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

Dr Chris Wareing

8th Symposium on Numerical Analysis of Fluid Flow and Heat Transfer
ICNAAM 2013, 21-27 September 2013, Rhodes, Greece

C J Wareing, M Fairweather, J Peakall, G Keevil, S Falle, R Woolley
University of Leeds, Leeds, LS2 9JT, United Kingdom

Overview

- Brief introduction to Carbon Capture and Storage
- The COOLTRANS Research Programme
- Near-field sonic dispersion of carbon dioxide (CO_2) from high pressure pipelines
  - Thermodynamic model
  - Numerical method
  - Large-scale Validation
- Bench-scale experiments to investigate particle behaviour
- Simulations of near-field sonic CO_2 releases with Lagrangian particle tracking – an application to buried pipelines.

Carbon Capture and Storage

UNIVERSITY OF LEEDS

- 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.
- But, storage sites, for example disused oil fields or saline aquifers are not usually close to the CO_2 emitter.

COOLTRANS Research Programme

UNIVERSITY OF LEEDS

- The electricity and gas global company National Grid's expertise in building and running safe and effective pipeline networks could play a critical role in helping the UK to meet its obligation to cut CO_2 emissions by 20 per cent by 2020 through provision of CO_2 transport services to support deployment of CCS technology.

- National Grid initiated the TRANSport of Liquid CO_2 (COOLTRANS) Research Programme to address knowledge gaps relating to the safe design and operation of onshore high pressure pipelines for transporting liquid CO_2 from industrial emitters to storage sites offshore.

- As part of this programme, the University of Leeds is undertaking research into the near-field sonic dispersion of CO_2 from an accidental puncture or rupture of the high pressure pipeline.

Near-field dispersion model

UNIVERSITY OF LEEDS

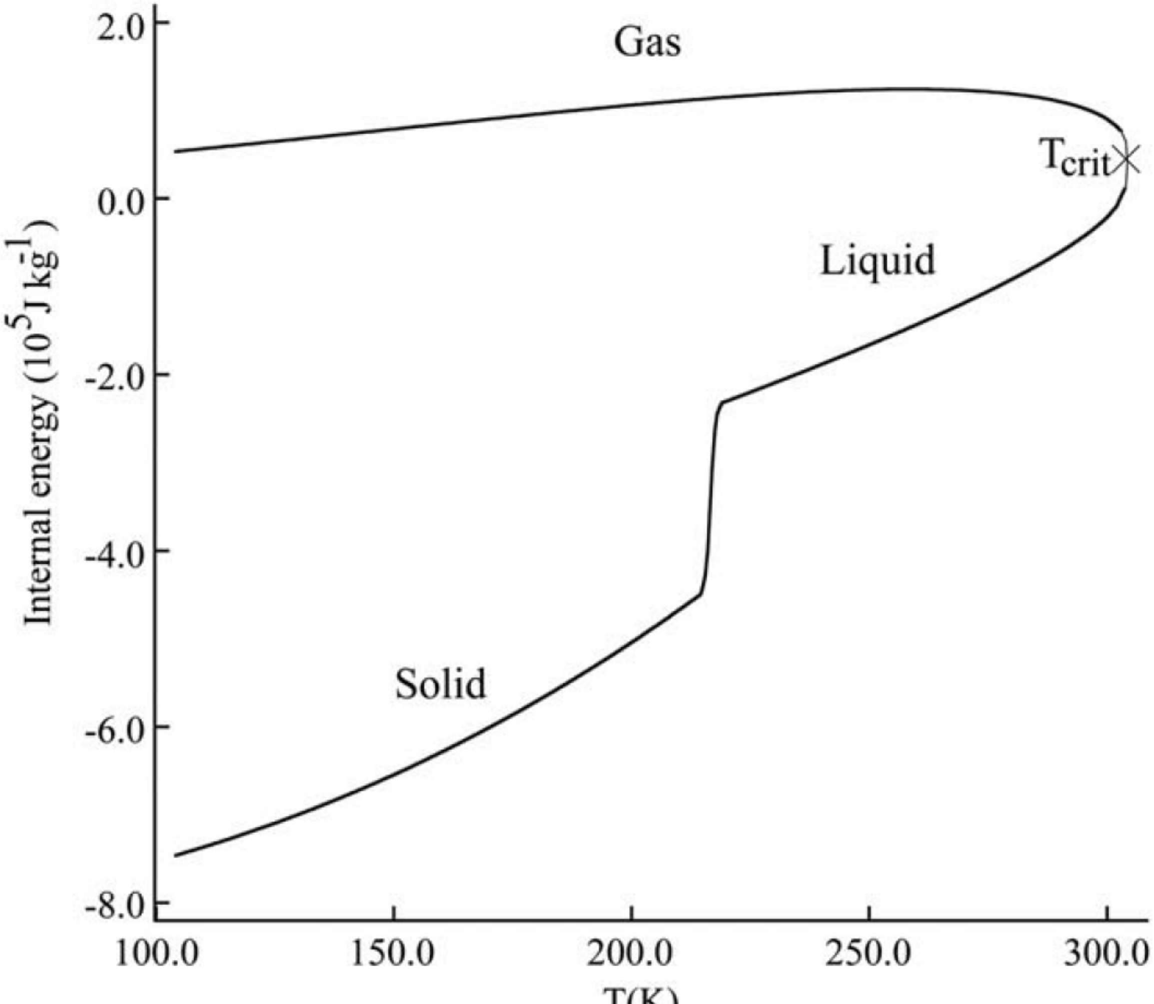
(Wareing et al. 2013, AIChE J. doi:10.1002/aic.14102)

- 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:-
    - 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

