Dispersion model predictions of the Jack Rabbit II chlorine release experiments

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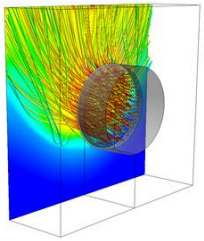
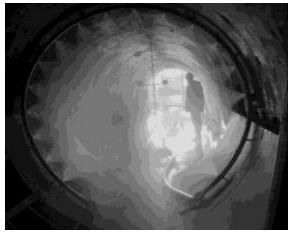
Outline

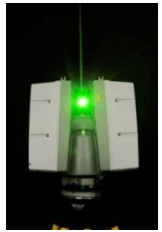
- Brief introduction to the Health and Safety Laboratory (HSL)
- Objectives
- Overview of models
  - DRIFT
  - PHAST
  - Computational Fluid Dynamics (CFD)
- Analysis of Jack Rabbit II data from 2015 trials
  - Comparison to Chlorine Institute Pamphlet 74 Guidance
- Model validation
- Conclusions and Future Directions

Brief Introduction to HSL

- Multi-disciplinary laboratory
  - Exposure control
  - Toxicology
  - Fire and process safety
  - Human factors etc.
- 80% work for government, 20% commercial
- Approx. 400 staff
- 550 acre test site
- Fire galleries and burn hall
- Impact track and drop tower
- Wind tunnel
- Thermal test chamber, etc.

Objectives

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 Models

1. **DRIFT** version 3.7.2
   - Used by HSE for land-use planning purposes in the UK
   - Validated against many field and wind-tunnel dispersion datasets
2. **PHAST** version 7.11
   - Comprehensive hazard analysis software, widely used by industry
   - Validated against many field and wind-tunnel dispersion datasets

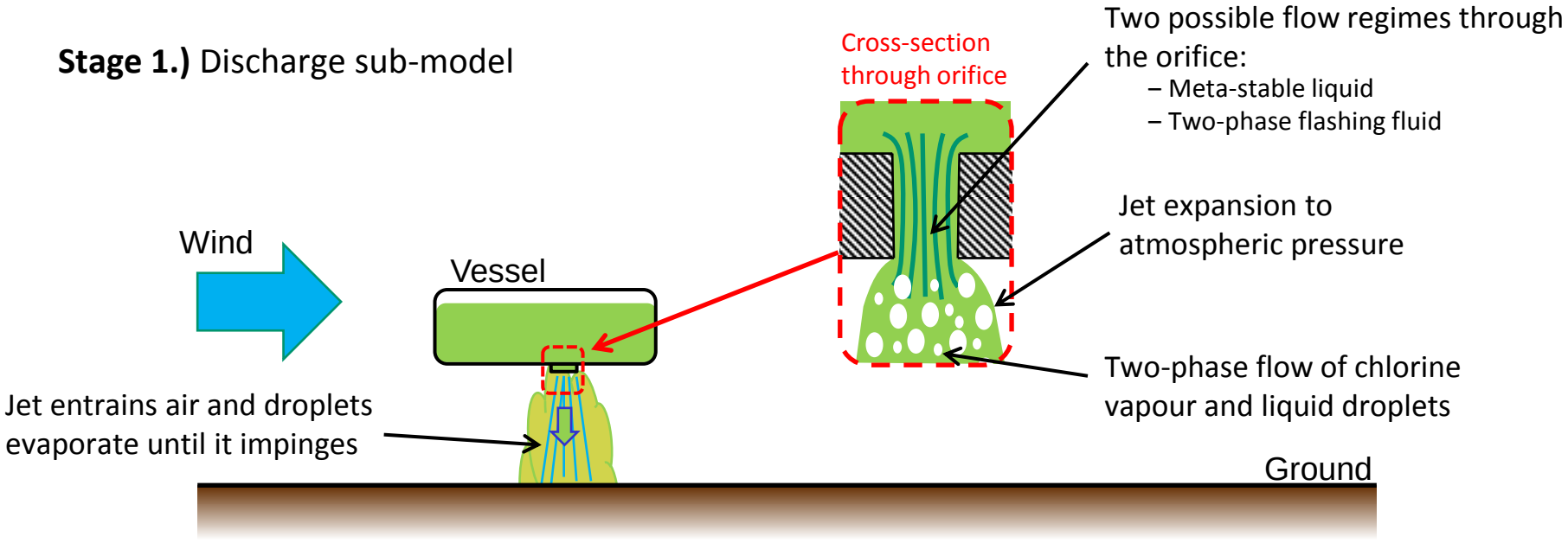
Integral-type dispersion models

Computer run-time: seconds

3. **CFX** version 17
   - General-purpose CFD software for fluid flow analysis, widely used by engineering consultancies
   - Previously validated by HSL for various two-phase jets and liquid sprays
   - Computer run time: hours to days on multiple CPUs

