**Institute of Particle Science and Engineering**
FACULTY OF ENGINEERING

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# Numerical Modelling of Turbulent Particle-Laden Sonic $CO_2$ Jets with Experimental Validation

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# Overview

- Brief introduction to Carbon Capture and Storage

- Near-field sonic dispersion of carbon dioxide ($CO_2$) from high pressure pipelines
  - Non-ideal thermodynamic model
  - RANS numerical method

- Bench-scale experiments to investigate particle behaviour

- Comparison to simulations of near-field sonic $CO_2$ releases with Lagrangian particle tracking and agglomeration model.

# Carbon Capture and Storage

- Climate change has emerged as society's biggest ever environmental challenge. Carbon Dioxide ($CO_2$) in the upper atmosphere reflects the Sun's heat back down to Earth, further warming the atmosphere like a greenhouse.

- Carbon Capture and Storage (CCS) presents a viable short-term option to reducing $CO_2$ emissions.

- The simple premise is that $CO_2$ is captured at the emitter (e.g. power plant or industrial source) and then stored, thereby avoiding release into the atmosphere and exacerbating any man-made climate change.

- Storage sites, e.g. saline aquifers, are not usually close to the $CO_2$ emitter and high pressure pipelines are required.

- In assisting with the preparation of safety cases for such pipelines, the University of Leeds undertook research into the near-field sonic dispersion of $CO_2$ from an accidental pipeline puncture or rupture.
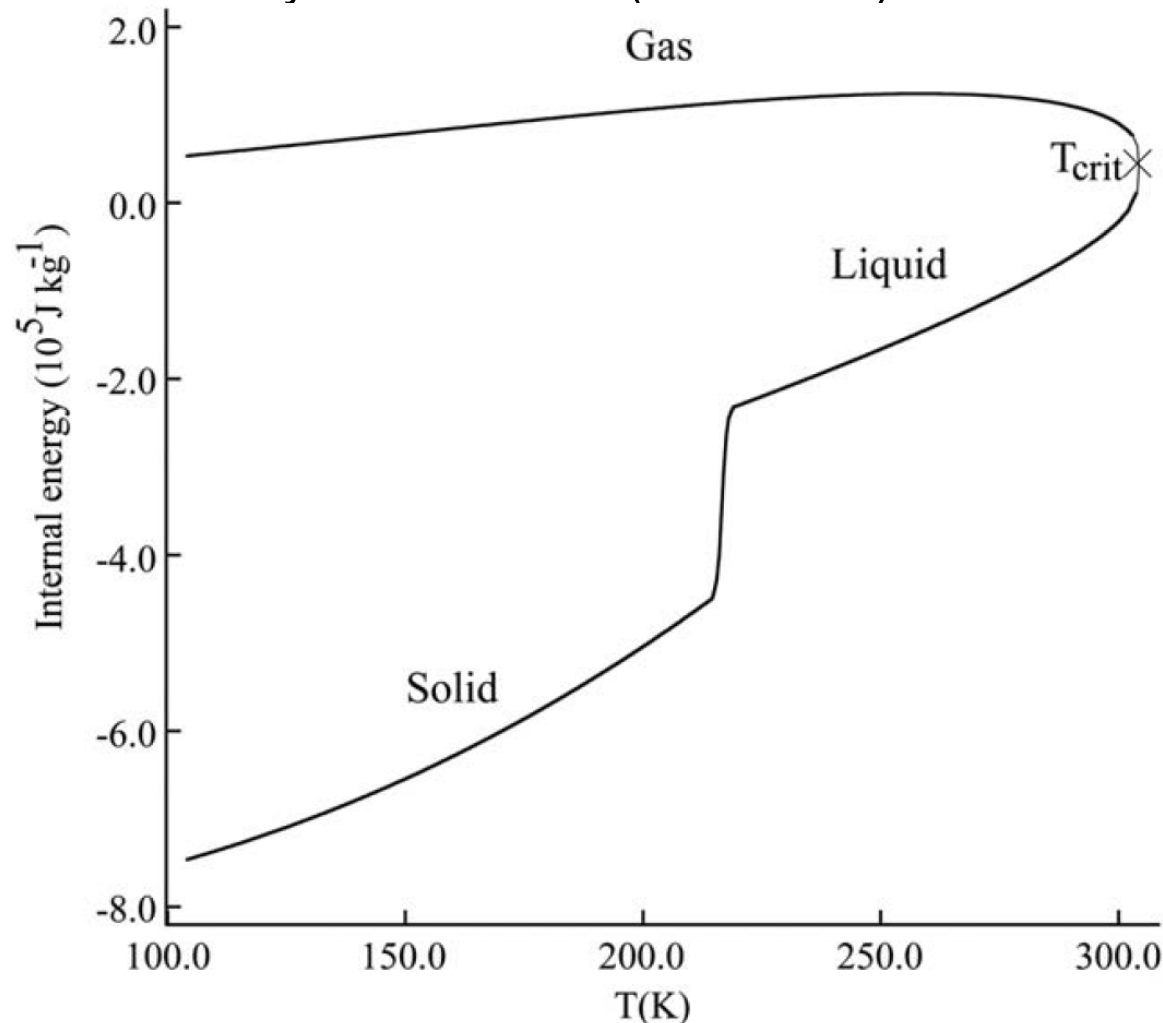
# Near-field dispersion model

