School of Physics & Astronomy / SCAPE
FACULTY OF MAPS / ENGINEERING

UNIVERSITY OF LEEDS

Numerical simulation of cryogenic machining with CO_2

Applying expertise from the carbon capture and storage sector

Monday 15th January 2018, Nuclear AMRC, Sheffield

C J Wareing, S Van Loo, S A E G Falle and M Fairweather
University of Leeds, Leeds, LS2 9JT, United Kingdom
C.J.Wareing@leeds.ac.uk S.VanLoo@leeds.ac.uk M.Fairweather@leeds.ac.uk

My background…

UNIVERSITY OF LEEDS

- Research Fellow at the University of Leeds, interested in:
  - Computational fluid hydrodynamics and magnetohydrodynamics
  - Multi-phase, particle-laden flows with complex equations of state
- Applications in Astrophysics, Applied Maths, Chemical and Mechanical Engineering
  - Star formation, evolution and death
  - Hall/Electron MHD turbulence
  - Carbon capture and storage – high pressure CO_2 transport pipelines
  - Cryogenic machining with CO_2
- Industry collaboration though National Grid's COOLTRANS Project (2011-15) and 2 EU projects
- Currently, an ongoing collaborative effort with the Nuclear AMRC to understand the fundamental behaviour of CO_2 in cryogenic machining, through thermodynamics and simulations

C.J.Wareing@leeds.ac.uk

Overview

Carbon capture and storage aims to capture CO_2 at emission from power source or other and store it, avoiding atmospheric release and climate effects.

- COOLTRANS – National Grid carbon capture and storage research programme.
  - **Required pragmatic quantified risk assessment (QRA) models**
  - **Robust source conditions for use in far-field CFD studies**
- Leeds: near-field sonic dispersion of CO_2 from high pressure pipelines
  - Developed thermodynamic model and numerical method
  - Modelled venting, puncture and rupture releases to validate approach
  - Application to full-scale ruptures to establish risks for HSE approval and UK CCS competition
  - Measuring and modelling particle evolution in turbulent sonic CO_2 jets
- Collaboration with Nuclear AMRC – applying the same model and method at smaller scales

Near-field dispersion numerical method

- Adaptive, finite-volume grid algorithm with rectangular mesh

- Grid adaption achieved by successive overlaying of refined layers of computational mesh
  - For steep gradients in variables, e.g. at **Mach shock**, mesh more refined. Generation of fine grids in regions of high spatial and temporal variation
  - Conversely, coarser grids allowed where flow field is smooth

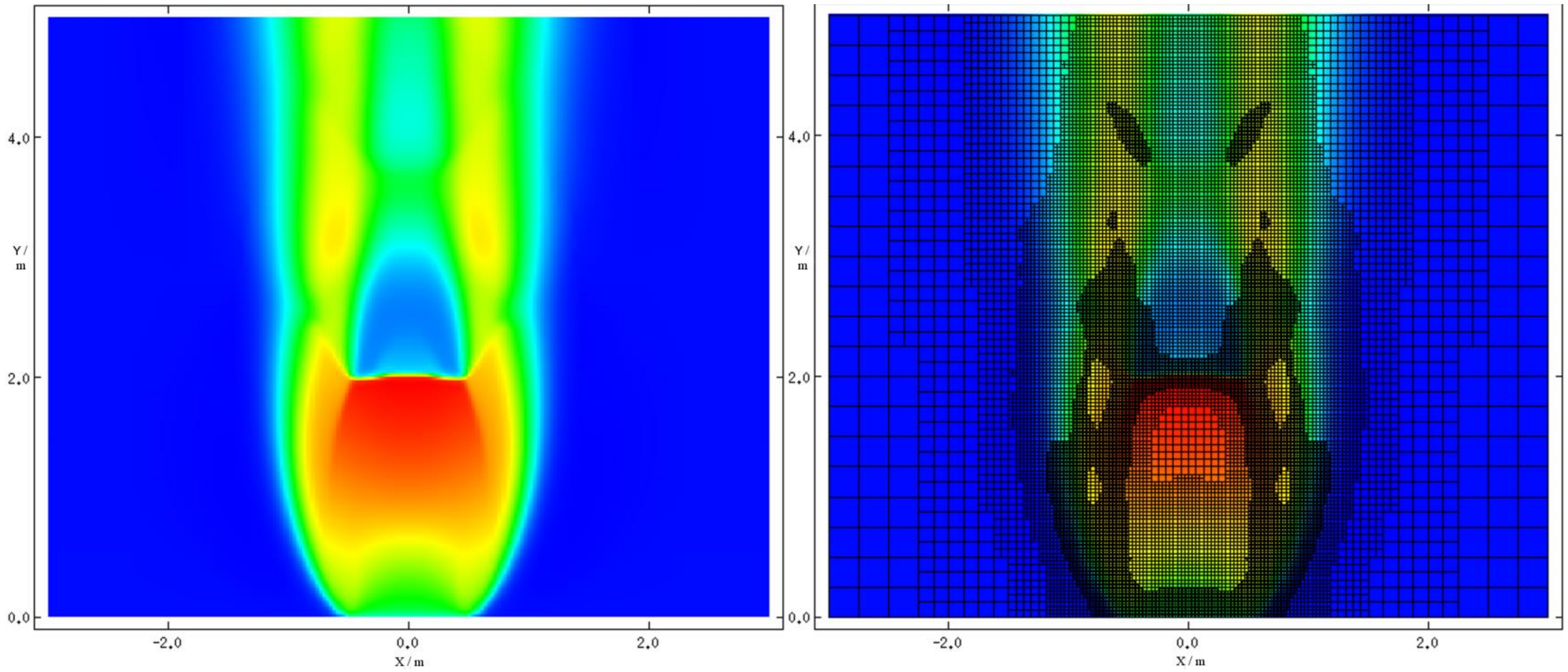
- ***k*-ε turbulence model available**, including compressibility correction
- Second-moment Reynolds stress turbulence model also available, including round-jet correction

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

- Efficient, general-purpose shock-capturing, upwind, second-order-accurate Godunov numerical scheme with Harten, Lax, van Leer Riemann solver

- Compared to FLUENT, this method is considerably **faster** and **able to model solid CO_2**
  (FLUENT uses the NIST REFPROP database, or GERG, which is limited to gas and liquid CO_2 above the triple point temp.)

Near-field dispersion numerical method



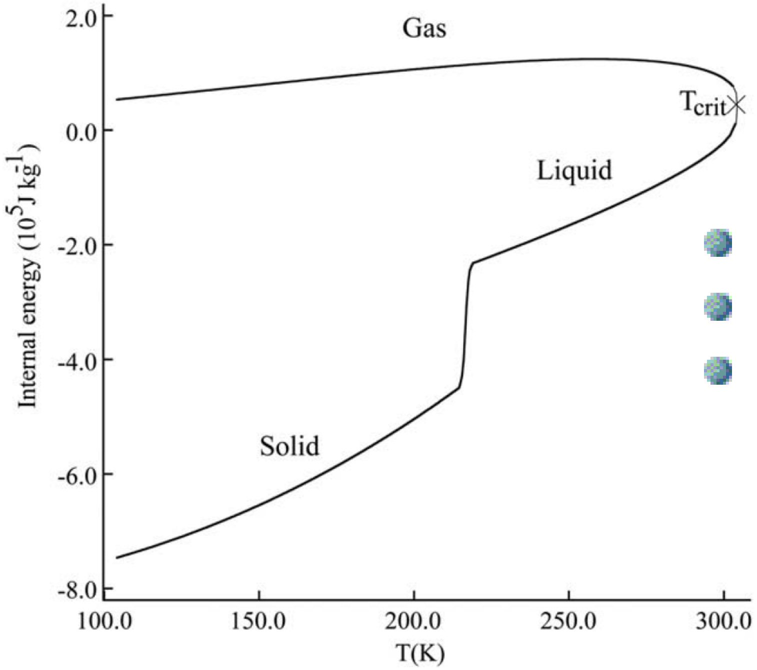
Adaptive mesh refinement grid mapped onto mean velocity predictions in the region of a Mach disc

- **Expensive computations**
- Require supercomputer for large-scale pipeline simulations.
- Desktop for small-scale simulations – e.g. cryogenic machining.

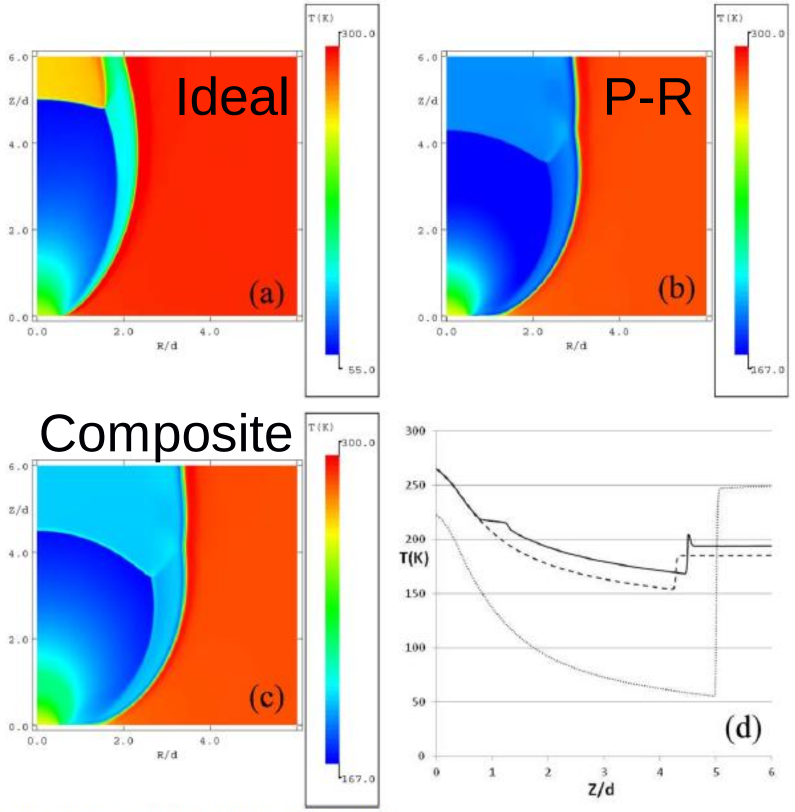
Note the axis units are in release diameters.