Overview of DRIFT and PHAST Models

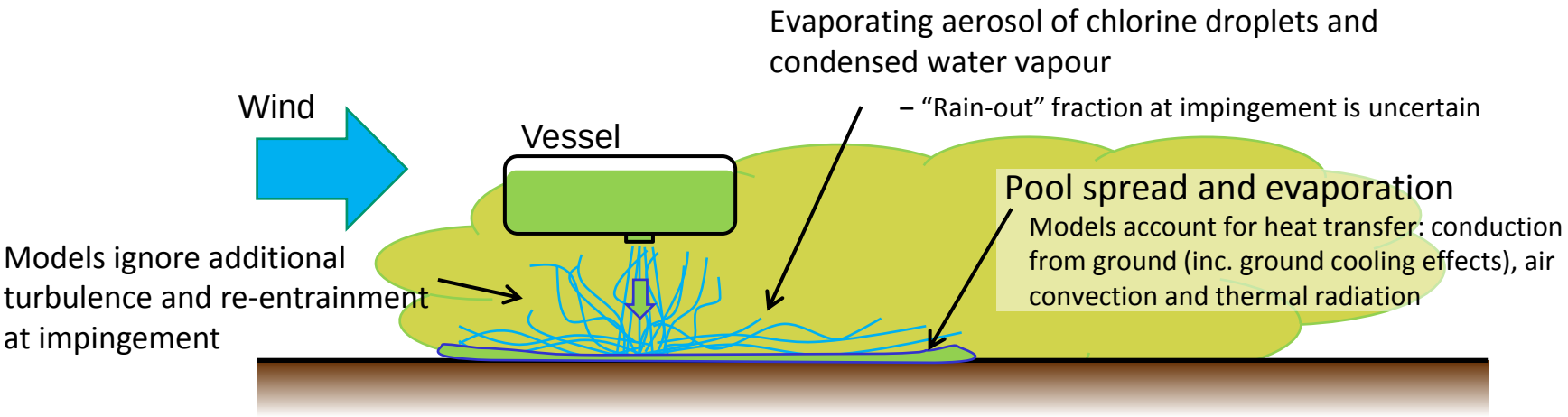
Stage 1.) Discharge sub-model



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

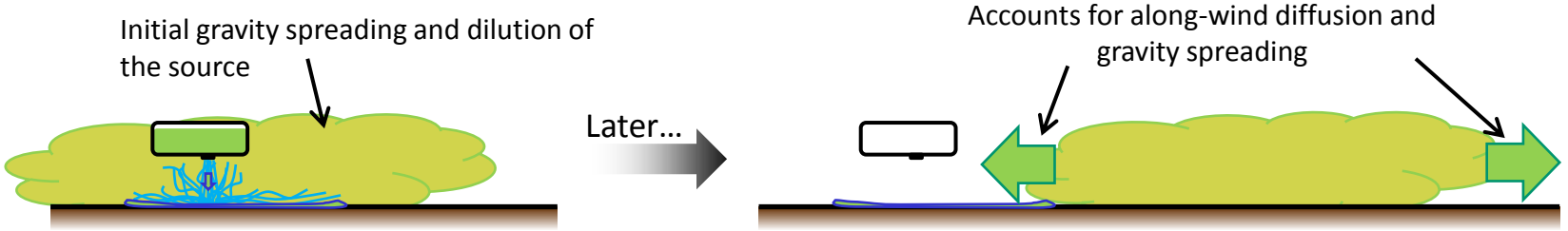


Model sensitivity tests performed to assess impact of liquid rain-out and pool formation

Overview of DRIFT and PHAST Models

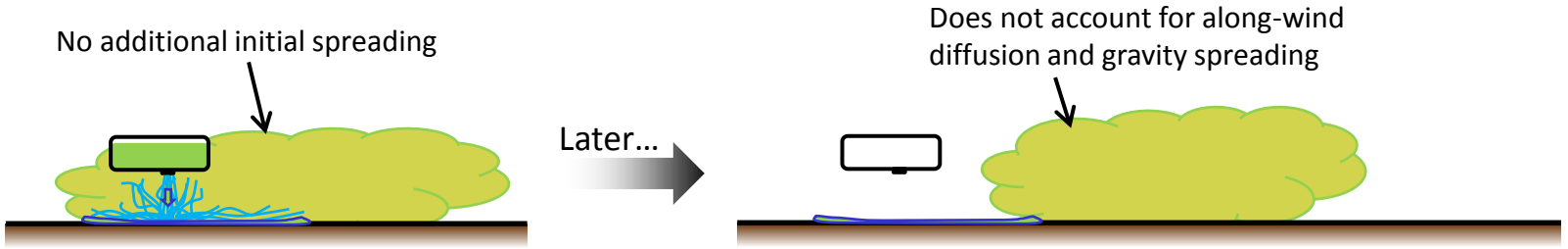
Stage 3.) Modelling dispersion of cloud

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

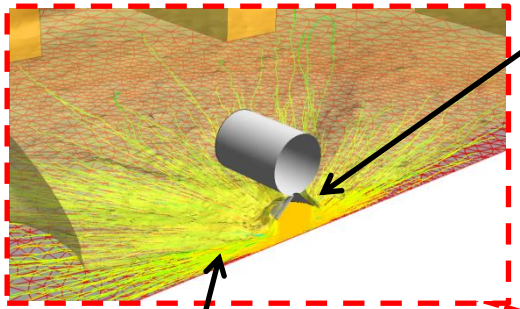
PHAST



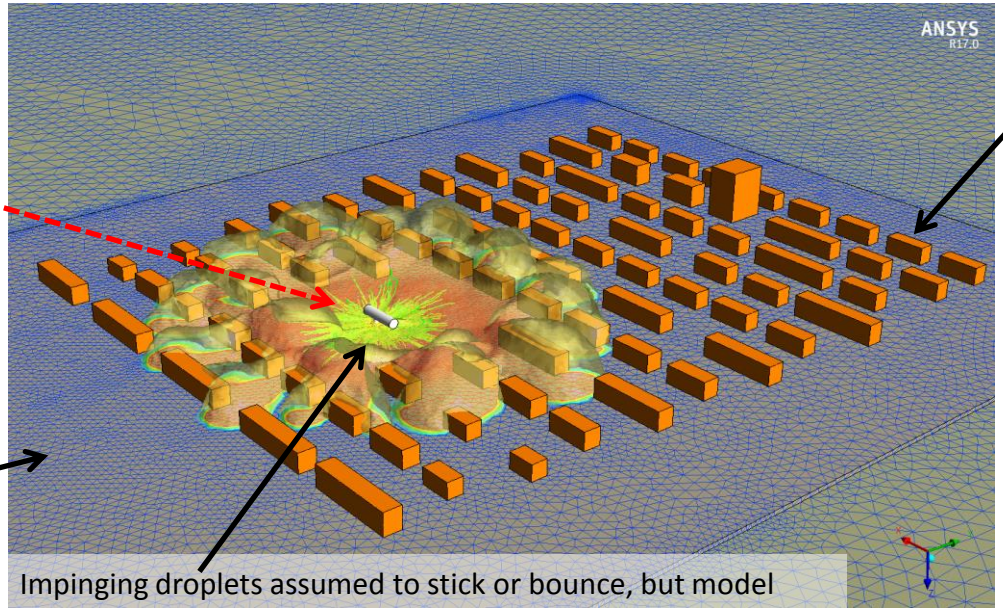
- PHAST can produce clouds that spread laterally more than along-wind, and over-predict concentrations in near-field
- Found to under-predict extent of cloud in stable conditions
- New PHAST version 8.0 (not used here, released in late 2017) accounts for along-wind diffusion and gravity spreading

