RANS Modelling of Turbulent Particle-Laden Sonic CO_2 Jets

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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

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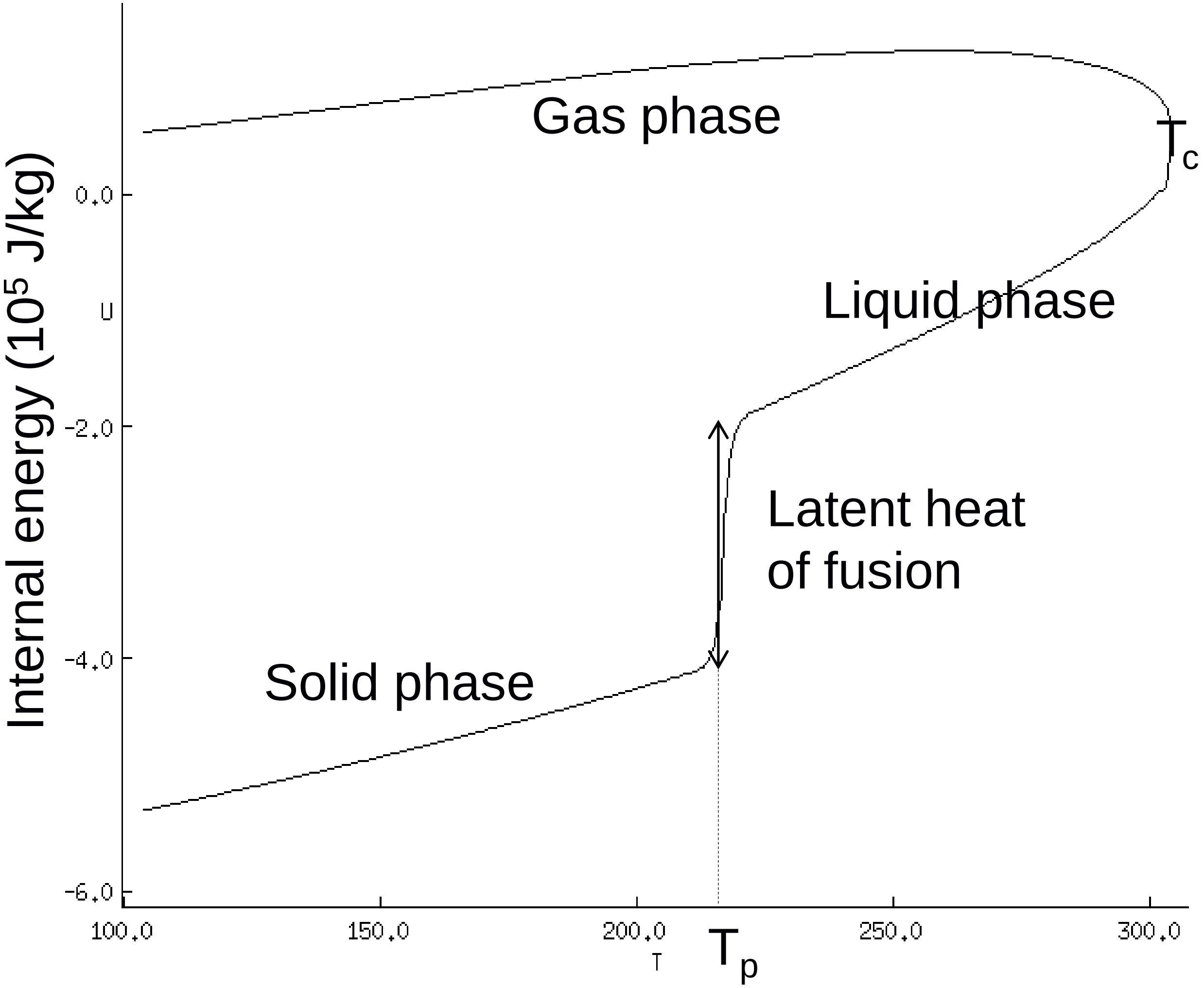
- Climate change has emerged as society’s biggest ever environmental challenge. Carbon Dioxide (CO_2) in the upper atmosphere reflects the Sun’s heat back down to Earth, further warming the atmosphere like a greenhouse.
- Carbon Capture and Storage (CCS) presents a viable short-term option to reducing 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:
    - 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:-
        - Gas phase: Peng-Robinson equation of state;
        - Liquid phase and vapour pressure: Span & Wagner equation of state;
        - Solid phase: Jager and Span equation of state
        - Latent heat of fusion: 204.932 kJ/kg (NIST/DIPPR).
    - 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 at coexistence along the saturation line.
- T_c marks the critical temperature.
- The triple point (T_p) 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 round jets.
  - 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