Thermodynamic model

- Novel **composite equation of state for pure CO_2** employing:
  - Peng-Robinson (1976) equation of state (EoS) in gas phase
  - Tabulated data derived from Span and Wagner (1996) EoS for liquid phase and vapour pressure. Span and Wagner underpins GERG/REFPROP.
  - Accurate **solid CO_2 equation of state: Jager and Span (2012)**
- Calculations undertaken using Helmholtz free energy in terms of temperature and molar volume, as all other thermodynamic properties can be readily obtained from it



- Internal energy on saturation line
- T_{crit} marks critical temperature
- Triple point can be identified by steep connection between liquid and solid phases – latent heat of fusion



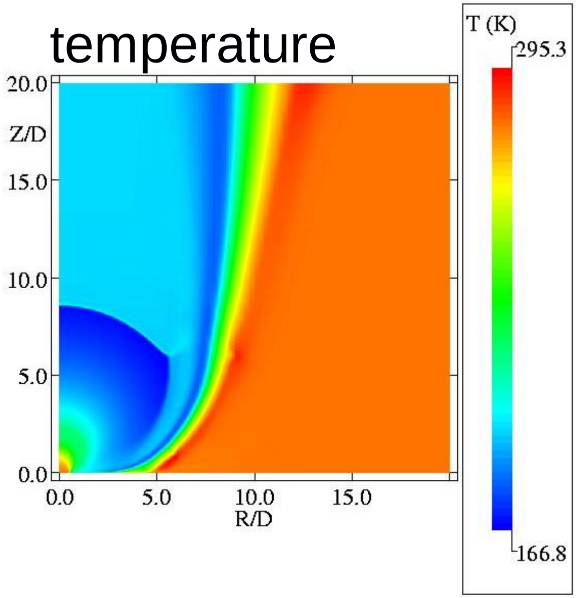
Temperature in the near-field of the flow domain.

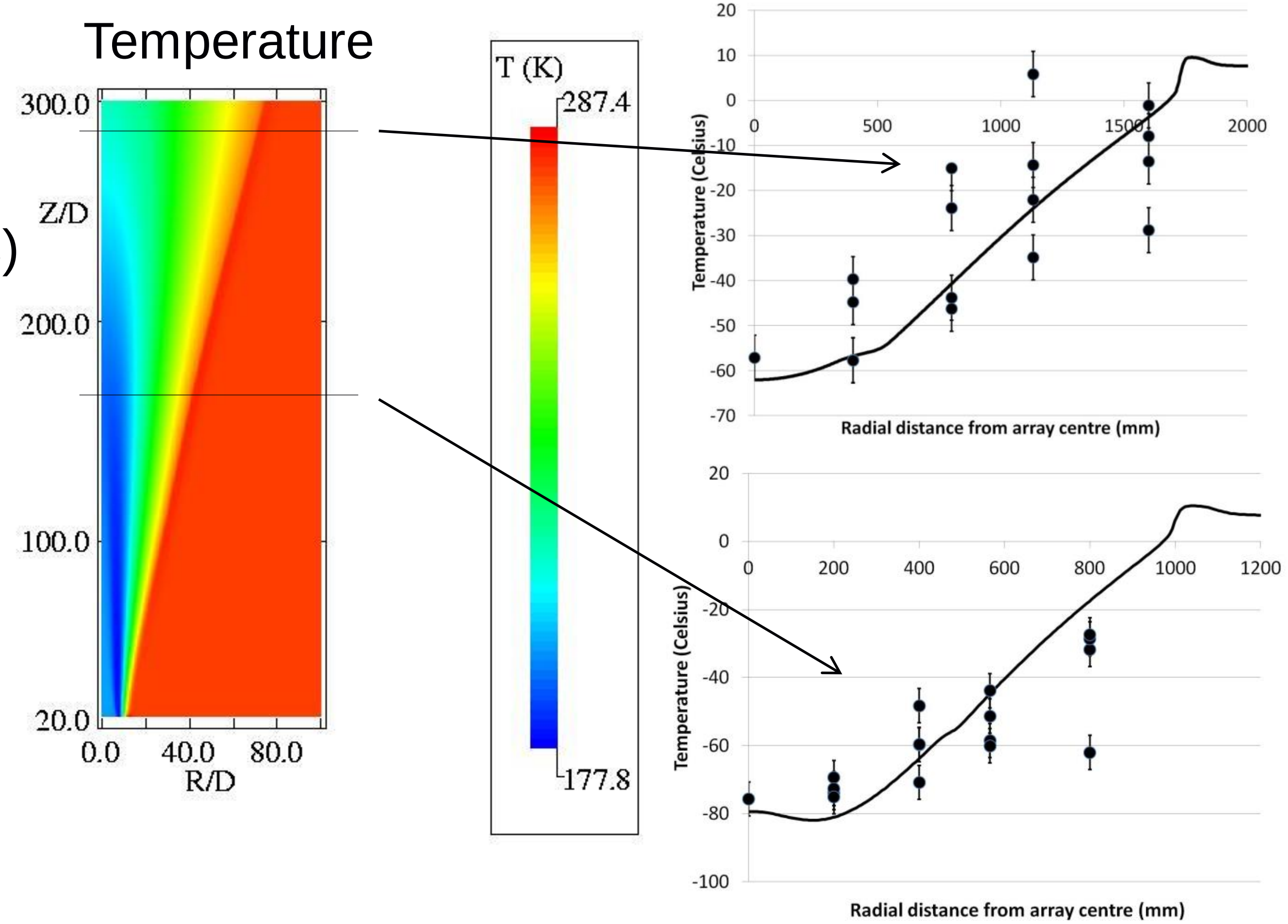
Ideal, or Peng-Robinson EoSs alone, do not work!

Validation – venting a 25mm pipe

- Dense phase release from a 150bar reservoir.
- Steady state release conditions achieved by supplying a driving pressure
- Measuring planes at 4m (165 nozzle diameters) and 7m (288D)

