Comparisons of the predictions of the gas dispersion model DRIFT against data for hydrogen, ammonia and carbon dioxide

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DRIFT gas dispersion model

- Integral model
  - Gaseous and two-phase dispersion in the atmosphere
  - Based upon Webber et al (1992)
  - Extended by Tickle and Carlisle (2008) to include
    - Momentum jets
    - Buoyant gas dispersion
    - Longitudinal dispersion for finite-duration and time-varying releases
- Decarbonisation technologies
  - Increased focus on
    - Hydrogen
    - Ammonia
    - Carbon dioxide

Model fitness for purpose

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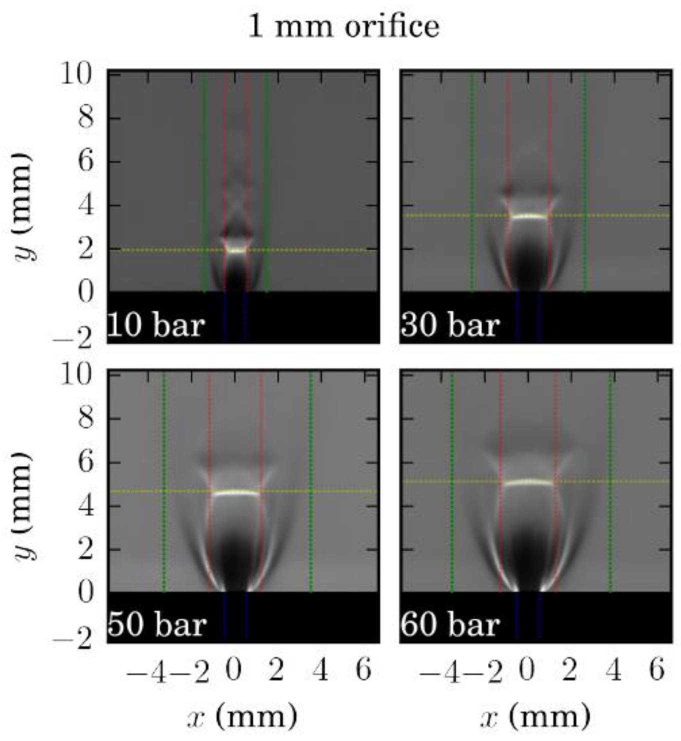
- Model Evaluation Guidelines
  - Scientific Model Evaluation
  - Model Verification
  - Model Validation
- New validation of DRIFT for
  - Hydrogen - molecular weight and high pressure
  - Ammonia – including ammonia aerosol composition and interactions with water
  - Carbon Dioxide – including solid phase (dry ice) and sublimation

Hydrogen jet data

- Papanikolaou and Baraldi (2011)
  - Hydrogen gas
  - 1 mm nozzle
  - 98.1 bara
  - Horizontally directed
  - Centreline concentration and axial velocity measurements
- DRIFT
  - Pseudo-source model of Birch et al (1987)
  - Validated for methane jets up to ~70 bar



