CFD results for near-field dispersion in Jack Rabbit II

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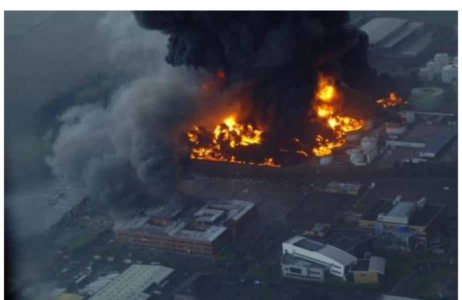
Outline

- Background
- Aims
- CFD model setup
- Uncertainties
- Jack Rabbit II 2015
  - Sensitivity tests for Trial 1
  - Results for Trials 2 to 5
- Jack Rabbit II 2016 Trial 7
- Hypothetical scenario
- Future work

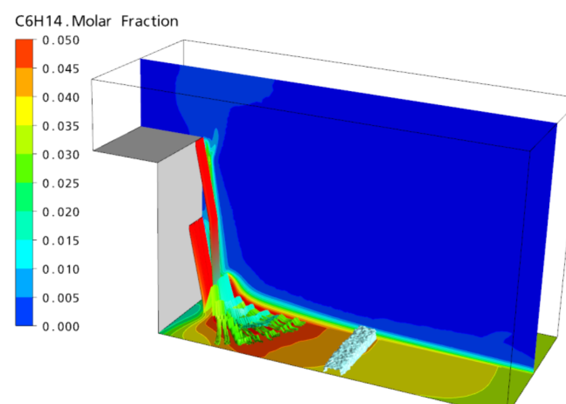
Background

- CFD can help to understand complex near-field dispersion behavior
- Example 1: Buncefield incident investigation – gasoline tank overfilling



Guidance on source terms published in FABIG TN12

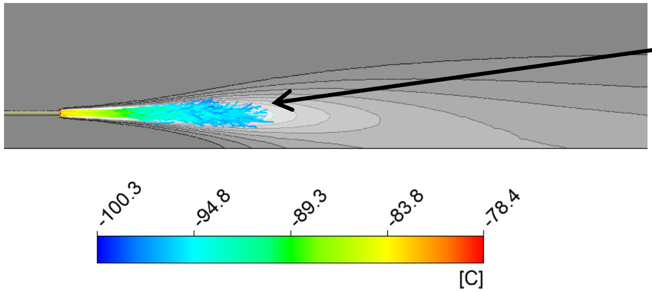
CFD used to determine the flow rate of flammable vapor from gasoline cascade



Background

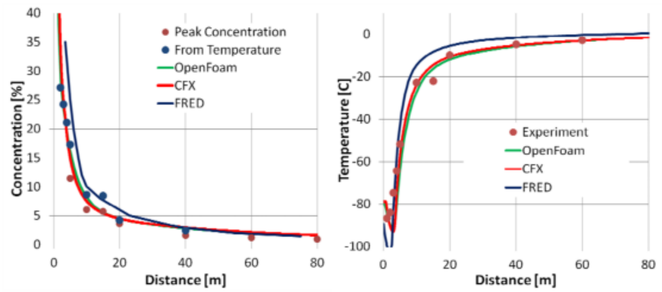
- Example 2: understanding potential hazards from carbon capture and storage – releases of pressure-liquefied carbon dioxide from pipelines

INERIS experiments (France)



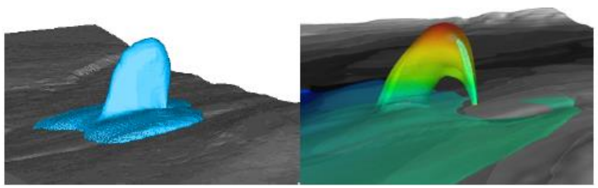
CFD model calculates sublimation rate of dry-ice particles in the jet

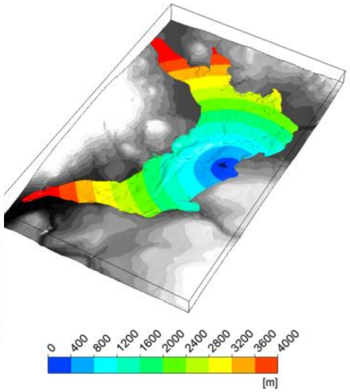
Dalian University of Technology experiments (China)



Model validation

Demonstration case with terrain



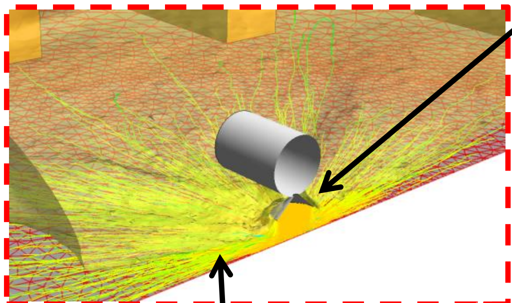


Aims

- Use CFD to help understand near-field dispersion in Jack Rabbit II trials
  - Interaction of two-phase flashing jet with the ground and nearby obstacles
- Identify which factors are important, using sensitivity tests
- Study hypothetical cases which could not be tested experimentally
  - e.g. extended mock urban array with additional (hypothetical) Conex containers
- Help inform the development of simpler/faster models

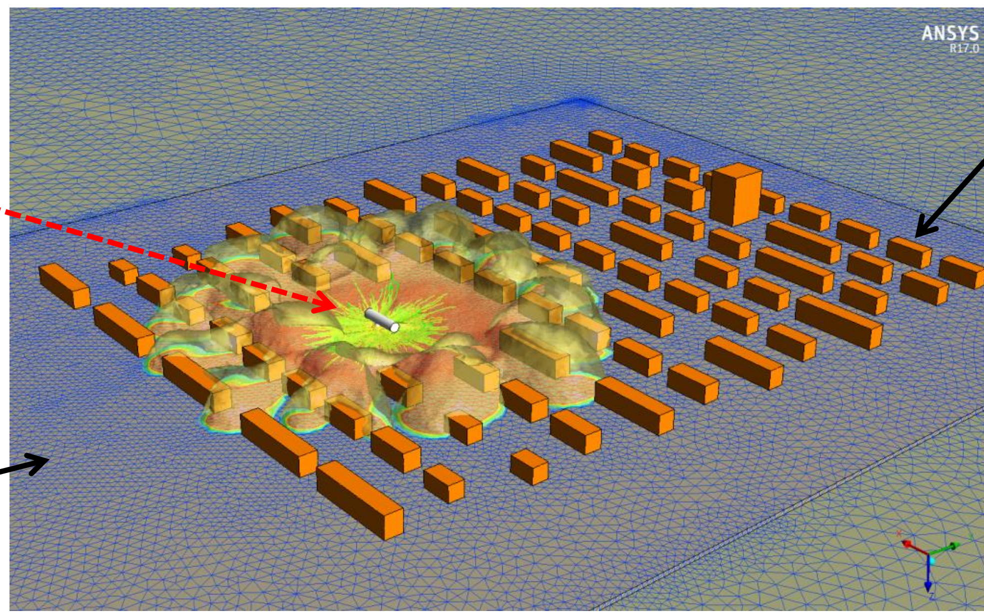
CFD Model Setup

Cross-section through source



Expanded jet of vapor and evaporating chlorine droplets (Lagrangian particles): post-expansion jet source conditions taken from PHAST or Rick Babarsky's source model

Model accounts for turbulence generation and any re-entrainment in the jet source



Conex blocks resolved in model geometry

RANS turbulence model solves for mean flow (SST model)
No wind-meandering model applied

Ground and all solid surfaces assumed to be smooth

Unstructured mesh
Approx. 1 – 2 M nodes
Particles: 1000 /second
Run time approx. 12 hrs on 34 CPUs for simulating first 10 minutes of JRII experiment

CFD code: ANSYS-CFX version 17

CFD Model Uncertainties

1. Discharge conditions
2. Interaction of chlorine jet with concrete pad
3. Pool formation and evaporation
4. Chlorine droplet size
5. Dry deposition of vapor
6. Atmospheric conditions

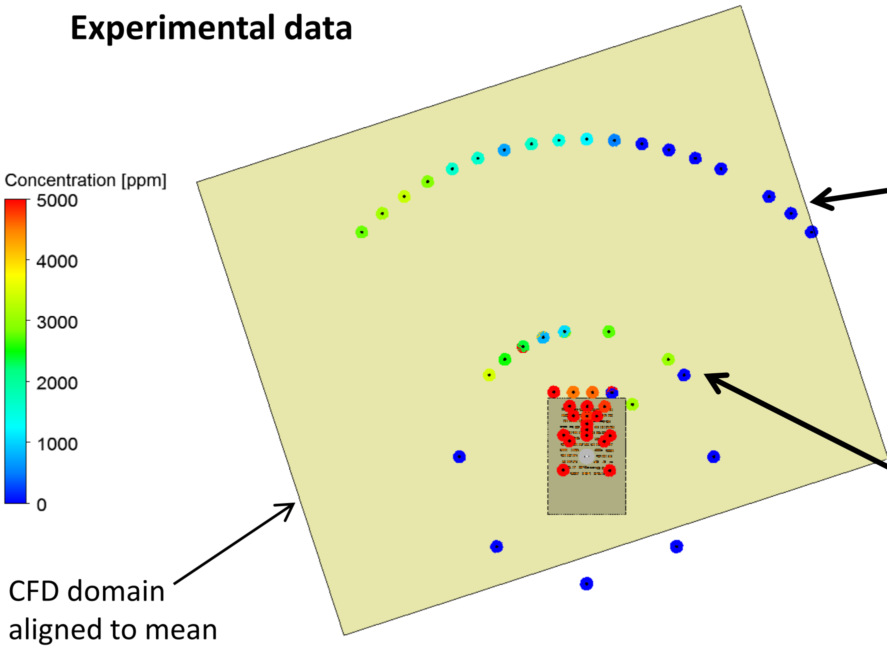
} Model Physics

7. Mesh resolution
8. Particle count
9. Time-step

} Model Numerics

Presentation of results

Trial 1
Experimental data

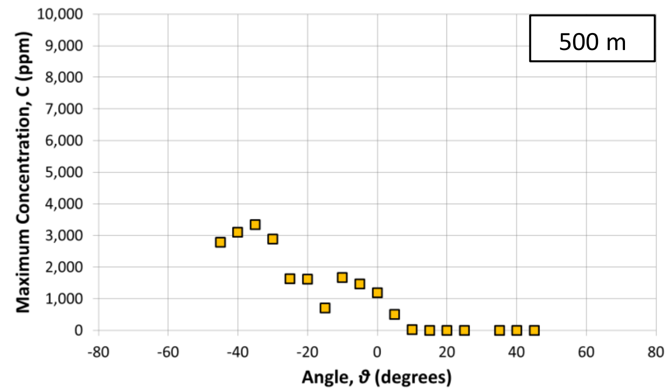


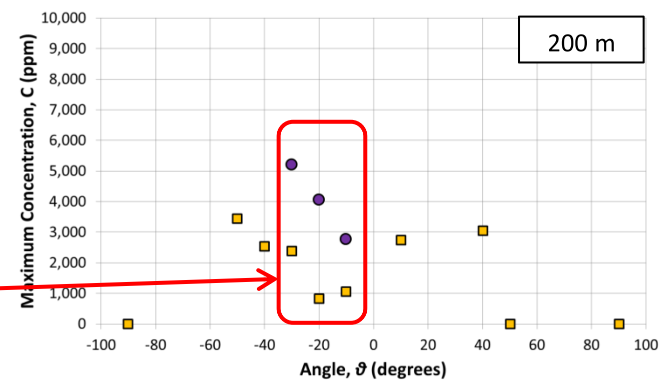
CFD domain aligned to mean wind direction (900 × 750 × 20 m)

Wind vector **2.0 m/s** -18°

Release size 4509 kg

In the following slides, CFD results are compared to the experimental data for max concentration at 200 m and 500 m





Higher concentrations measured by Canary than MiniRAE at the same locations

Measured maximum concentration (MiniRAE)

Measured maximum concentration (Canary)

CFD Model Uncertainties

HSE

1. Discharge conditions
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5. Dry deposition of vapor
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} Model Physics

7. Mesh resolution
8. Particle count
9. Time-step

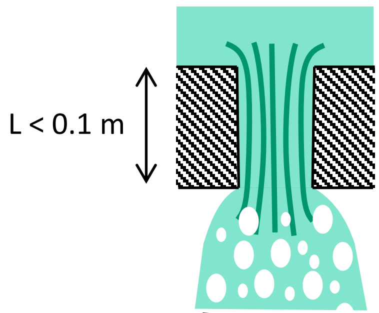
} Model Numerics

1.) Discharge Conditions

Three different conceptual models for providing the mass flow rate:

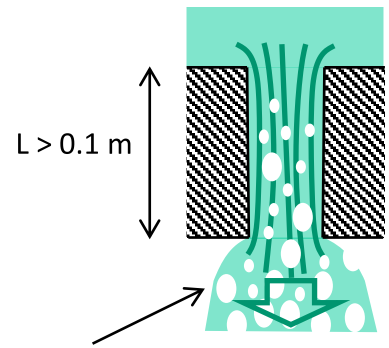
Britter, Weil, Leung & Hanna (2011)

1.) Meta-stable liquid



Conditions at point where jet has expanded to atmospheric pressure is used to set CFD input conditions

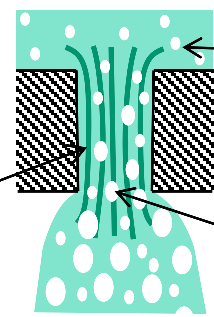
2.) Flashing in orifice



Choked flow, lower mass release rate when flashing in the orifice

Spicer & Miller (2017) MLM* model

3.) Modified meta-stable liquid

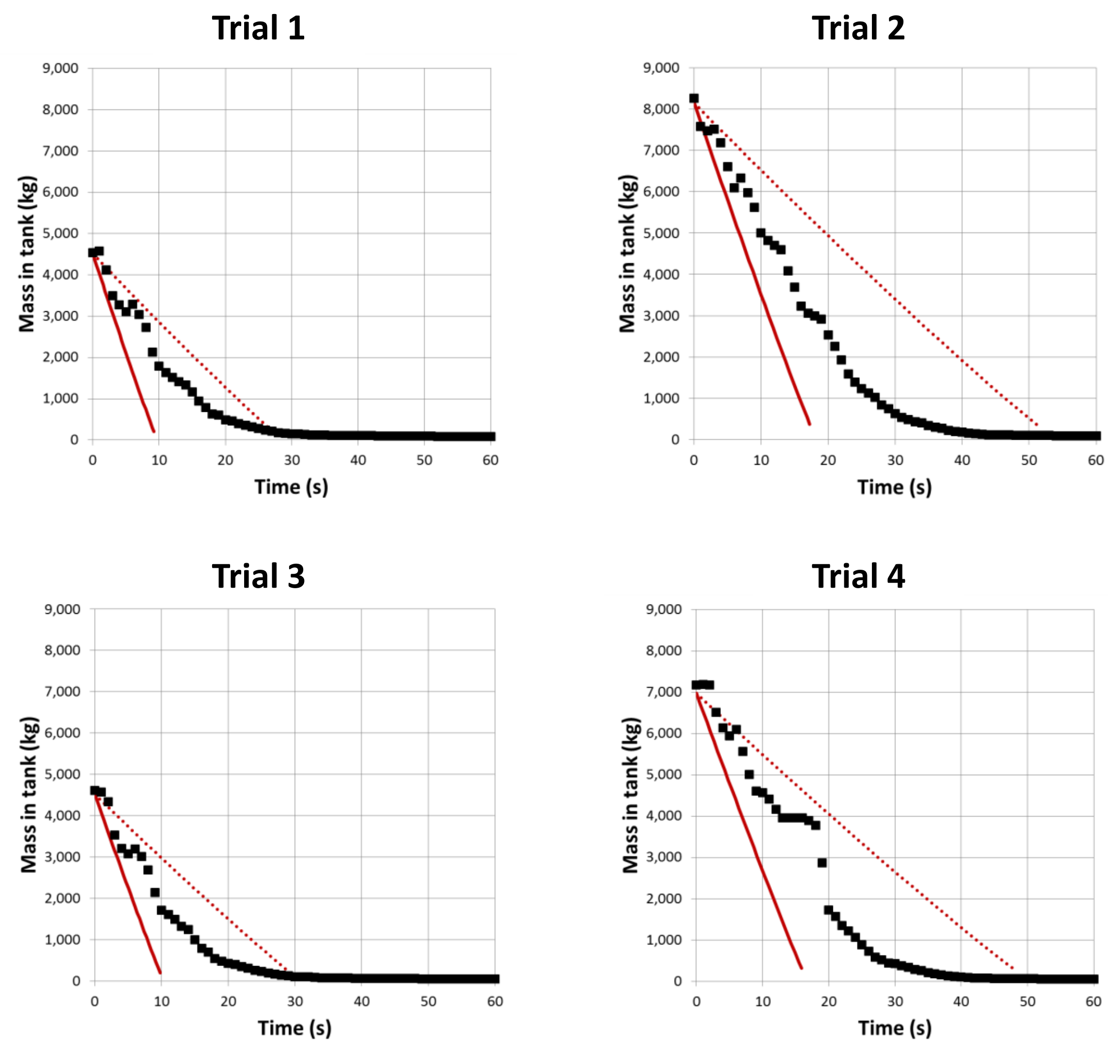


Flashing inside the vessel (liquid swell) when the orifice is relatively large

Orifice length is too short for much flashing to take place, but mass flow rate is reduced due to presence of two-phase fluid in vessel