- Thermodynamic model: *(Wareing et al. 2013, AIChE J. **59**, (2013) 3928-3942)*

  - Near-field dispersion of $CO_2$ in the gas, liquid and solid phases into dry air.

  - Novel composite equation of state for pure $CO_2$ employing:-

    - the Peng-Robinson equation of state in the gas phase;

    - tabulated data derived from the Span & Wagner equation of state for the liquid phase and vapour pressure;

    - and NIST/DIPPR data for the solid phase and latent heat of fusion.

  - Calculations were undertaken using the Helmholtz free energy in terms of temperature and molar volume, as all other thermodynamic properties can be readily obtained from it.

  - Homogeneous equilibrium model, but a simple sub-model for relaxation to equilibrium is required for the solid phase, as it would appear that the particles are not sufficiently small enough to be in equilibrium.

# Near-field dispersion model

- Thermodynamic model (continued):



• Internal energy on the saturation line.

• $T_{crit}$ marks the critical temperature.

• The triple point can be identified by the steep connection between the liquid and solid phases – the latent heat of fusion.
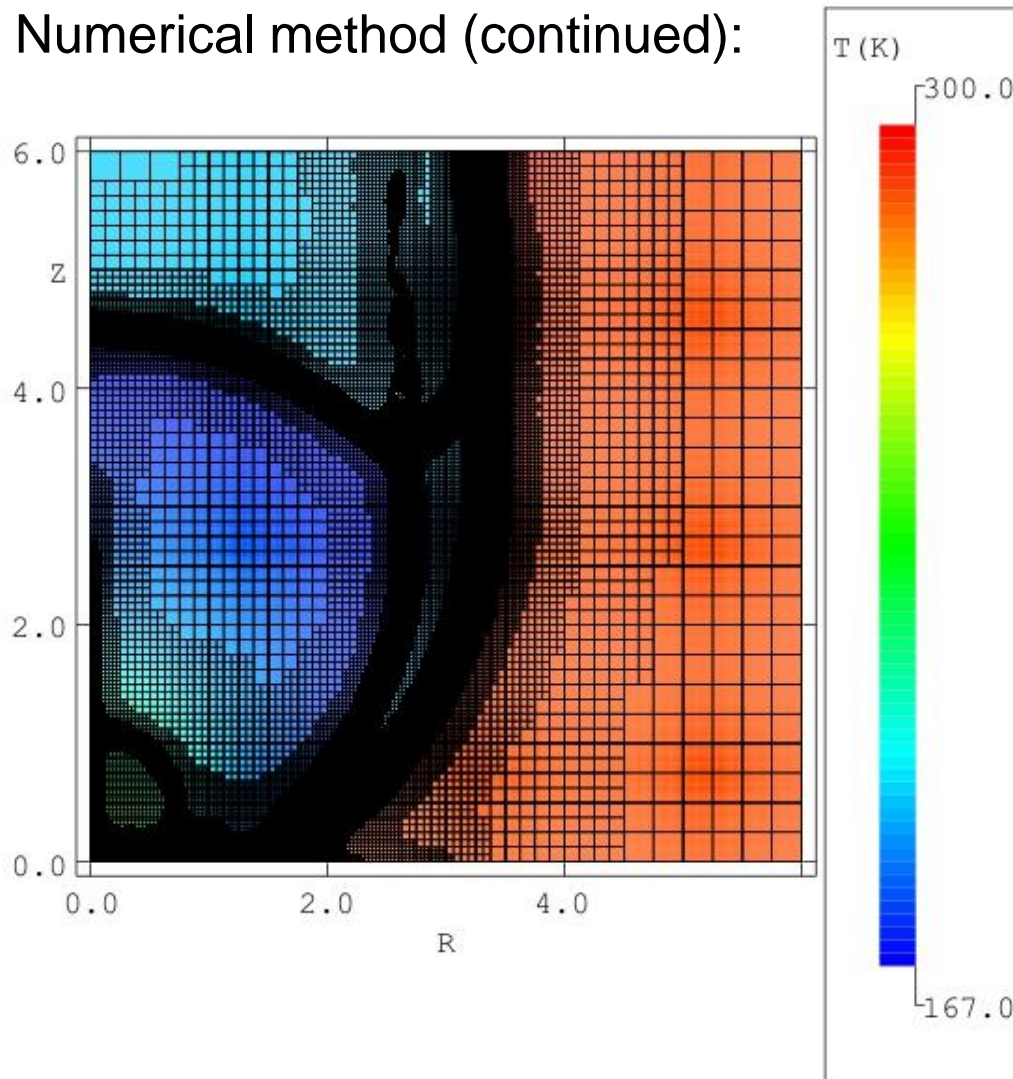
# Near-field dispersion model

