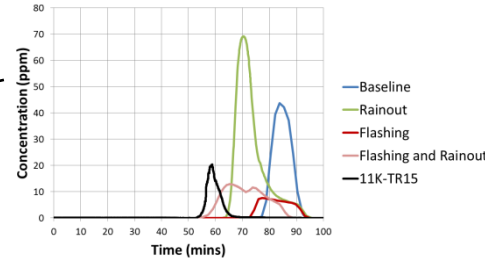
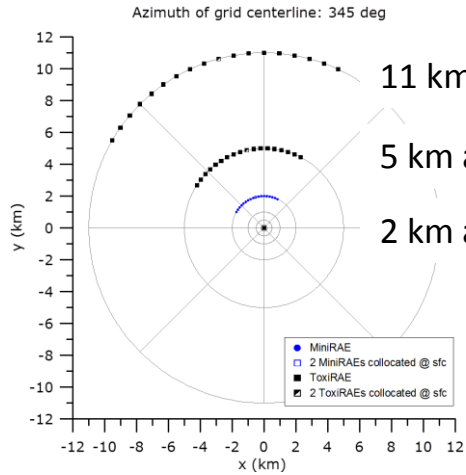
- Metastable liquid for outflow (not “flashing”)
- No rainout: chlorine aerosol remains airborne

Time-Varying Concentration Predictions



Note: concentration scales on vertical axes **different** in each graph

Time-Varying Concentration Predictions



Note: concentration scales on vertical axes **different** in each graph

The next slide shows the same four graphs for Trials 1 – 5, but only for two Drift sub-models: Baseline and Rainout

50

Trial 1

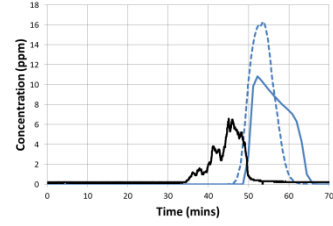
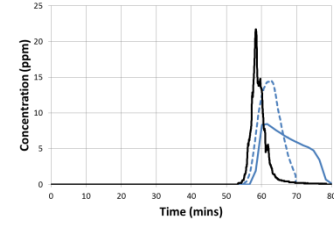
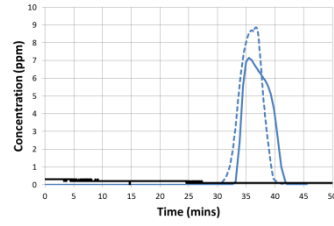
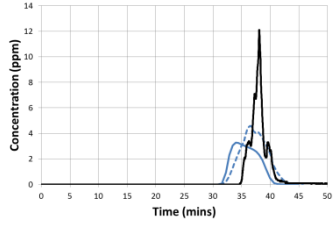
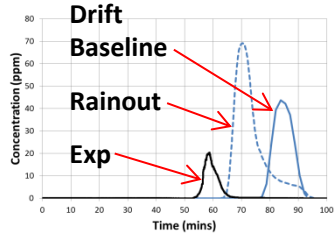
Trial 2

Trial 3

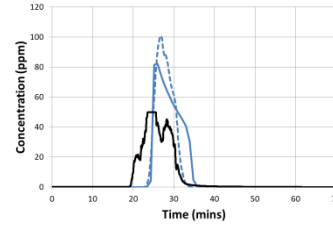
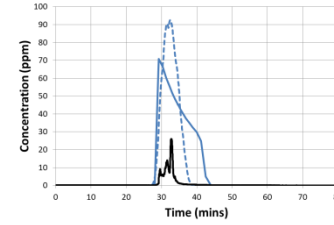
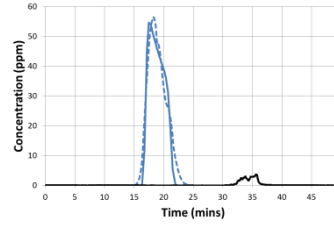
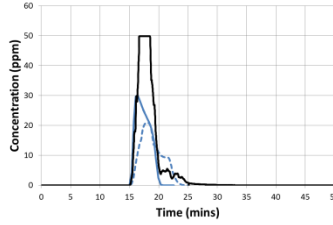
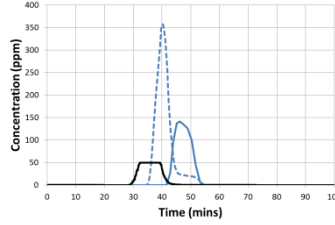
Trial 4

Trial 5

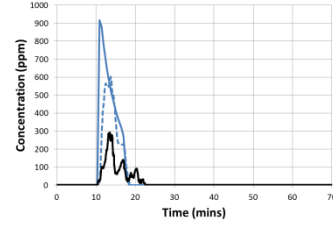
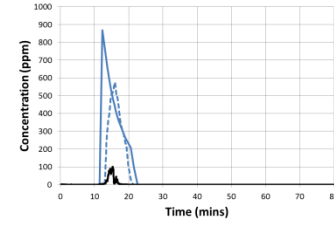
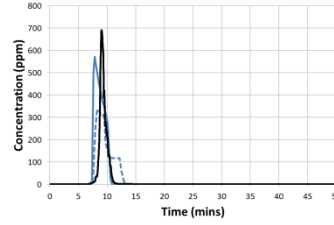
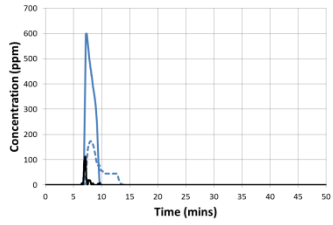
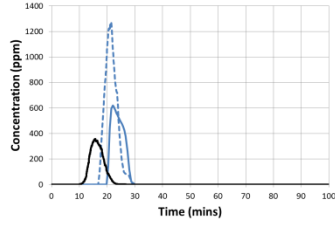
11 km



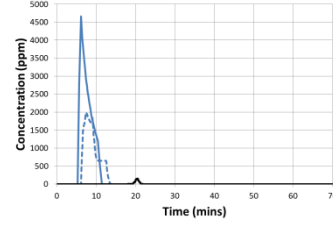
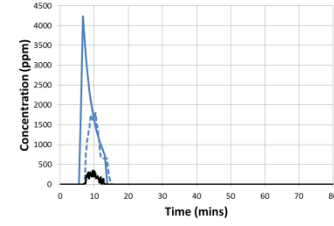
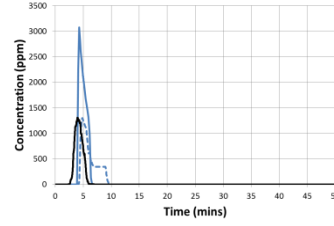
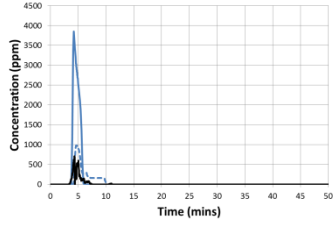
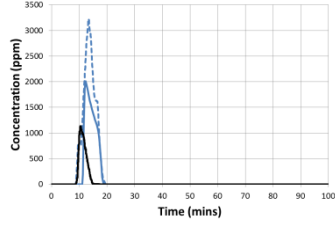
5 km



2 km



1 km



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