Flow rate calculated from meta-stable liquid model using average two-phase fluid density

1.) Discharge Conditions



PHAST meta-stable liquid

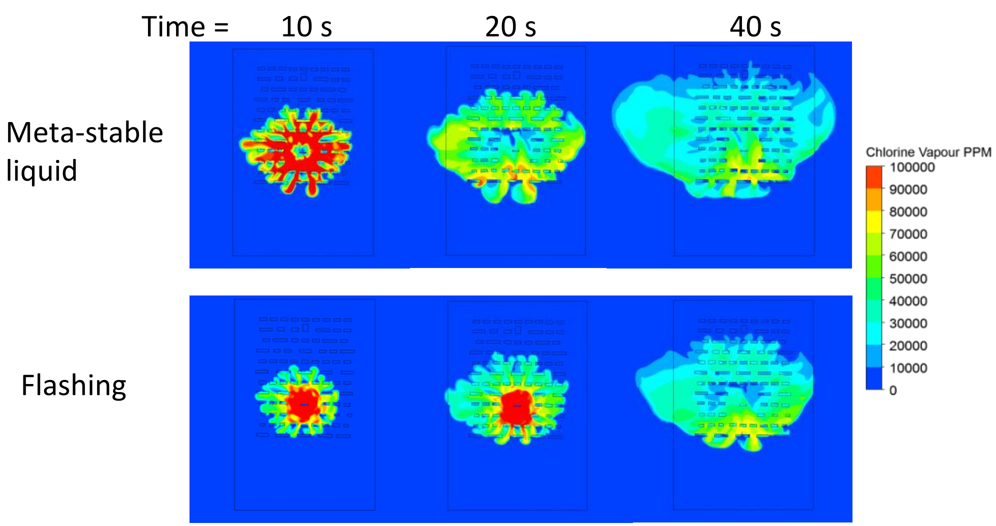
PHAST flashing in orifice

Measurements from load cell data

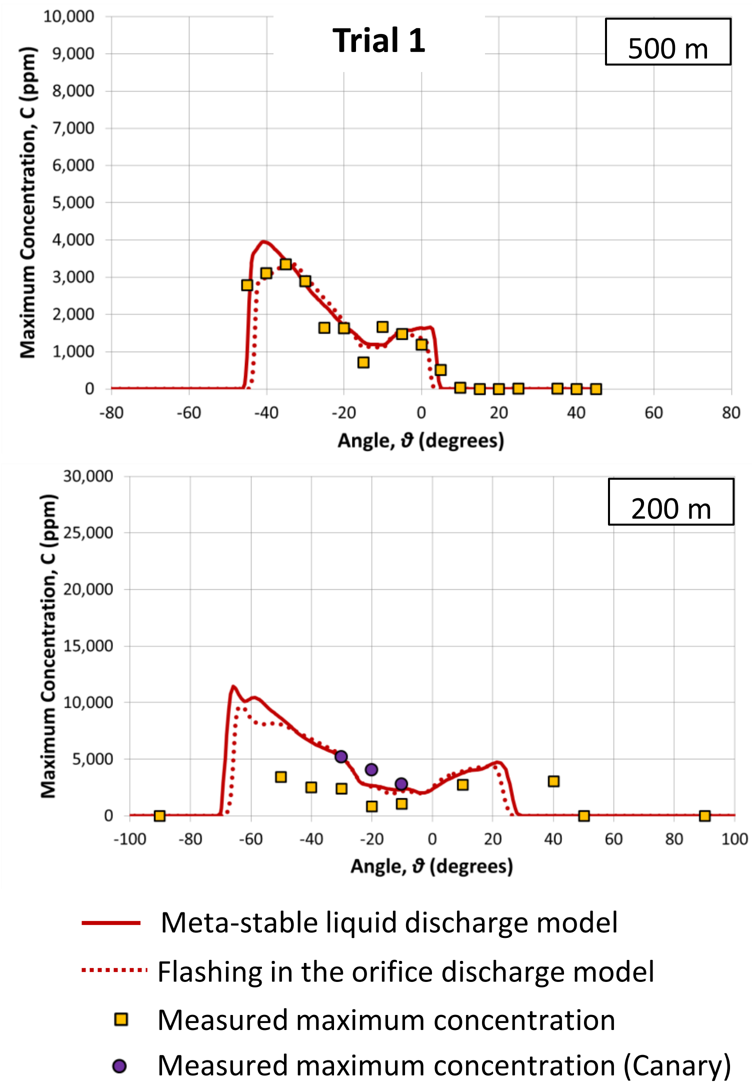
Sensitivity test performed using CFD model on Trial 1 to investigate effect of using the two discharge models:

a) Meta-stable liquid
b) Flashing in the orifice

1.) Discharge Modelling



Chlorine concentrations at ground level



Conclusion

Choice of discharge model of either:

a) Meta-stable liquid

b) Flashing in the orifice

has modest effect on the maximum concentrations in the near-field

CFD Model Uncertainties

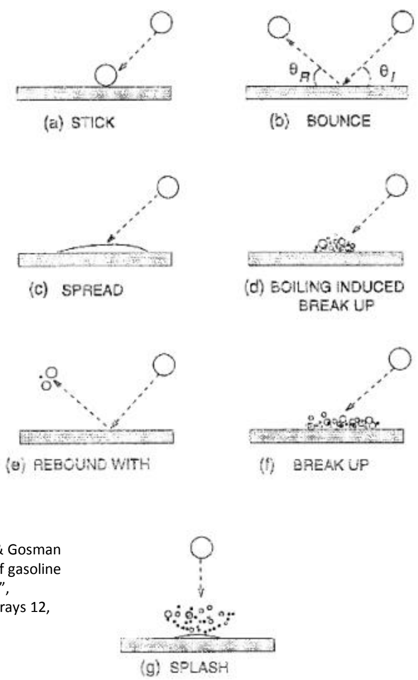
1. Discharge conditions
2. Interaction of chlorine jet with concrete pad
3. Pool formation and evaporation
4. Chlorine droplet size
5. Dry deposition of vapor
6. Atmospheric conditions

Model Physics (items 1–6)

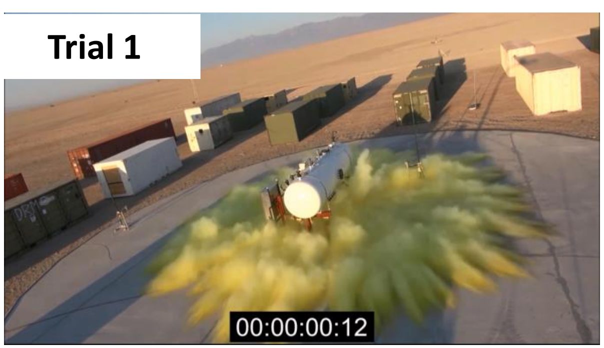
7. Mesh resolution
8. Particle count
9. Time-step

Model Numerics (items 7–9)

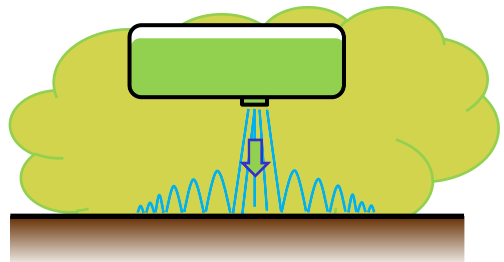
2.) Interaction of chlorine jet with pad



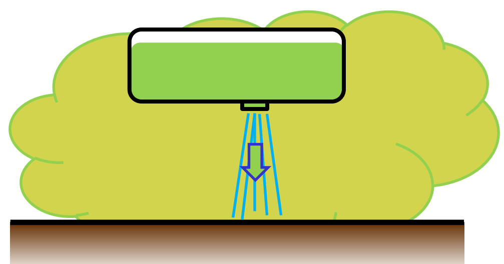
From: Bai, Rusche & Gosman (2002) “Modeling of gasoline spray impingement”, Atomization and Sprays 12, p1-27



Three approaches tested:

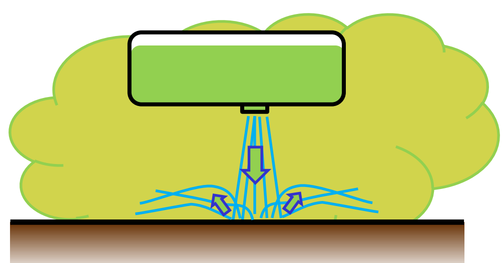


1.) Droplets bounce elastically



2.) Droplets lose all momentum on impact (droplets stick)

Particle-tracking is halted on impact
No further evaporation of droplets



3.) 50% of droplets splash back

Droplets in downward jet stick to pad. Additional droplets released upwards in hemispherical direction from 1 m diameter area of pad. Splashing droplets contain 50% of initial mass, 50% of velocity and have diameter 10µm.

2.) Interaction of chlorine jet with pad

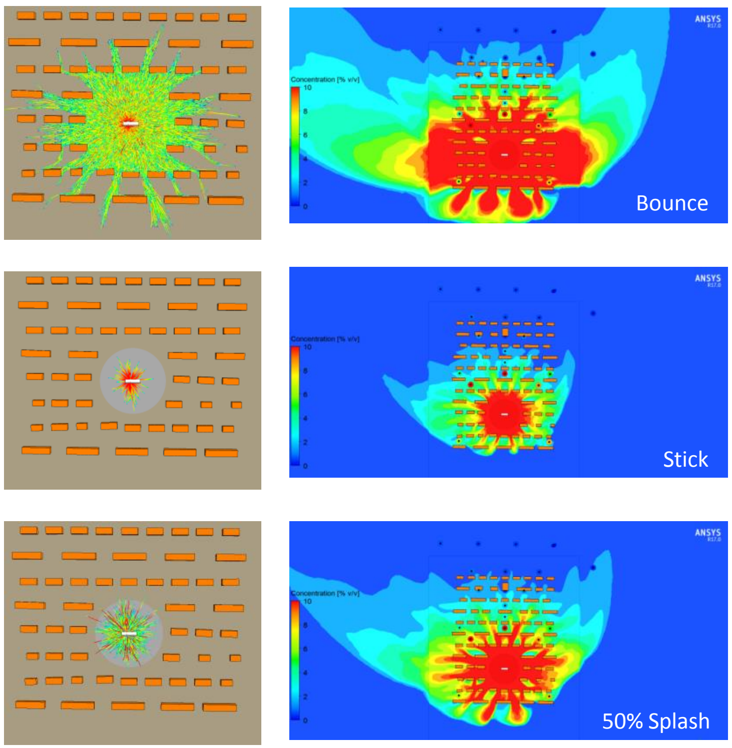
Droplet trajectories

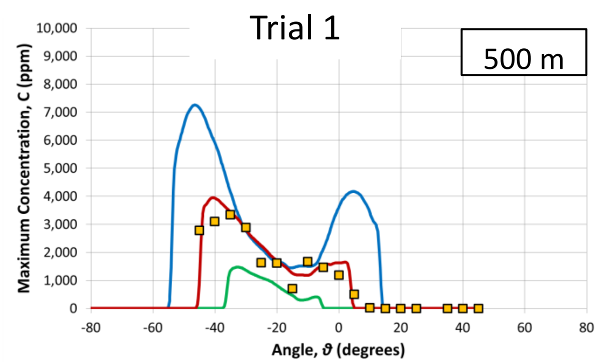
Maximum concentrations at height of sensors (h = 30 cm)

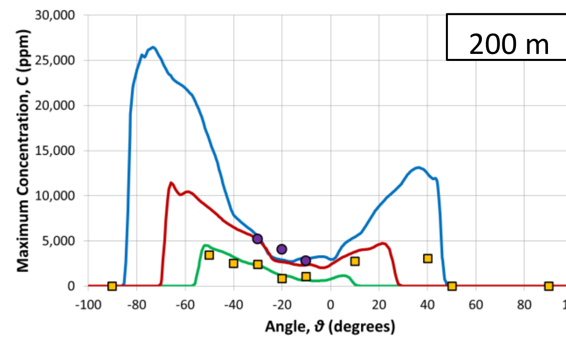
1.) Droplets bounce

2.) Droplets stick

3.) 50% Splash







- Droplets bounce elastically
- Droplets stick on impact
- 50% of droplets splash
- Measured maximum concentration (MiniRAE)
- Measured maximum concentration (Canary)

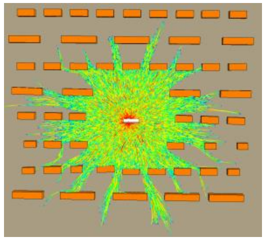
Conclusion

Choice of droplet impingement conditions has a strong effect, but…

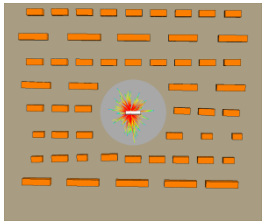
2.) Interaction of chlorine jet with pad

Droplet trajectories

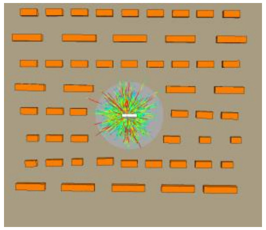
1.) Droplets bounce



2.) Droplets stick

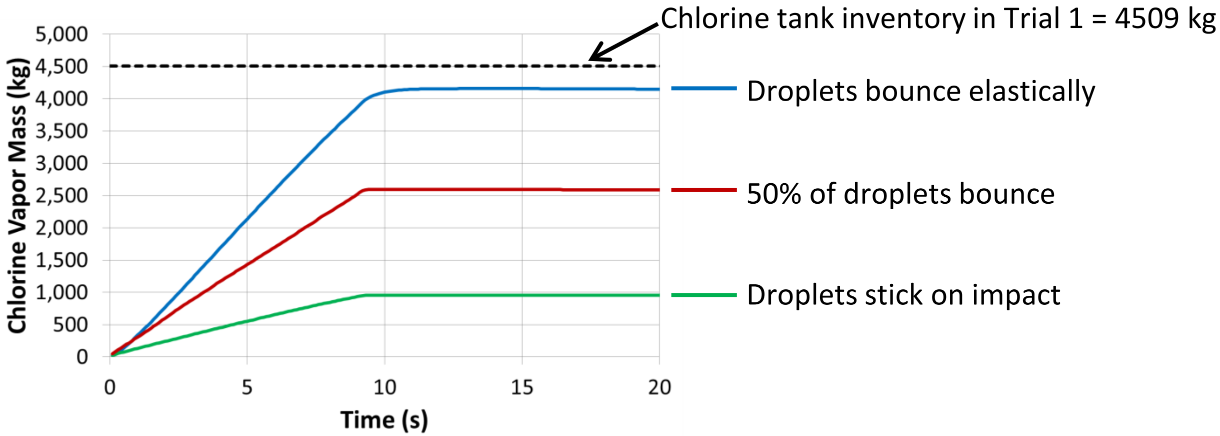


3.) 50% Splash



Problem

- Chlorine droplets "disappear" in the CFD model when they hit a surface
- No further evaporation of the droplets once they contact the surface
- Total mass of chlorine vapor released in model depends on droplet behavior



Solution

- Include pool evaporation in the CFD model to account for remaining mass of chlorine

CFD Model Uncertainties

Model Physics

1. Discharge conditions
2. Interaction of chlorine jet with concrete pad
3. Pool formation and evaporation
4. Chlorine droplet size
5. Dry deposition of vapor
6. Atmospheric conditions