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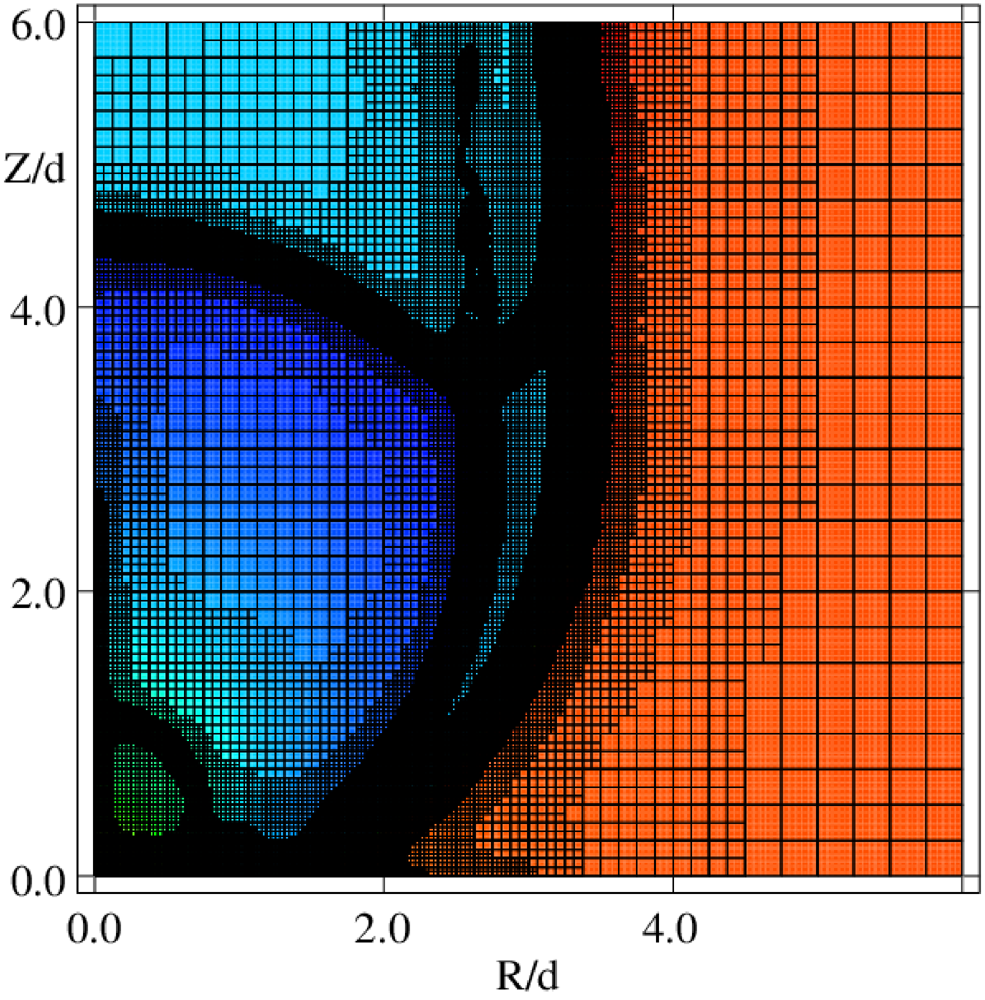
- Numerical method (continued):



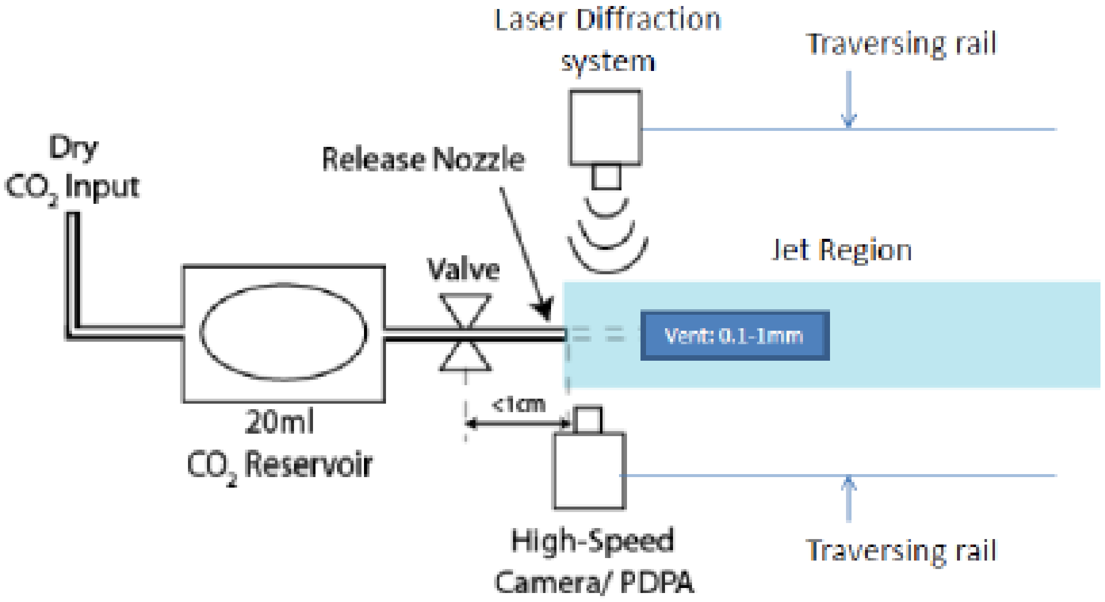
- Adaptive meshing around the Mach shock in a dense high pressure release of CO_2.

