School of Chemical and Process Engineering
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High pressure CO_2 CCS pipelines: Comparing dispersion models with multiple experimental datasets (including impurities)

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Overview

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How to shed light on the risks of CO_2 pipeline transport?

- ***Numerical simulation*** **of the near-field sonic dispersion of CO_2 with impurities from high pressure pipelines**
    - Numerical method
    - Thermodynamic equation of state, with impurities
    - Validation – 100% liquid CO_2 releases
        - Free releases into air
        - Punctures and ruptures of buried pipelines.
- Comparison to available experimental data with impurities
    - Centreline and radial comparisons with two turbulence models
    - Pure CO_2 with varying liquid fraction
    - CO_2 with impurities: methane CH_4, nitrogen N_2
- Conclusions

Near-field dispersion model

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- Numerical simulations: method:
  - Adaptive, finite-volume grid algorithm with 2D or 3D rectangular mesh.
  - Axisymmetric cylindrical coordinate r-z grid.
  - 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 models:-
    - standard k-ε model with a compressibility correction.
    - Reynolds stress second moment closure model.
  - 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 method

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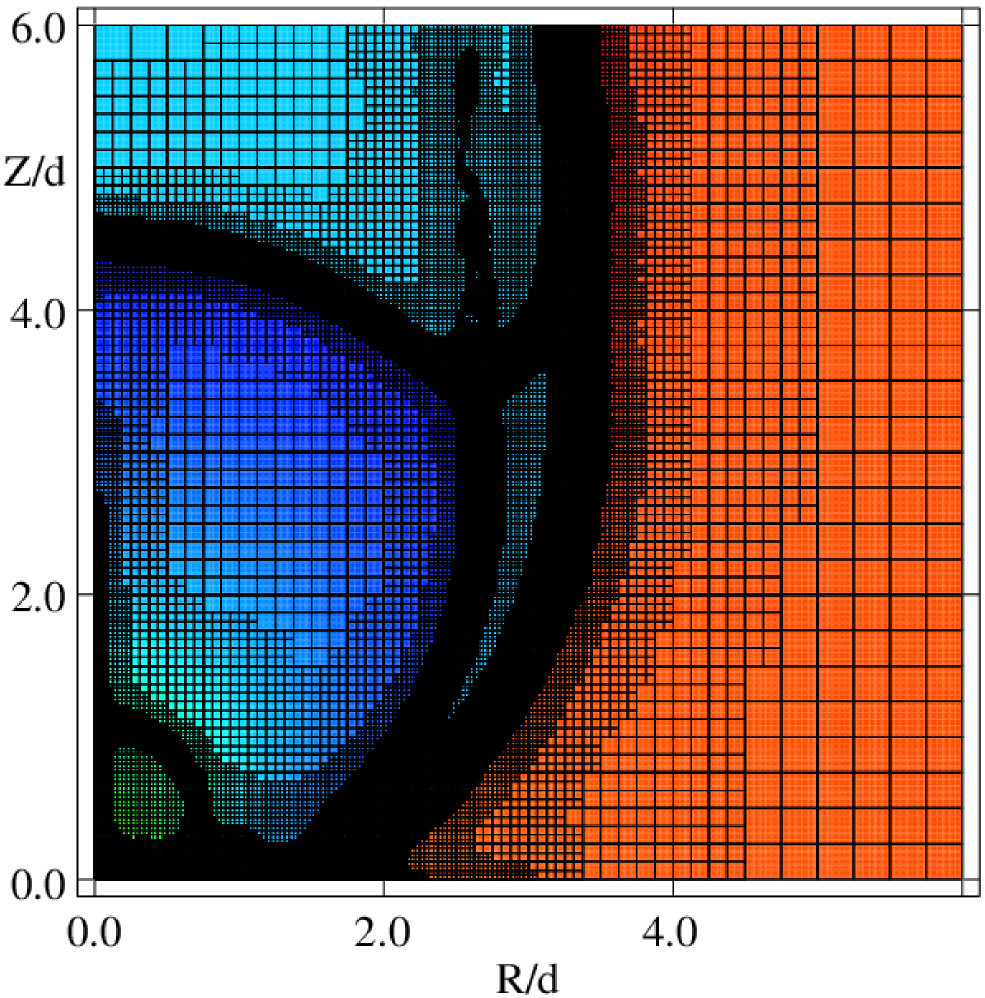
- Numerical method (continued):



- **Very expensive computations**

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

Still require hundreds of CPU hours on hundreds of processors

Total: 128x150hrs: **20,000 CPUhrs per case.**

Note the axis units are in release diameters.