Model Numerics

7. Mesh resolution
8. Particle count
9. Time-step

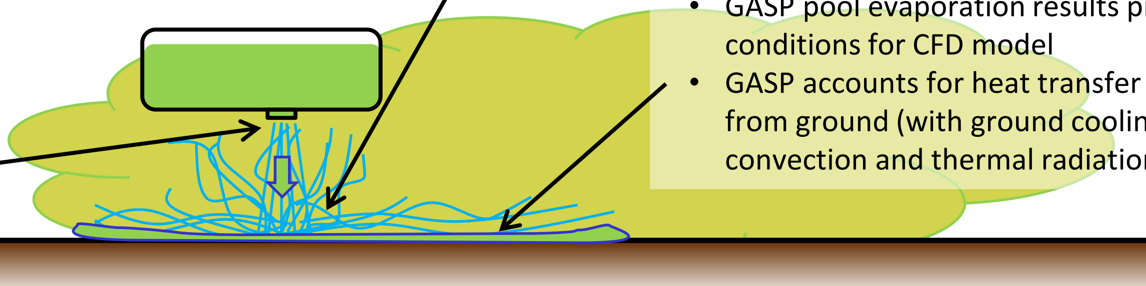
3.) Pool Formation and Evaporation

Wetted concrete pad

Assumed that either:
- Droplets bounce elastically
- 50% of droplets splash
- Droplets stick on impact

Pool spread and evaporation
- Accounts for remaining mass of chlorine
- GASP pool evaporation results provide source conditions for CFD model
- GASP accounts for heat transfer inc. conduction from ground (with ground cooling effects), air convection and thermal radiation

CFD jet source is approx. 80% liquid + 20% vapor

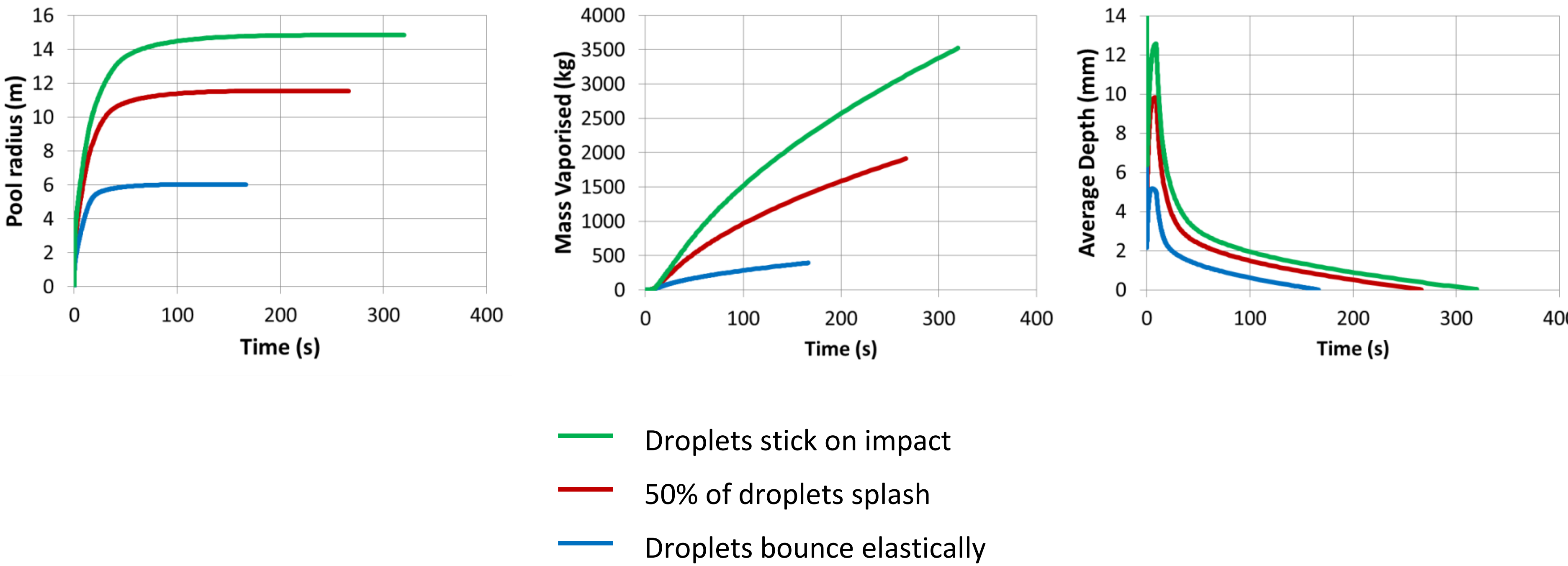


Limitations:

- GASP model is uncoupled from CFD: it uses a pre-defined atmospheric wind profile, not the local air velocity predicted by CFD

3.) Pool Formation and Evaporation

GASP pool evaporation model results

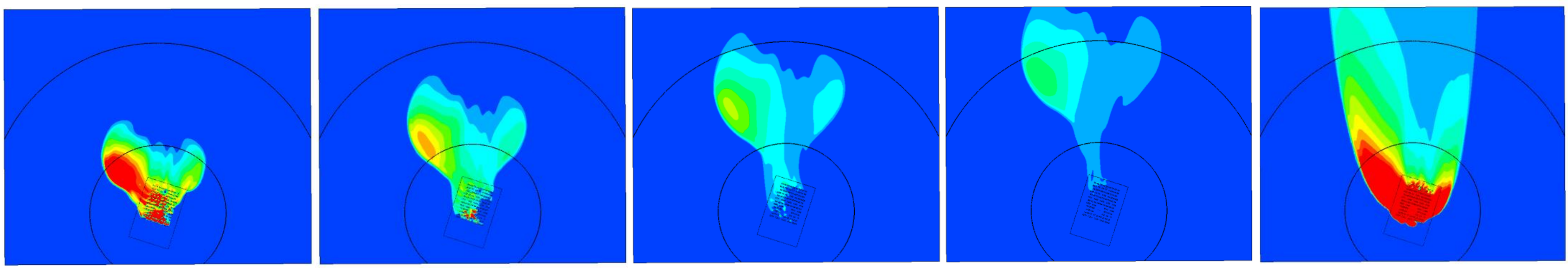


3.) Pool Formation and Evaporation

CFD results for 50% splash

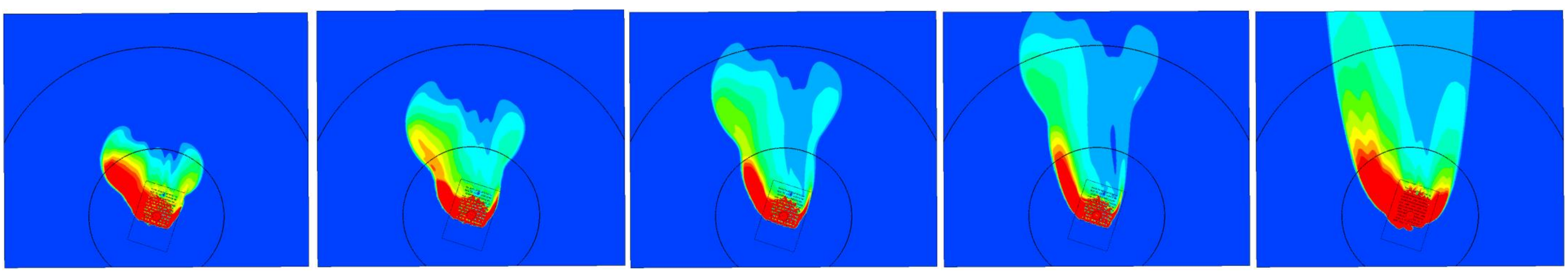
Without Pool

Time = 2 mins | 3 mins | 4 mins | 5 mins | Max concentrations

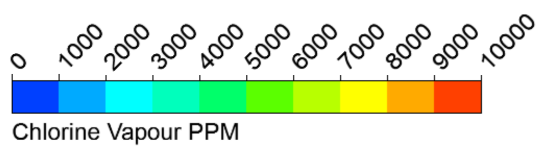


With Pool

Time = 2 mins | 3 mins | 4 mins | 5 mins | Max concentrations



Chlorine concentrations at ground level

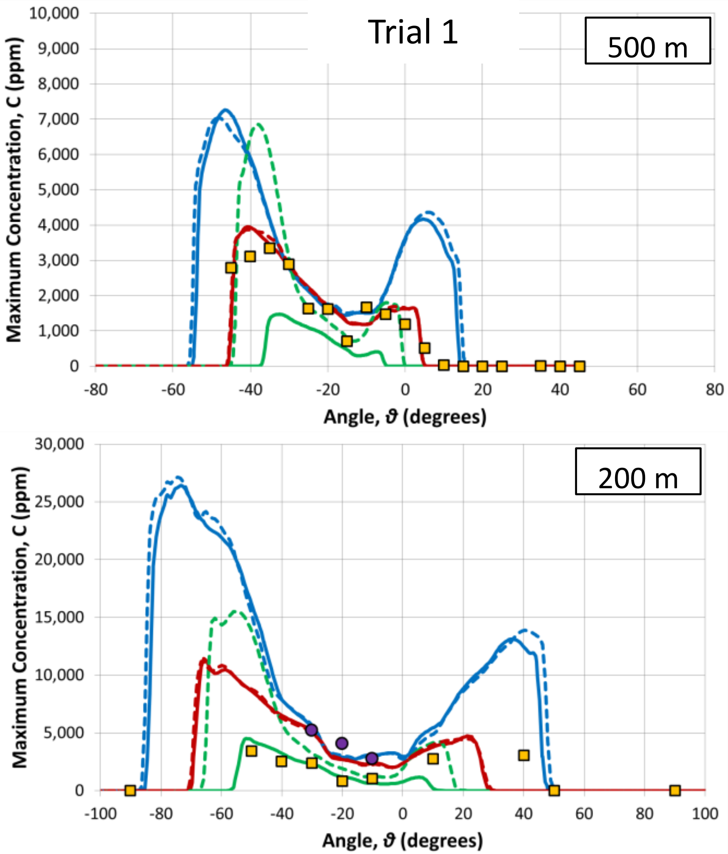


3.) Pool Formation and Evaporation

Droplets bounce: Without pool With pool

Droplets stick: Without pool With pool

50% splash: Without pool With pool



Measured maximum concentration (MiniRAE)

Measured maximum concentration (Canary)

Conclusion

When 50% of droplets (or more) remain as aerosol

- Pool source has relatively little effect on max concentrations in near-field

When there is no aerosol

- Pool source has significant effect

Pool evaporation is likely to have significant effect on time-integrated concentration (i.e. dose) and far-field concentrations

CFD Model Uncertainties

1. Discharge conditions
2. Interaction of chlorine jet with concrete pad
3. Pool formation and evaporation
4. Chlorine droplet size
5. Dry deposition of vapor
6. Atmospheric conditions

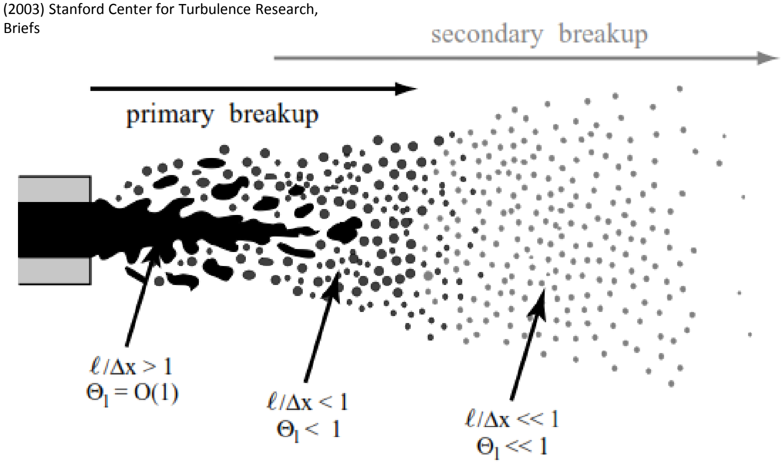
} Model Physics (items 1–6)

7. Mesh resolution
8. Particle count
9. Time-step

} Model Numerics (items 7–9)

4.) Chlorine Droplet Size

From: Herrmann (2003) Stanford Center for Turbulence Research, Annual Research Briefs

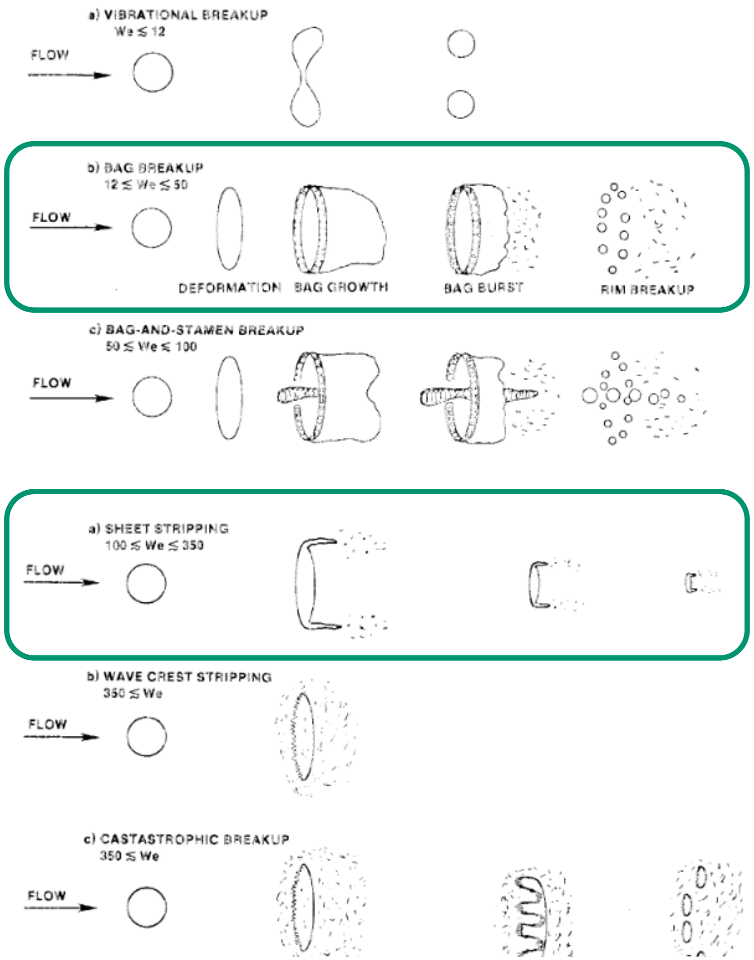


Secondary droplet breakup model tested:

- Reitz & Diwakar (1987) "Structure of high-pressure fuel sprays", SAE technical Paper 870598

Bag breakup: $(We > We_{crit})$: $r_{stable} = \frac{We_{crit}\,\sigma}{\rho_F\,V_{slip}^2}$

Stripping $(We/\sqrt{Re} > C_{s1})$: $r_{stable} = \frac{2\,C_{s1}^{\,2}\,\sigma^2}{\rho_F^2\,V_{slip}^3\,\nu_F}$

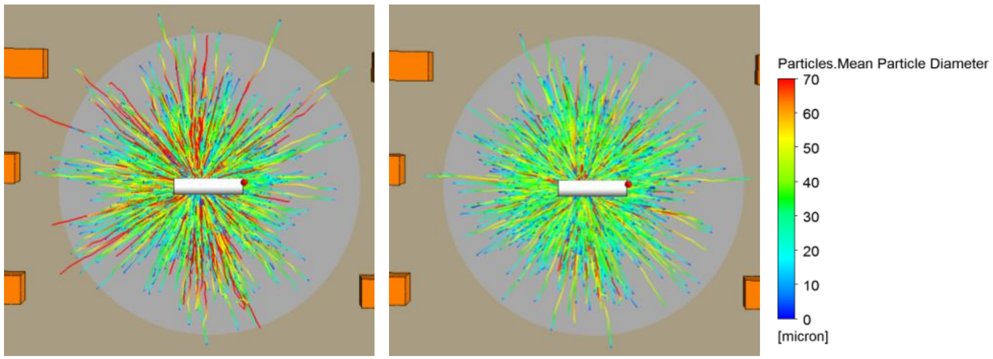


From: Pilch & Erdman (1987) "Use ofbreakup time data and velocity history data to predict the maximum size of stable fragments for acceleration-induced breakup of a liquid drop" Int. J. Multiphase Flow, 13(6), p741-757