Note the axis units are in release diameters.

Particle experiments

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.

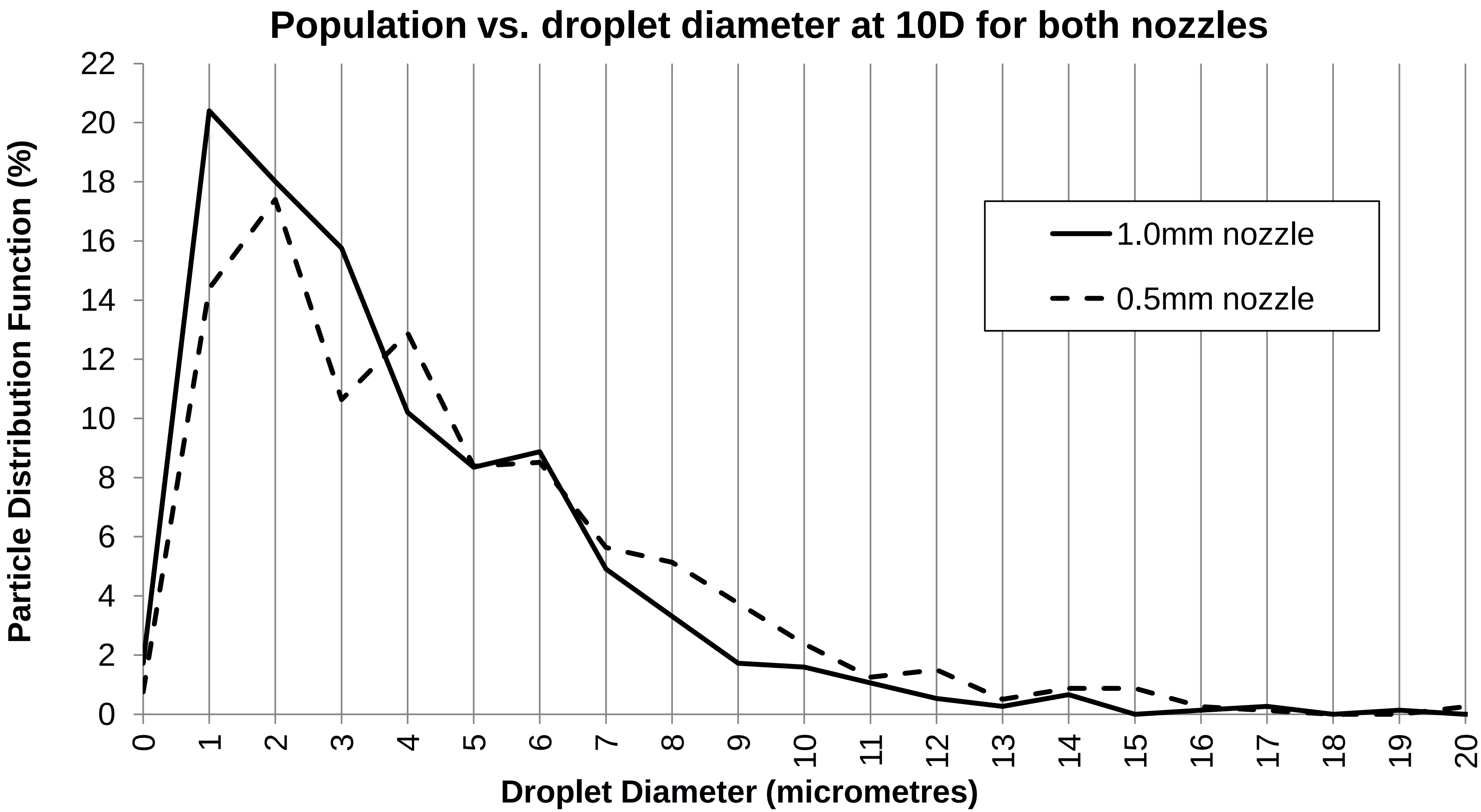


Experimental results - movie

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

Individual particles are visible.