UNIVERSITY OF LEEDS

- 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

UNIVERSITY OF LEEDS

The RANS equations closed with a $k - \epsilon$ turbulence model are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad \text{continuity,}$$

$$\frac{\partial \rho C}{\partial t} + \nabla \cdot (\rho C \mathbf{u}) - \nabla \cdot (\mu_T \nabla C) = 0 \quad \text{scalar transport,}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) + \nabla P - \nabla \cdot \tau = \mathbf{s}_p \quad \text{momentum,}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + P)\mathbf{u} - \mathbf{u} \cdot \tau] - \nabla \cdot (\mu_T T \nabla S) = 0 \quad \text{energy,}$$

$$\frac{\partial \rho k}{\partial t} + \nabla \cdot (\rho k \mathbf{u}) - \nabla \cdot (\mu_T \nabla k) = s_k \quad \text{turbulence energy,}$$

$$\frac{\partial \rho \epsilon}{\partial t} + \nabla \cdot (\rho \epsilon \mathbf{u}) - \nabla \cdot (\mu_\epsilon \nabla \epsilon) = s_\epsilon \quad \text{turbulence energy dissipation rate}$$

where S is the entropy per unit mass.

Near-field dispersion model

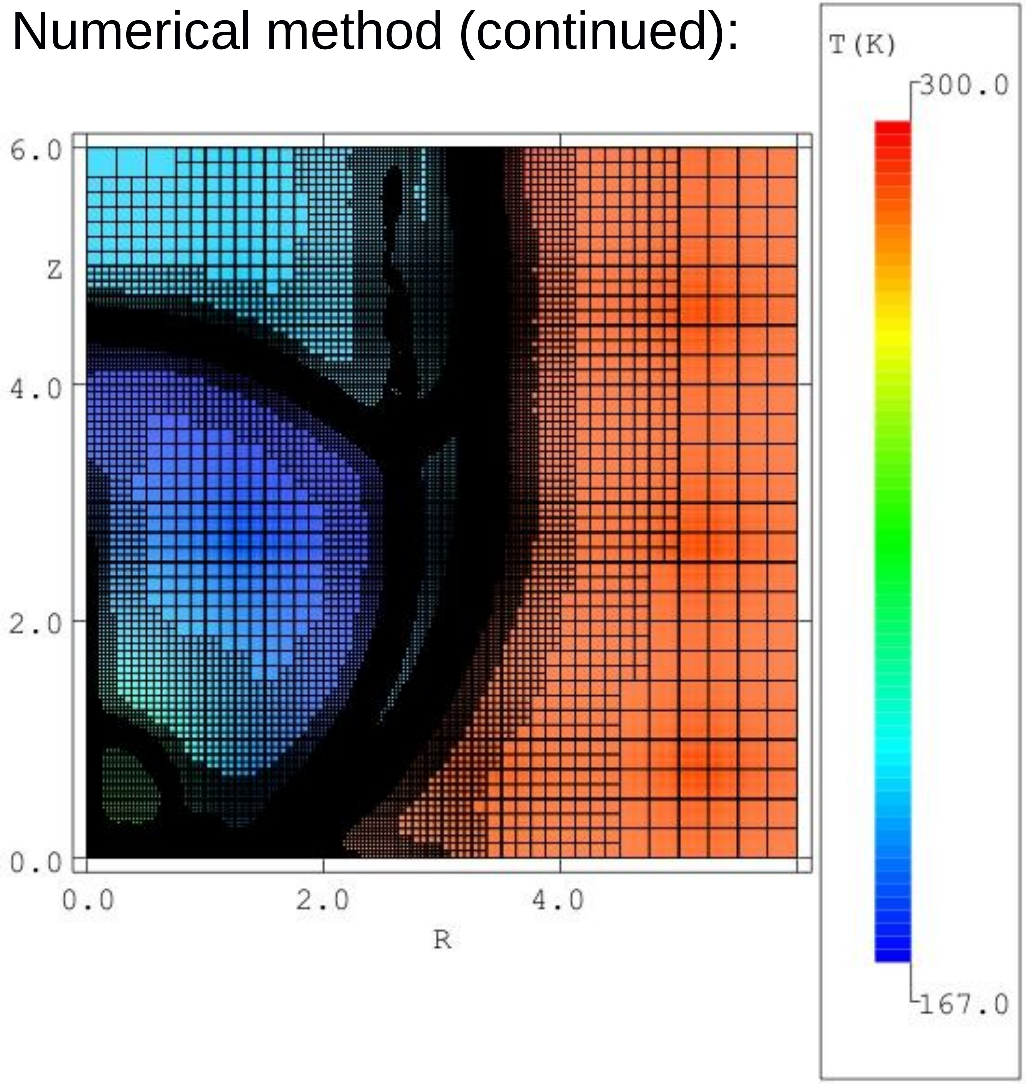
UNIVERSITY OF LEEDS

- 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: we employ a standard k-ε model, but since performance is poor for prediction of compressible flows, we include a compressibility correction according to Sarkar et al (1991).
  - 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

UNIVERSITY OF LEEDS

- Numerical method (continued):