- RANS numerical method:

  - Adaptive, finite-volume grid algorithm with 2D or 3D rectangular mesh.

  - Grid adaption achieved successive overlaying of refined layers of computational mesh.

  - Where steep gradients of variable exist, such as at the Mach shock in this case, the mesh is more refined. This technique enables the generation of fine grids in regions of high spatial and temporal variation. Conversely, coarser grids are allowed where the flow field is smooth.

  - Turbulence model: Reynolds stress with modifications for compressible flows.

  - Lagrangian particle tracker and particle distribution function.

  - Solutions obtained for the time-dependent, density-weighted equations.

  - Efficient, general-purpose shock-capturing, upwind, second-order-accurate Godunov numerical scheme with a HLL Riemann solver.

# Near-field dispersion model

- Numerical method (continued):



• Adaptive meshing around the Mach shock in a dense high pressure release of $CO_2$.
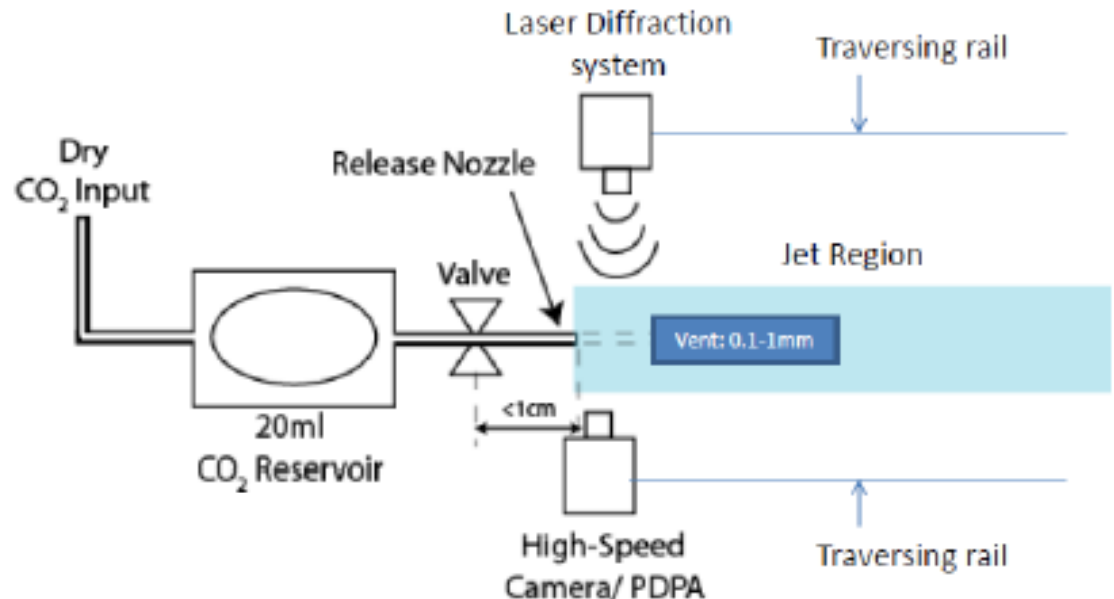
Note the axis units are in release diameters.