Near-field temperature



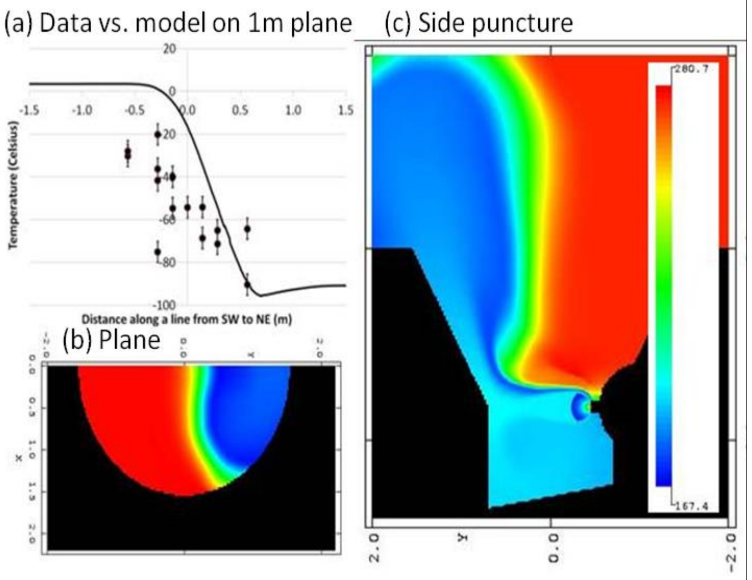


Far-field region up to 300D (7.5m) from the release

Wareing et al., Int. J. Greenhouse Gas Control, ***20****, 254-271 (2014)*

Further validation and application

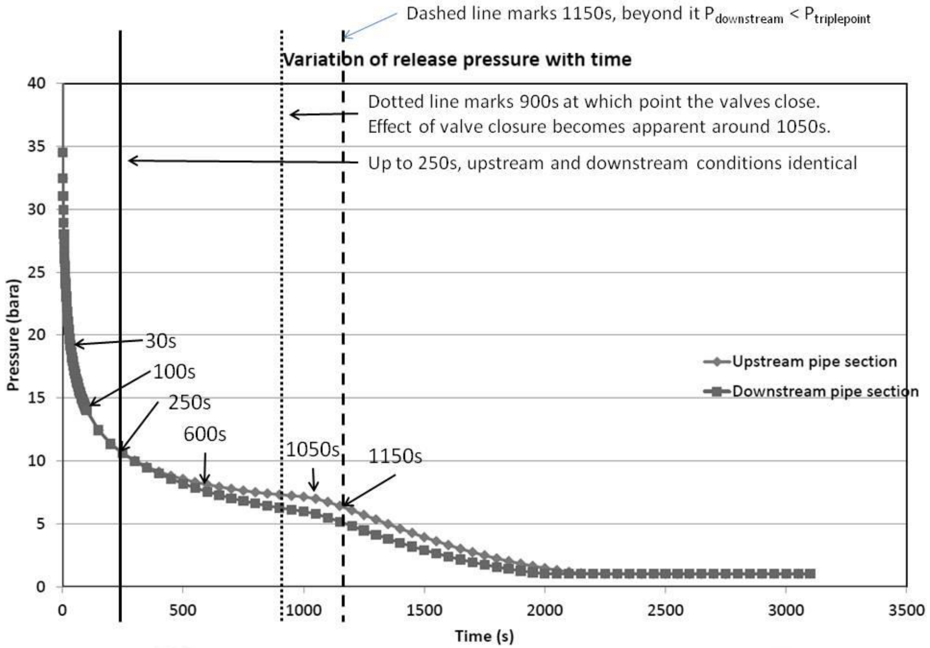
Validation - Punctures

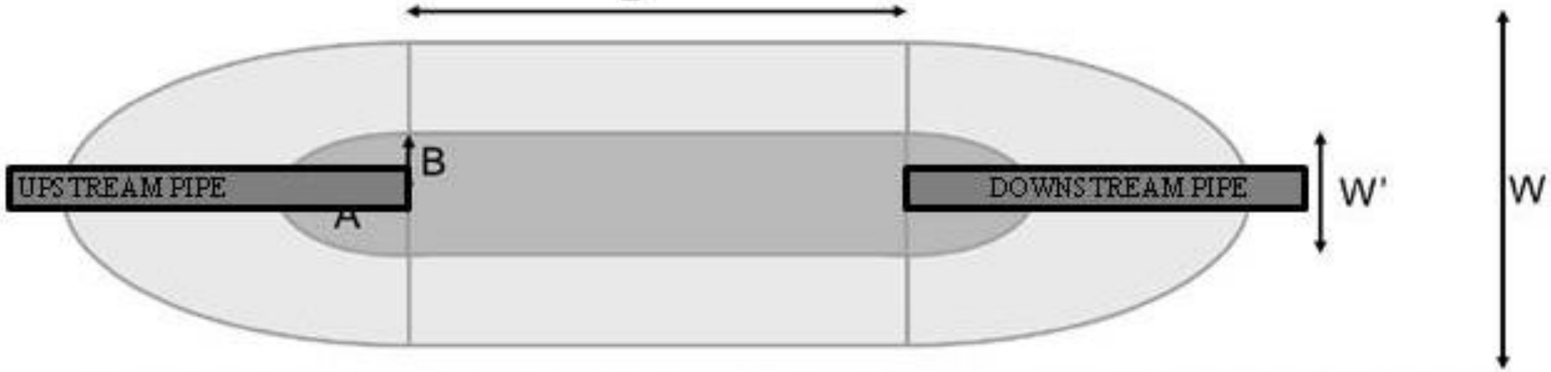


Wareing et al., Int. J. Greenhouse Gas Control, **29**, 231 (2014)

Application – full-scale rupture

- **0.6m diameter pipeline**.
- Pipeline pressurised to **150bar**.
- **Preformed craters** based on observations of real craters.
- **12m section of pipeline**.
- Experimental measurements on arrays above ground level.



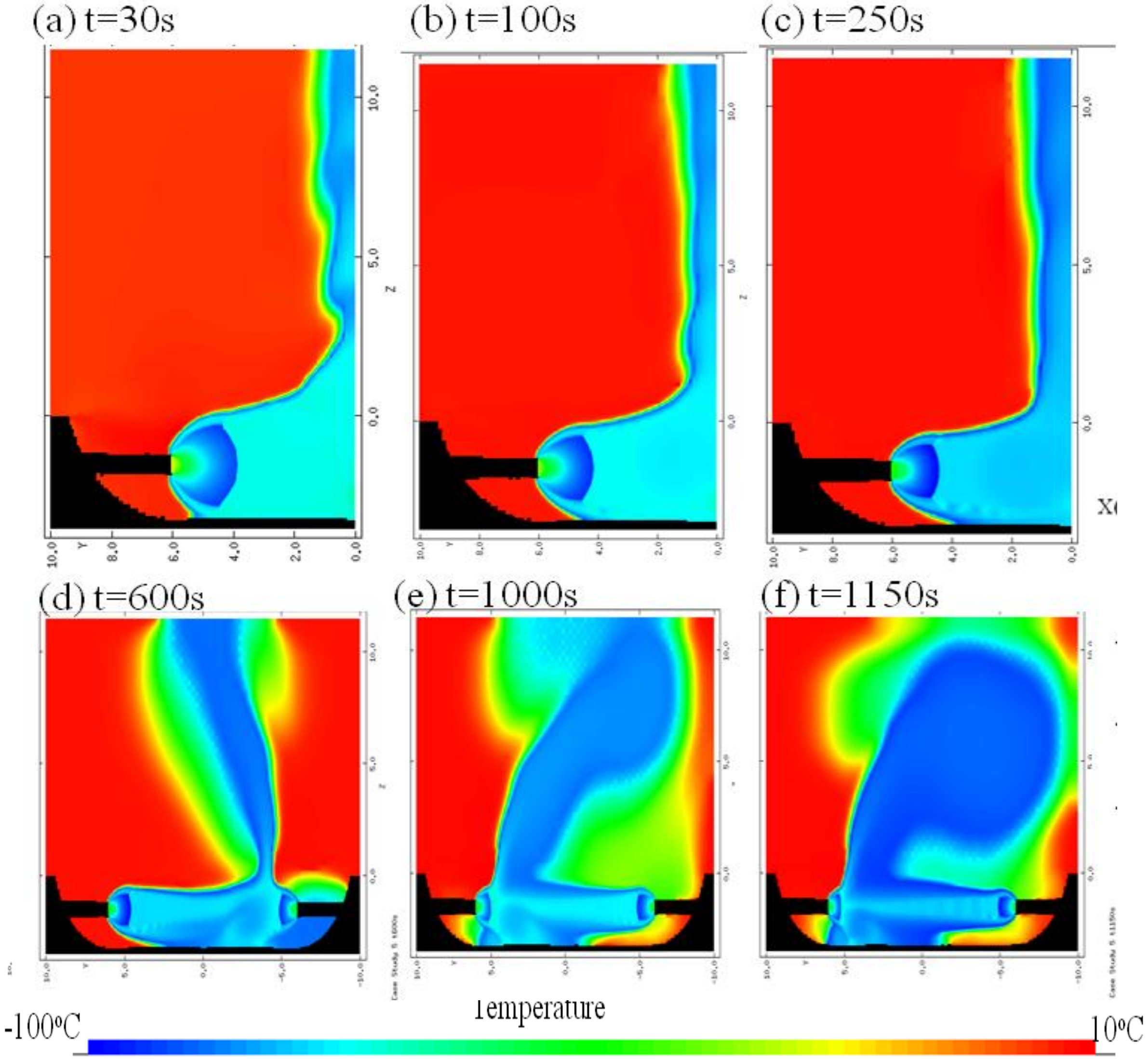


L = crater length, W = crater width, L'=length of flat base, W'=width of flat base,
D = crater depth, θ = wall angle, A = semi-major axis of base ellipse, B = 0.5 W'

Ruptures – full scale results

Pipeline diameter, D=0.6 m

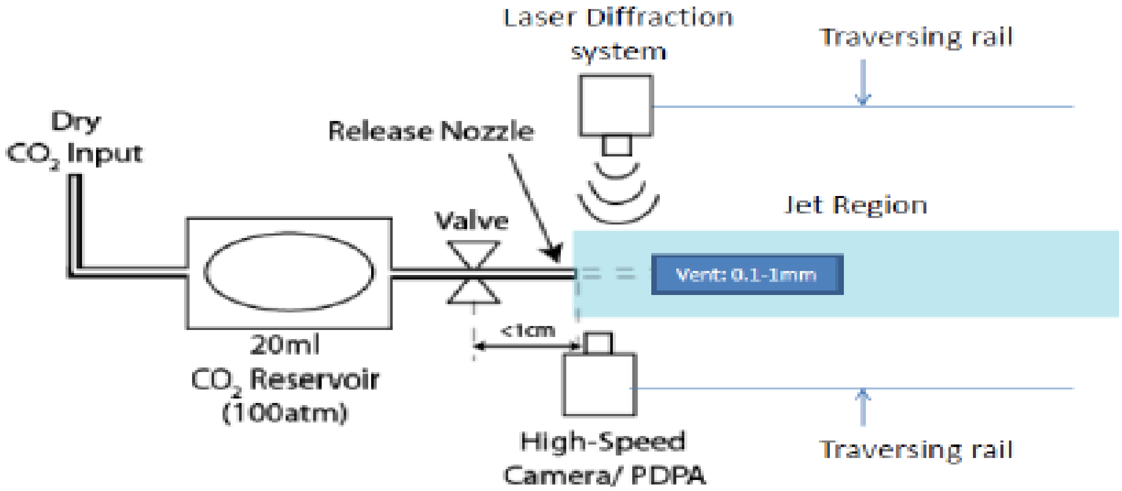
COSHER Project (Carbon Dioxide, Safety, Health & Environmental Risk), http://www.cosher.net/en/



Wareing et al., Int. J. Greenhouse Gas Control, **42**, Paper 1: p701, Paper 2: p712 (2015)

Problem – how do the CO_2 snow particles behave?