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

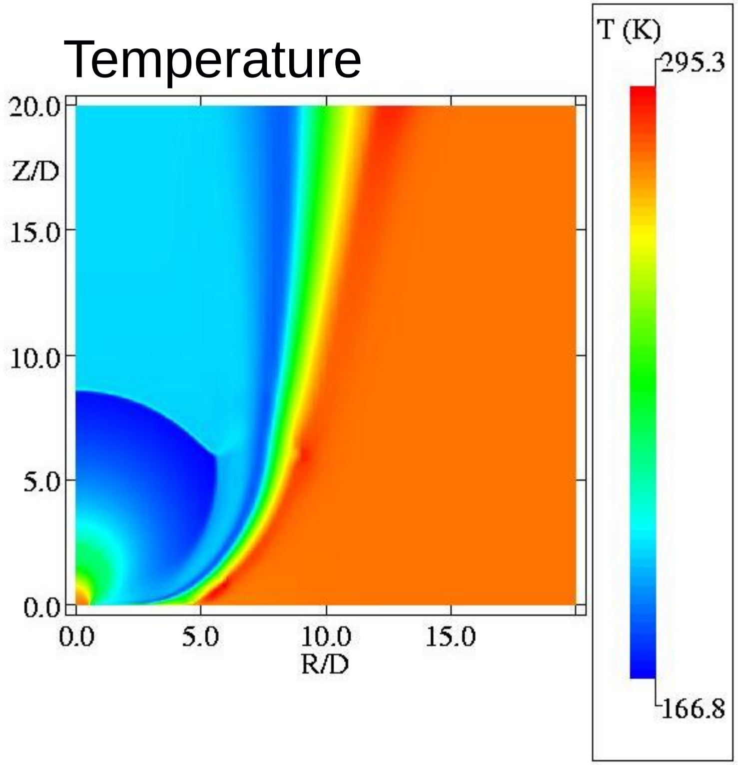
Note the axis units are in release diameters.

Validation: dense phase release

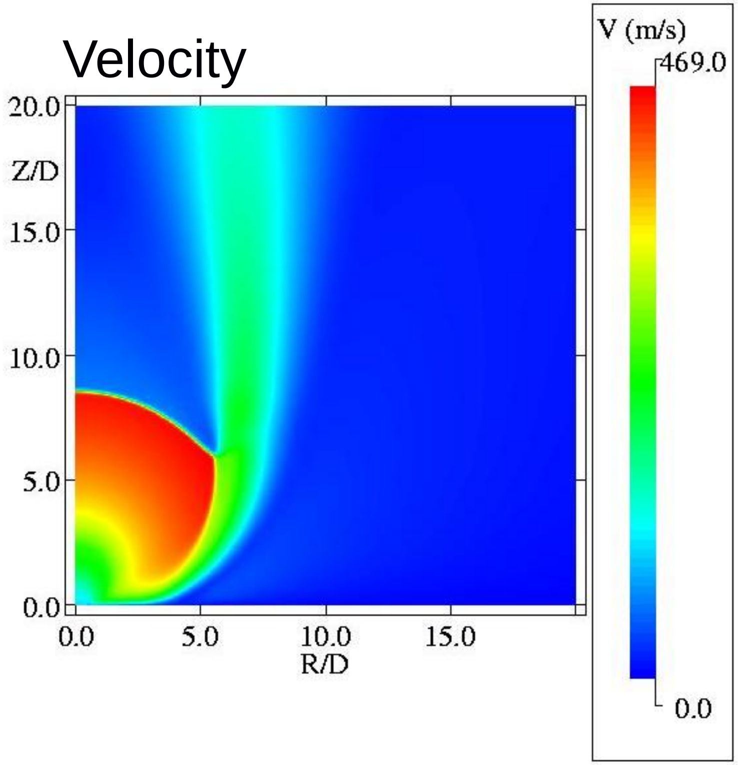
UNIVERSITY OF LEEDS

- 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)

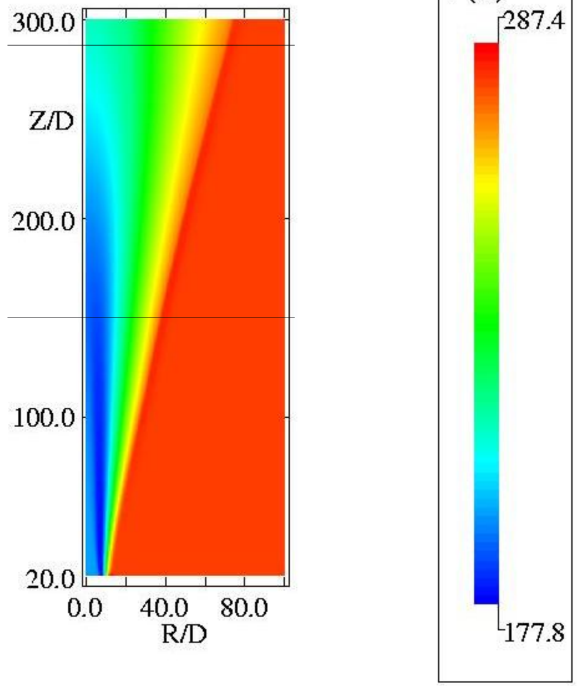
Validation: dense phase release

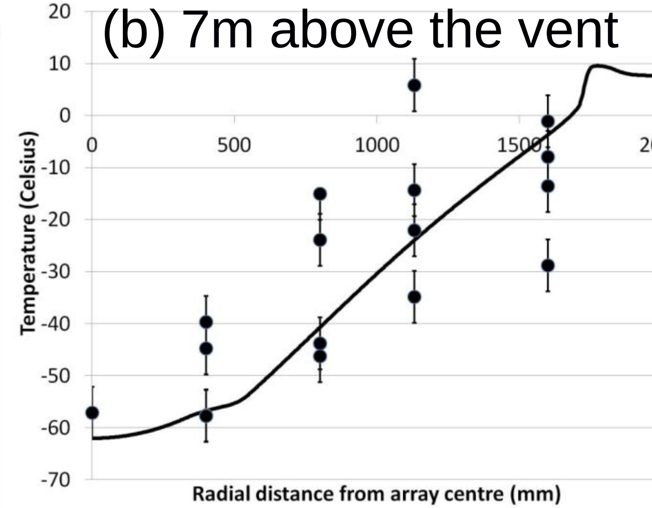
UNIVERSITY OF LEEDS

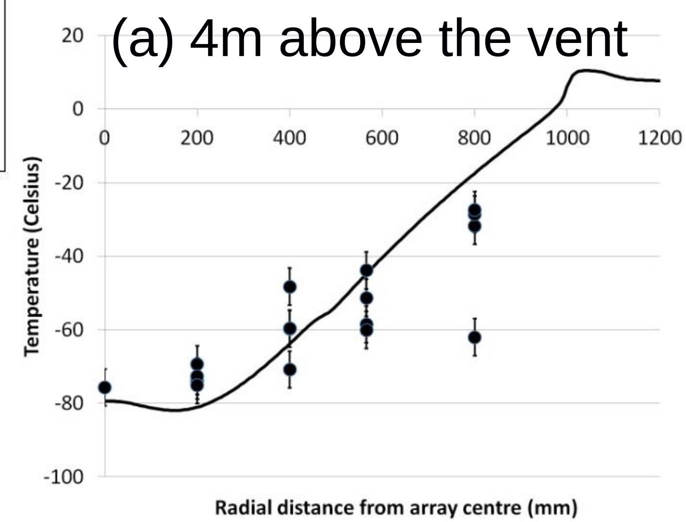
Measuring planes at:

- 4m (165D)
- 7m (288D)

Temperature







Predictions

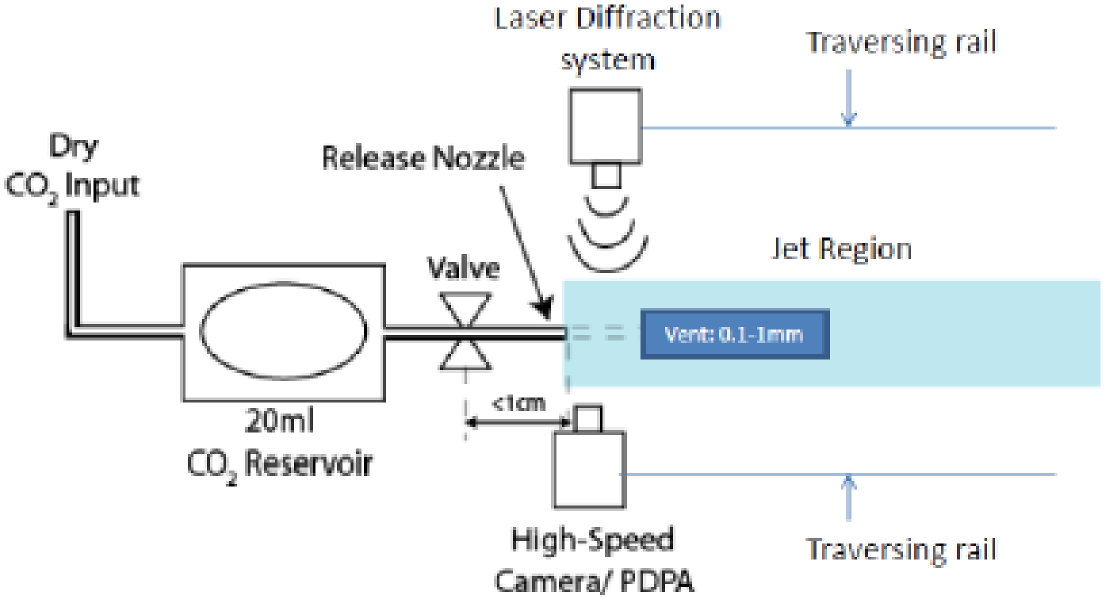
- Core temperatures good.
- Jet widths good.
- Some cross-wind effects.

Particle experiments

UNIVERSITY OF LEEDS

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

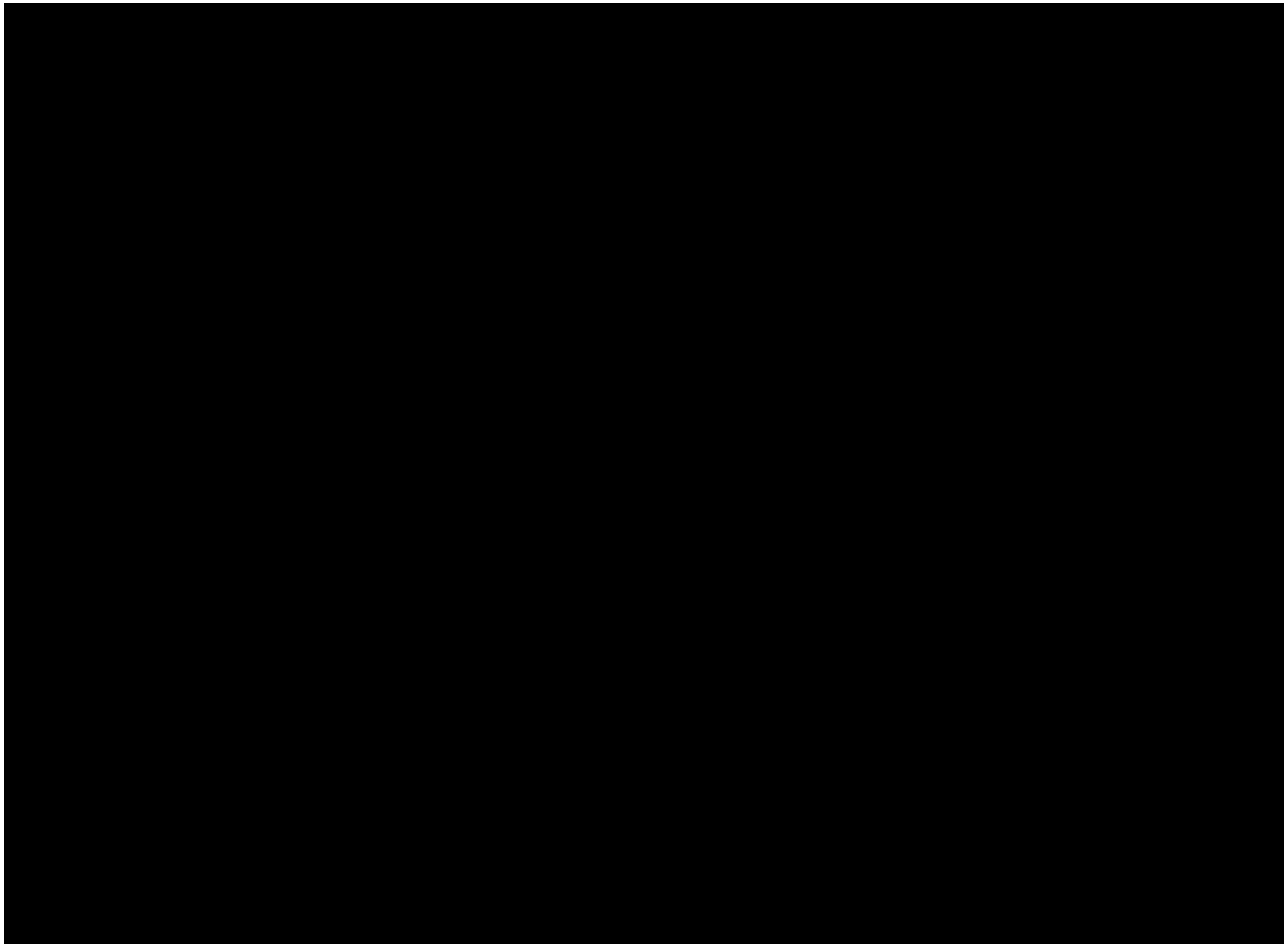
- **Solution:** Laboratory-scale experiments in a ventilated chamber
  - 20ml canister of liquid CO_2 pressurised to 68.9 bar at ambient temp.
  - Connected to a nozzle at one end of a Perspex box 50x50x500mm.
  - Two nozzles flush with inside of box: 0.5mm and 1.0mm in diameter (D).
  - Phase Doppler 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