**Problem: where do the particles go? No clear information available.**

- **Solution:** Laboratory-scale experiments in a ventilated chamber
  - 20ml canister of liquid $CO_2$ pressurised to 68.9 bar at ambient temp.
  - Connected to a nozzle at one end of a Perspex box 50x50x500mm.
  - Two nozzles flush with inside of box: 0.5mm and 1.0mm in diameter (D).
  - Phase Doppler Particle Anemometry used to measure particle sizes and velocities along the sonic release.
  - Data obtained at 3D, 5D, 6D, 10D, 20D, 30D, 50D and 100D.
  - Experiment mimics a pipeline discharge.

# Results - movie

A high-speed camera movie of a release into a dry atmosphere.

Individual particles are visible.

# Results – initial particle distribution
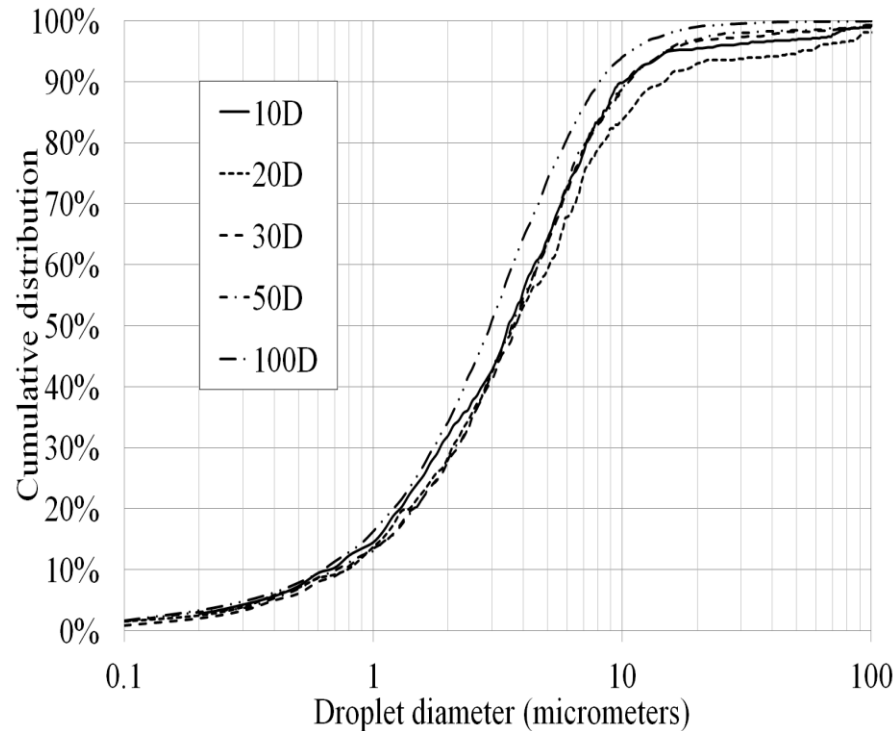
**Population vs. droplet diameter at 10D for both nozzles**

*Y-axis: Particle Distribution Function (%)*
*X-axis: Droplet Diameter (micrometres)*

Legend:
— 1.0mm nozzle
- - 0.5mm nozzle

- Initial particle distribution post-Mach shock is centred on 1-2 micrometres.
- These particle sizes are in agreement with Weber number predictions.