Hecht, Li and Ekoto (2015)
Sandia National Labs, SAND2015-3211C

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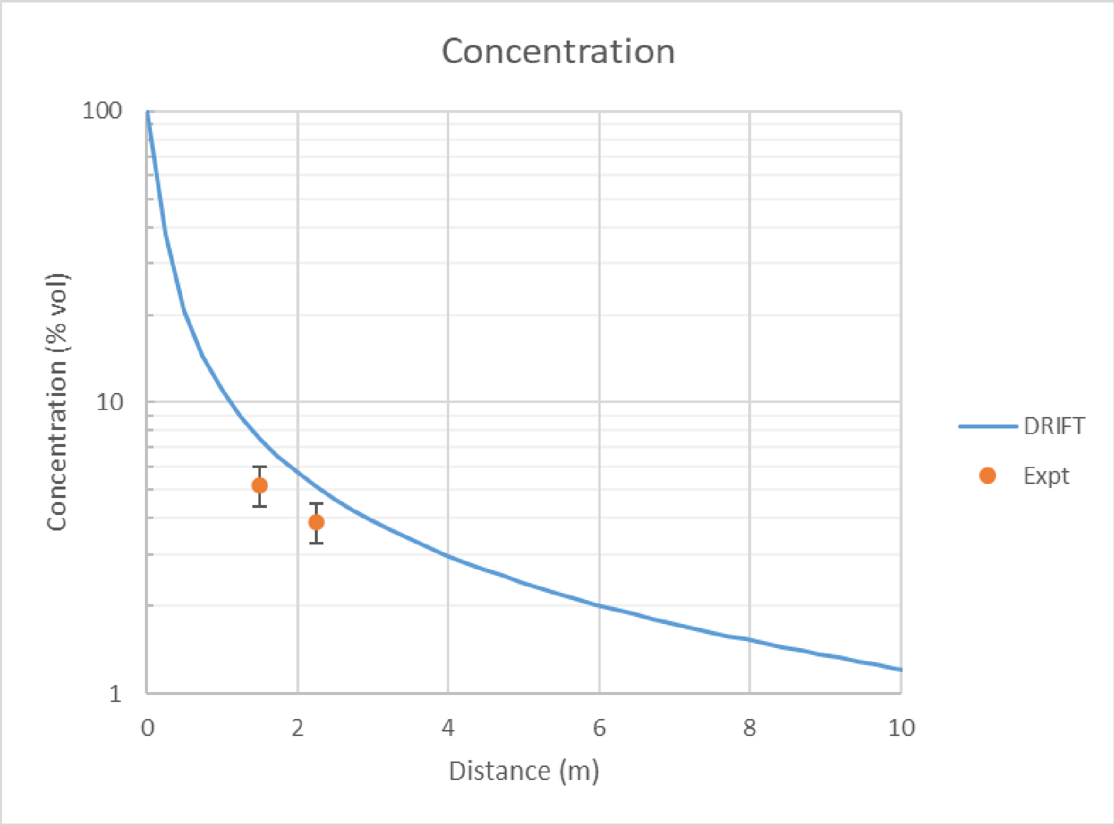
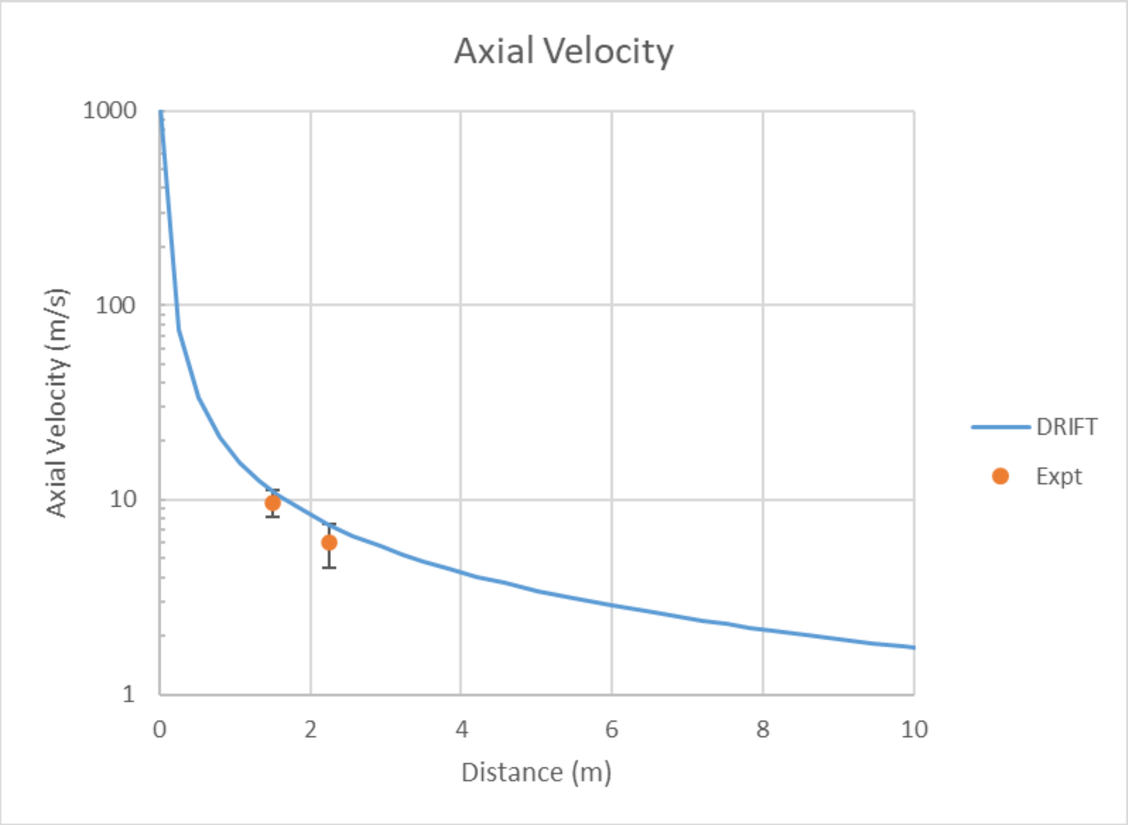
Hydrogen jet predictions





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Hydrogen jet prediction findings