CFD Model

Cross-section through source



Expanded jet of vapour and evaporating chlorine droplets (Lagrangian particles): source conditions taken from PHAST



Conex blocks resolved in model geometry
(whereas DRIFT/PHAST modelled mock urban array as uniform region of increased surface roughness)

Model accounts for additional turbulence and re-entrainment at impingement

Ground and all solid surfaces assumed to be smooth

SST turbulence model

Mesh: 1 – 2 million nodes

Impinging droplets assumed to stick or bounce, but model does not account for evaporating liquid pool

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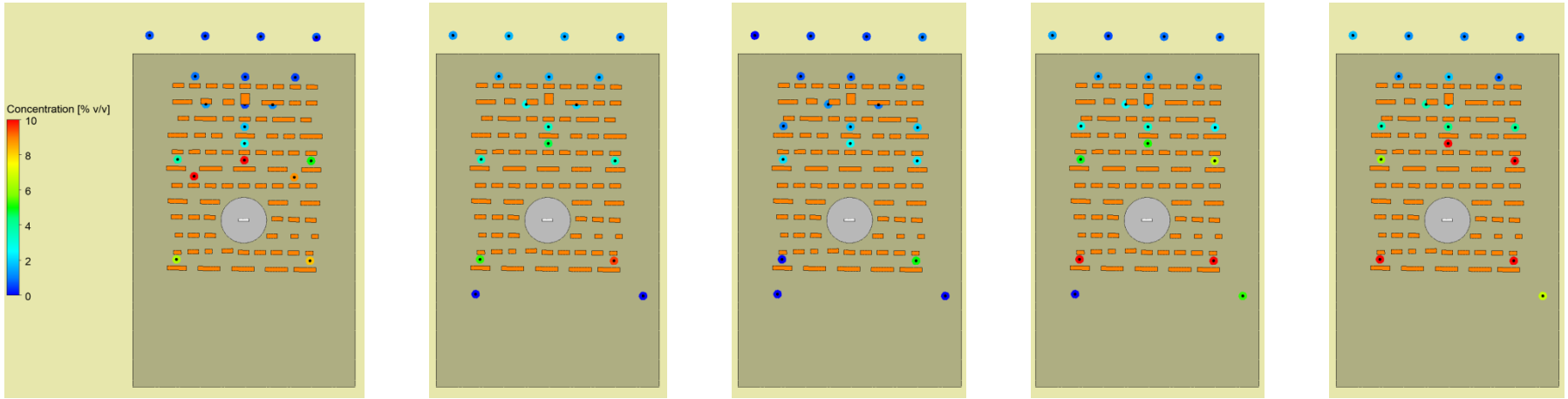
Jack Rabbit II Trials (2015)

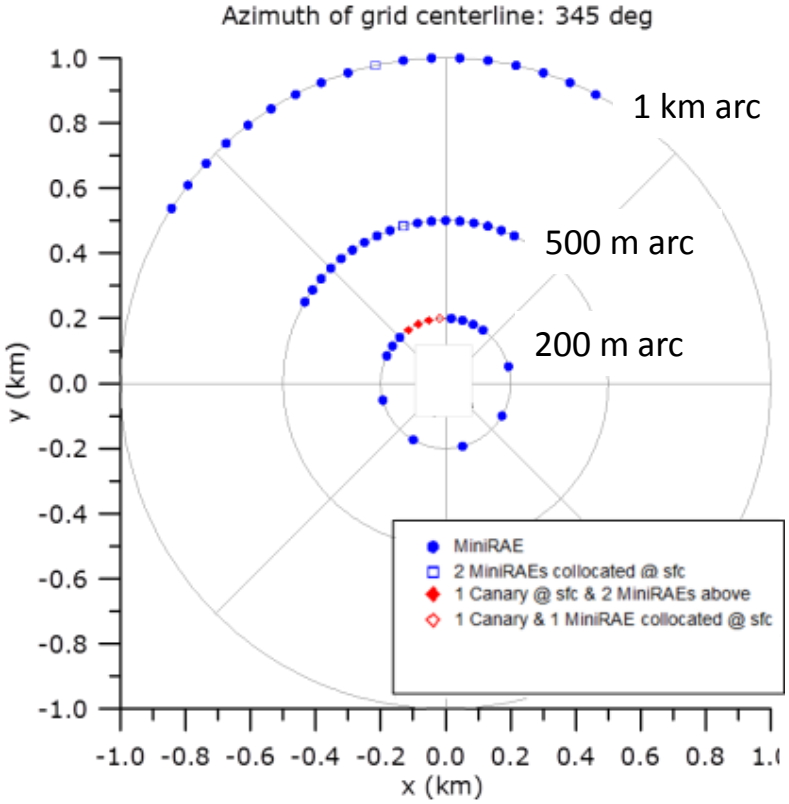
Trial	Chemical Amount (kg)	Initial Tank Pressure (barg)	Wind direction offset to urban array (deg)	Wind Speed (m/s)	Atmospheric Temperature (°C)	Relative Humidity (%)	Atmospheric Pressure (Pa)	Pasquill Stability Class
1	4509	6.50	-18	2.0	17.7	39.2	87,350	F
2	8151	6.06	-7	4.2	22.7	33.6	87,512	C → B
3	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 ?