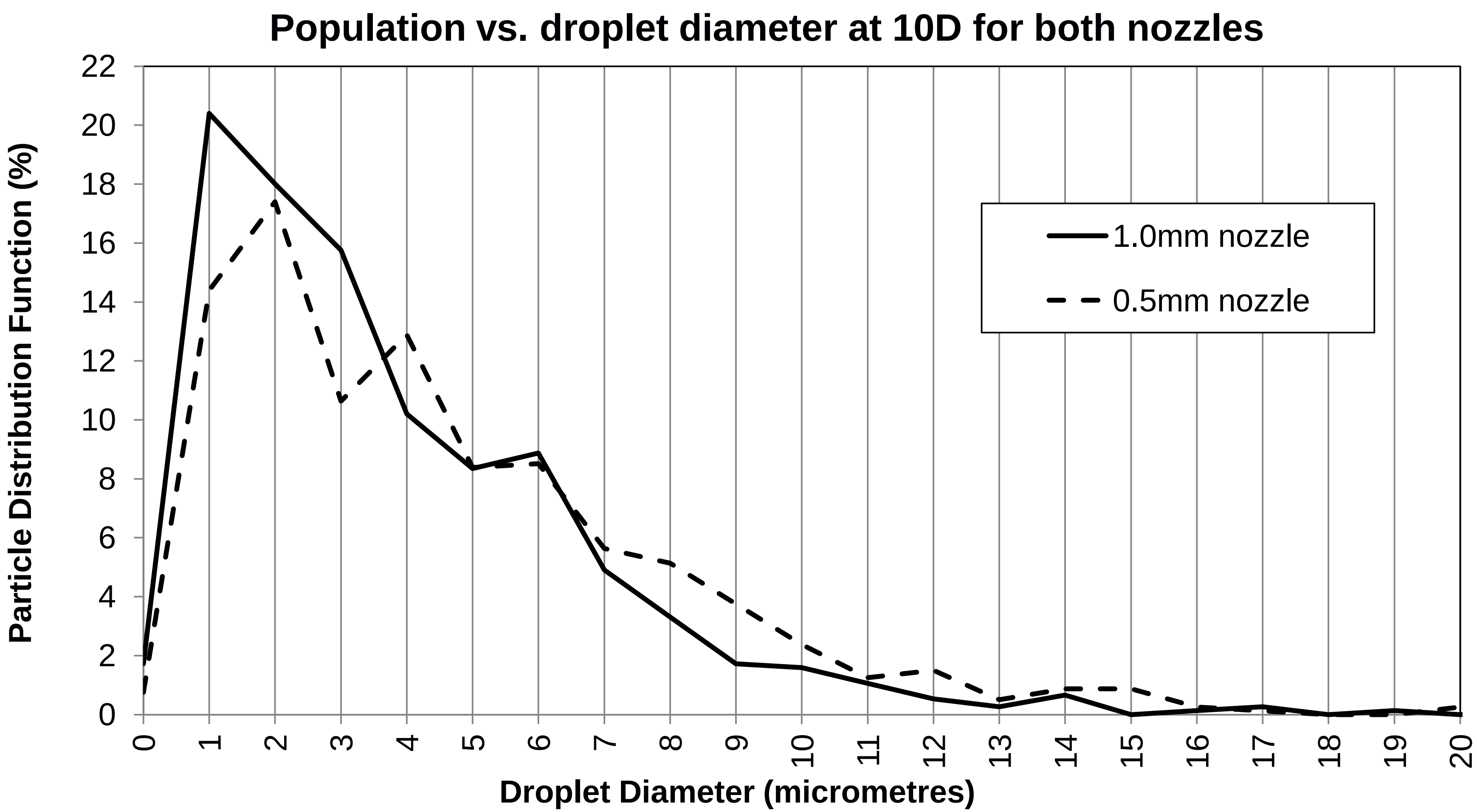
UNIVERSITY OF LEEDS

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



Individual particles are visible.