4.) Chlorine Droplet Size

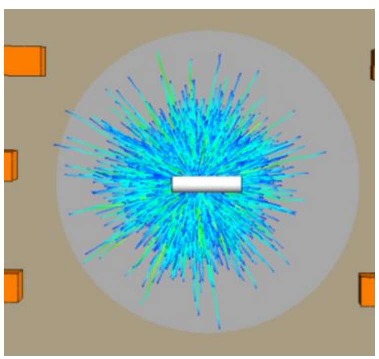
HSE

Plan view of chlorine droplet trajectories colored by droplet diameter



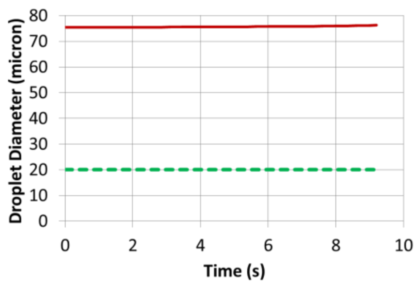
DNV correlation without breakup

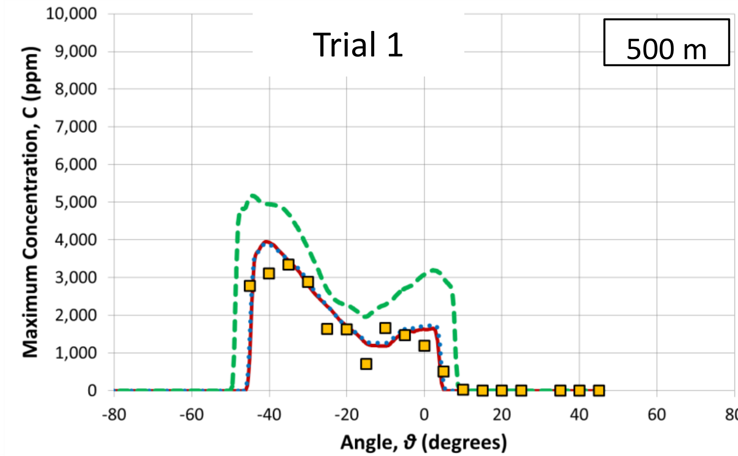
DNV correlation with breakup

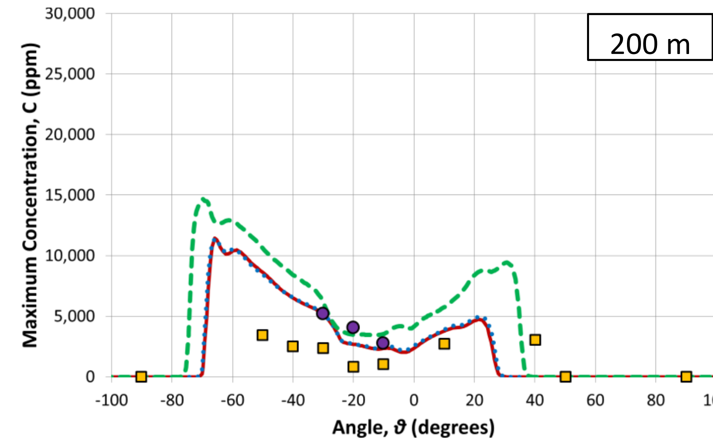


20 micron

Droplet size decreases as droplets evaporate in all three cases







- DNV Phase III JIP droplet correlation without secondary breakup
- DNV Phase III JIP droplet correlation with secondary breakup
- 20 micron (Hanna *et al*. 2008 railcar incident analysis)
- Measured maximum concentration (MiniRAE)
- Measured maximum concentration (Canary)

Conclusion

Reducing droplet size to 20 µm increases concentrations

CFD Model Uncertainties

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Model Physics

7. Mesh resolution
8. Particle count
9. Time-step

Model Numerics

5.) Dry Deposition

HSE

$$F = -V_d C$$

Deposition flux applied to all solid surfaces in CFD model

Deposition velocity

Chlorine concentration (calculated by CFD model)

Assumed to be the upper range in estimates of V_d = 5 cm/s

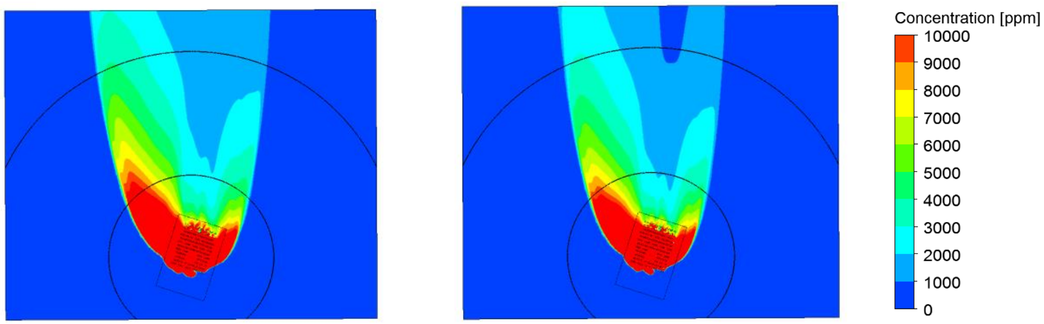
Suggested values of v_d for chlorine in the literature range from 0.5 cm s^{-1} (EPA, 2005) to 2 cm s^{-1} (Sehmel, 1984), to as high as 5 cm s^{-1} (Hanna and Chang, 2008). For large releases, such as that occurring in Graniteville, Hanna and Chang (2008) have suggested that v_d may also vary as a function of the concentration of the depositing gas. Surfaces near the release that are exposed to extremely high concentrations could quickly become saturated with chlorine or undergo a chemical transformation which then limits additional deposition. Furthermore, Hill

From Buckley *et al*. (2012) “A case study of chlorine transport and fate following a large accidental release”, https://www.osti.gov/scitech/servlets/purl/1053021

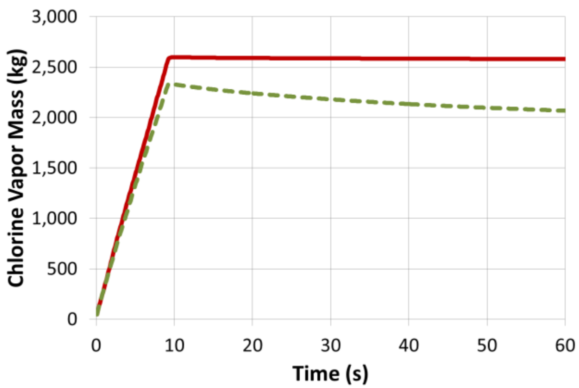
5.) Dry Deposition

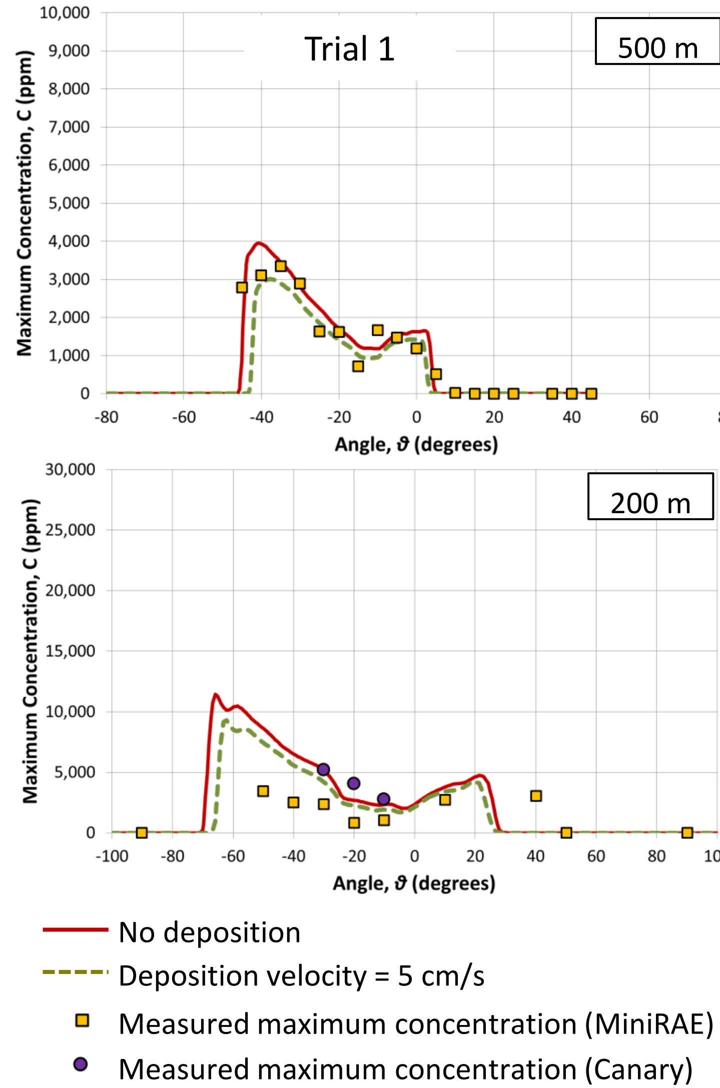
No vapor deposition

Deposition velocity = 5 cm/s



Maximum concentrations at ground level





Conclusion

A high vapor deposition velocity of 5 cm/s causes a modest reduction in concentrations in the near-field … but it is likely to have a significant effect on the far field concentrations

CFD Model Uncertainties

1. Discharge conditions
2. Interaction of chlorine jet with concrete pad
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} Model Physics (items 1–6)

7. Mesh resolution
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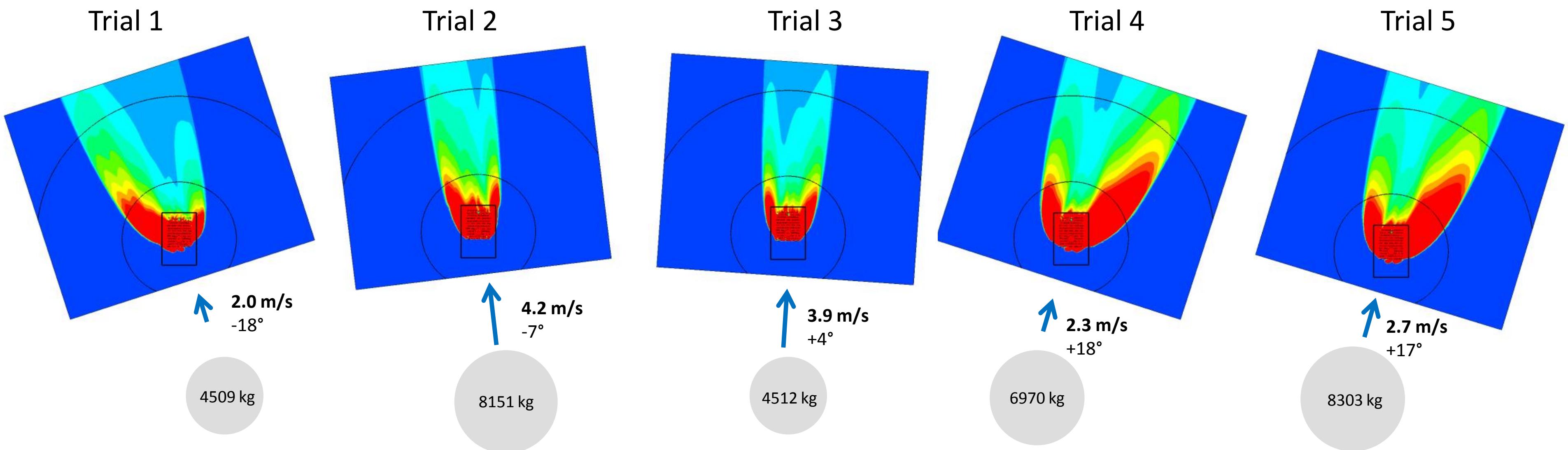
} Model Numerics (items 7–9)

Atmospheric Conditions

- CFD model uses constant wind direction and log-law velocity profile, neutral Pasquill D-class
- Incorporating wind fluctuations in RANS-based CFD models is an open research question
- Some approaches tested (e.g. FLACS) but not widely accepted for predictive modelling
- Potential problems
  - RANS models cause turbulent fluctuations imposed at the inlet to decay with distance
  - Are coherent turbulent structures required for the inlet profile? How should these be defined? Is forcing required to sustain fluctuations?
  - Standard RANS models also cannot sustain realistic atmospheric boundary layers over several kilometers
- LES is preferable for modelling atmospheric boundary layers with realistic fluctuations, but it may have grid-resolution issues for the high-speed jet source

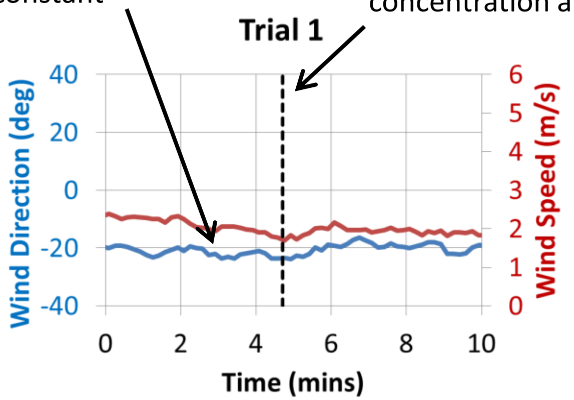


Atmospheric Conditions

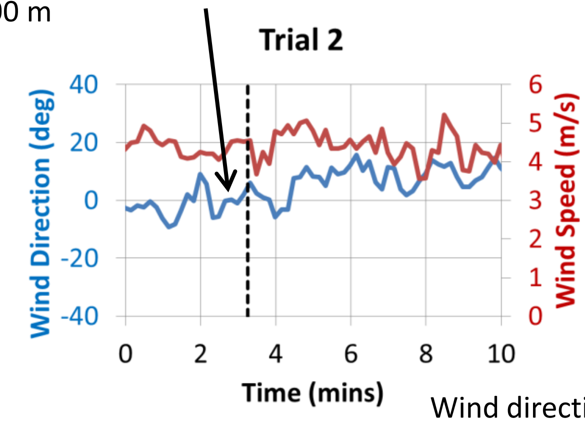
Wind speed and direction measurements from PWIDS 19, located 100m upwind of release point (apart from Trial 3)

Wind direction fairly constant

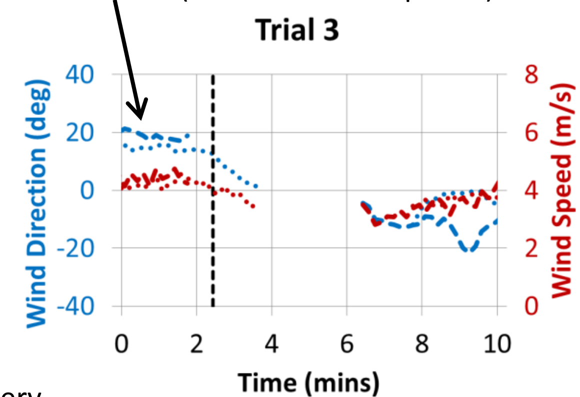
Arrival time of max concentration at 500 m

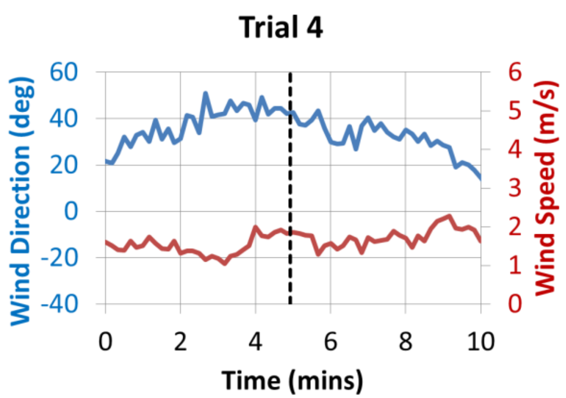


Wind direction more variable

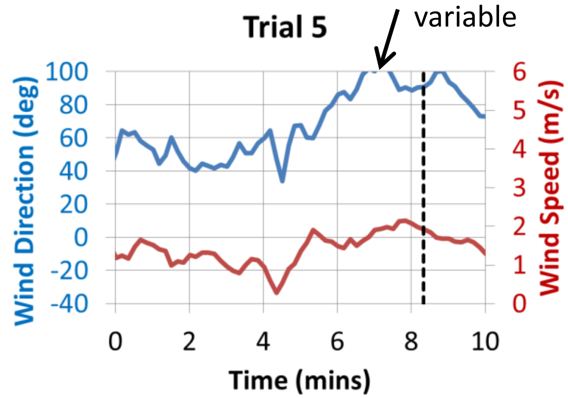


PWIDS 19 failed, results shown for PWIDS 25 and 31 (1 km and 2 km upwind)