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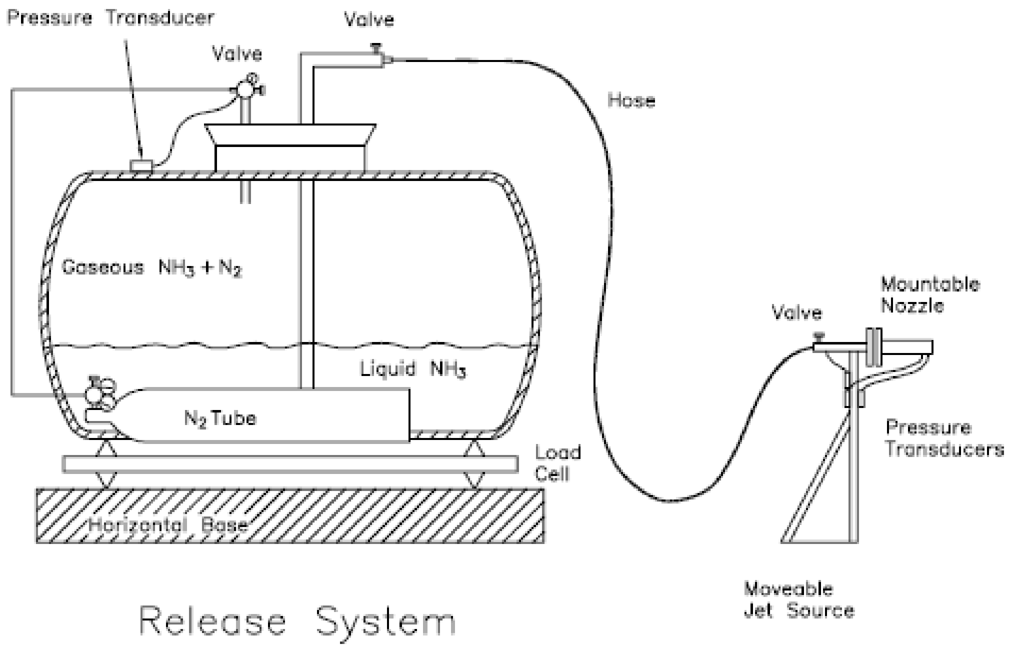
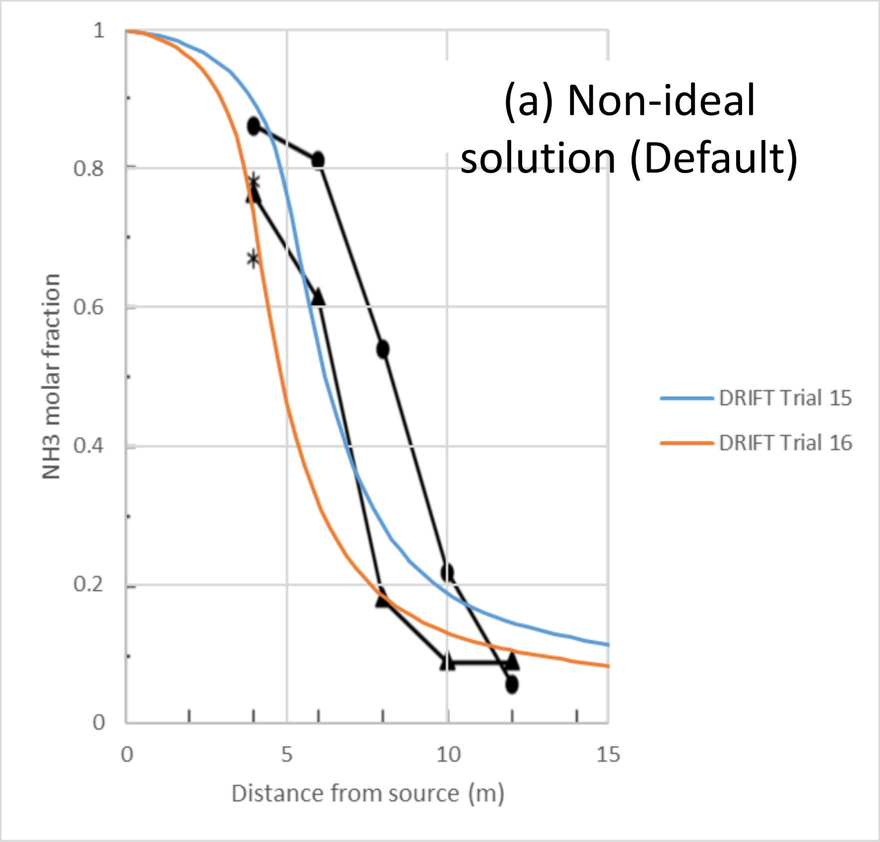
- Velocity prediction within +1 standard deviation of measurements
- Concentration prediction within +50% of measurements
- No tuning of model to these data
- Possible scope for improving predictions in this case by allowing for different spreading rates of scalar (mass, species) and vector quantities (momentum) in jet. Not done – avoid specific tuning to this data.
- Acceptable overall agreement given the high pressure of the release and the low molecular weight