- **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
  - Designed to mimic pipeline discharge
  - Experimental scale is very close to that of cryogenic machining!



Particle evolution model

- Motion of particles computed using **Lagrangian particle tracker**
- Viscous drag in the low Reynolds number regime included
- Turbulent shear agglomeration model
  - Reproduces observed agglomeration in the 1.0mm diameter case
- Particle mass changes according to

$$\frac{1}{m_p}\frac{\mathrm{d}m_p}{\mathrm{d}t} = \frac{[p_\infty - p_s(T_\infty)]}{\tau_t p_s(T_\infty)}\left[\mathrm{s}^{-1}\right]$$

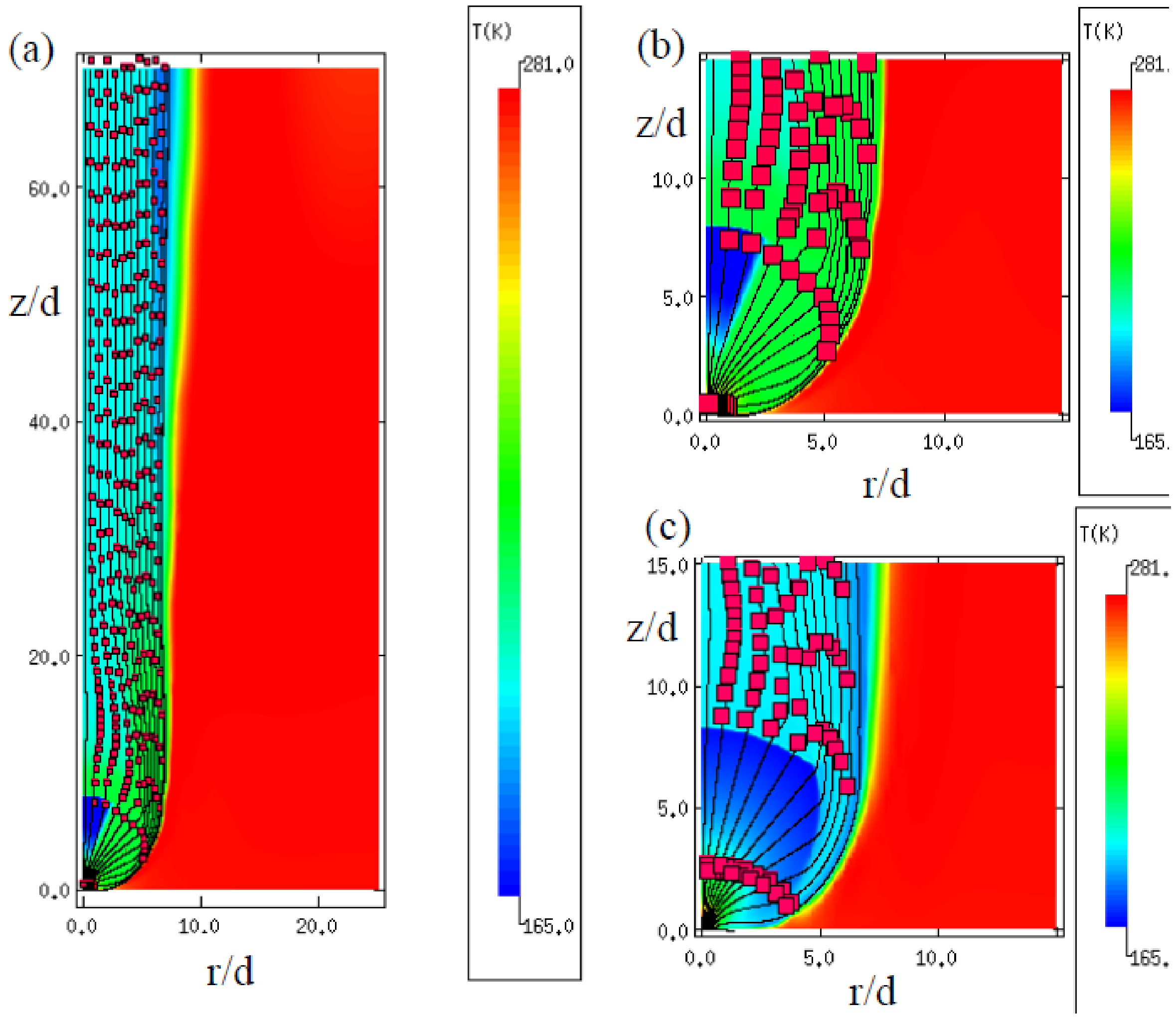
- Thus defining a thermal relaxation time

$$\tau_t = \frac{\rho_p r_p^2 L^2 w_v}{3\kappa R T_\infty^2}[\mathrm{s}]$$

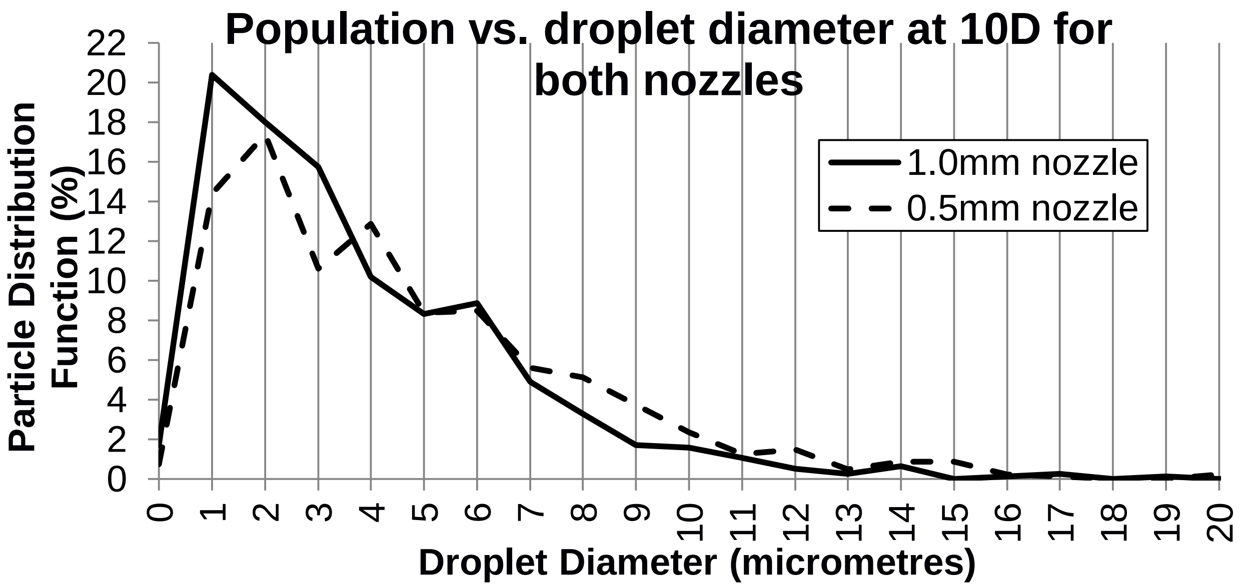
- **Fluid and particles two-way coupled** through fluid-temperature dependent particle relaxation model

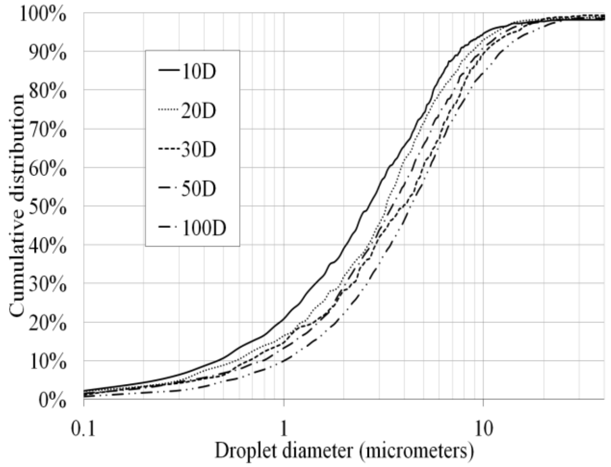
Particle results from simulation and experiment

UNIVERSITY OF LEEDS



Wareing et al., Procedia Engineering, **102**, 1621 (2015)





- 1.0mm nozzle: agglomeration!
- No agglomeration for 0.5mm nozzle.

Collaboration with the Nuclear AMRC

Specification

UNIVERSITY OF LEEDS

“The Nuclear AMRC wishes to gain more fundamental knowledge on the behaviour of multiphase CO_2 jets for the purpose of cooling machining processes”

- Phase 1
  - **Deliverable**: preliminary simulation of two nozzle geometries, one of which employing previous free-jet Leeds geometry
  - Fixed diameter and mass-flow
  - Simulation to extend to 30 nozzle diameters downstream
- Phase 2
  - **Deliverable**: 6 2D simulations with refinements from experiment. Variation of pipe pressure, nozzle shape and diameter. 1 3D simulation repeating the refined 2D base case.