Experimental results – initial distribution



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

Experimental results – particle behaviour 1

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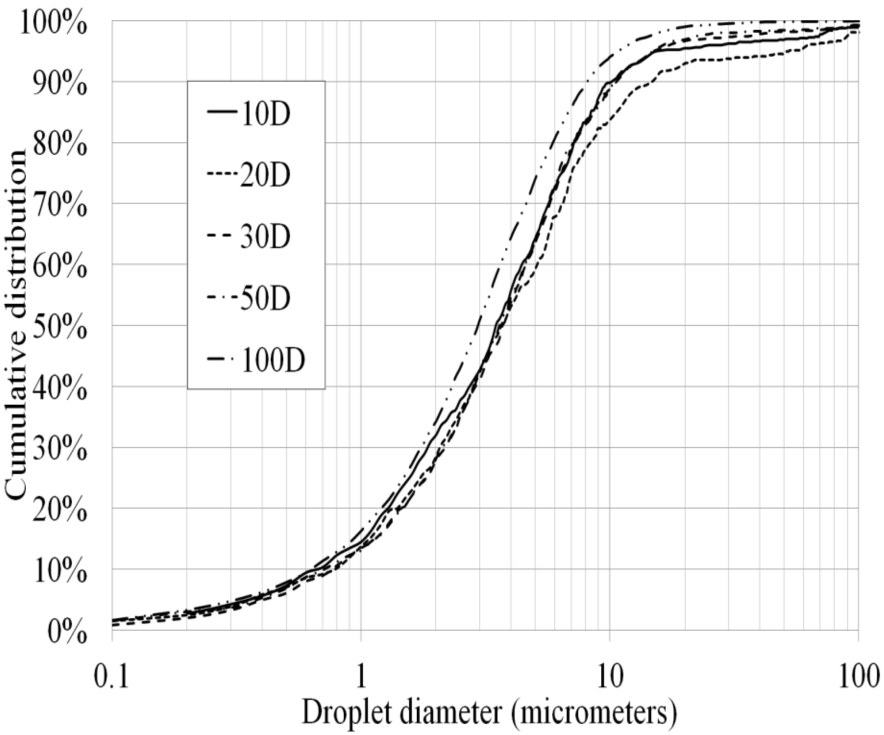
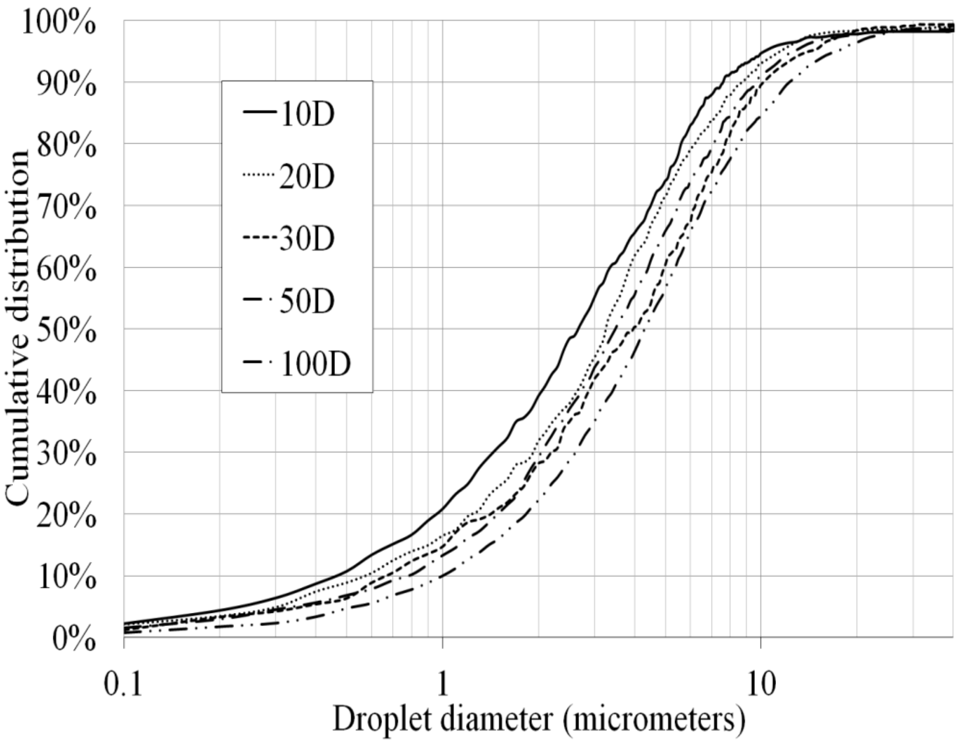
- 0.5mm nozzle: no agglomeration