# Results – particle behaviour along jet
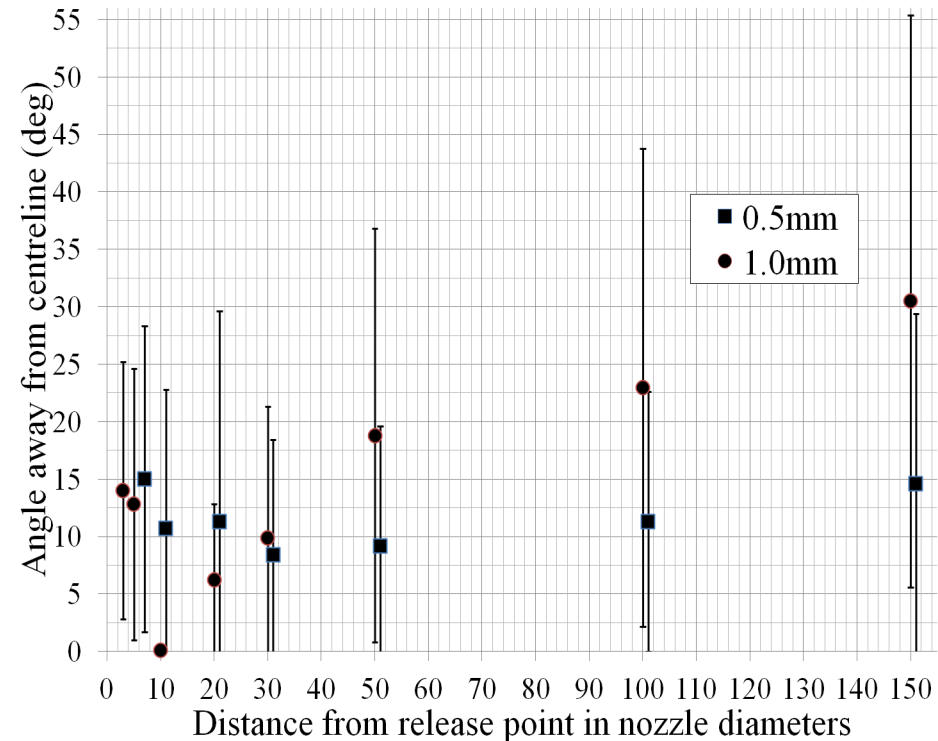
- 0.5mm nozzle: no agglomeration
- 1.00mm nozzle: agglomeration!
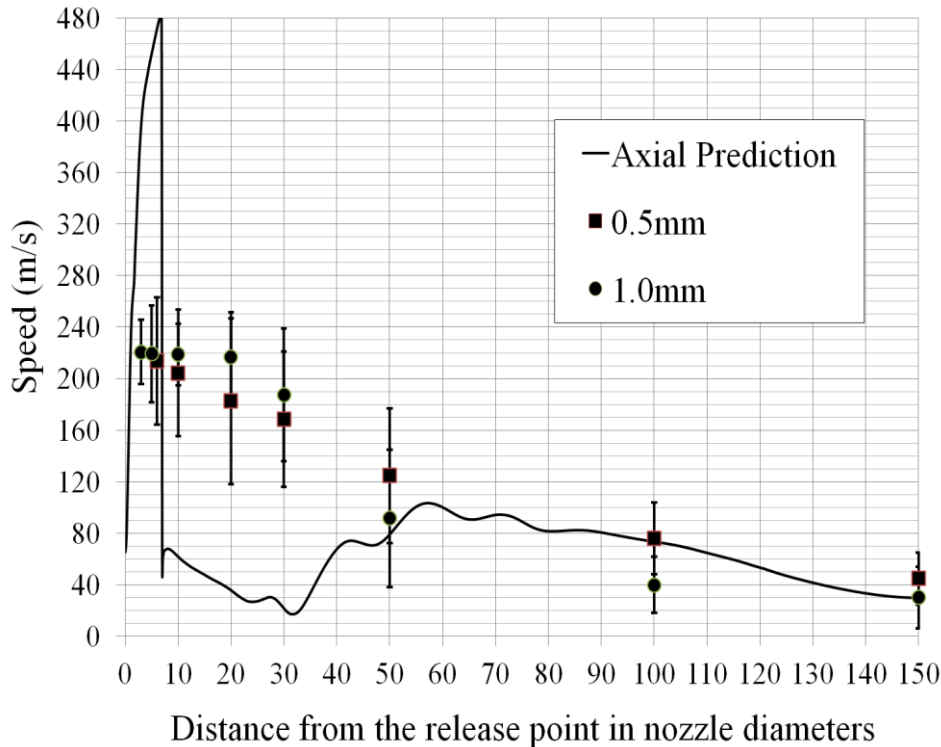