Specification

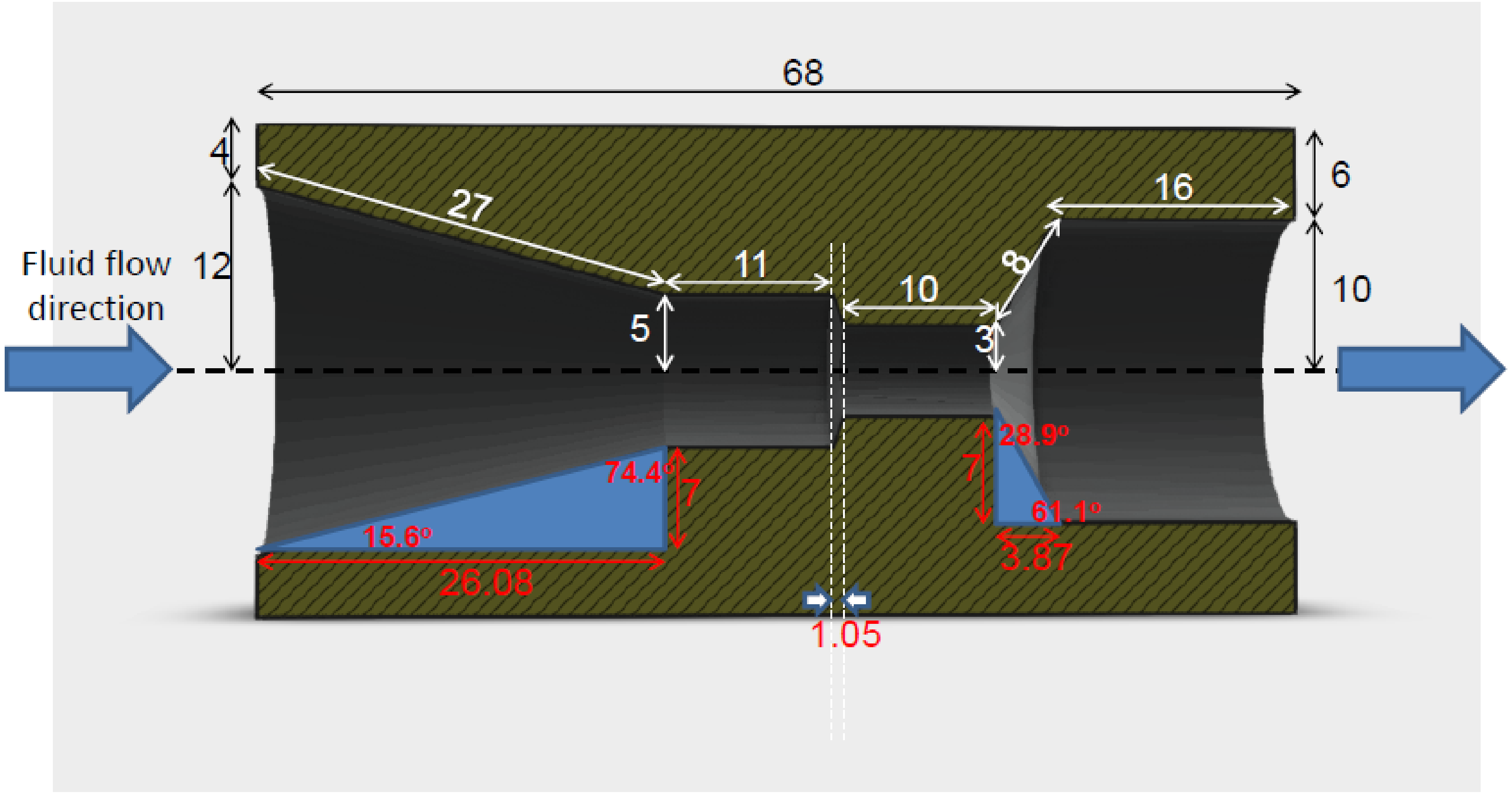
- Early information from kick-off meeting:-
  - Gaseous CO_2 at P,T = 35bar, 20^{o}C combines with liquid CO_2 at P,T = 65bar,-7^{o}C approximately 1m from tool tip
  - Combination mechanism covered by NDA
  - Pipework from there to tool tip is not uniform
- Known nozzle diameter: 0.6mm. Mass-flow: 10 kg/hr
- Assume flow into tool is saturated equilibrium CO_2 thermodynamic condition closest to post-combination conditions. Hence, in 6mm pipe:

  Pressure, Temp, solid fraction = 2.9518e6 Pa, 267 K, 0.0725 kg/kg
- By Bernoulli, refined nozzle condition is:

  Temp. = 249.47 K, Press. = 1.7558 Pa, solid fraction = 0.12911 kg/kg,
  Density = 86.443 kg/m^3, Velocity = 188.20 m/s, mass-flux = 10 kg/hr

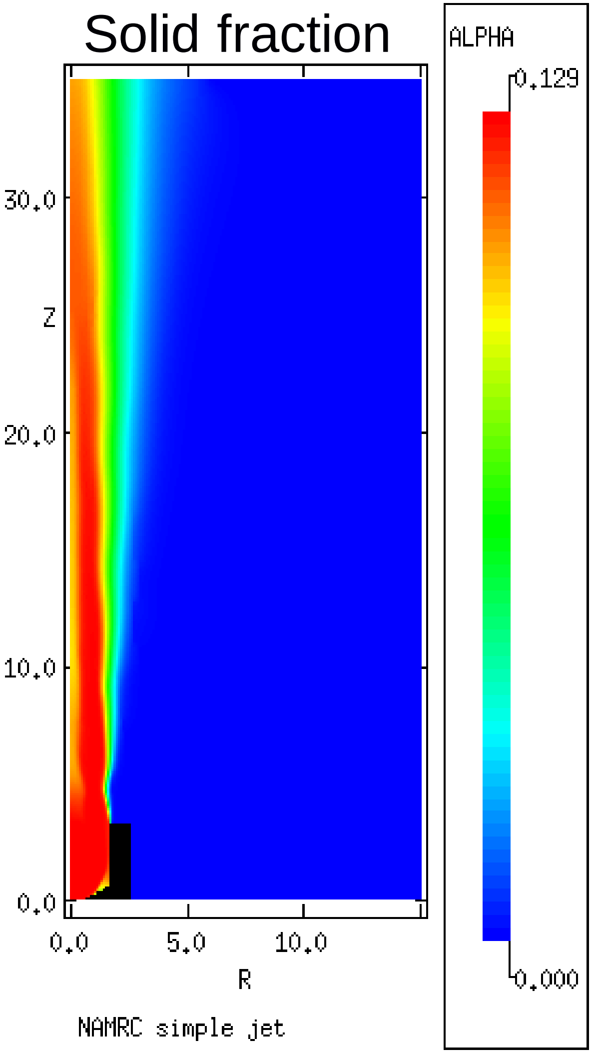
Complex nozzle geometry

Nozzle dimensions (Units: 1/10ths of a mm)

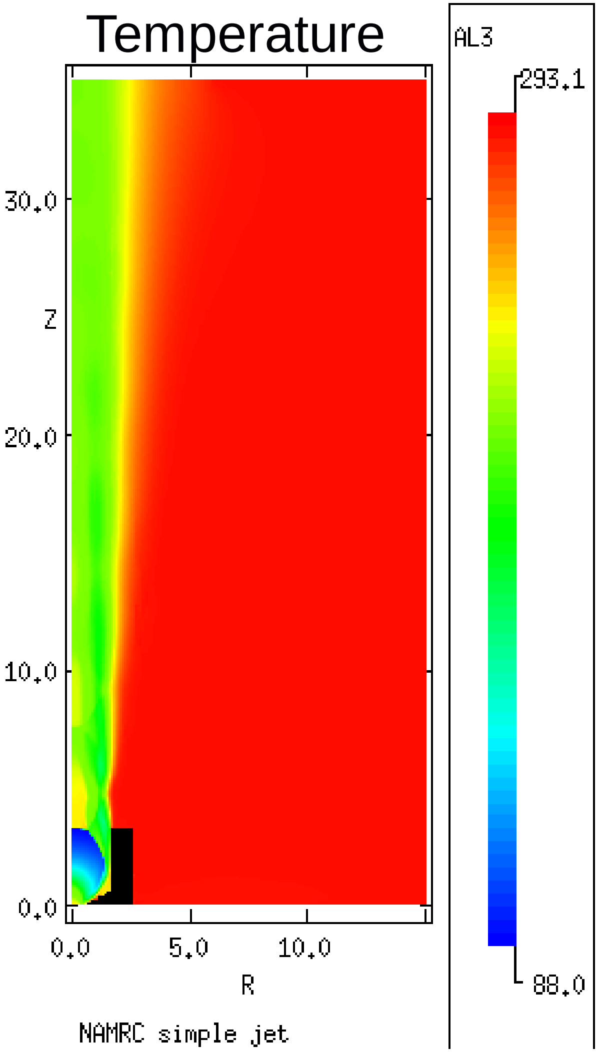


Imported via Autodesk 360 viewer: https://a360.autodesk.com/viewer/#
Imported measurements in **black** and **white**. Inferred measurements in **red**.