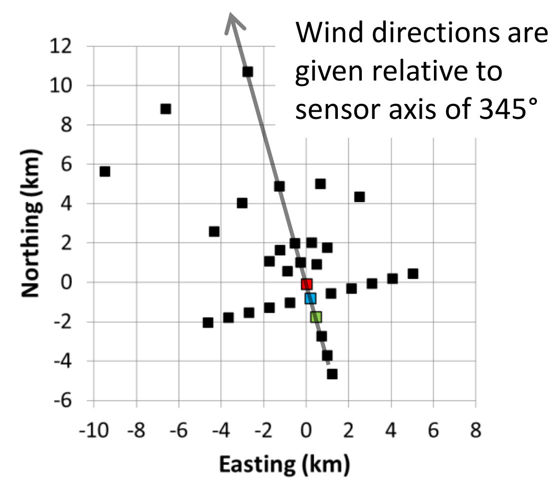




Wind direction very variable



Wind directions are given relative to sensor axis of 345°



Conclusion: Fixed wind direction reasonable for Trial 1, but less so for Trials 2 – 5

CFD Model Uncertainties

Model Physics:

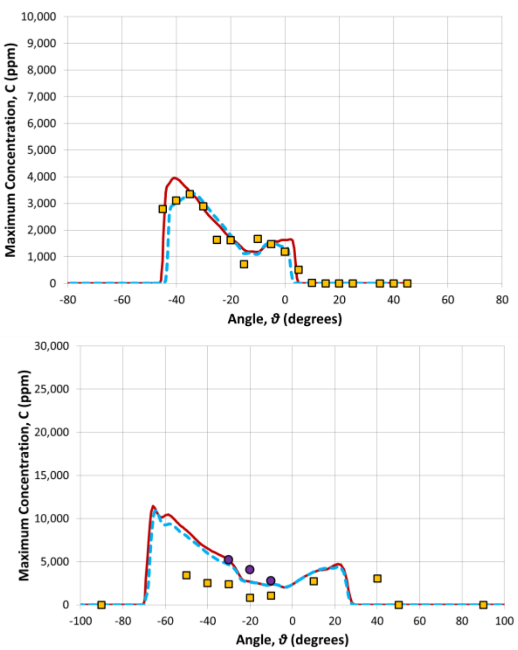
1. Discharge conditions
2. Interaction of chlorine jet with concrete pad
3. Pool formation and evaporation
4. Chlorine droplet size
5. Dry deposition of vapor
6. Atmospheric conditions

Model Numerics:

7. Mesh resolution
8. Particle count
9. Time-step

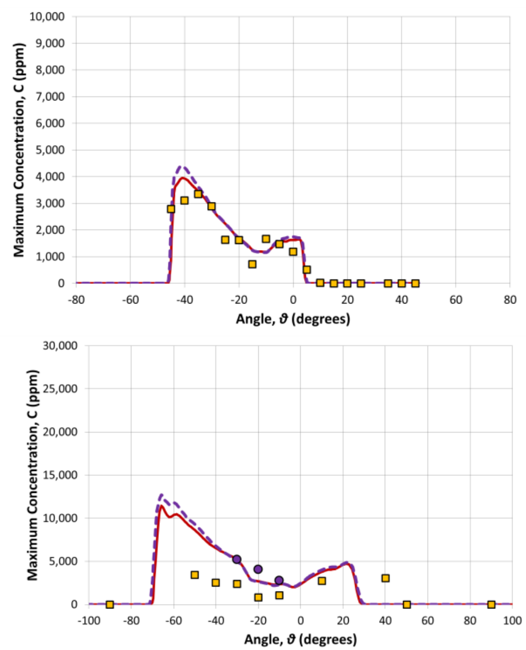
7 – 9.) Model Numerics

Mesh resolution



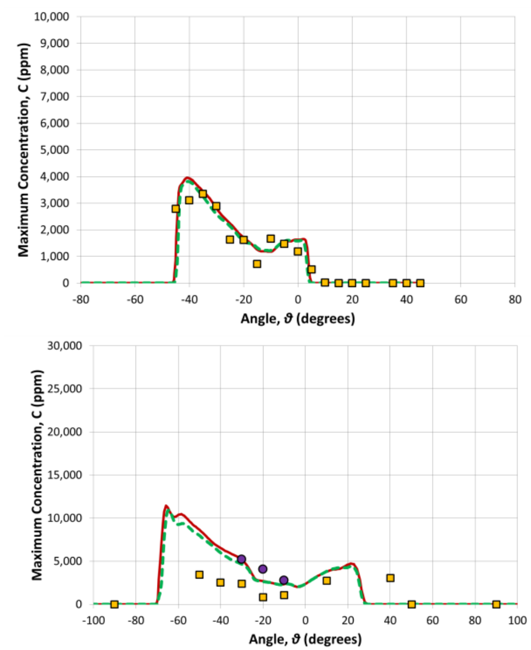
1.1 M nodes (12 hours)
2.5 M nodes (32 hours)

Particle count



1000 s^{-1} (12 hours)
2000 s^{-1} (13 hours)

Time-step



0.1s / 1.0 s (12 hours)
0.05 s / 0.5 s (26 hours)

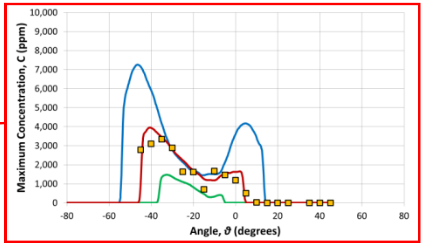
Computing time required on 24 CPUs

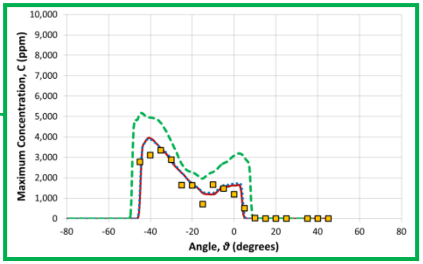
Later simulations used 2000 s^{-1} particles since only small increase in runtime required

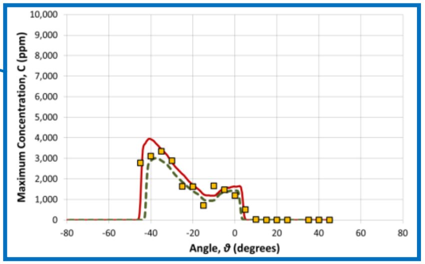
Summary of CFD Model Uncertainties

HSE

1. Discharge conditions ← Minor effect
2. Interaction of chlorine jet with concrete pad ← Largest effect
3. Pool formation and evaporation ← Minor effect
4. Chlorine droplet size ← Second largest effect
5. Dry deposition of vapor ← Third largest effect
6. Atmospheric conditions ← Not investigated



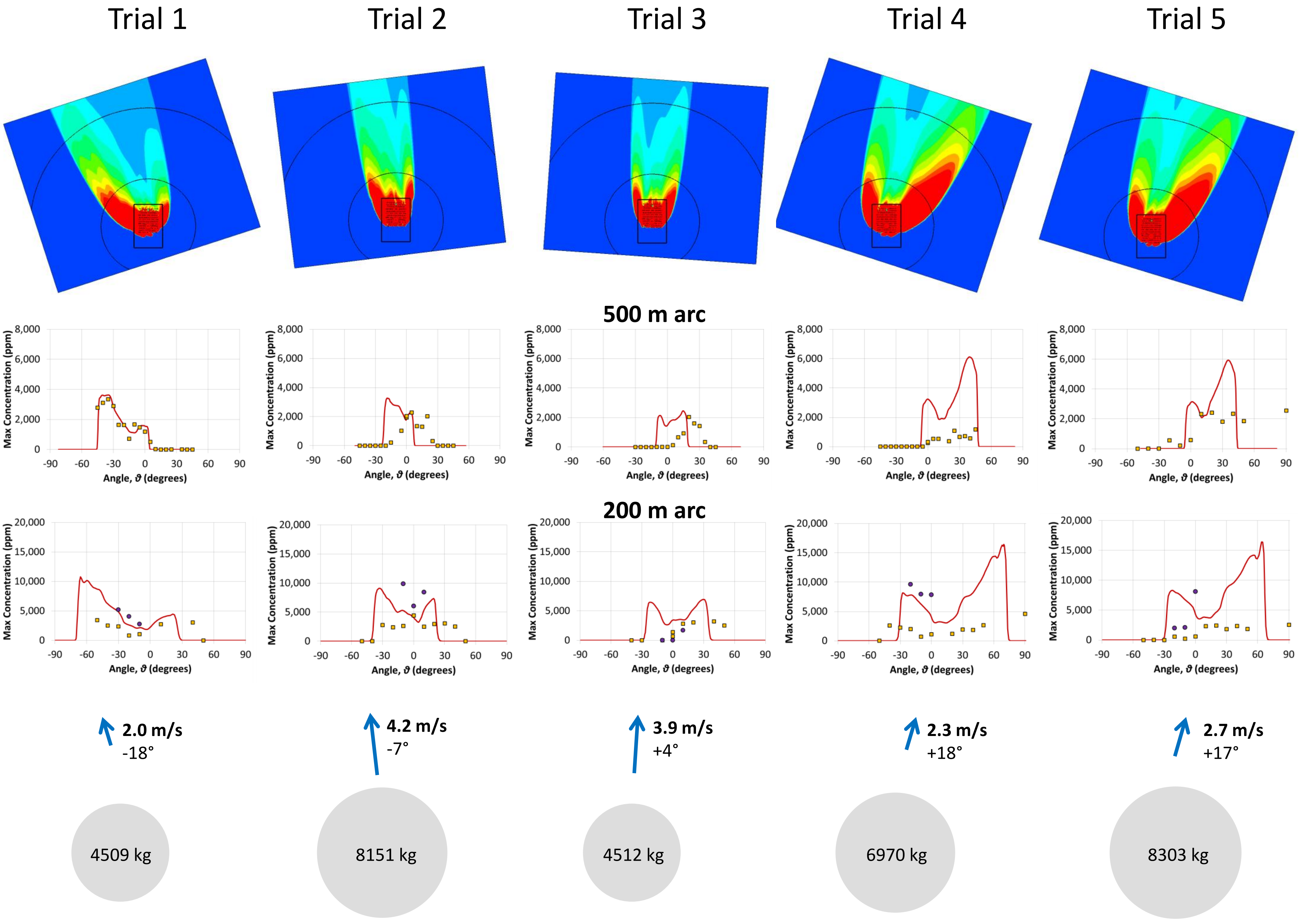




7. Mesh resolution
8. Particle count
9. Time-step

Results not fully mesh or time-step independent but compromise with CPU time
More particles used in later simulations

NB: influence of these effects on max. concentration in near-field may differ from their influence on the time-integrated dose or the far-field concentrations

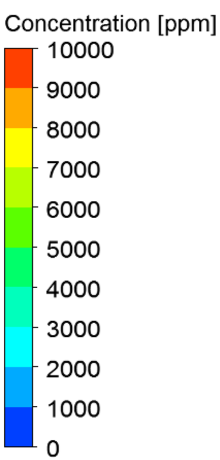


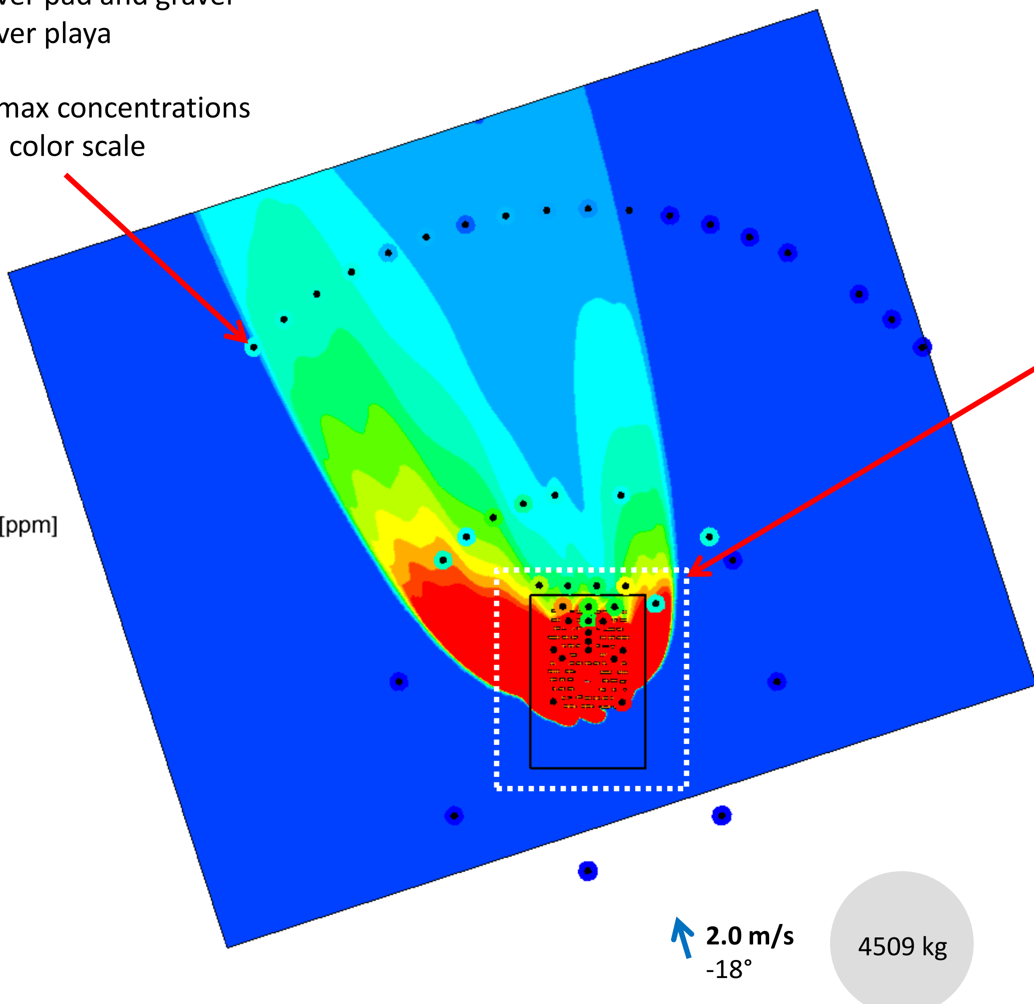
Trial 1
Trial 2
Trial 3
Trial 4
Trial 5
500 m arc
200 m arc
Max Concentration (ppm)
Angle, ϑ (degrees)
2.0 m/s
-18°
4.2 m/s
-7°
3.9 m/s
+4°
2.3 m/s
+18°
2.7 m/s
+17°
4509 kg
8151 kg
4512 kg
6970 kg
8303 kg

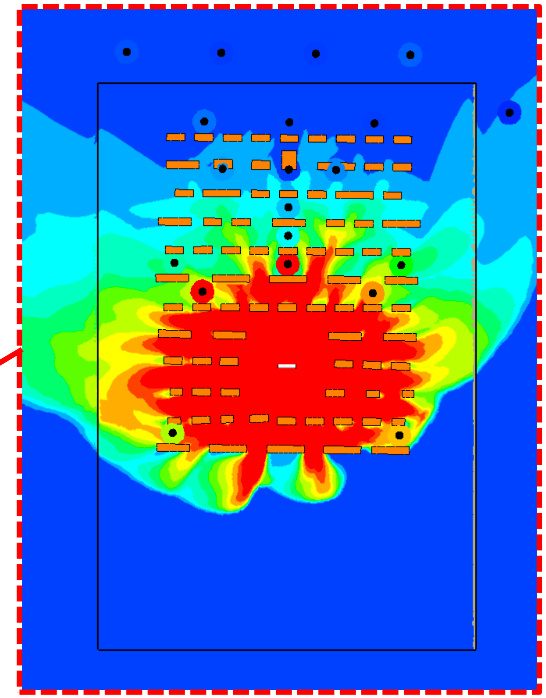
Jack Rabbit II 2015: Trial 1

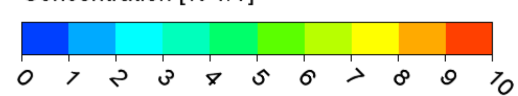
Maximum concentration contours at heights:
h = 10 cm over pad and gravel
h = 30 cm over playa

Measured max concentrations using same color scale









Higher concentration levels to help discern near-field behavior

Outline

- Background
- Aims
- CFD model setup
- Uncertainties
- Jack Rabbit II 2015
  - Sensitivity tests for Trial 1
  - Results for Trials 2 to 5
- Jack Rabbit II 2016
- Hypothetical scenarios
- Future work