- No change in PDF along the jet for the 0.5mm nozzle case.
- Shift of PDF -> evidence of agglomeration in 1.0mm nozzle case. Why?
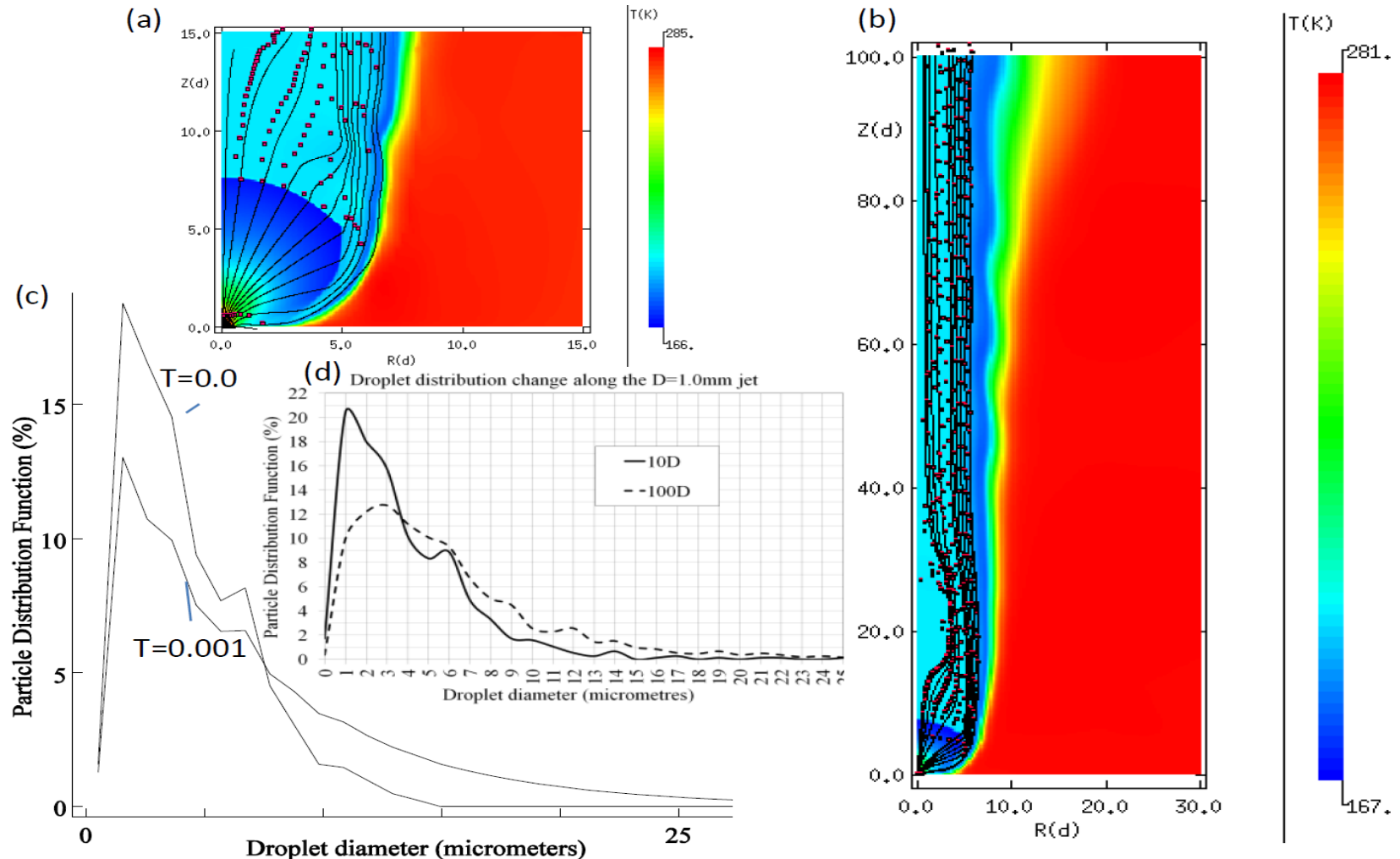
- Particles are not in equilibrium with the flow until at least 50D.