Phase 1 non-equilibrium results



Solid fraction



Temperature

Phase 2

#	Description
1	Base case repeated from Phase 1. Standard D=0.6mm nozzle, full hex key, nozzle conditions derived from treating the pipe as a ‘reservoir’ with above conditions. Extension adding particles.
2	High pressure of 38bar in the pipeline. No particles.
3	Low pressure of 33bar in the pipeline. No particles.
4	Half-height hex key socket. No particles.
5	D=1.0mm standard shape nozzle. No particles.
6	D=0.2mm sharp plate nozzle. No particles.
7	Repeat of base case in 3D. No particles.

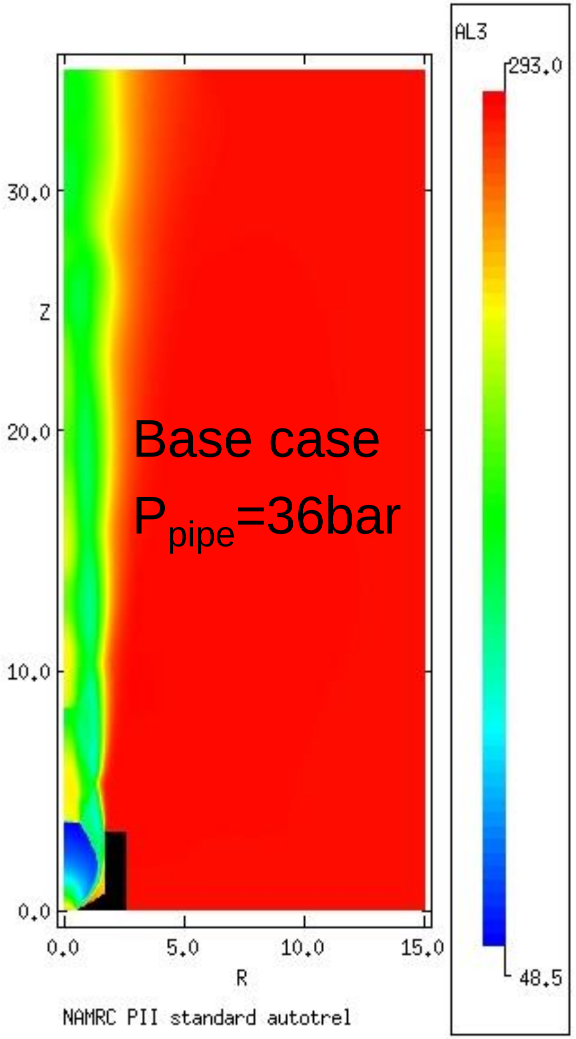
Phase 2

UNIVERSITY OF LEEDS

	Mass-flow [kg/hr]	Temp. [K]	Pres. [Pa]	Density [kg/m^3]	Solid density [kg/m^3]	Vel. [m/s]	CO$_2$ fraction [kg/kg]	Solid fraction [kg/kg]
1	42.96	244.24	20.053e5	57.02	1072	209.28	1.0	1.315e-3
2	43.82	243.66	21.099e5	50.42	1075	206.76	1.0	1.781e-3
3	51.93	244.81	18.397e5	61.69	1069	213.44	1.0	7.359e-4
4	As (1)							
5	135.95	244.84	20.175e5	57.32	1069	209.71	1.0	3.493e-3
6	5.409	243.87	20.046e5	57.11	1074	209.33	1.0	0.0e0
7	As (1)							

Phase 2 results: variation of pressure

Temperature

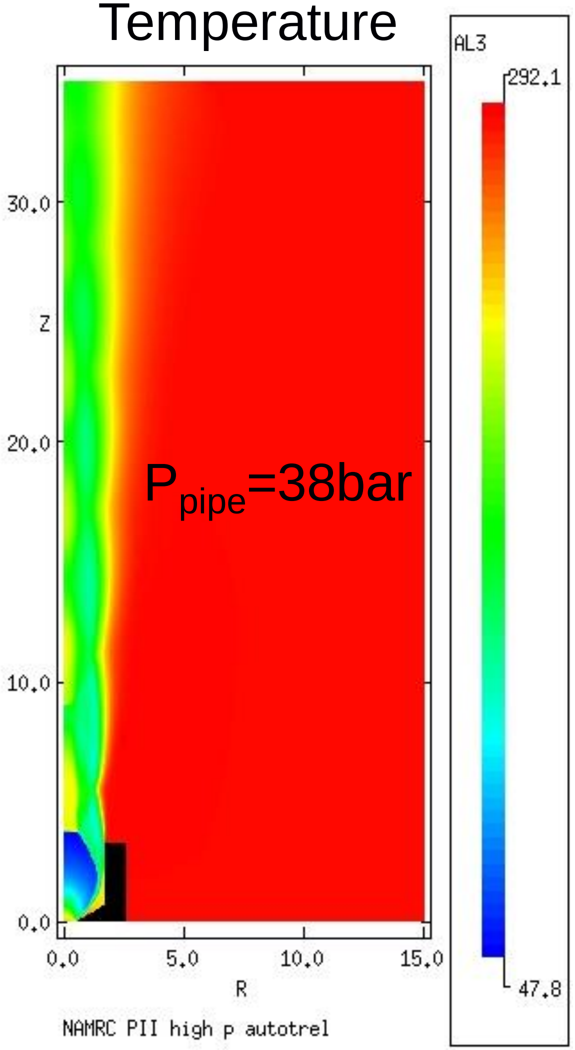


NAMRC PII standard autotrel

Base case

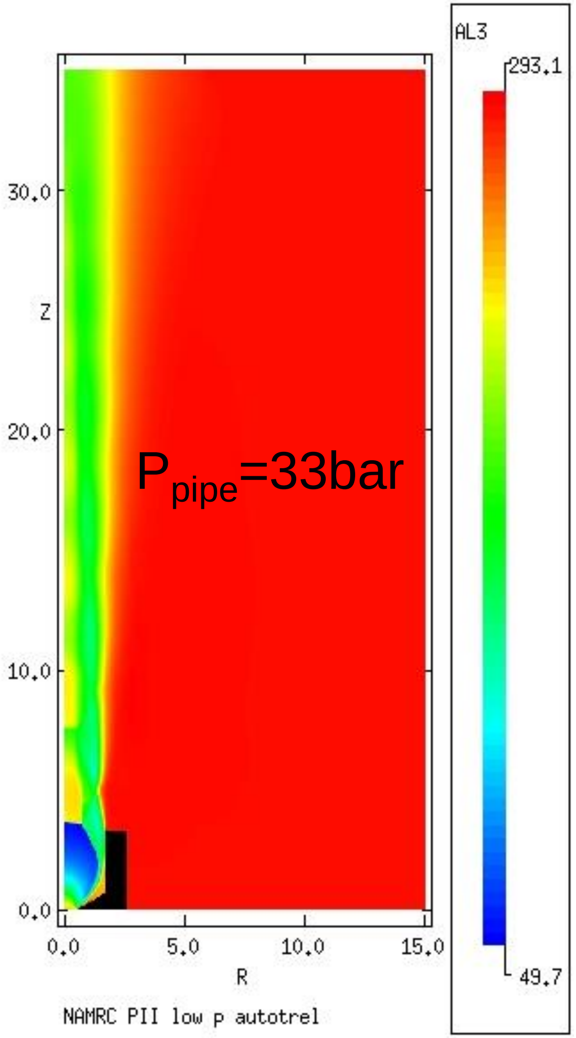
P_{pipe}=36bar

- Temperature distributions are nearly identical.