Near-field dispersion model

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- Equation of state : *(Version 1:Wareing et al., AIChE J. 59, 3928-3942 (2013).*
  - 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;
    - Version 1:NIST/DIPPR data for the solid phase and latent heat of fusion Version 2:Jager & Span equation of state for solid CO_2.
  - 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

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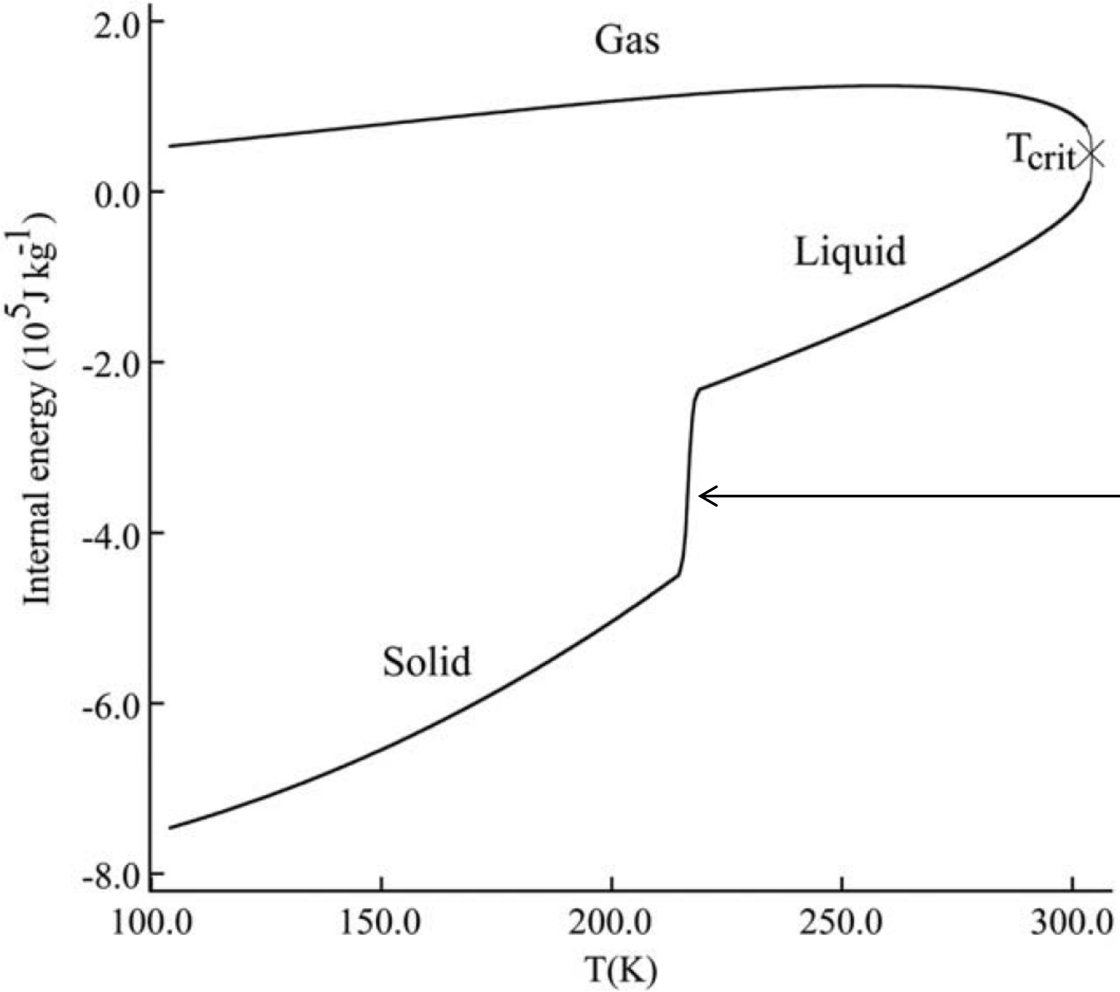
- Thermodynamic model (continued):