Measured concentrations in urban array

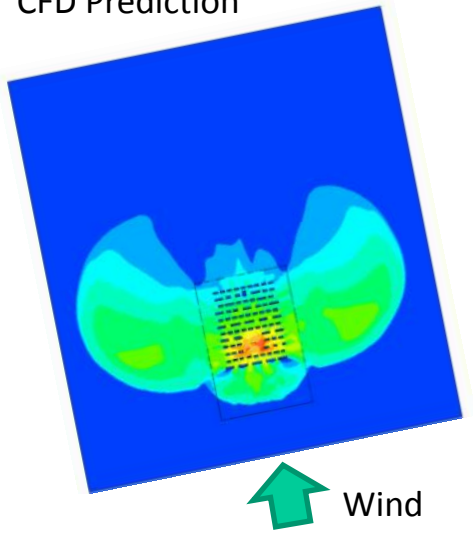


	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5
Wind vector	**2.0 m/s** -18°	**4.2 m/s** -7°	**3.9 m/s** +4°	**2.3 m/s** +18°	**2.7 m/s** +17°
Release size	4509 kg	8151 kg	4512 kg	6970 kg	8303 kg

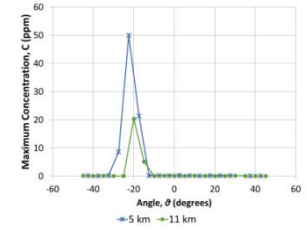
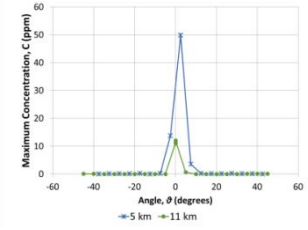
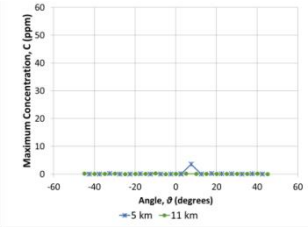
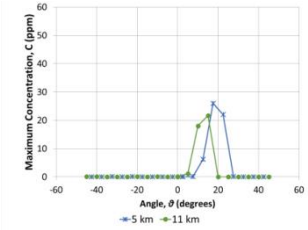
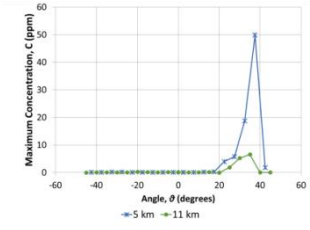
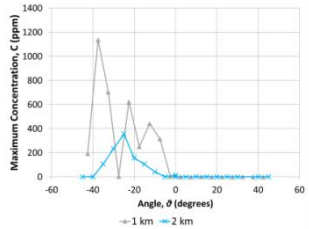
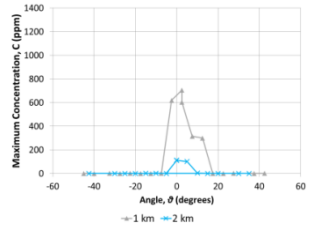
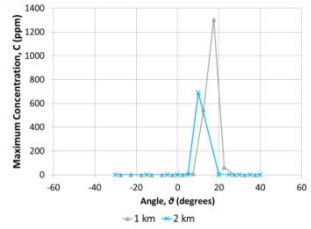
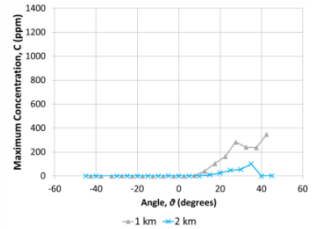
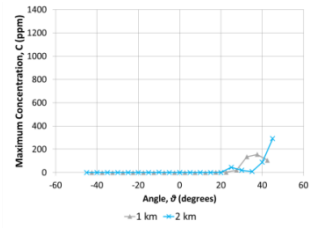
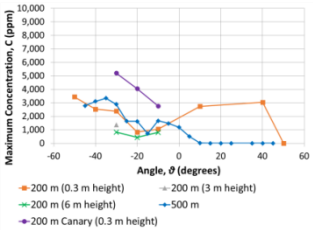
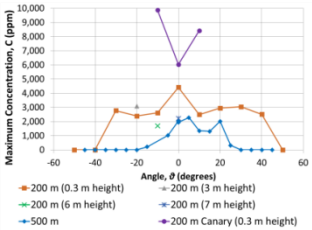
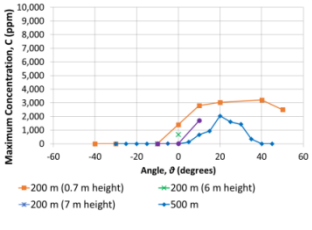
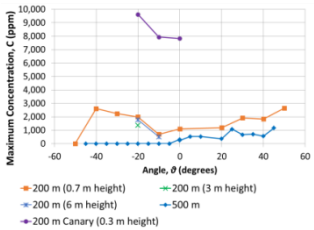
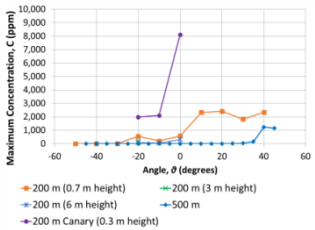
Measured concentrations in near field



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
				
				
				