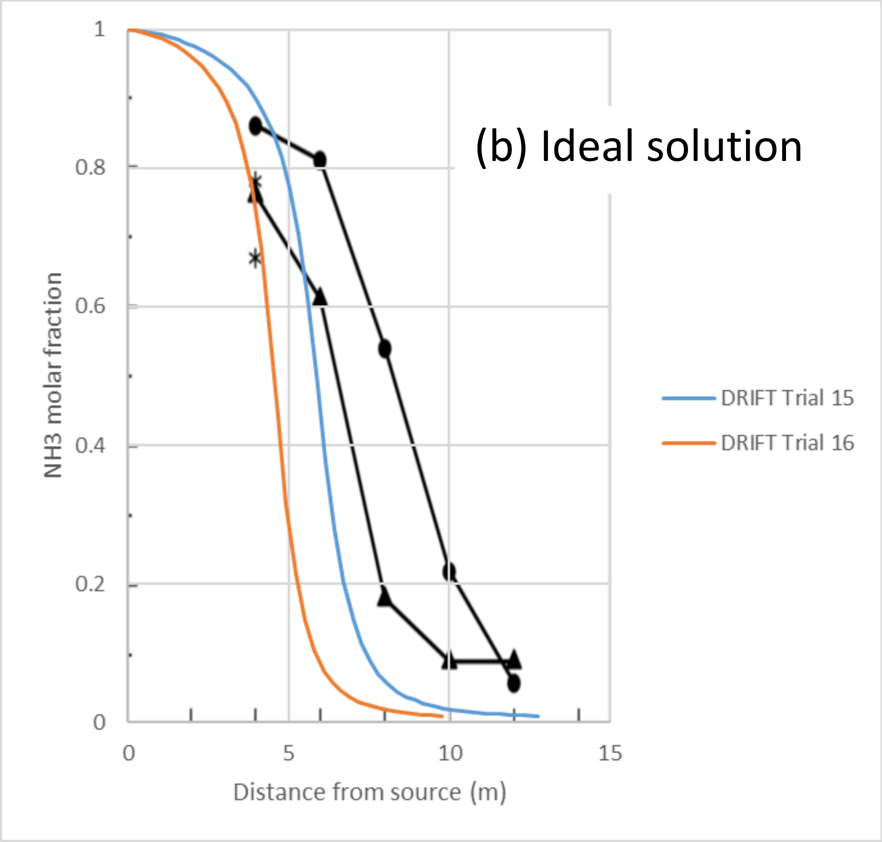
Ammonia field trials

- FLADIS ammonia field trials
  - Superheated anhydrous liquid ammonia
  - Dense jet to passive behaviour
  - Nielsen and Ott (1996), Nielsen et at. (1997)
  - Measurements
    - Aerosol composition at two distances (2 trials)
    - Centreline concentration - moving frame analysis (14 trials)



Ammonia aerosol composition predictions





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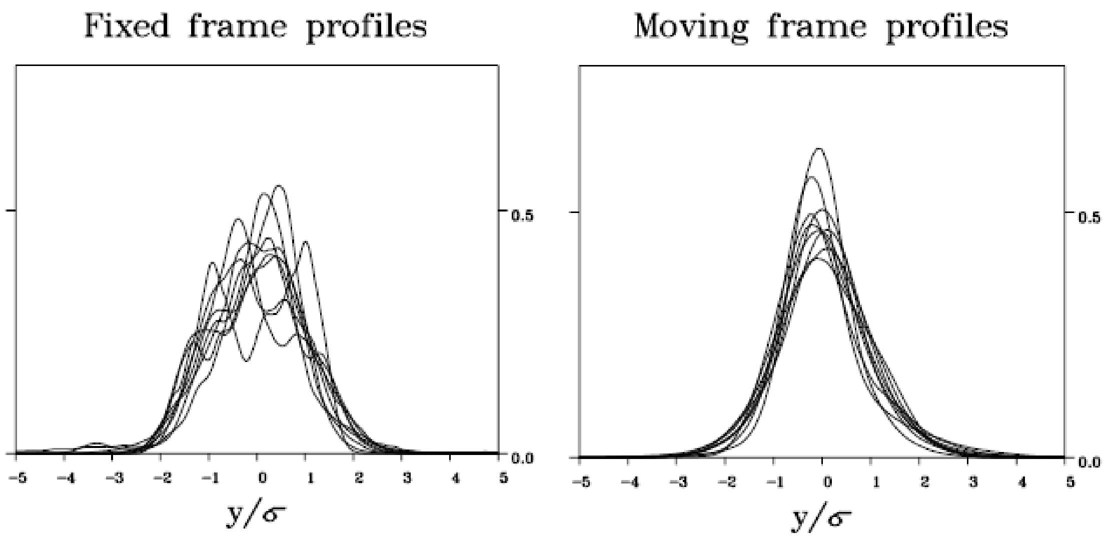
Moving frame analysis

- Subtract lateral plume meander:

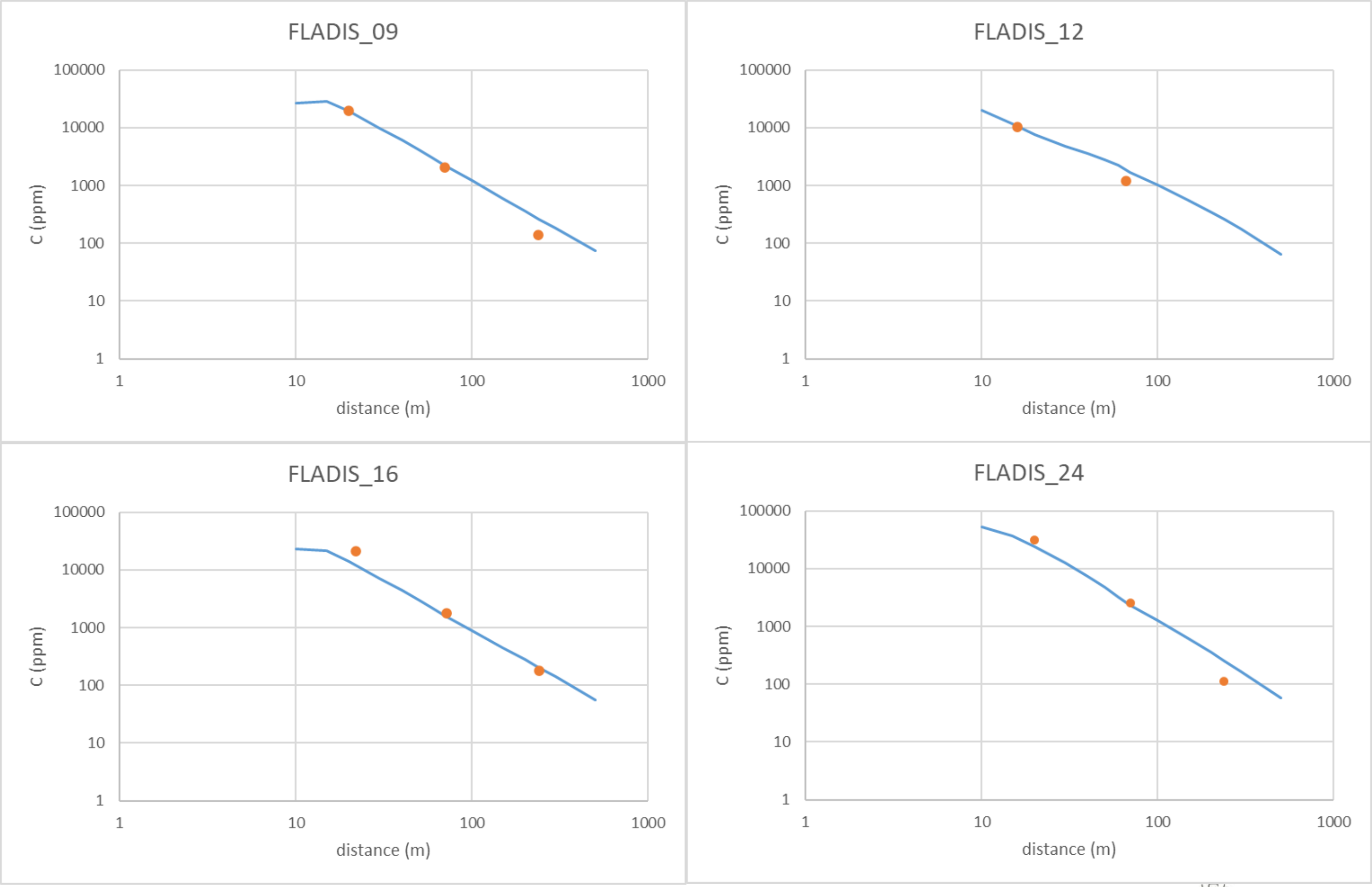
$$\bar{C}_m(y) \equiv \frac{1}{T}\int_0^T dt\, C(y + y_c(t), t)$$