- Supported by theoretical calculations of thermal and dynamic relaxation times for these specific nozzles.

- Instantaneous velocities are further away from the centreline in the 1.0mm case. Indications of particles following the turbulent motion?

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• Test of a turbulent shear agglomeration model using a turbulent shear agglomeration model (Saffman JFM **1** 16-30 1956).

# Conclusions

- Novel dispersion model covering the necessary range of pressures and temperatures in accidental releases of $CO_2$.

- Experimental work has allowed the investigation of particle behaviour in these sonic multi-phase releases.

  - Initial particle distribution has been measured.

  - Net agglomeration along the jet has been modelled by a turbulent shear agglomeration model with a Lagrangian particle tracker, particle distribution function and Reynolds stress turbulence model.

- Future work:

  - Experimental and numerical modelling of turbulent pipe flow.

  - Refinement of coupled particle motion and evolution models.

  - Supercritical releases and RESS cleaning processes.

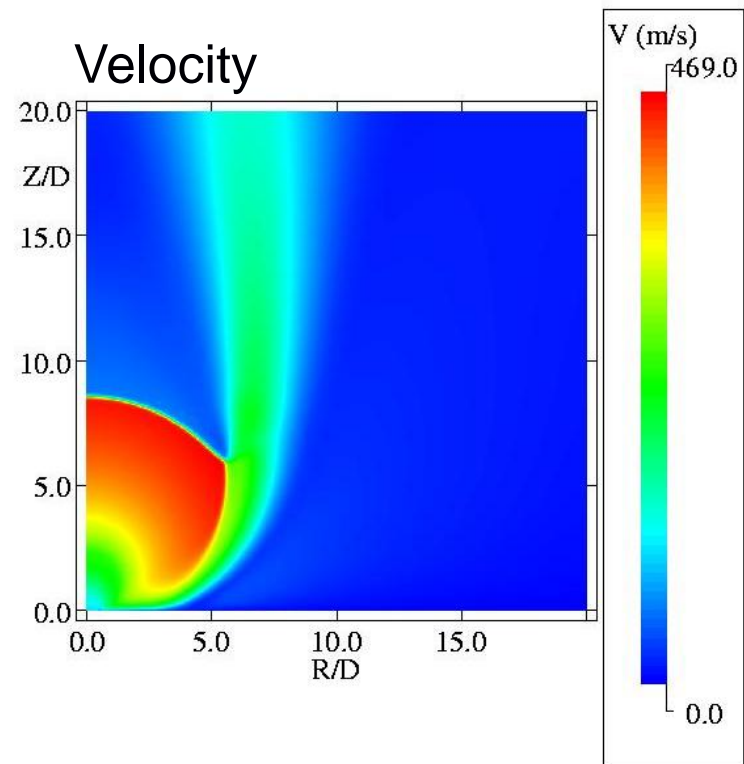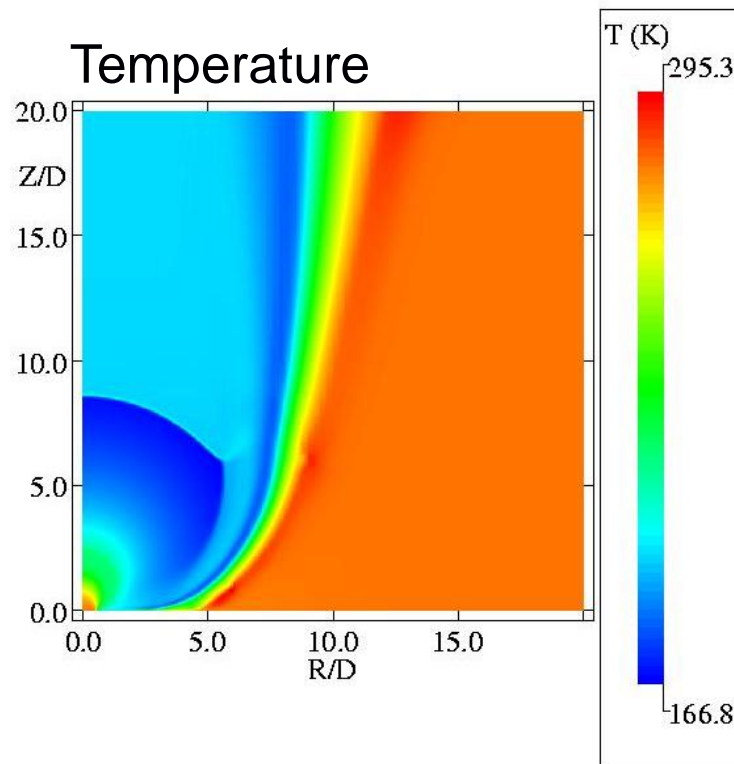**Thank you for listening.**