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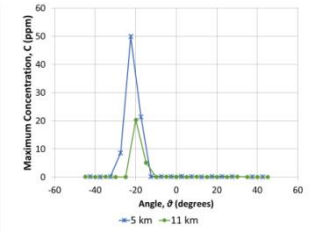
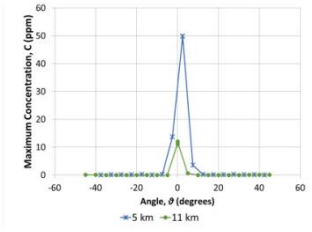
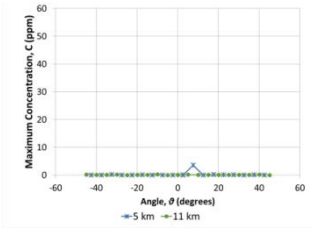
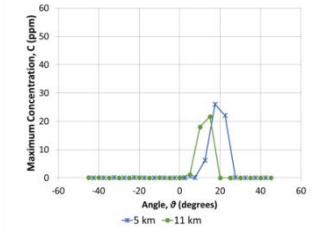
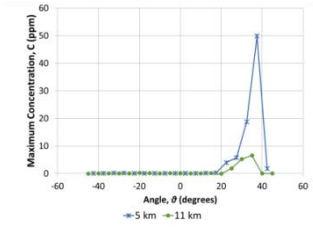
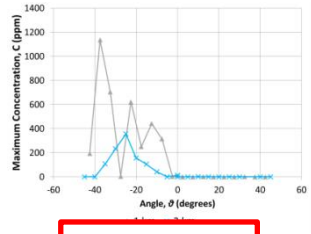
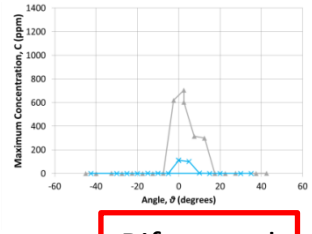
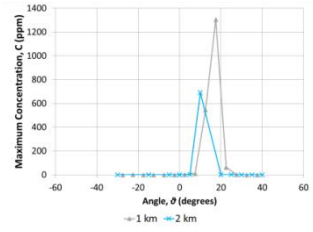
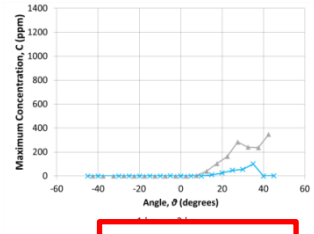
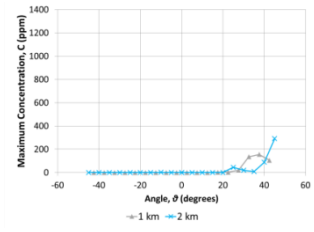
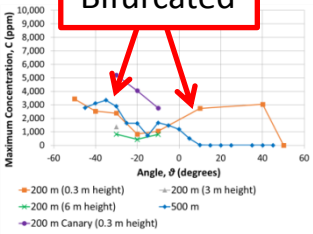
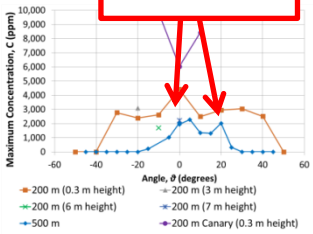
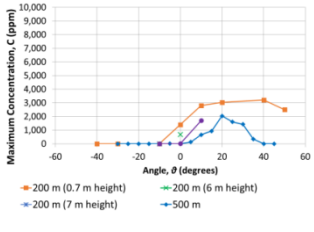
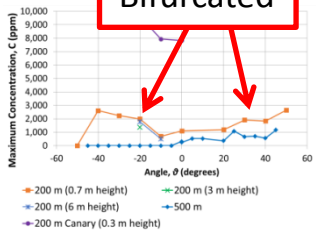
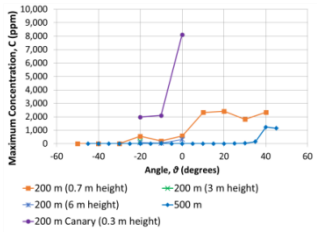
				