Results – initial particle distribution

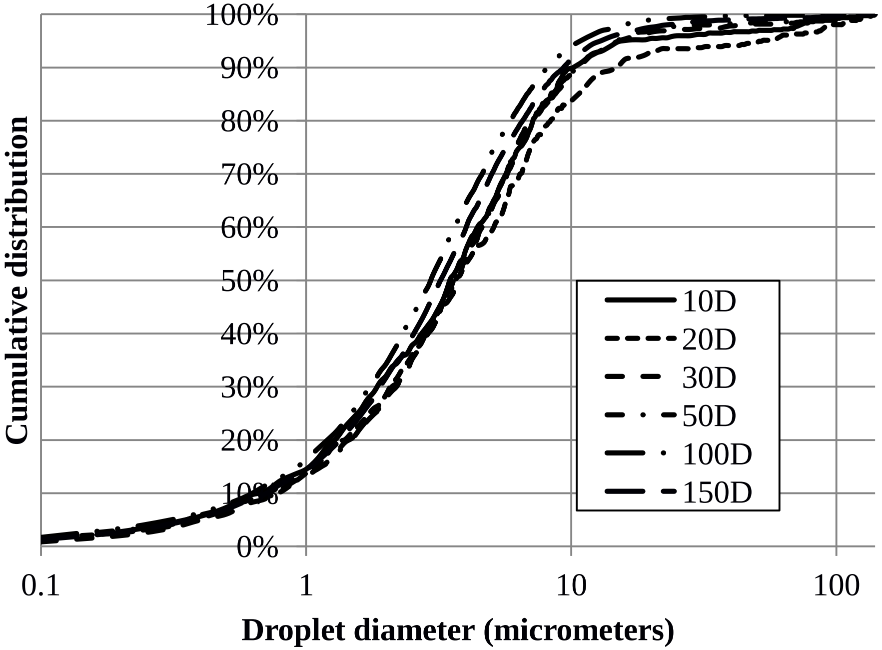


- Initial particle distribution post-Mach shock is centred on 1-2 micrometres.
- These particle sizes are in agreement with Weber number predictions.

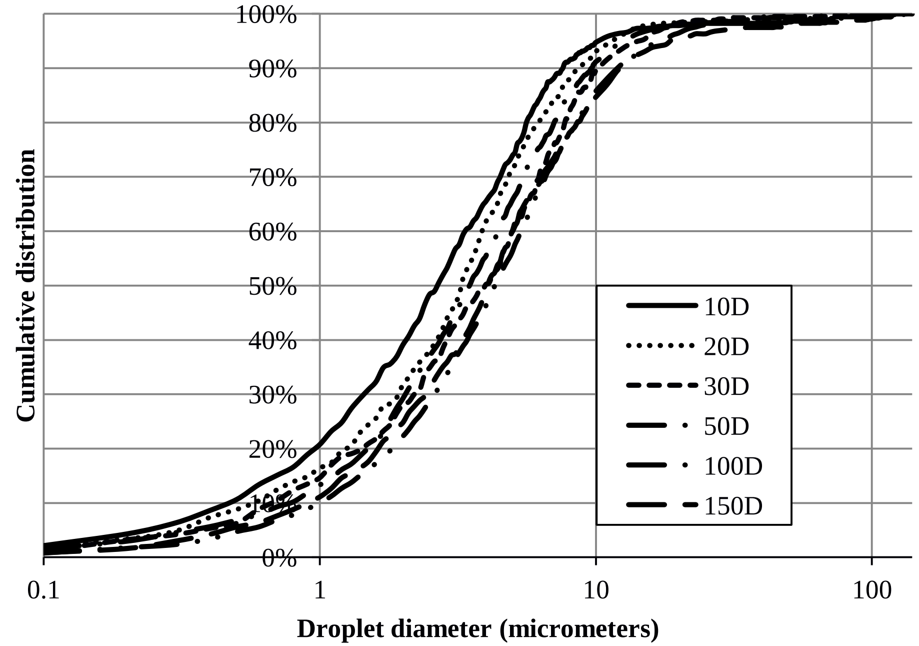
Results – particle behaviour along jet

UNIVERSITY OF LEEDS

- 0.5mm nozzle: no agglomeration



- 1.00mm nozzle: agglomeration!