$$y_c(t) = \int_{-\infty}^{\infty} dy\, y\, C(y, t)$$



Ott and Ejsing Jørgensen (2002): URAHFREP Lidar

Centreline concentration predictions(ammonia)



Centreline concentration (ammonia) statistical performance

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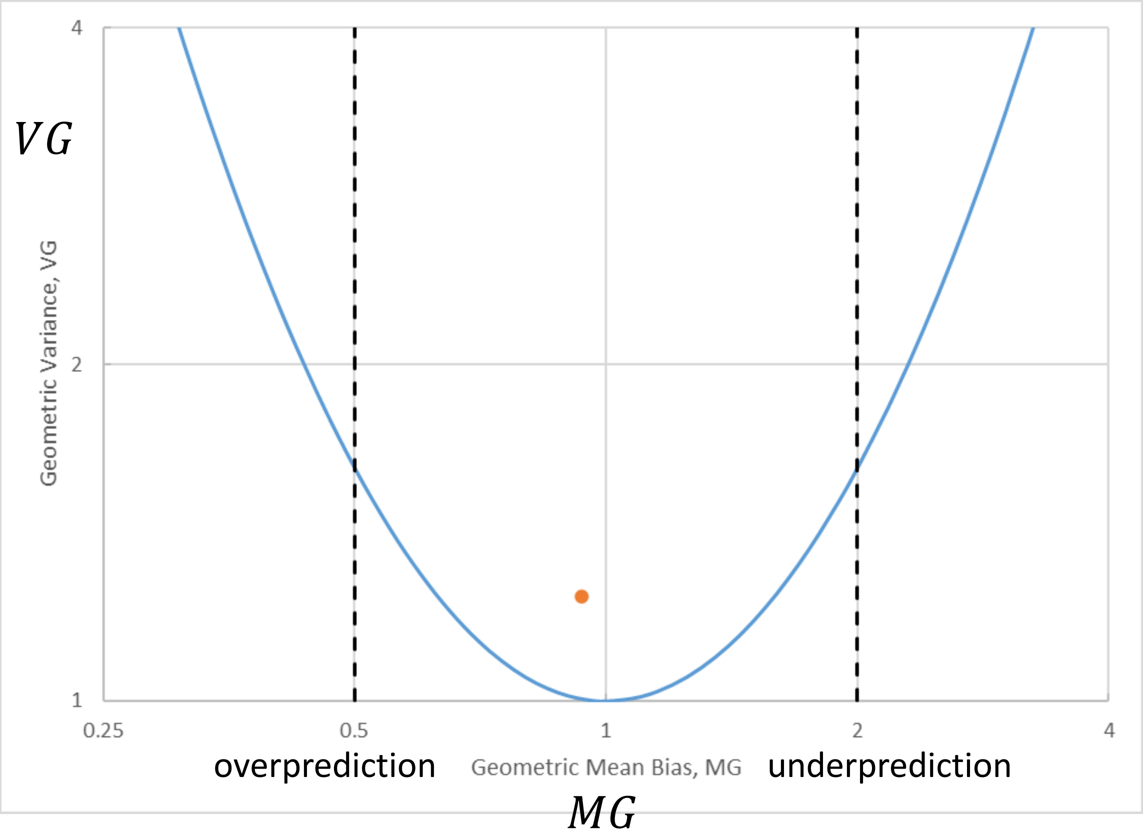
- Geometric Variance

$$VG = exp\left\langle\left[\log_e\left(\frac{C_m}{C_p}\right)\right]^2\right\rangle$$

- Geometric Mean Bias

$$MG = exp\left\langle\log_e\left(\frac{C_m}{C_p}\right)\right\rangle$$



Ammonia prediction findings

- Centreline concentrations
  - Short time-averaging gives good agreement with moving frame results
  - VG and MG well within the acceptable range typically used in model evaluation of dense gas dispersion models
- Non-ideal ammonia-water solution model (default in DRIFT)
  - Best agreement for the aerosol composition in near field – greater persistence of aerosol
  - Negligible impact on the predicted concentrations at greater distances in the FLADIS trials