				
Bifurcated 	Bifurcated 		Bifurcated 	
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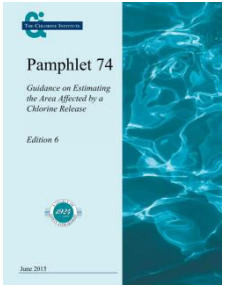
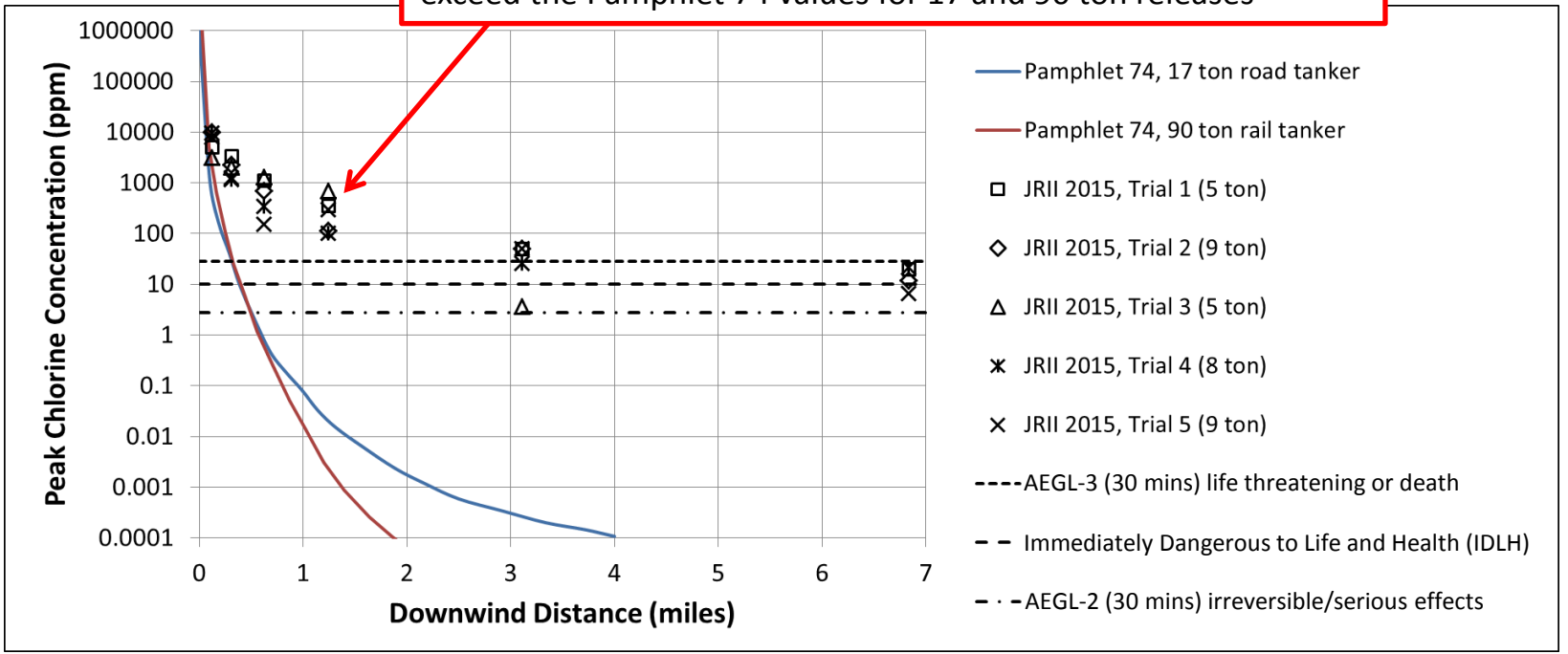
Chlorine Institute Pamphlet 74 (Edition 6)



Measured concentrations from JRII 2015 for 5 to 9 ton releases exceed the Pamphlet 74 values for 17 and 90 ton releases



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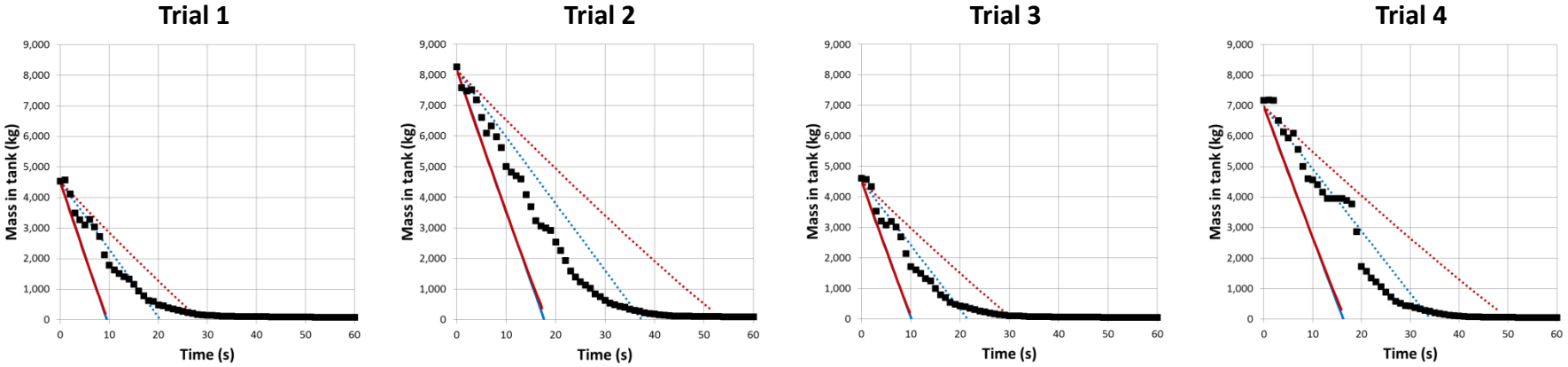
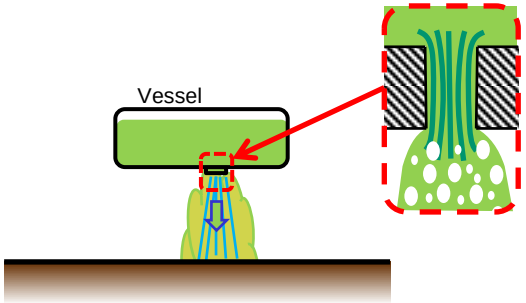
Model Validation: JRII 2015 Discharge