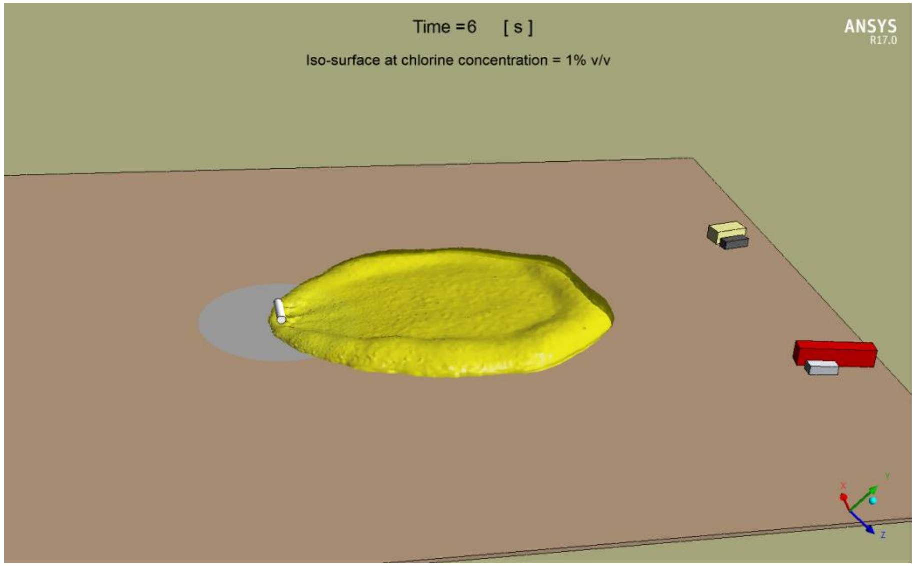
Jack Rabbit II 2016, Trial 7

Chlorine tank mass = 9067 kg; Mass released = 8339 kg

Release angle = 45 deg downwards

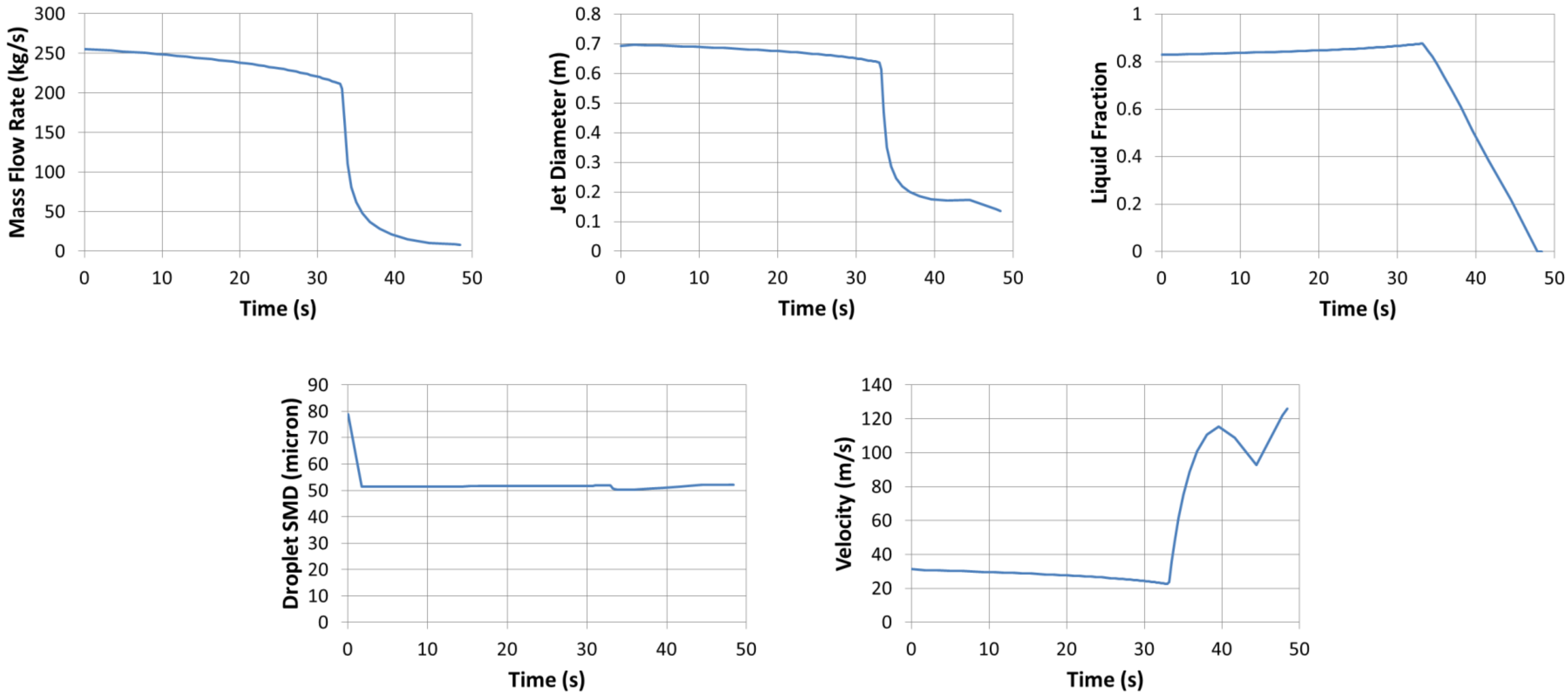
Wind speed = 4.5 m/s

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

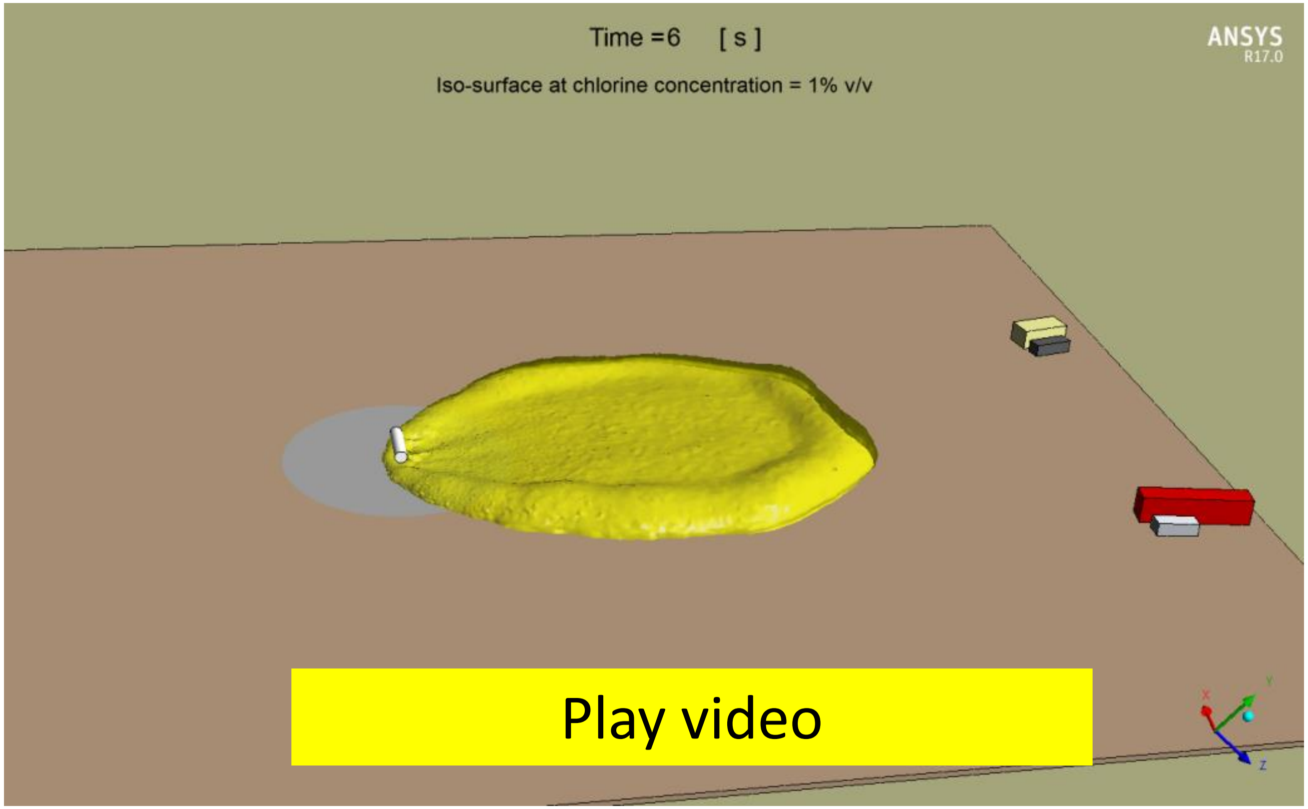


Jack Rabbit II 2016, Trial 7

Post-expansion jet source conditions for CFD model provided by Rick Babarsky (US Army)



Jack Rabbit II 2016, Trial 7



Outline

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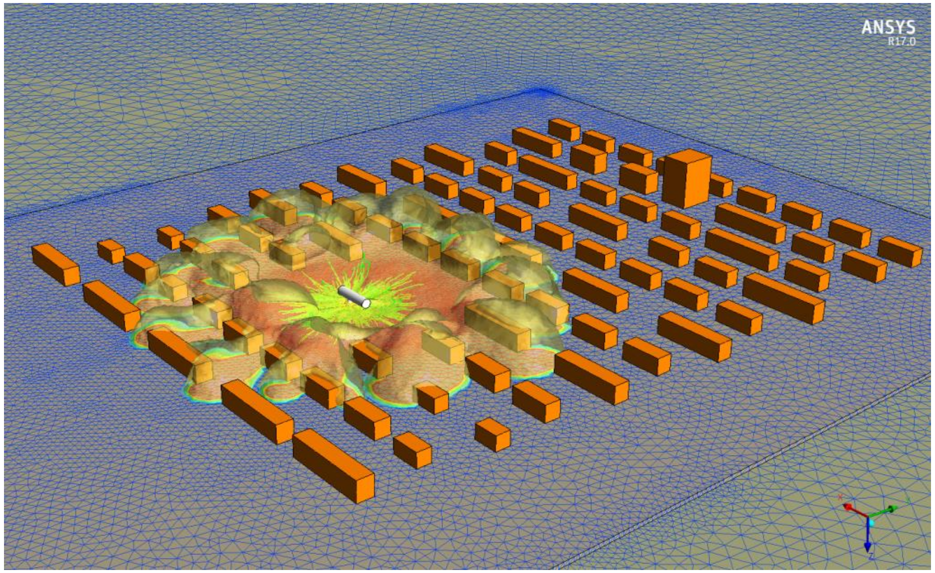
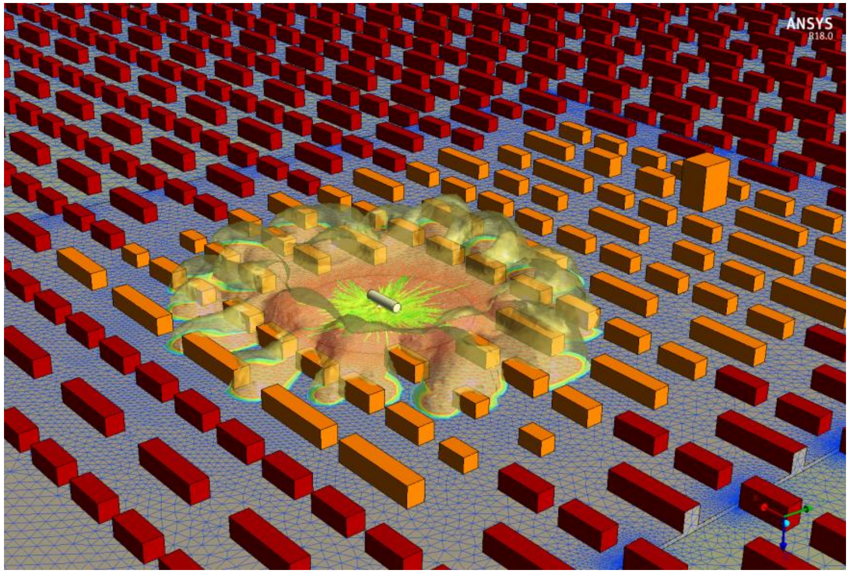
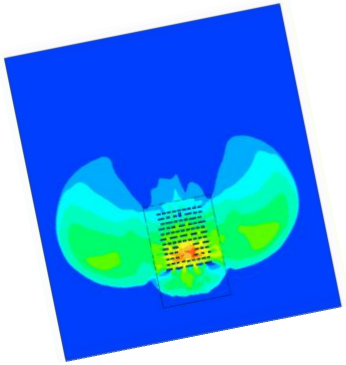
Hypothetical Scenario

JRII geometry



Extended urban array of Conexes





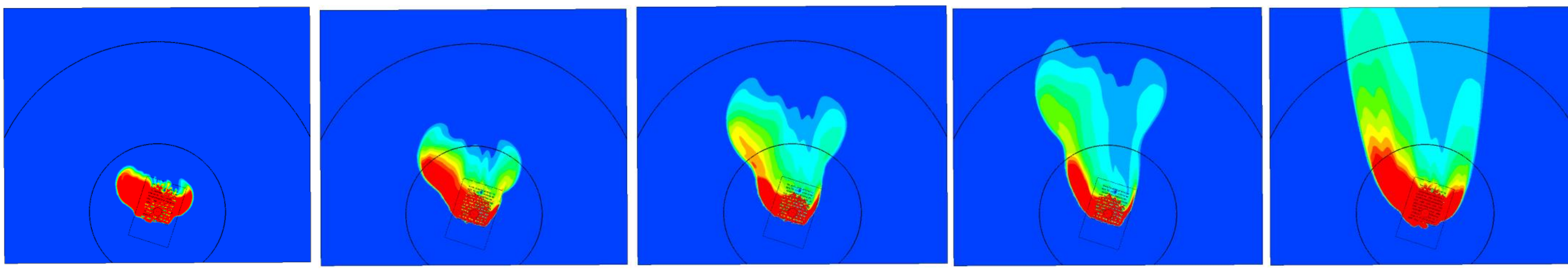
Questions:

- To what extent is this dispersion behavior influenced by the JRII urban grid?
- How would concentrations be changed if the urban grid extended further in all directions, like in a city?

Hypothetical Scenario

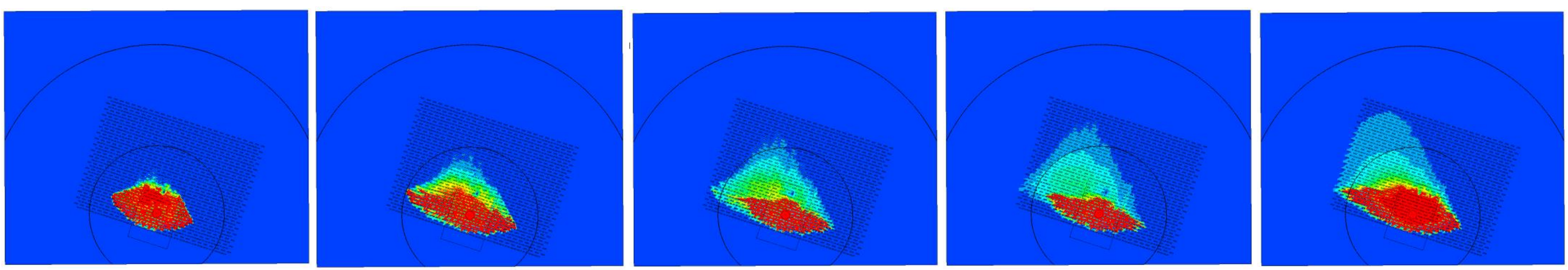
JRII 2015 Trial 1: CFD model with 50% splashing droplets, DNV droplet size, pool evaporation and zero deposition

Time = 1 mins | 2 mins | 3 mins | 4 mins | Max concentrations

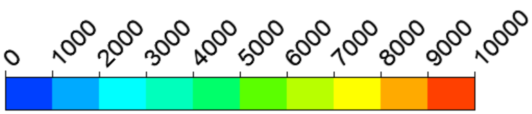


Extended urban array: CFD model identical to above except for the modified geometry