Carbon dioxide

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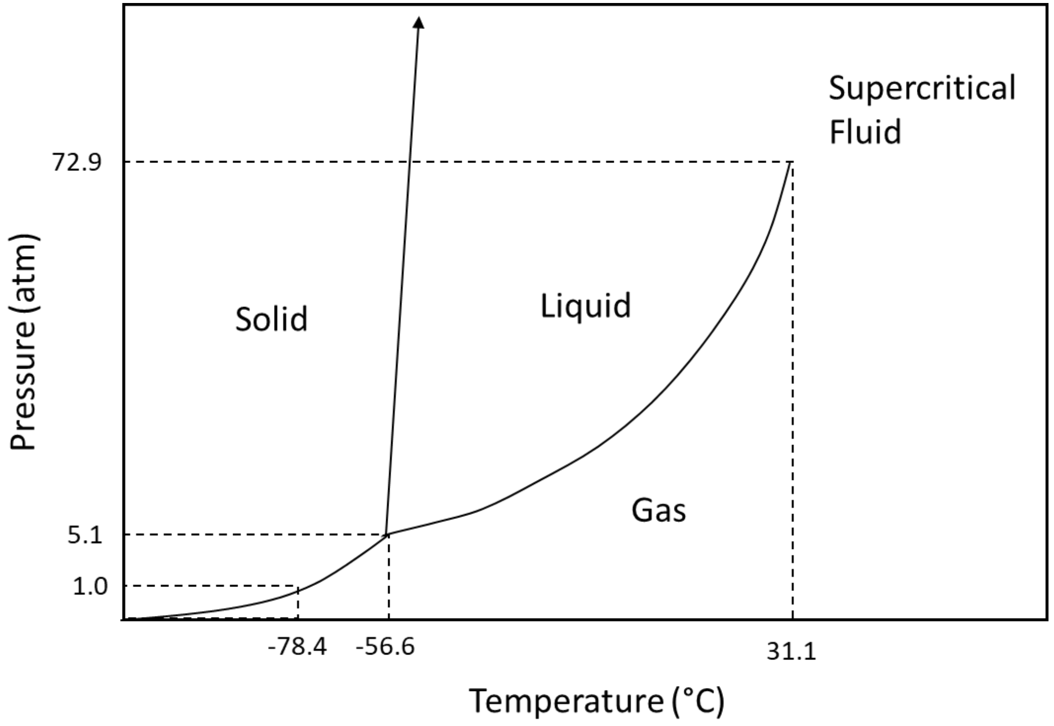
- Pressure liquefied storage/ transmission of CO_2
- Release
  - Two-phase jet of solid (dry-ice) and vapour at atmospheric pressure
- DRIFT thermodynamic model
  - Extended to include solid CO_2 aerosol following Witlox, Harper and Oke (2009) and Webber (2011)



Carbon dioxide field trials

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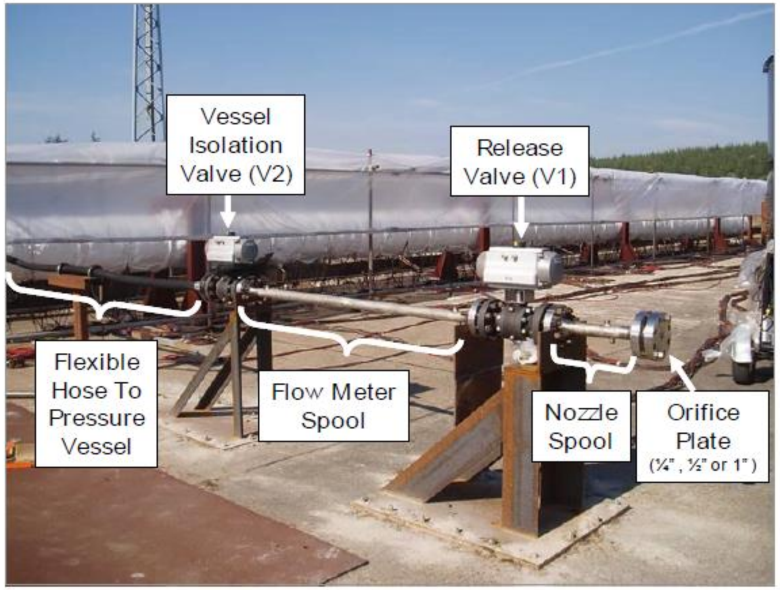
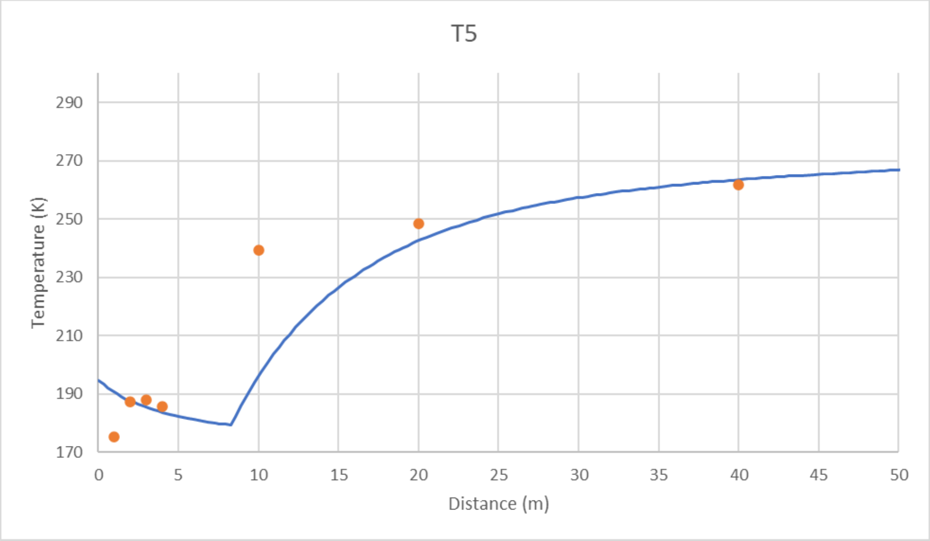
- CO2PIPETRANS JIP
  - Subset of data analysed by Witlox (2012)
  - Release from pressurized conditions
    - Pressure liquefied (6 cases)
    - Vapour (2 heated cases)
  - Expanded source conditions
    - Witlox (2012) using DNV ATEX model
  - Dispersion predictions using DRIFT
    - Temperature
    - Concentration