DRIFT meta-stable liquid

DRIFT flashing in orifice

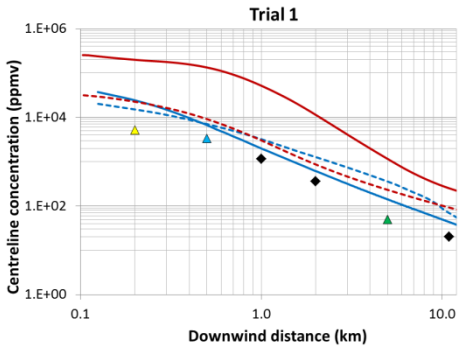
Results from HSE's STREAM outflow model

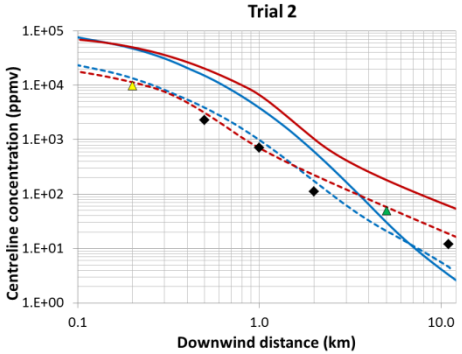
PHAST meta-stable liquid

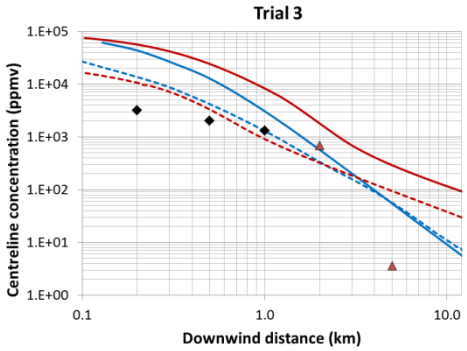
PHAST flashing in orifice

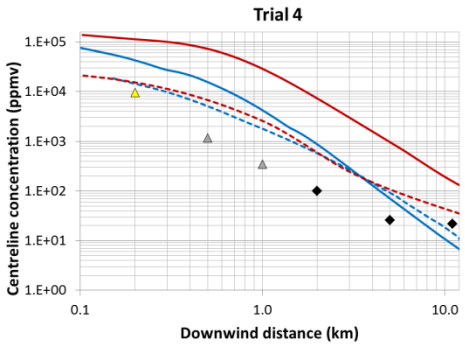
Measurements from load cell data

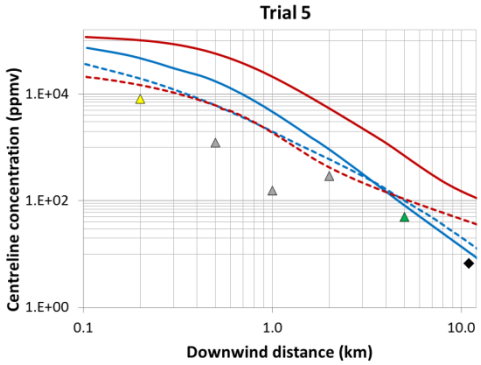
Model Validation: JRII 2015 Concentration









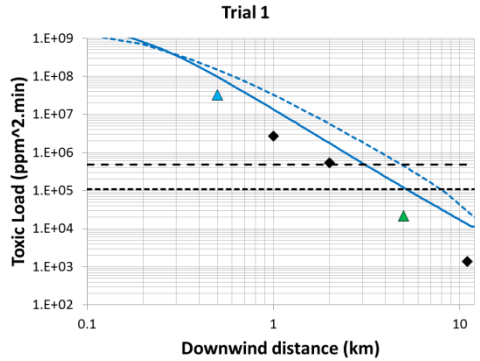


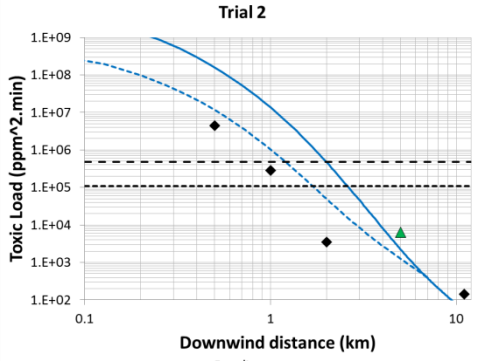
DRIFT without droplet rainout
DRIFT with droplet rainout
PHAST without droplet rainout
PHAST with droplet rainout

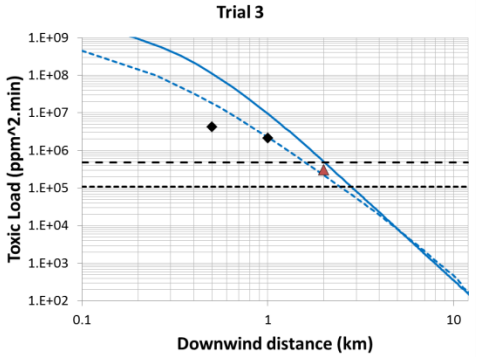
Both PHAST and DRIFT models assumed meta-stable liquid discharge from the vessel

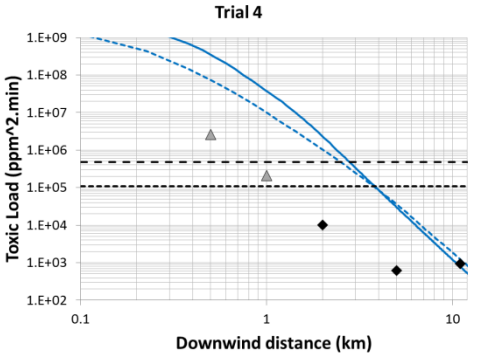
- Measured maximum arc-wise concentration
- Canary sensor data: only 3 sensors, may have missed plume maximum
- MiniRAE sensor saturated
- ToxiRAE sensor saturated
- Narrow plume passed between sensors: plume maximum may have been missed
- Plume passed beyond edge of arc: plume maximum may have been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

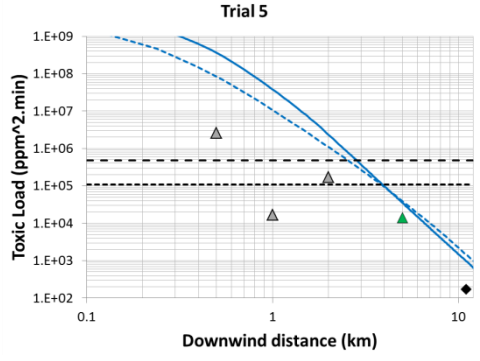
Model Validation: JRII 2015 Toxic Load











DRIFT without droplet rainout
DRIFT with droplet rainout
Specified Level of Toxicity (SLOT)
Significant Likelihood of Death (SLOD)