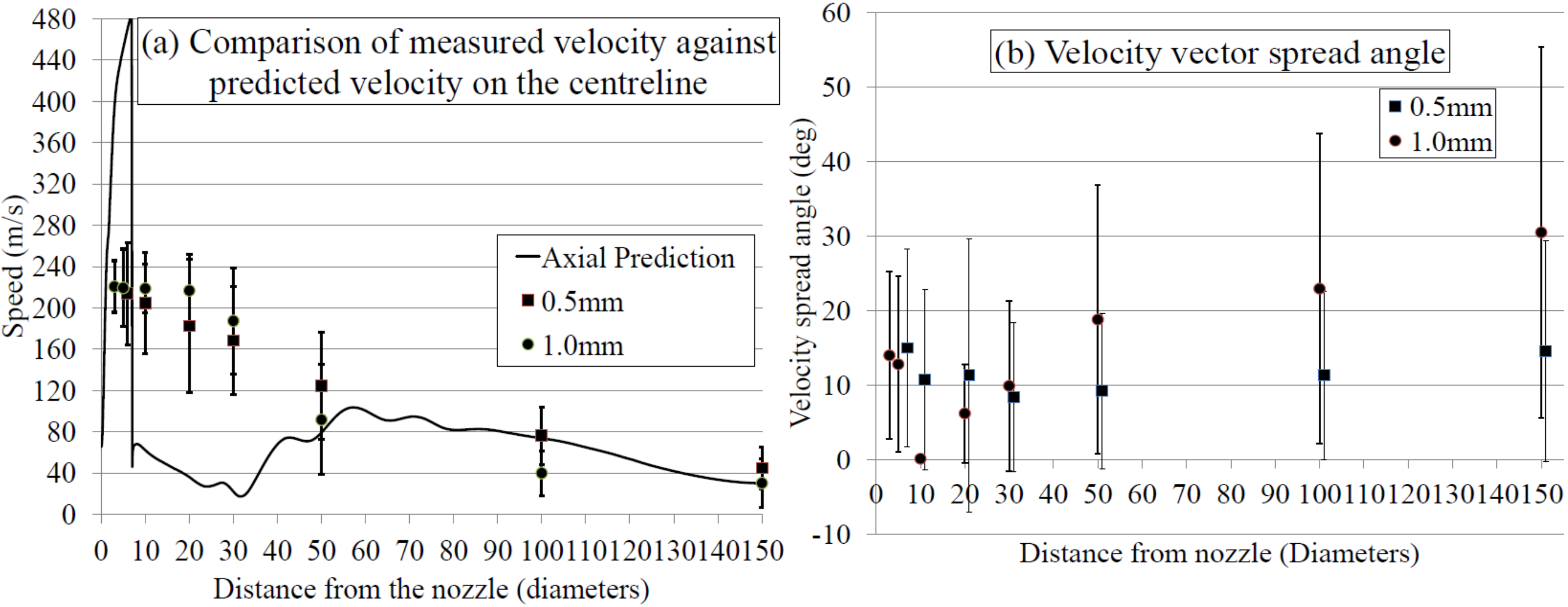
- 1.0mm nozzle: agglomeration!



- 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?

Experimental results – particle behaviour 2



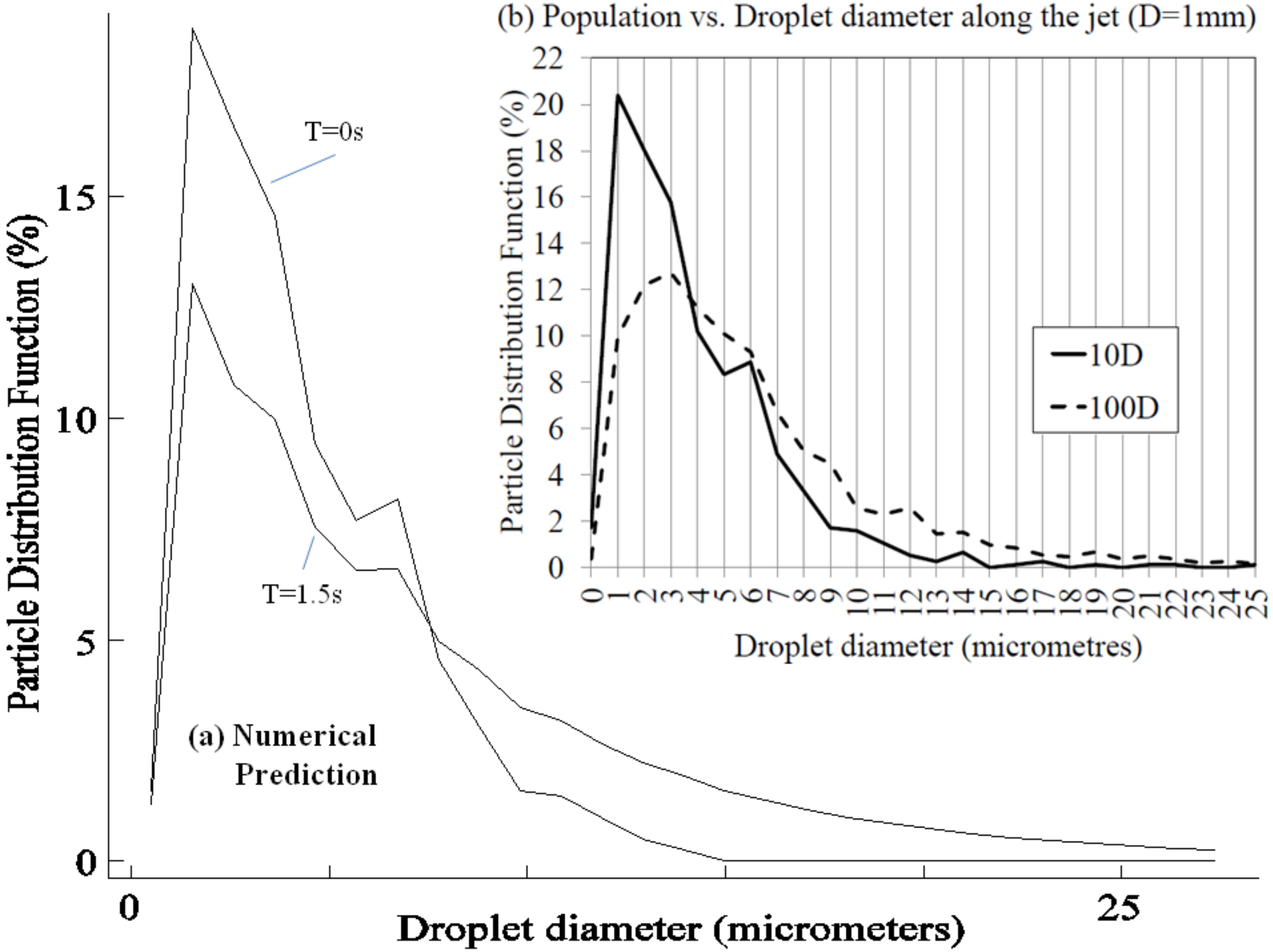
(a) Comparison of measured velocity against predicted velocity on the centreline