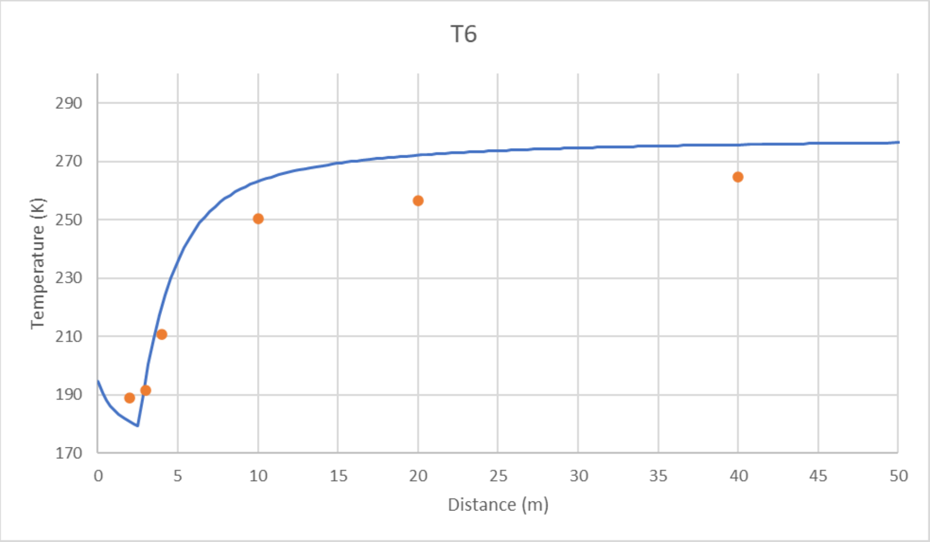


Test Rig (extract from DNV Report: 1st Release of Model Validation Data (BP Data) Overview Report, 2012)

Minimum temperature predictions (carbon dioxide)

- Depression below sublimation temperature of 194 K
- Rise in temperature after solid all sublimed





Maximum concentration (carbon dioxide) predictions

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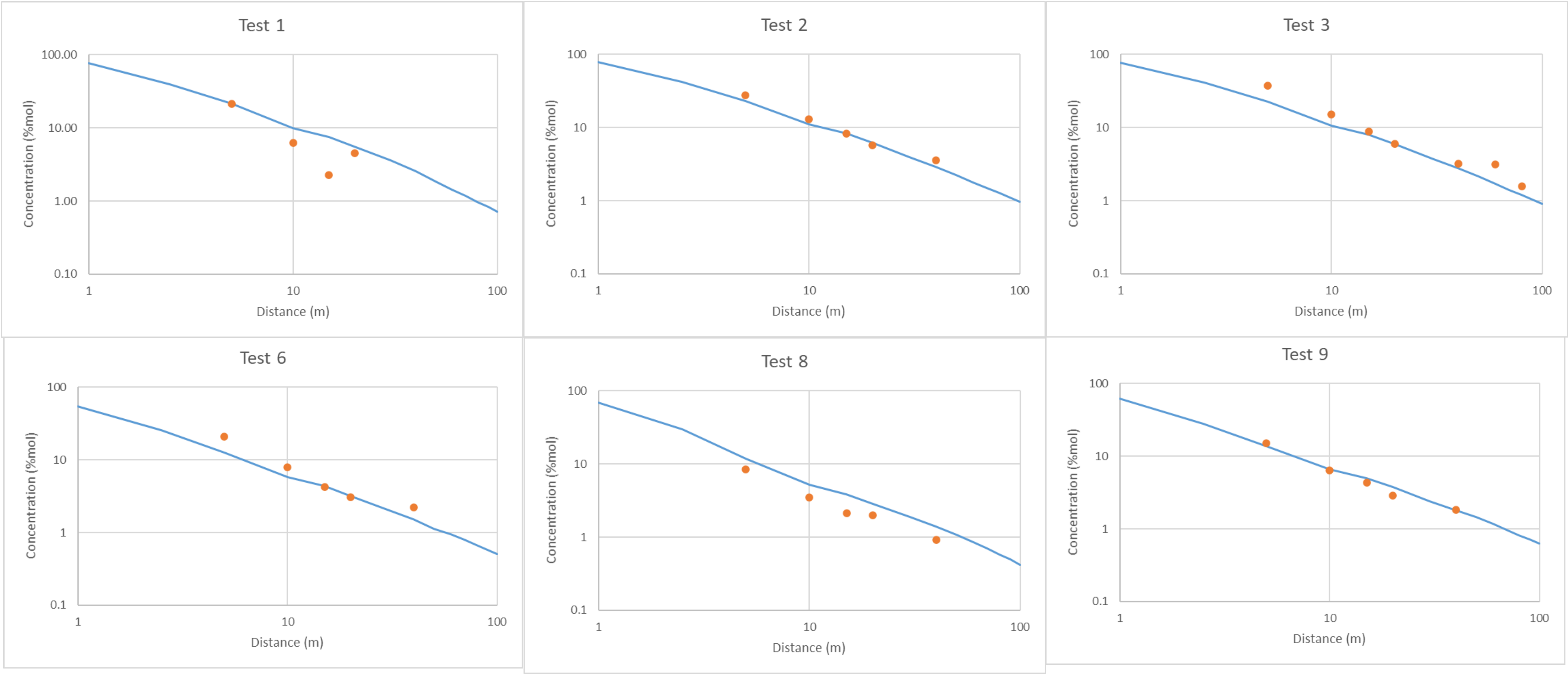