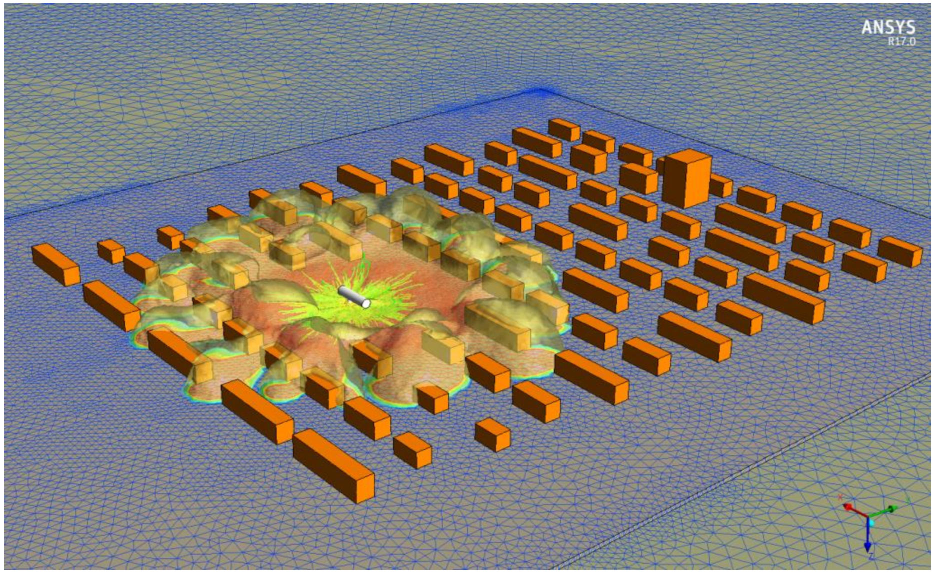
Time = 1 mins | 2 mins | 3 mins | 4 mins | Max concentrations

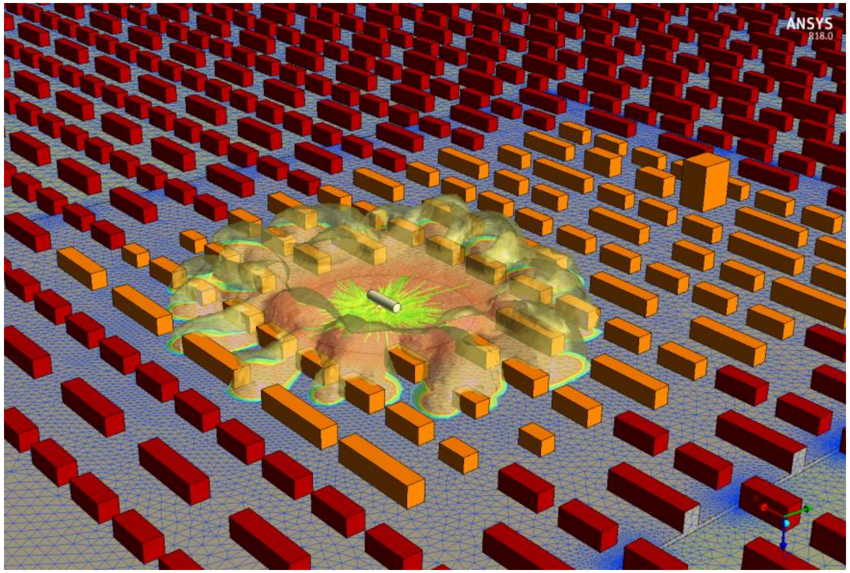


Chlorine concentrations at ground level



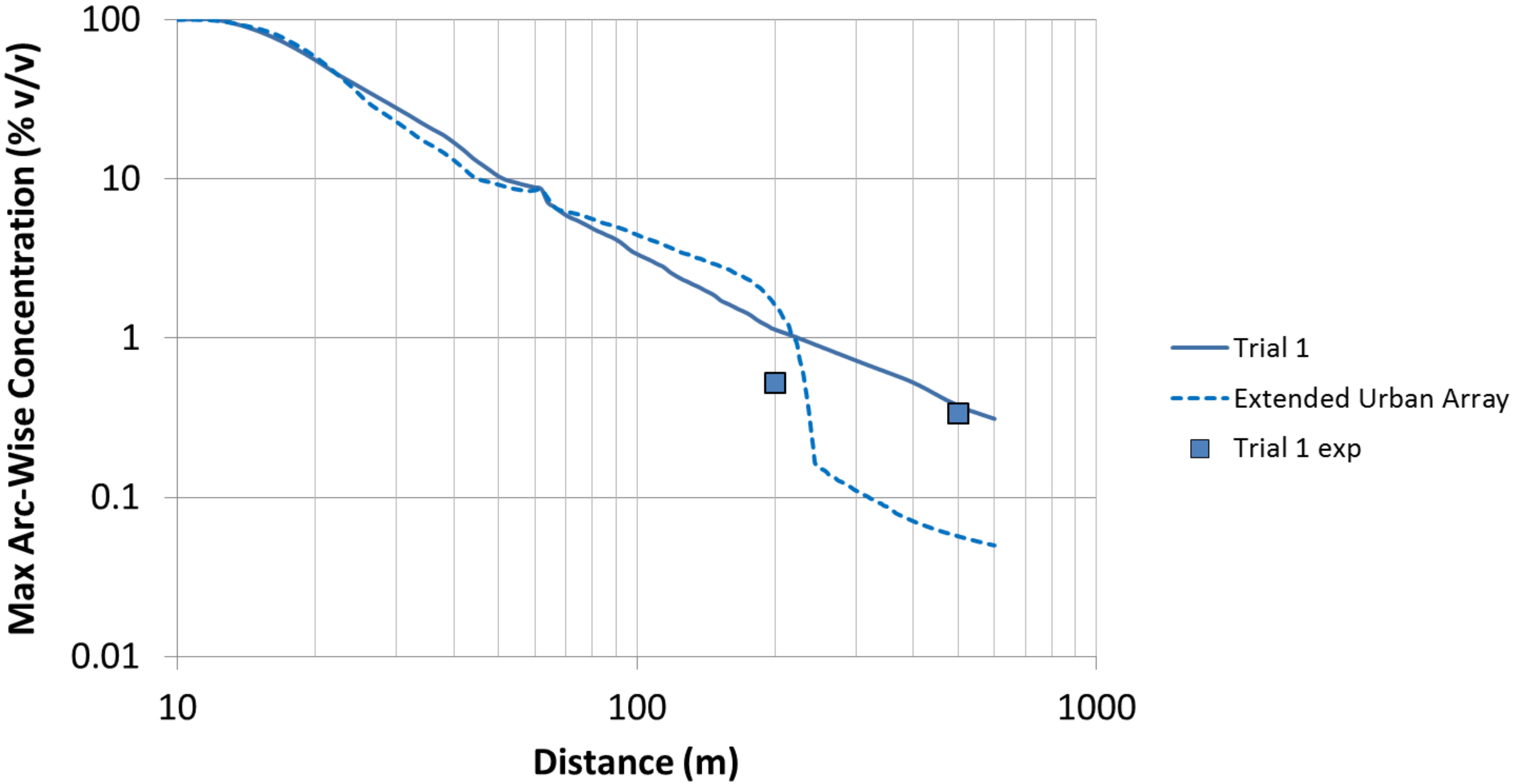
Hypothetical Scenario





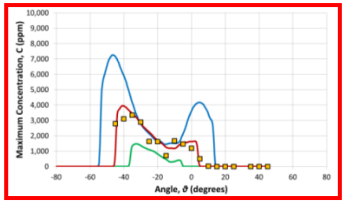
Play videos

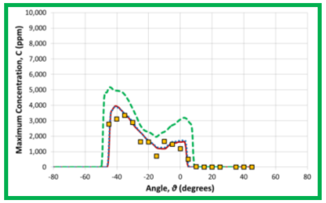
Max Arc-Wise Concentrations



Conclusions

- CFD model sensitivity tests for Trial 1 showed:

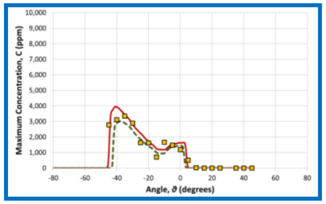




1.) Higher airborne aerosol fraction → higher concentrations

2.) Smaller droplets → higher concentrations

3.) Faster deposition rate → lower concentrations



Possible to "tune" concentrations up or down, according to the model choices

- CFD model with 50% splashing, DNV Phase III JIP droplet size correlation and no deposition gave good agreement with measured max concentrations in Trial 1
- Same model gave reasonably good results in Trials 2 and 3, worse in Trials 4 and 5
- Extending the urban array had a strong effect on the predicted near-field dispersion behavior
- Limitations of the model: wind assumed constant (no meandering), atmospheric stability assumed neutral and pool evaporation model uncoupled from CFD

Future Directions

- Try to reduce model uncertainties (bound values) using:
  - JRII data: analysis of pool size
  - Lab test data: deposition experiments

- Integrate pool evaporation model into CFD model

- Use the CFD model to help refine integral or operational models?
  - Source terms for road/rail tanker releases
  - Resistance terms for cloud spread in different directions with urban grids

- CFD for visualization: what would a 90 ton railcar release look like?

Acknowledgements

DISCLAIMER:

- This work 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)
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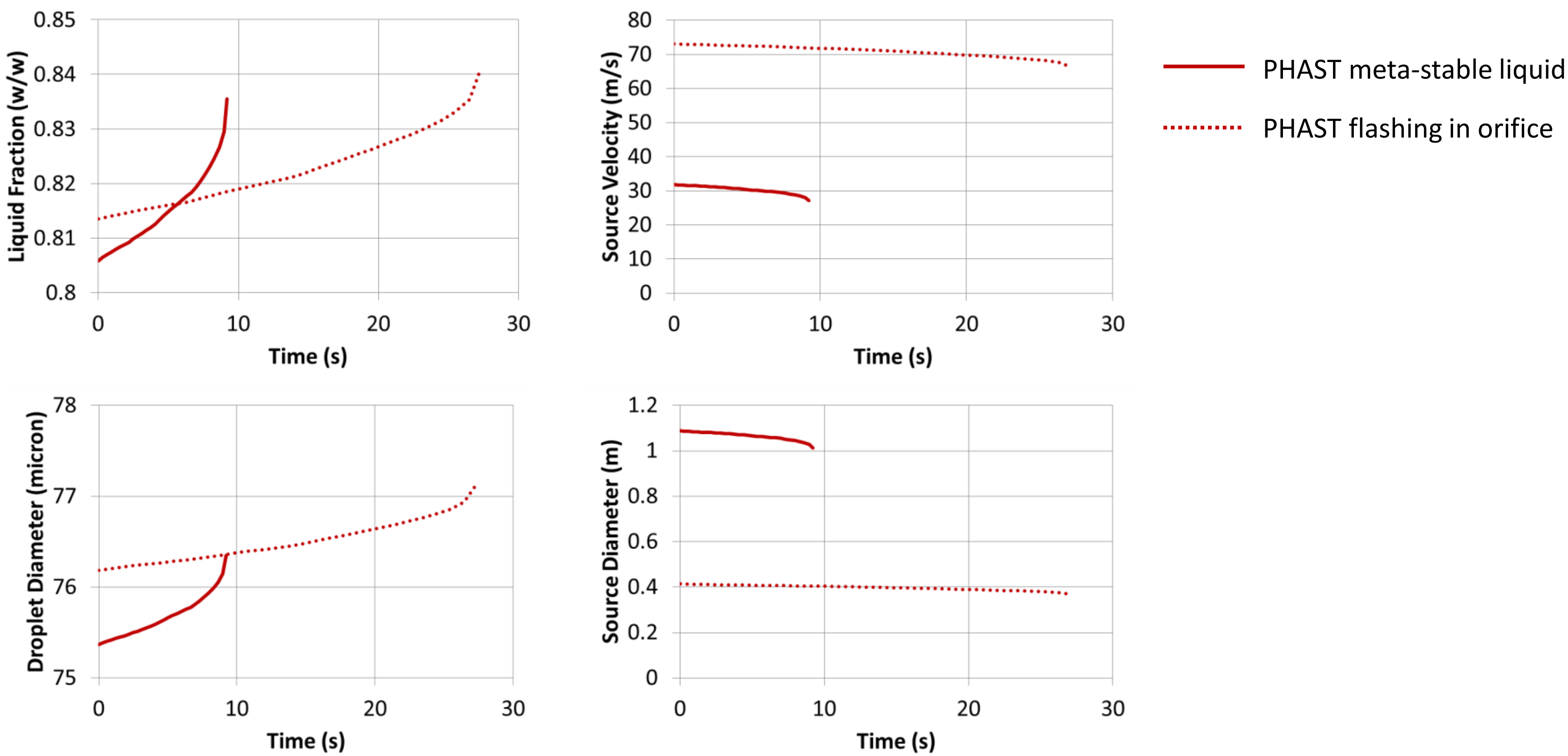
- Ronald Meris (DTRA)
- Steven Hanna (Hanna Consultants)
- Joseph Chang (RAND)
- Thomas Spicer (Arkansas University)
- Richard Babarsky (US Army)
- Nathan Platt, Jeffry Urban and Kevin Luong (IDA)
- Jeffrey Weil (NCAR)
- John Boyd (ARA)
- Steven Herring (DSTL)
- Andy Byrnes (UVU)

Additional Slides…

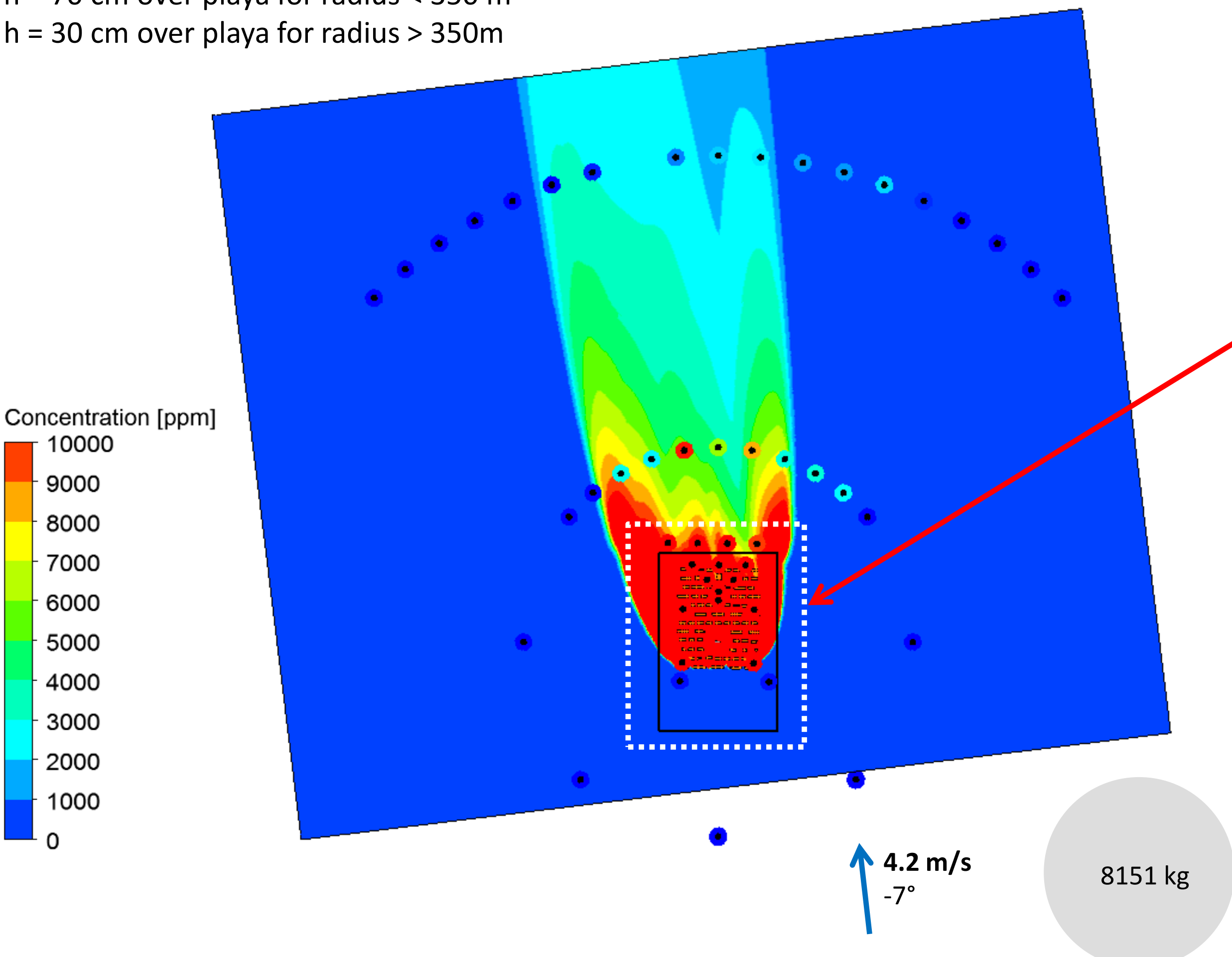
1.) Discharge Conditions

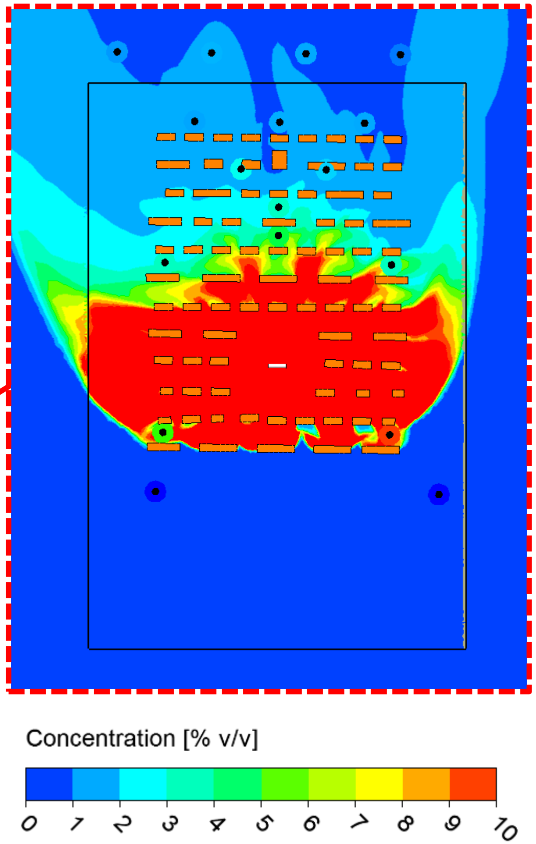
PHAST post-expansion jet source conditions used as inputs for CFD model in Trial 1