(b) Velocity vector spread angle

- 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?

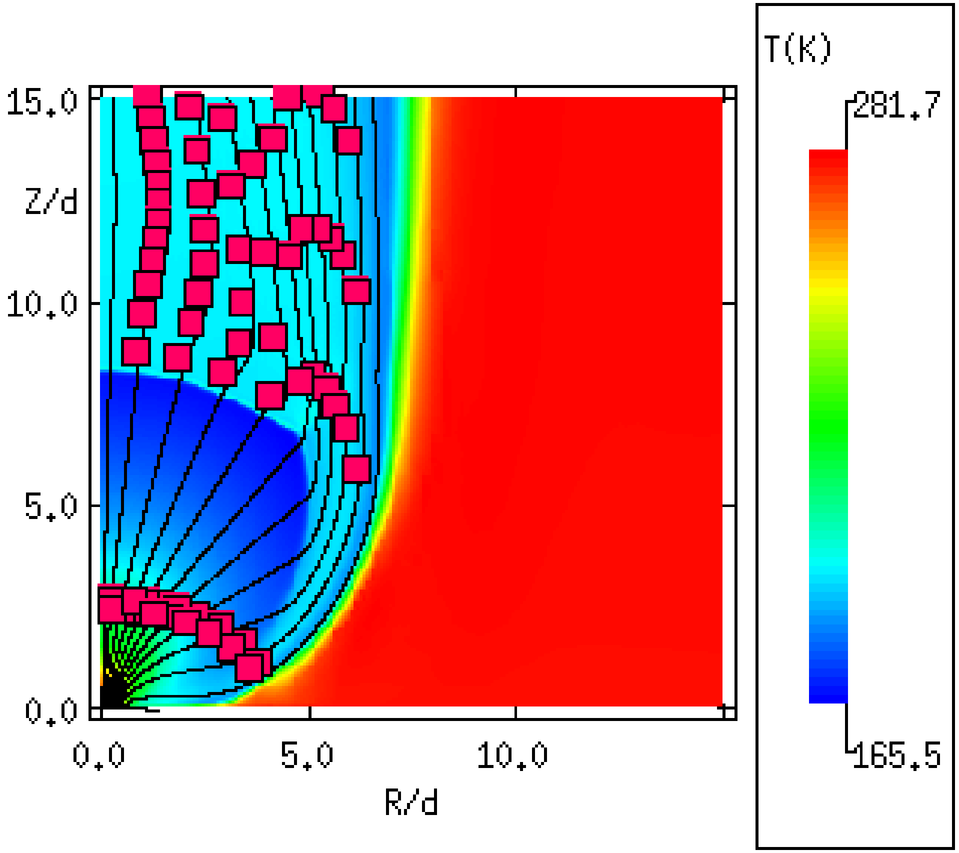
Numerical results – agglomeration model

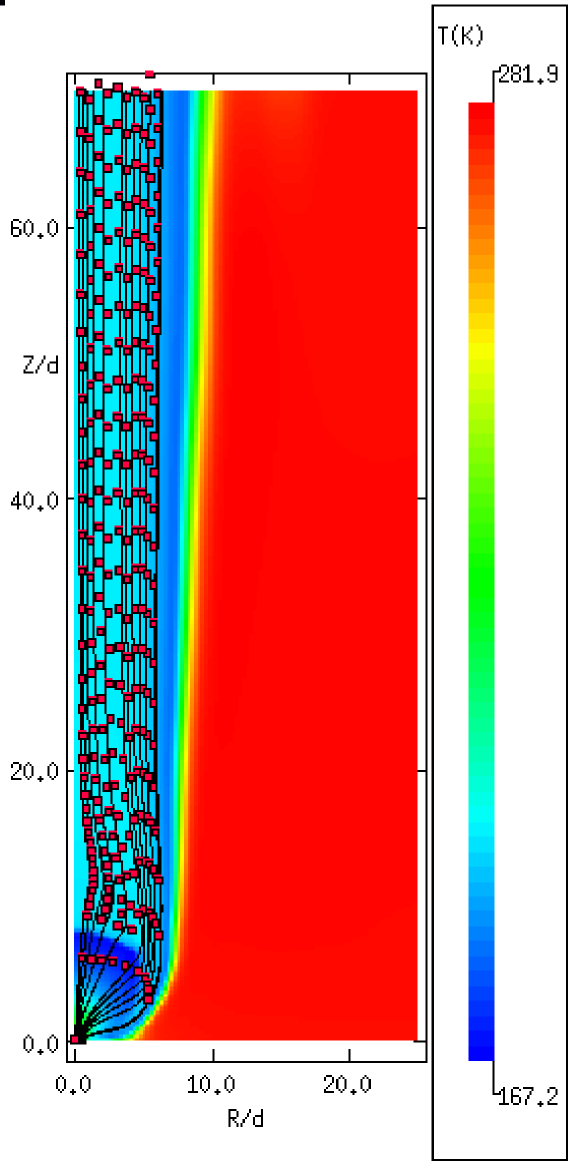
- Test of using the turbulent shear agglomeration model according to (Saffman JFM **1** 16-30 1956).



Numerical results – fluid model with particles