NAMRC PII high p autotrel

P_{pipe}=38bar

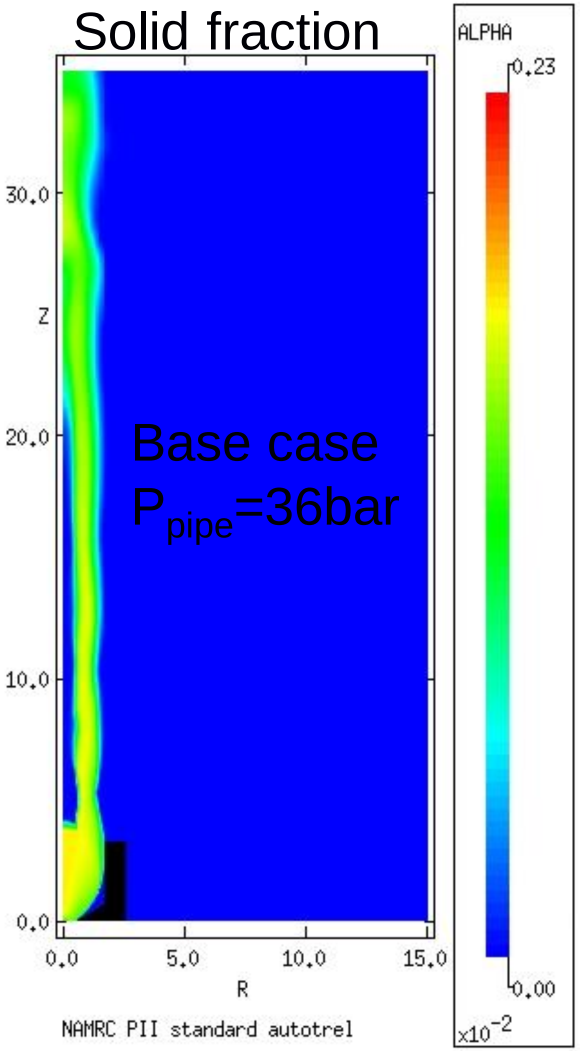


NAMRC PII low p autotrel

P_{pipe}=33bar

Phase 2 results: variation of pressure

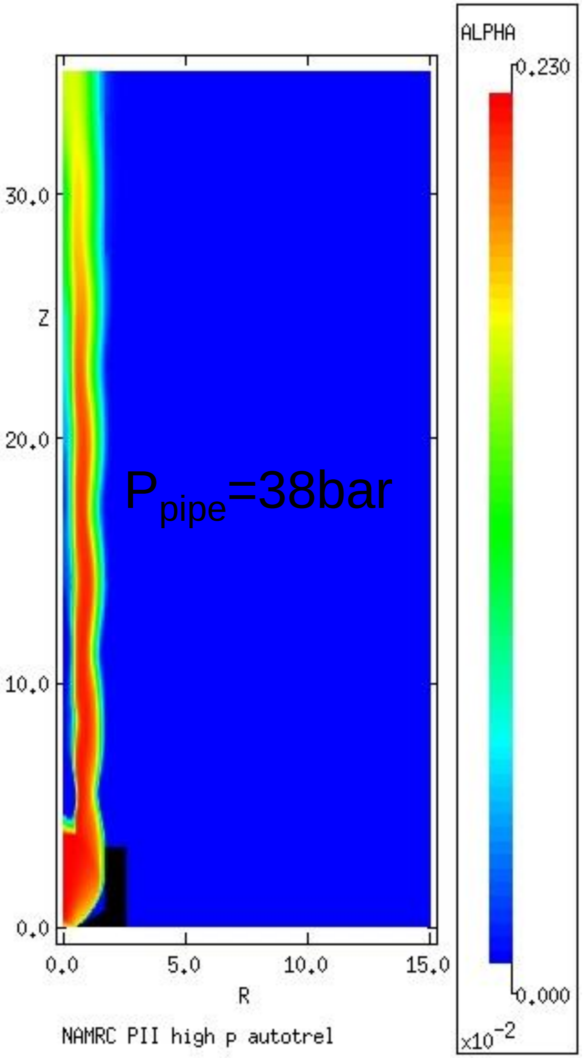
Solid fraction



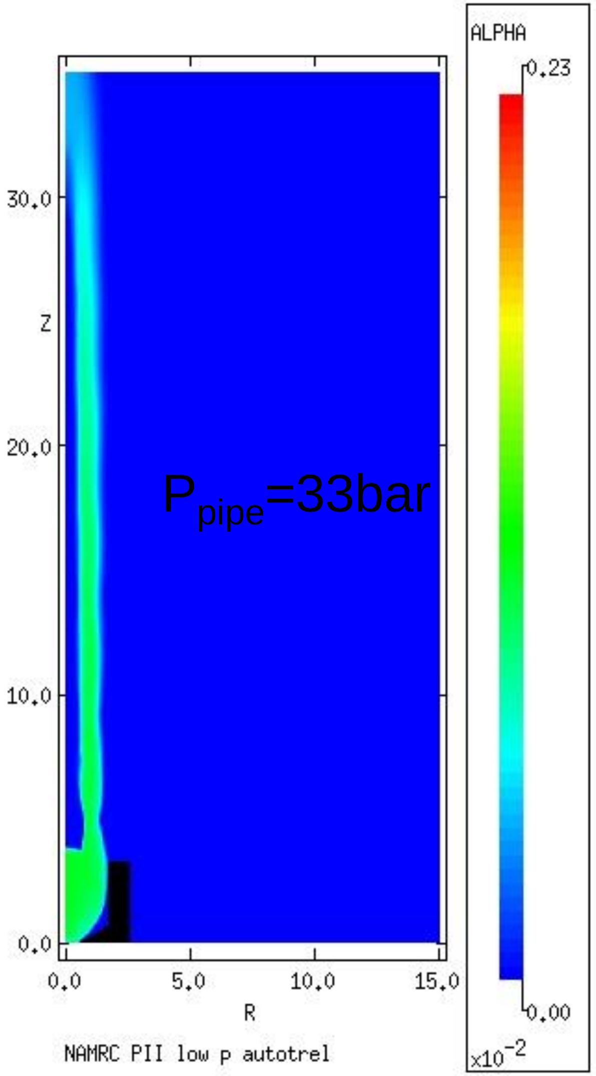
Base case

P_{pipe}=36bar

- High pressure case has **1/3 more** condensed phase;
- Low pressure case **1/3 less**.