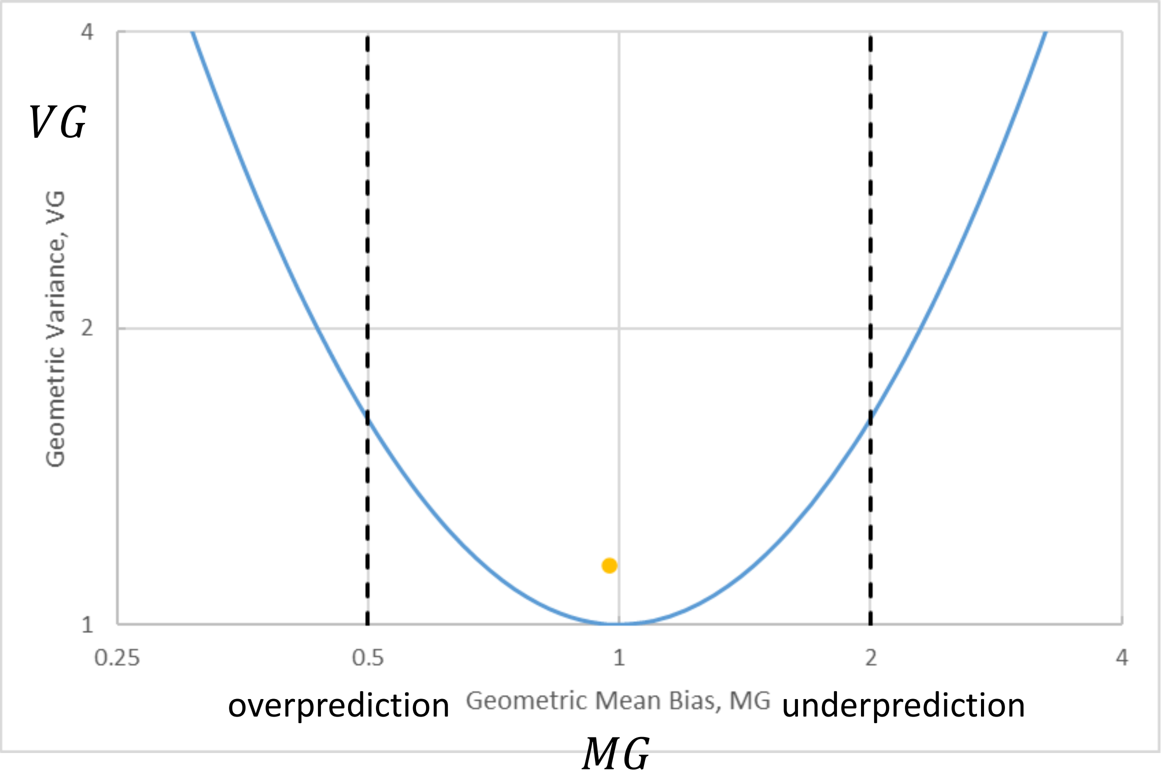
Maximum concentration (carbon dioxide) statistical performance

- Geometric Variance

$$VG = exp\left\langle\left[\log_e\left(\frac{C_m}{C_p}\right)\right]^2\right\rangle$$

- Geometric Mean Bias

$$MG = exp\left\langle\log_e\left(\frac{C_m}{C_p}\right)\right\rangle$$



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Carbon dioxide predictions findings

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- Solid CO_2 predicted to sublime over distances of less than 10 m for the trials
- Minimum temperature comparisons
  - Depression below sublimation temperature for solid CO_2 cases followed by temperature rise
  - Tendency for measurements to rise sooner than predictions
  - Sensitivity to small spatial offset/fluctuations
- Maximum concentration comparisons
  - Good agreement of model centreline concentrations with maximum measured value
  - VG and MG well within acceptable range typically used in model evaluation of dense gas dispersion

Conclusions

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- Good overall agreement with the datasets for hydrogen, ammonia and carbon dioxide support the use of DRIFT for these substances
- No tuning of the model to any of these datasets
- Comparisons based upon short time-averaged model results
- Possible future work
  - Investigate the effects of longer time-averaging on predictions
  - Comparison with other available datasets for these substances

Any questions?

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- Thank you for your time

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