- Axisymmetric near-field Mach Shock structure and far-field jet structure with stream lines.
- Red squares indicate particle locations.





Numerical results – velocity comparisons

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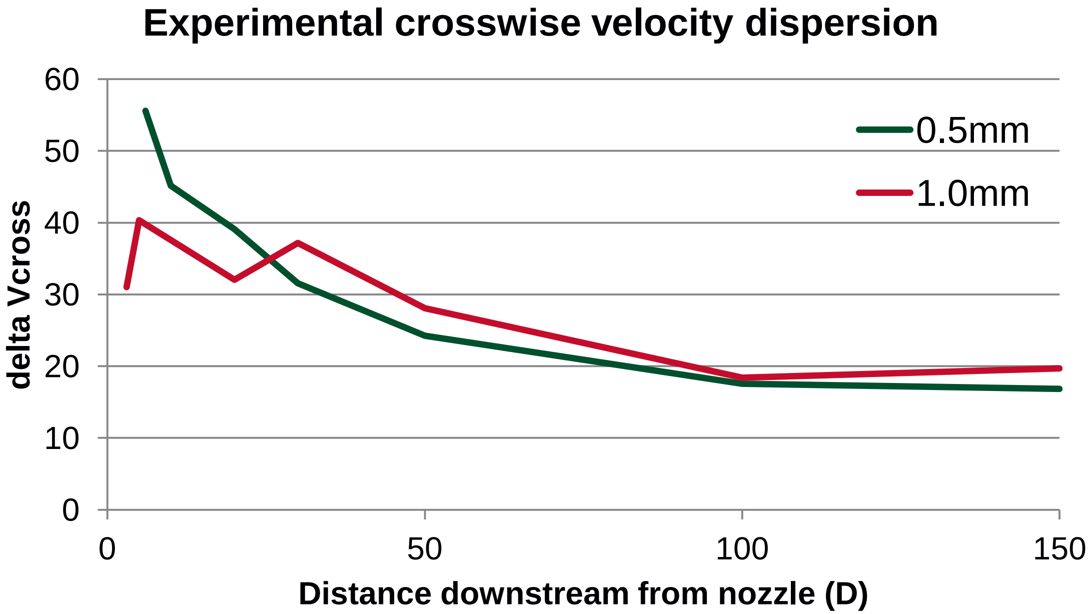
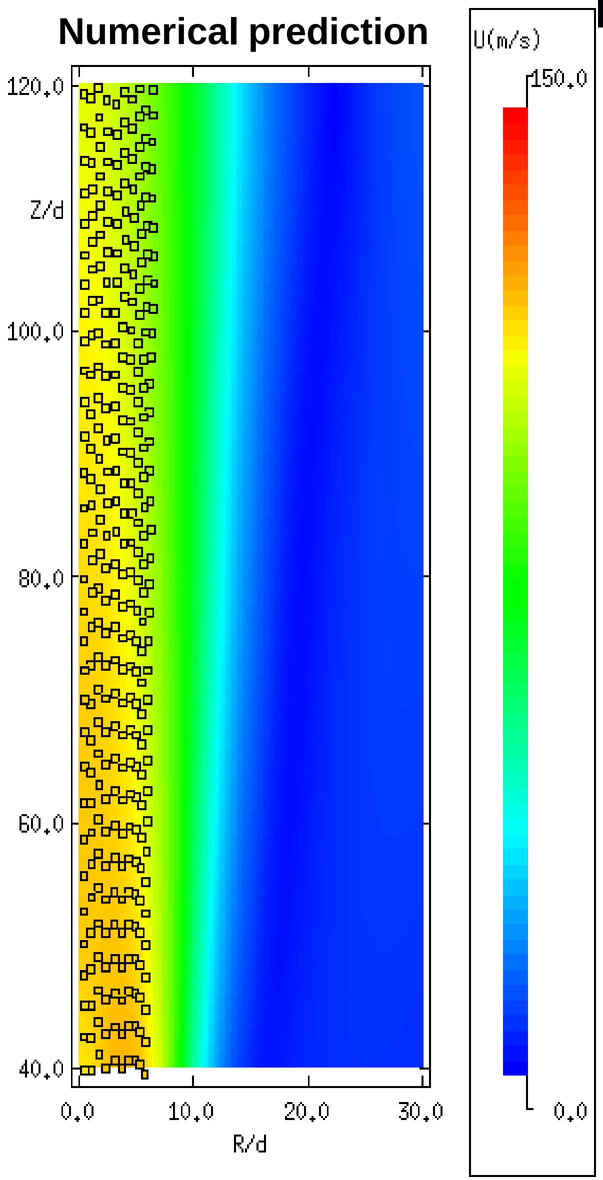
- Axisymmetric prediction of particle velocity shows good agreement with fluid velocities.