**Any questions or comments?**

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# Validation: dense phase release

- Dense phase release from a 150bar reservoir through 25mm (D) vent pipe.
- Steady state release conditions achieved by supplying a driving pressure



Temperature

Velocity

Near-field shock containing region: 20D x 20D (0.5m x 0.5m)
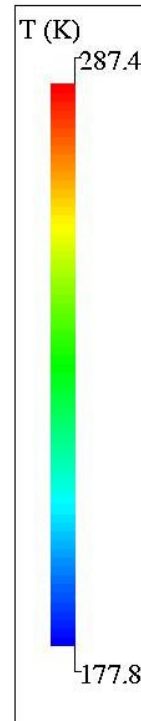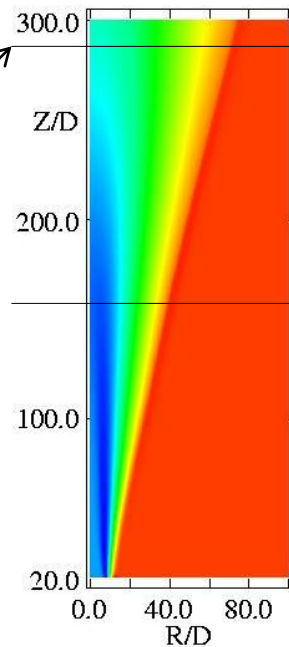
# Validation: dense phase release

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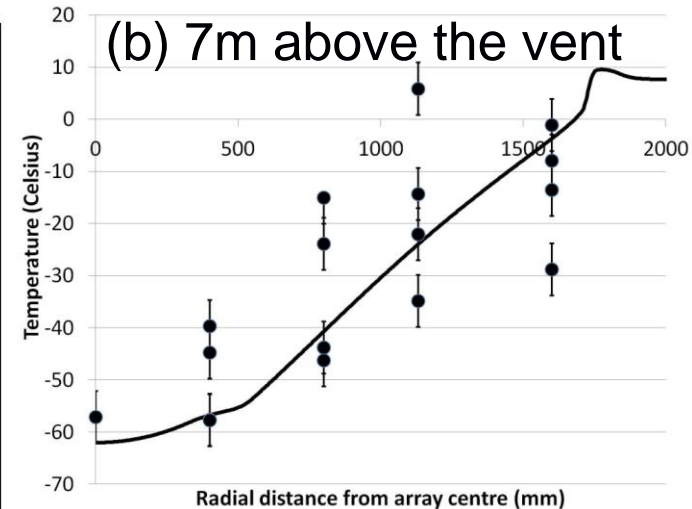Temperature

Measuring planes at:
- 4m (165D)
- 7m (288D)

**Predictions**
- Core temperatures good.
- Jet widths good.
- Some cross-wind effects.

T (K)

(b) 7m above the vent

(a) 4m above the vent

*Wareing et al. IJGGC **20** (2014) 254-271*