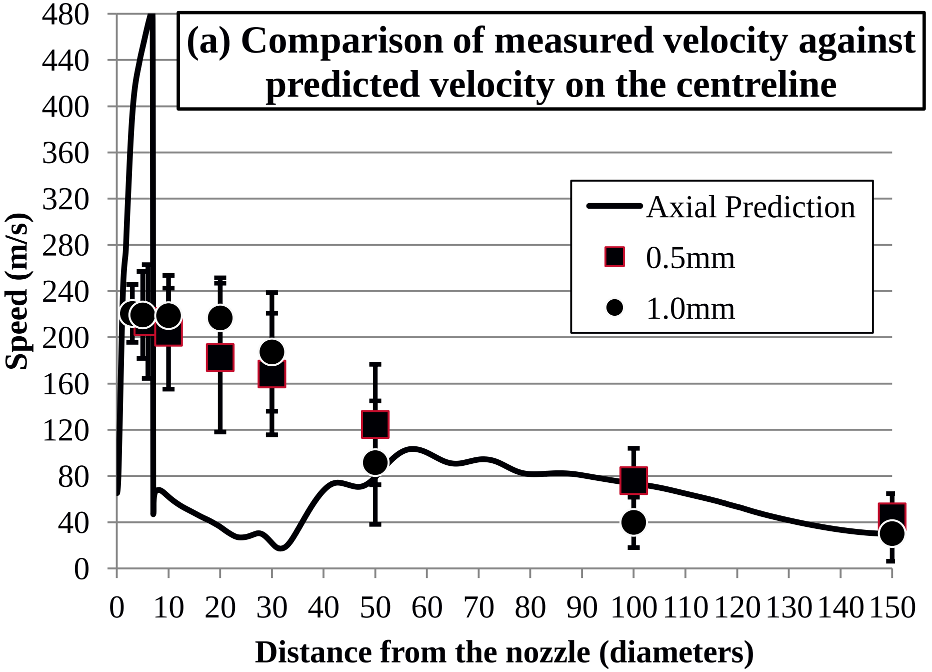


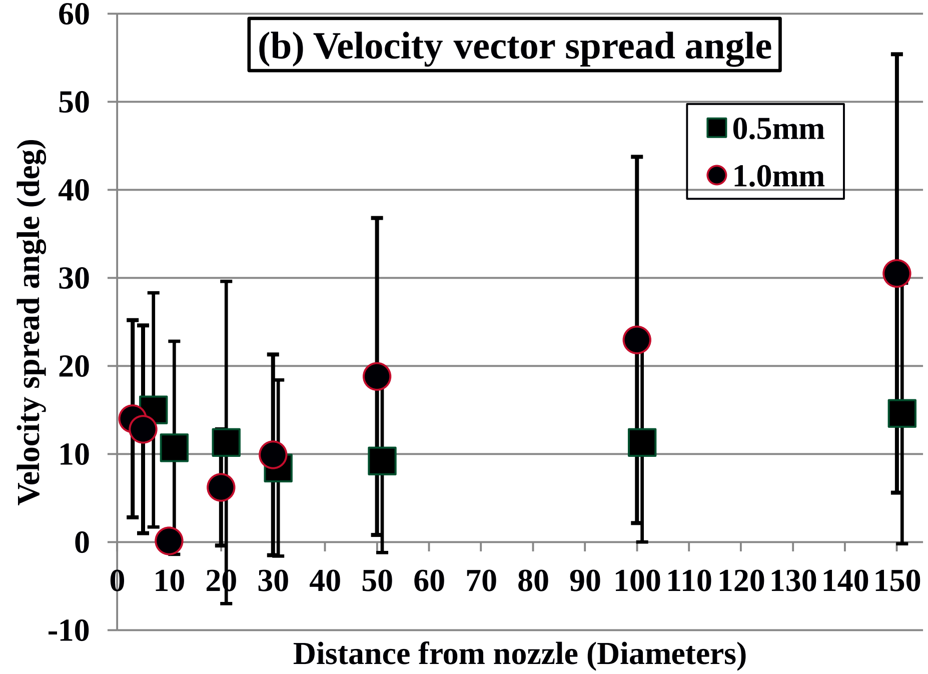
- No change in PDF along the jet for the 0.5mm nozzle case.
- Shift of PDF -> evidence of agglomeration in 1.0mm nozzle case.

Why?

Results – particle behaviour along jet

UNIVERSITY OF LEEDS



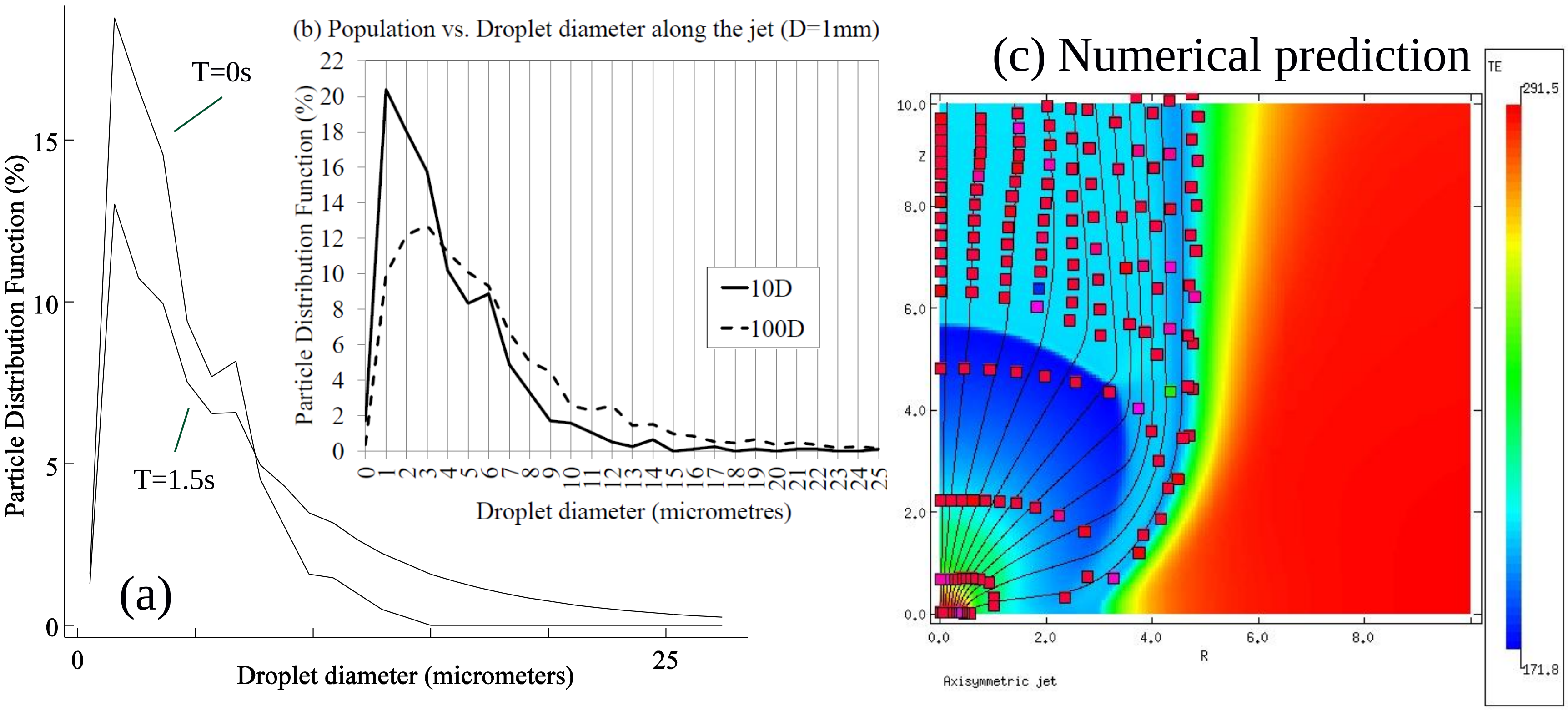


- Particles are not in equilibrium with the flow until at least 50D.
- Supported by theoretical calculations of thermal and dynamic relaxation times for these specific nozzles.
- Instantaneous velocities are further away from the centreline in the 1.0mm case. Indications of particles following the turbulent motion?