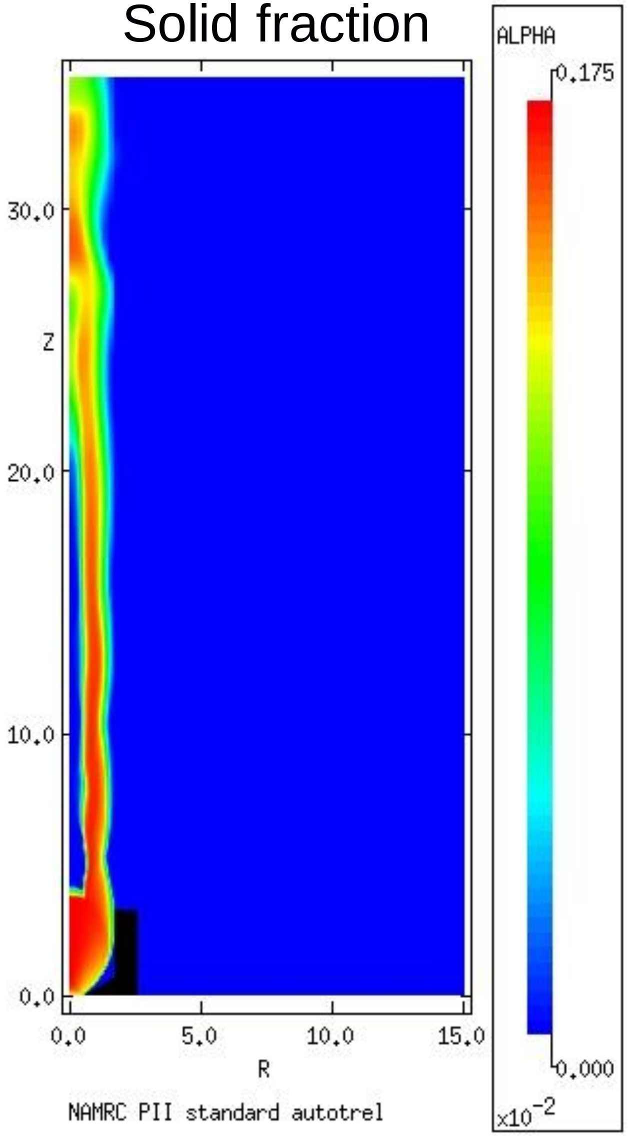
P_{pipe}=38bar



P_{pipe}=33bar

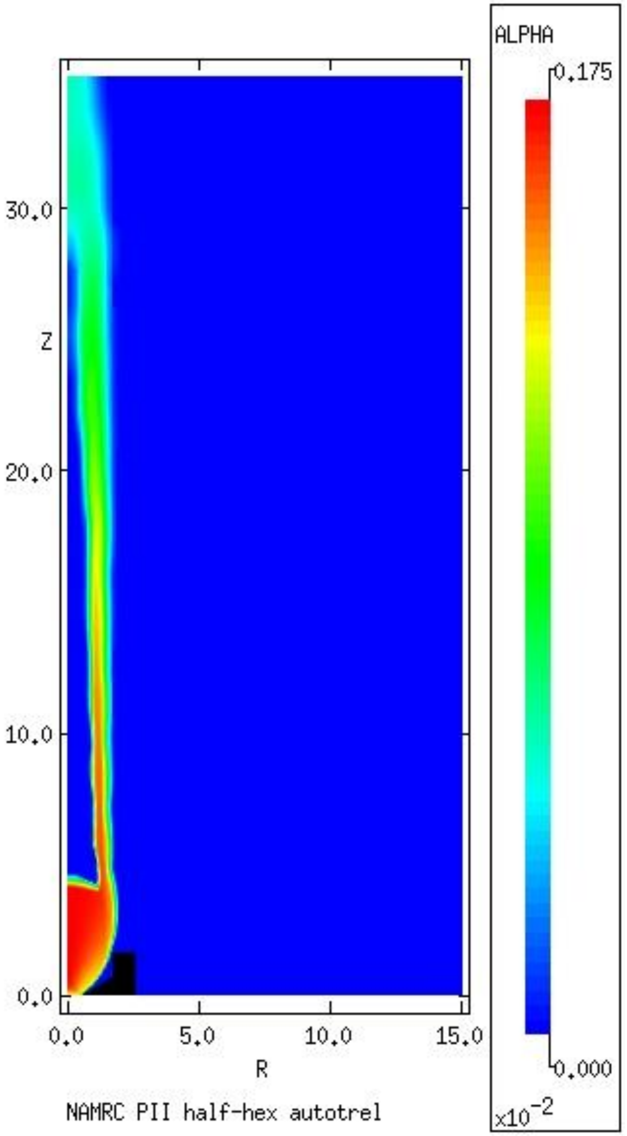
Phase 2 results: hex-key height

Solid fraction

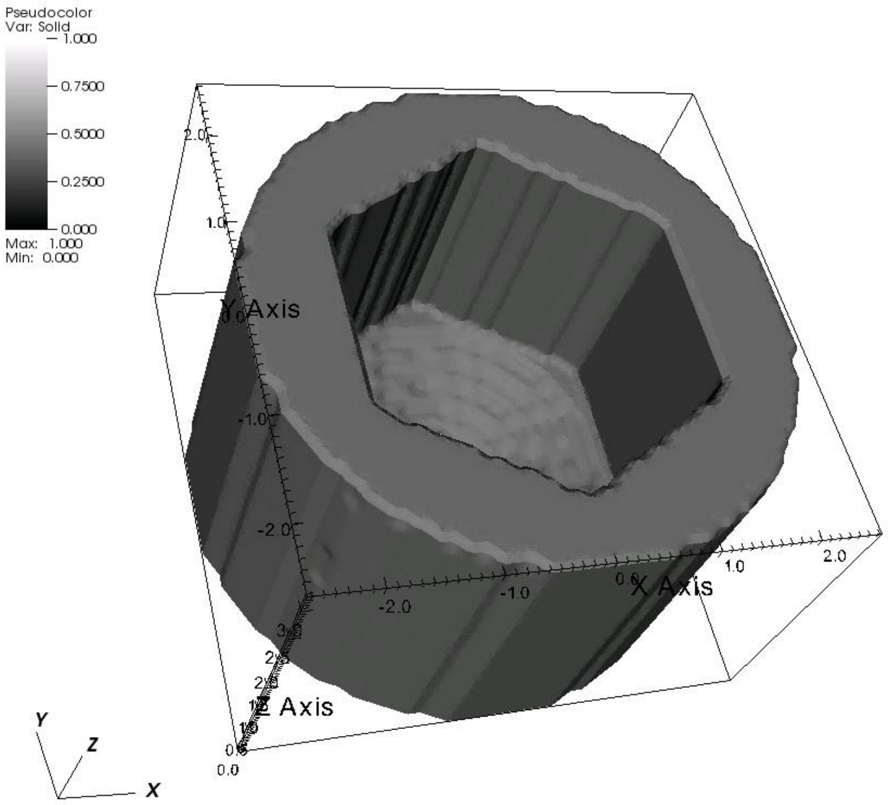


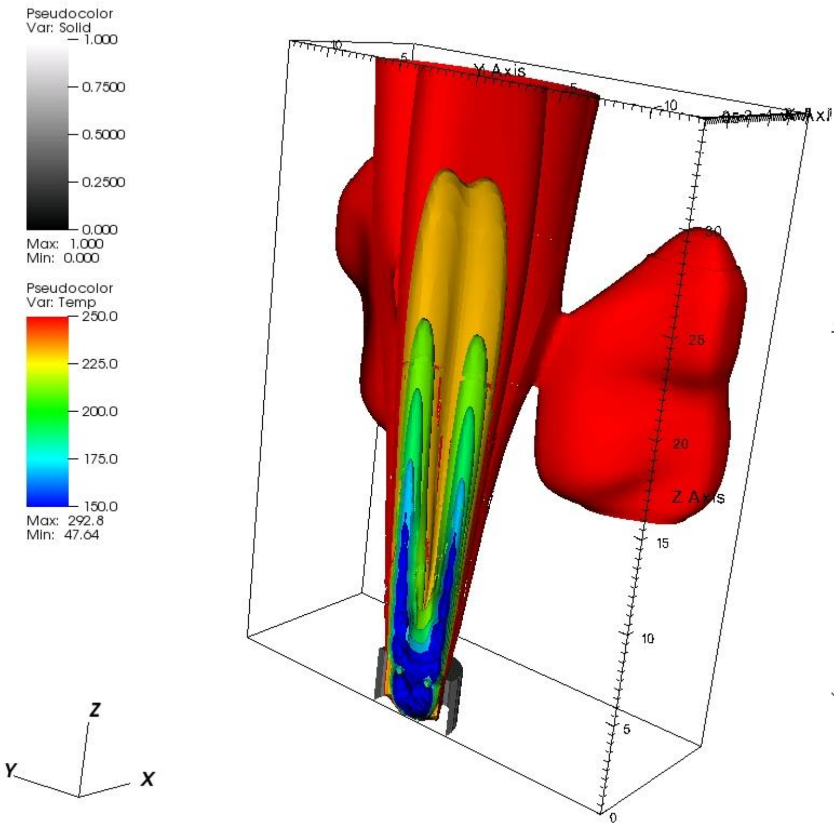
- Narrower mixing region leads to lower amounts of solid CO_2 in the mixing region and evaporation sooner

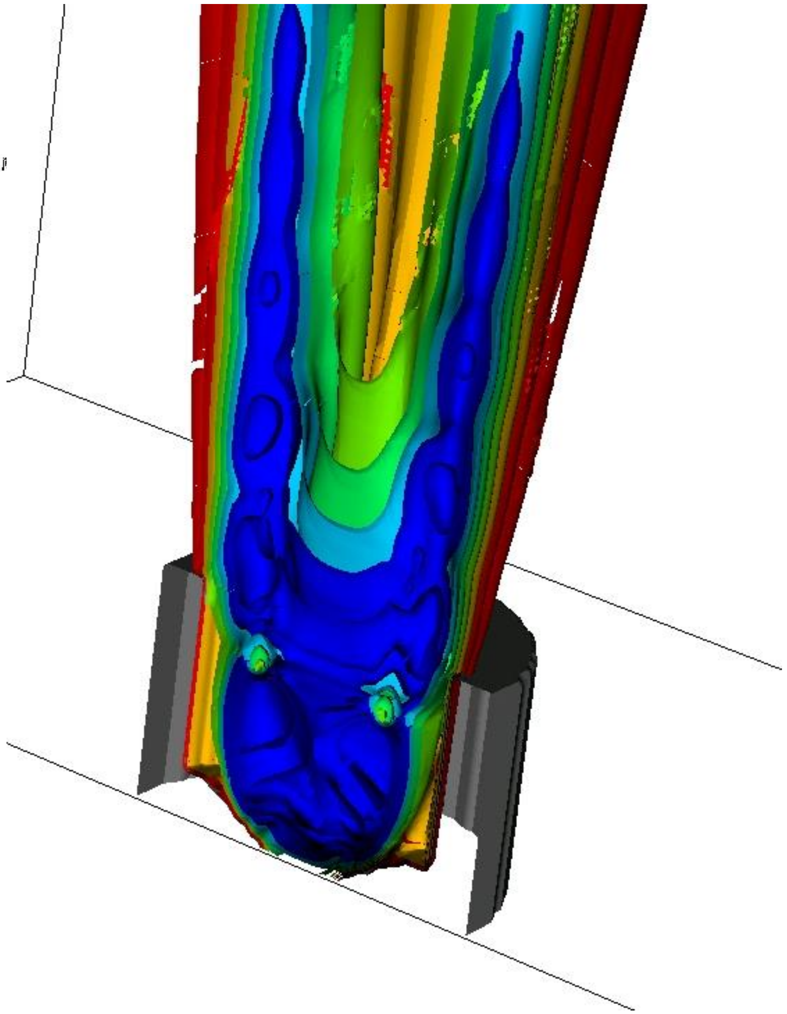
- These results would suggest that a **half-height hex key socket will result in lower amounts of solid CO_2** at the operating plane.



Phase 2: 3D simulation







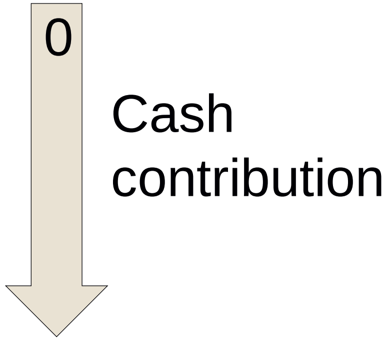
Executive summary

UNIVERSITY OF LEEDS

- Nozzle conditions can be estimated from Bernoulli, and can be refined by experimental measurements of the flow in the pipe upstream from tool.
- Non-equilibrium effects are present – solid flow is inertia-dominated
  - Over the region of interest, solid and gas flow are detached
  - Gas flow rapidly becomes ‘hot’ at ~ -20^{o}C, solid particle flow is cold ~ -80^{o}C
- Mach shock is around the size of the hex key socket in this D=0.6mm case
- Hex key acts to focus flow and increase solid fraction at 30 diameters
  - Lines present in close-up photography are likely to be a result of ‘hex’ key shape
- Nozzle simulations have shown solid fraction does not change through simulations – to increase solid fraction, maximise condensed phase flow in supply line.
  - Phase 2 simulations have shown supply line pressure is important.
- A better model is required to explore this more accurately - EPSRC research grant application

Grant proposal in progress, at an early stage

- EPSRC standard grant proposal, to examine:
  - Extended thermodynamic equation of state – supercritical / MQL
  - Multi-fluid Direct Numerical Simulation flow scheme
  - Tuned fundamental particle experiments with Phase Doppler Particle Anemometry
  - Impinging jets and heat transfer
  - Outputs: optimal use and refined machine and tool design
- Various opportunities for involvement exist
  - Advisory Board membership, guiding research questions
  - Provision of existing data or relevant facilities
  - Full collaboration, e.g. a range experiments for validation purposes



We invite people to talk to us about becoming involved