- Velocity dispersion analysis of cross-wise **experimental** velocity indicates slightly higher levels of turbulence in the region 30-150D for the 1.0mm nozzle, but not conclusive.





Numerical results – agglomeration

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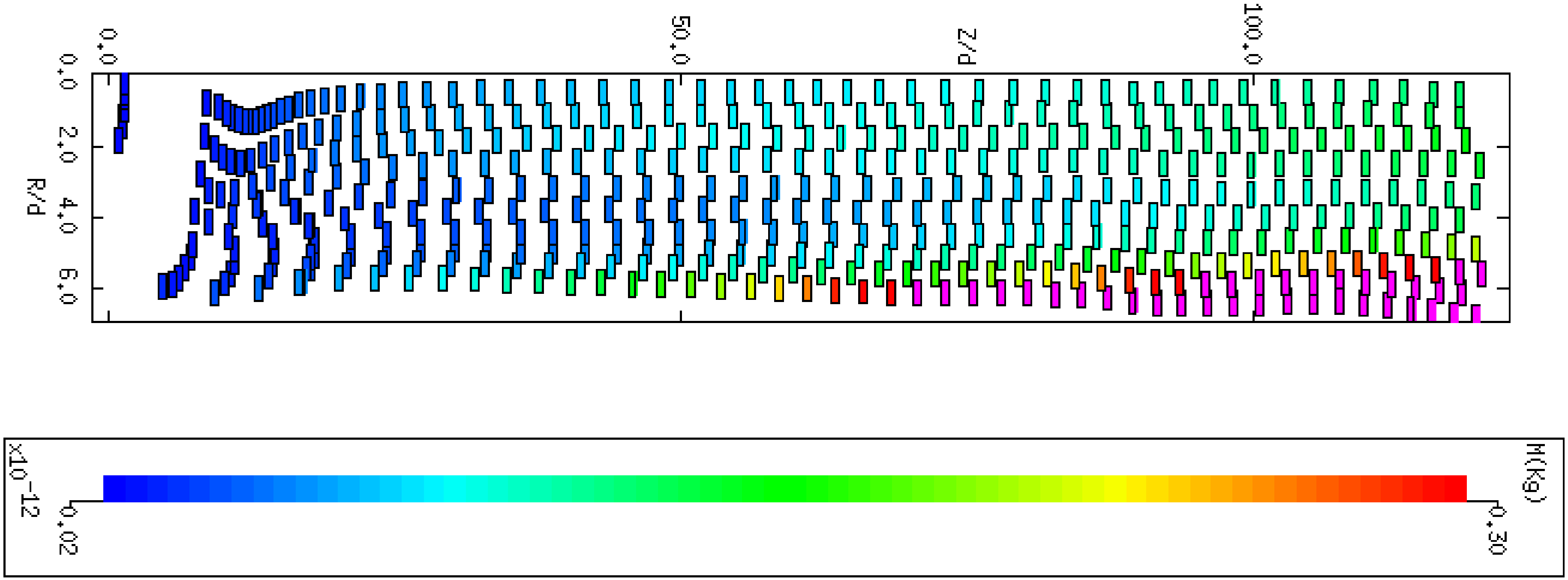
- Using the turbulent shear agglomeration model, the simulation is able to reproduce the agglomeration observed along the 1.0mm jet.



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.
  - Velocity dispersion analysis is supportive, but inconclusive.
- Future work:
  - Refined and extended experiments.
  - Refinement of coupled fluids, particle motion and evolution models.
  - Application to supercritical releases and RESS cleaning processes.

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Thank you for listening.

Any questions or comments?

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