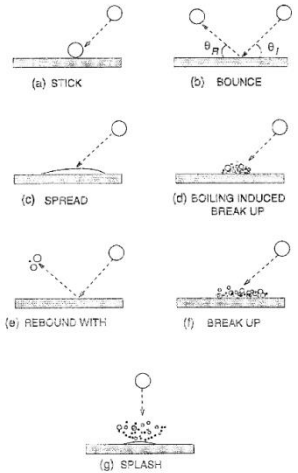
$$Toxic\ Load = \int C^n dt$$

Results presented here using UK HSE value n = 2.0
(USA value is n = 2.75)

- Measured maximum arc-wise concentration
- Canary sensor data: only 3 sensors, may have missed plume maximum
- MiniRAE sensor saturated
- 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

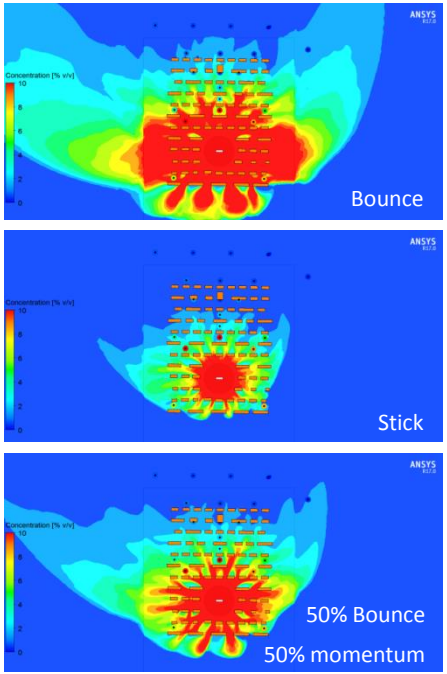
CFD Analysis of source conditions

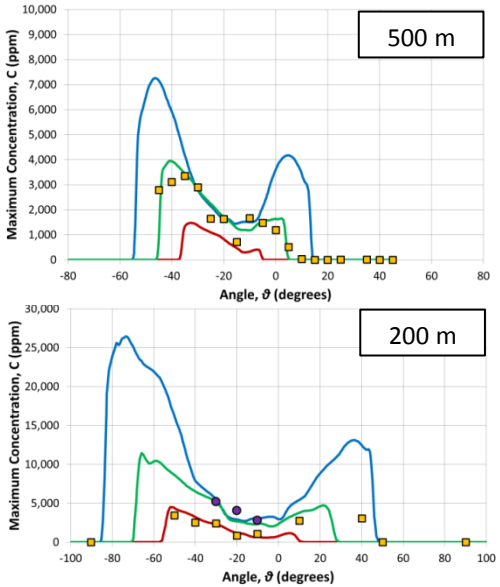
Choice of droplet impingement conditions has a strong effect



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

Maximum concentrations at height of sensors in Trial 1

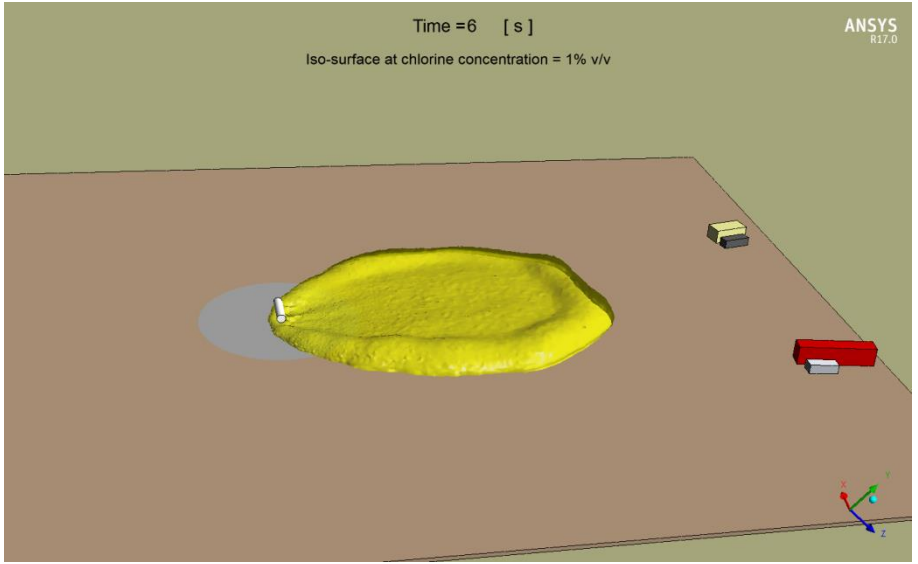




- Droplets bounce elastically
- Droplets stick on impact
- 50% of droplets bounce with 50% of momentum
- Measured maximum concentration (MiniRAE)
- Measured maximum concentration (Canary)

CFD Simulation of JRII 2016 Trial 7

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



Play Videos

Outline

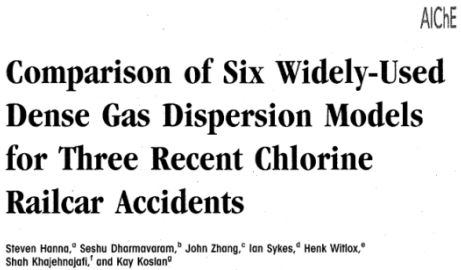
- Brief introduction to the Health and Safety Laboratory (HSL)
- Objectives
- Overview of models
  - DRIFT
  - PHAST
  - Computational Fluid Dynamics (CFD)
- Analysis of Jack Rabbit II data from 2015 trials
  - Comparison to Chlorine Institute Pamphlet 74 Guidance
- Model validation
- Conclusions and Future Directions

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 used to process JRII 2015 data has been investigated
  - No significant influence on results
- Wind speed, wind direction and atmospheric stability conditions in JRII 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 Khajehnajafi,[f] and Kay Koslan[g]

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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

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Data from the Jack Rabbit II test program is available on request (email: Jack.Rabbit@st.dhs.gov)