Results – particle behaviour along jet

UNIVERSITY OF LEEDS

- Test of a turbulent shear agglomeration model using the k-epsilon turbulence model (Saffman JFM **1** 16-30 1956).



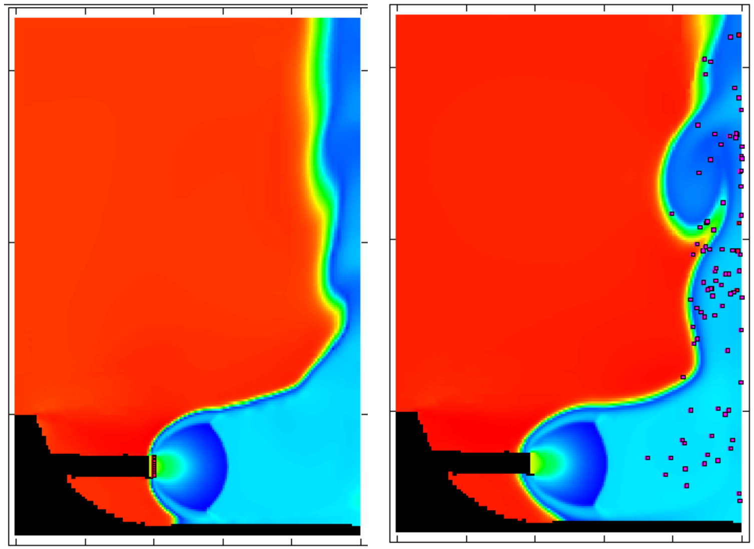
- Numerical agglomeration model is able to reproduce this agglomeration.
- Experimental velocity variation thus reflects turbulence in the jet.

Application to a large-scale scenario

UNIVERSITY OF LEEDS

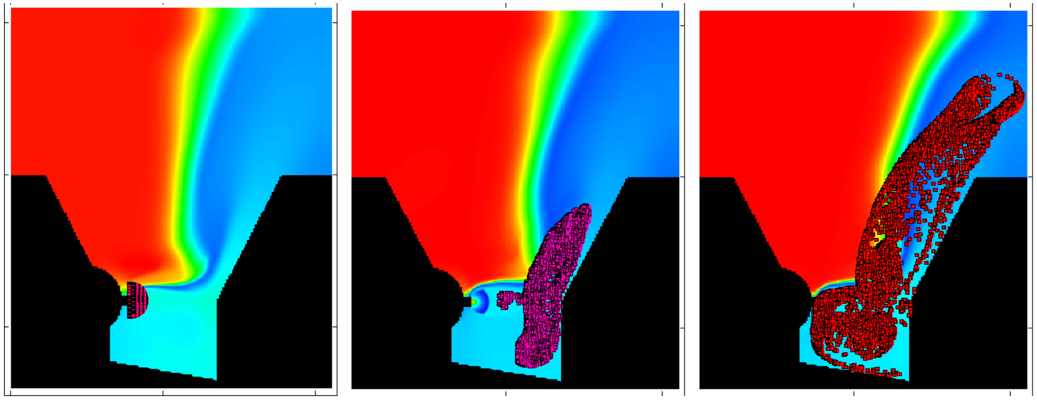
• Lagrangian particle tracker, initial distribution imposed from labscale measurements. Non-equilibrium effects allowed for through particle relaxation time according to viscous drag.

A Rupture Case



• Particles in equilibrium with flow.
• No particles embedded into wall.
• Minimal deposition in the crater.

A Puncture Case



• Particles not in equilibrium with flow.
• Particle distribution imposed post-shock.
• ~1% of particles embedded in wall.
• But, what about the particles swirling?

Conclusions

UNIVERSITY OF LEEDS

- Novel dispersion model covering the necessary range of pressures and temperatures in accidental releases of CO_2.
- Validated against large-scale experimental releases.
- 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.
  - For these small nozzles, particles are initially out of equilibrium.
- Applied to large-scale scenarios for accidental or operational releases in CCS scenarios.
- Future work:
  - Experimental and numerical modelling of turbulent pipe flow.
  - Refinement of particle motion and evolution models.

Thank you for listening

Any questions or comments?

UNIVERSITY OF LEEDS

Contact details: Dr Chris Wareing
C.J.Wareing@leeds.ac.uk
+44 113 343 1619

The Don Valley CCS Project is co-financed by the European Union's European Energy Programme for Recovery. The sole responsibility of this publication lies with the author. The European Union is not responsible for any use that may be made of the information contained therein.

COOLTRANS Partners:
National Grid Carbon Ltd, GL Noble Denton, The UK Health and Safety Laboratory, Pipeline Integrity Engineers, Atkins Global, Penspen Integrity
UK University partners: Leeds, Manchester, Newcastle, Nottingham, University College London, Warwick.

National Grid Carbon Ltd
National Grid Carbon Ltd is a non-regulated, independent subsidiary of National Grid, created to develop carbon dioxide transportation infrastructure in the UK. National Grid is an international electricity and gas company and one of the largest investor-owned energy companies in the world.

GL Noble Denton
GL Noble Denton are independent advisors providing consulting, design, assurance and project execution services, combining excellent engineering and analytical skills with operational experience of offshore, maritime and onshore oil and gas assets.