Jack Rabbit II 2015: Trial 2

Maximum concentration contours at heights:
h = 10 cm over pad and gravel
h = 70 cm over playa for radius < 350 m
h = 30 cm over playa for radius > 350m

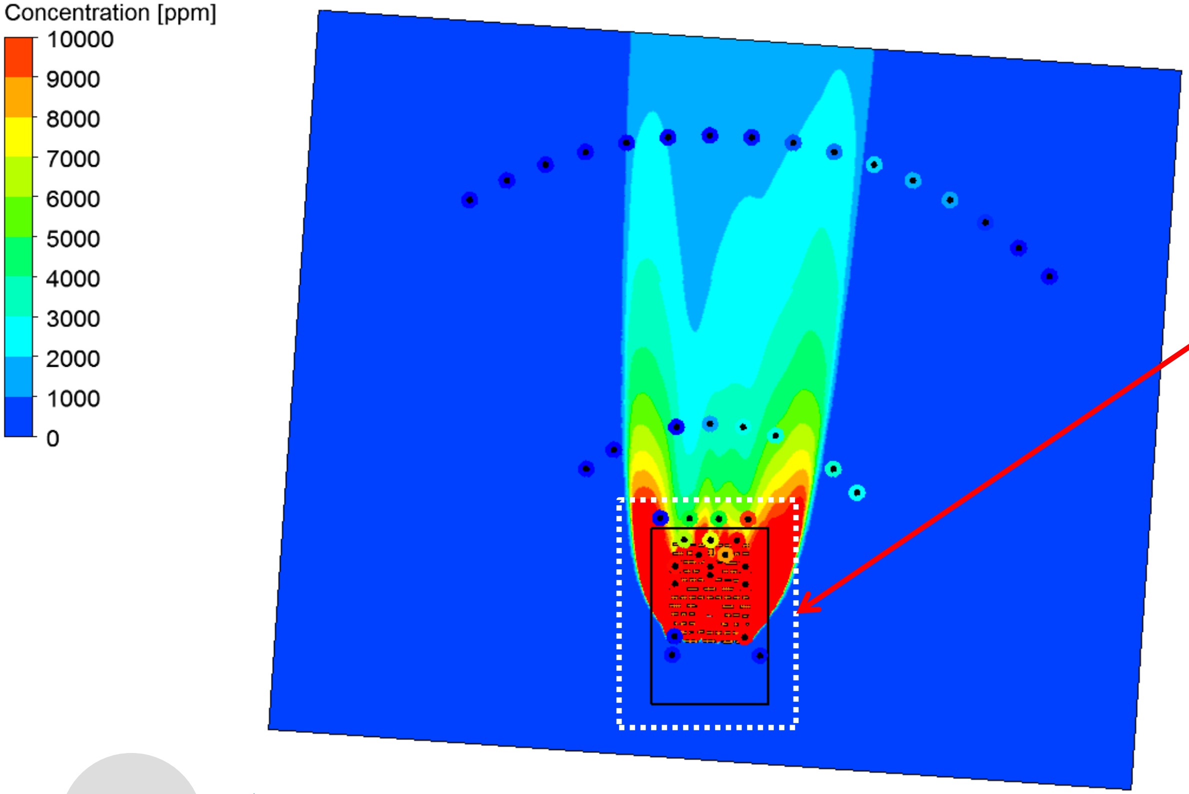


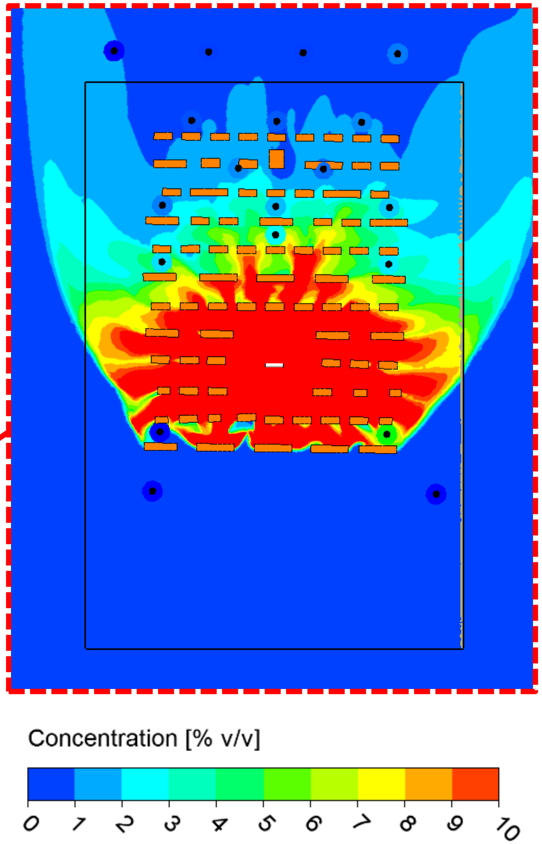


Higher concentration levels to help discern near-field behavior

Jack Rabbit II 2015: Trial 3

Maximum concentration contours at heights:
h = 10 cm over pad and gravel
h = 70 cm over playa for radius < 350 m
h = 30 cm over playa for radius > 350m





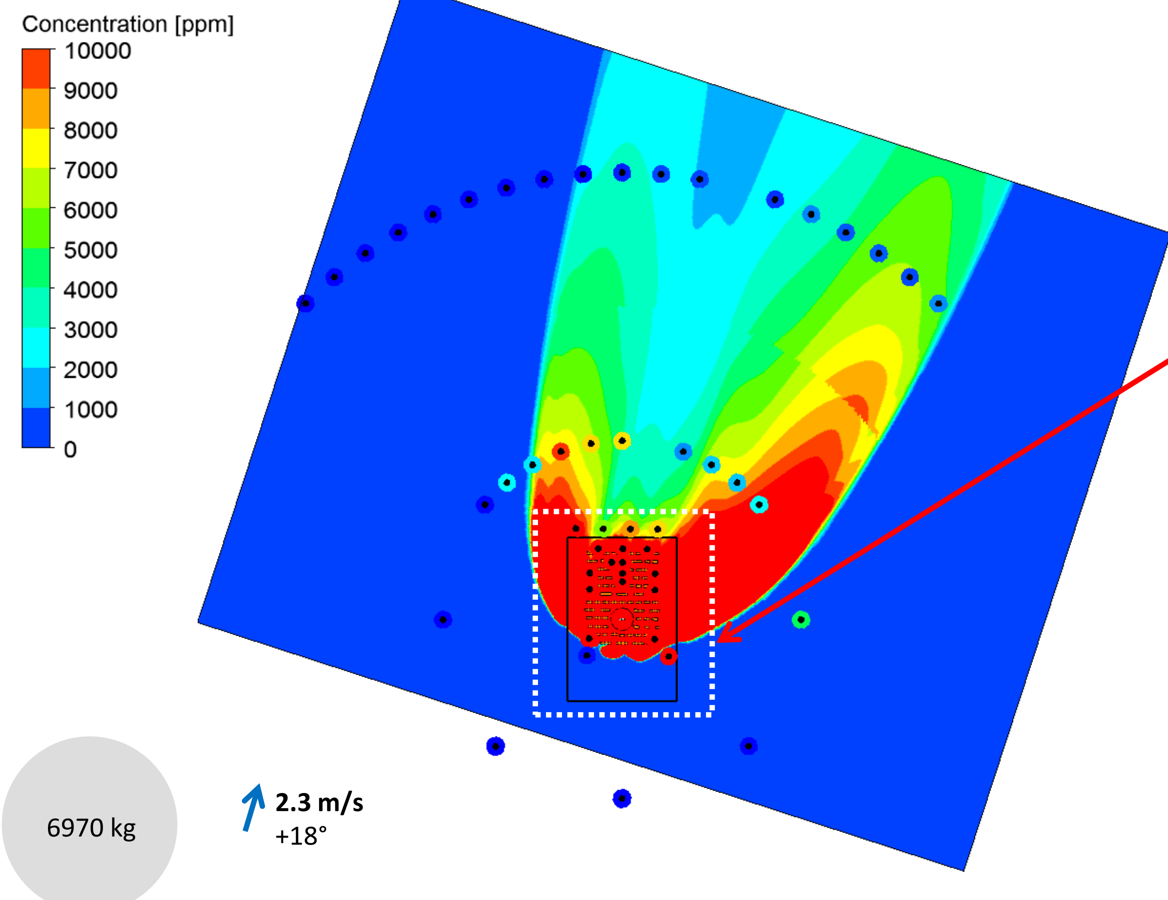
Higher concentration levels to help discern near-field behavior

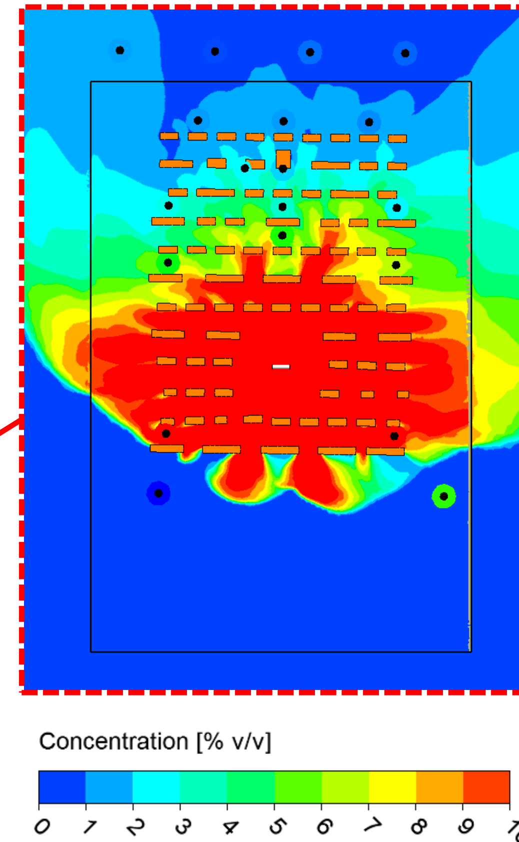
4512 kg

3.9 m/s
+4°

Jack Rabbit II 2015: Trial 4

Maximum concentration contours at heights:
h = 10 cm over pad and gravel
h = 70 cm over playa for radius < 350 m
h = 30 cm over playa for radius > 350m

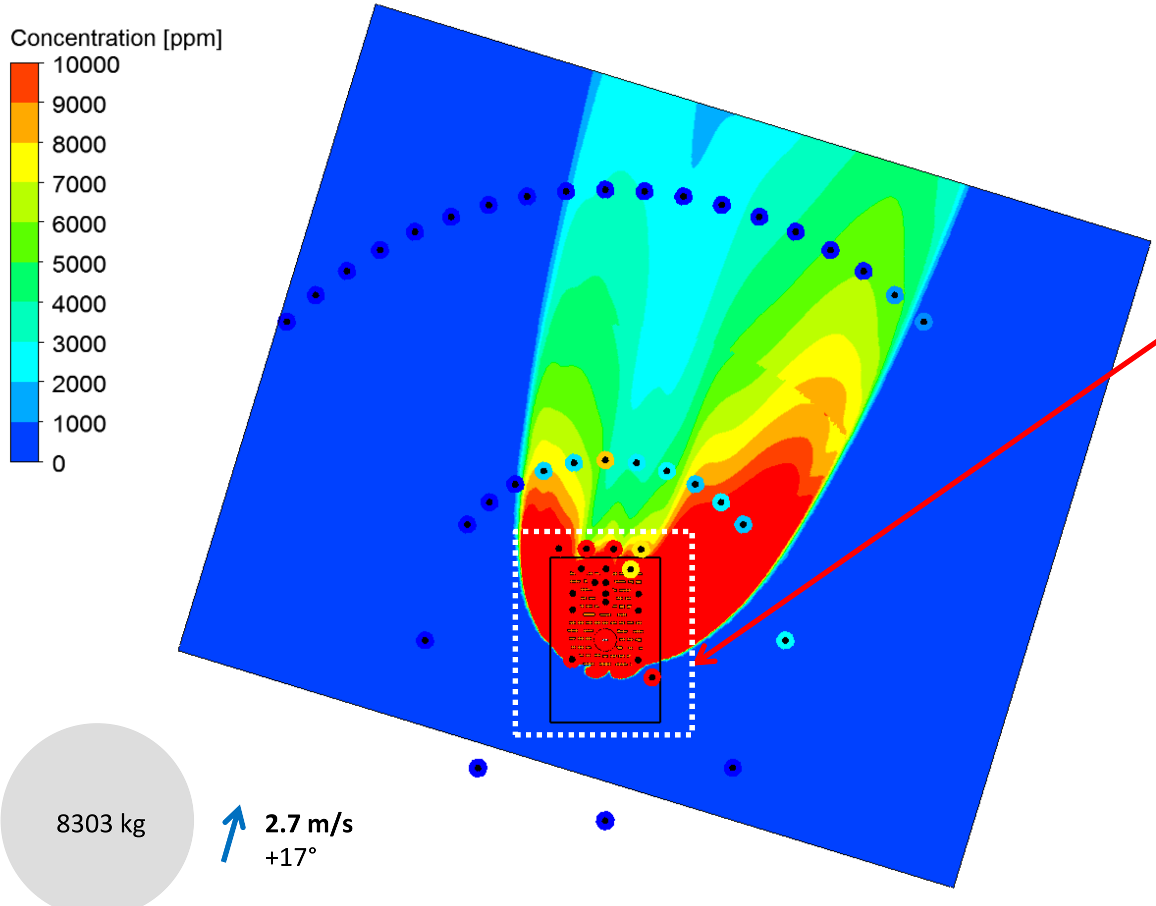


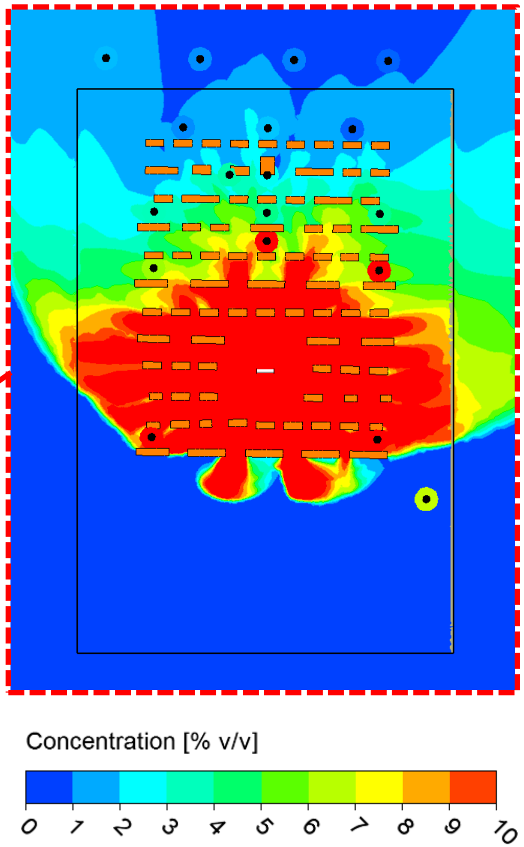


Higher concentration levels to help discern near-field behavior

Jack Rabbit II 2015: Trial 5

Maximum concentration contours at heights:
h = 10 cm over pad and gravel
h = 70 cm over playa for radius < 350 m
h = 30 cm over playa for radius > 350m





Higher concentration levels to help discern near-field behavior

Max Arc-Wise Concentrations