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

Near-field dispersion model

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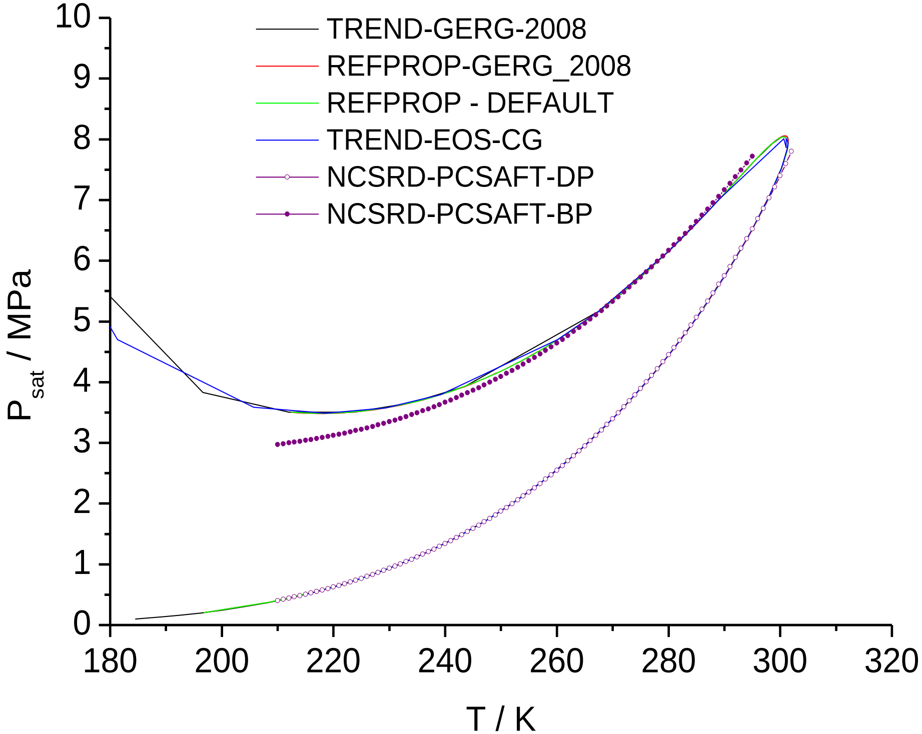
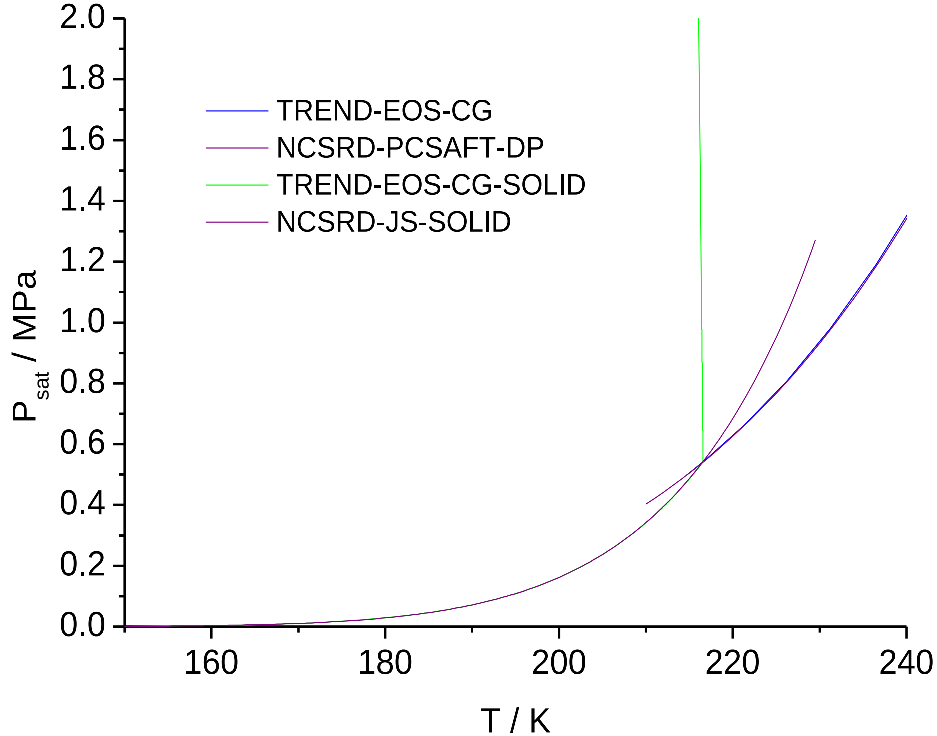
- Version 3: For **impure** CO2, developed by NCSRD, CO2QUEST
  - Implemented by means of a P and T loop-up table
  - SAFT-based methods above T_{triple}, Jager & Span EoS below T_{triple}





Comparison P-T Phase-Space Predictions of a 96% CO_2 / 4% N_2 mixture

Venting: free liquid phase

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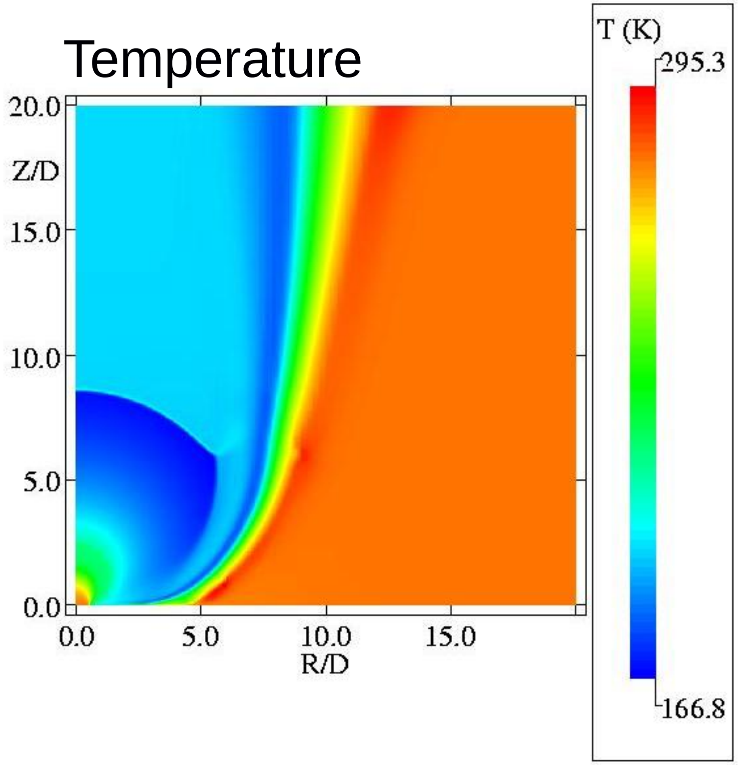
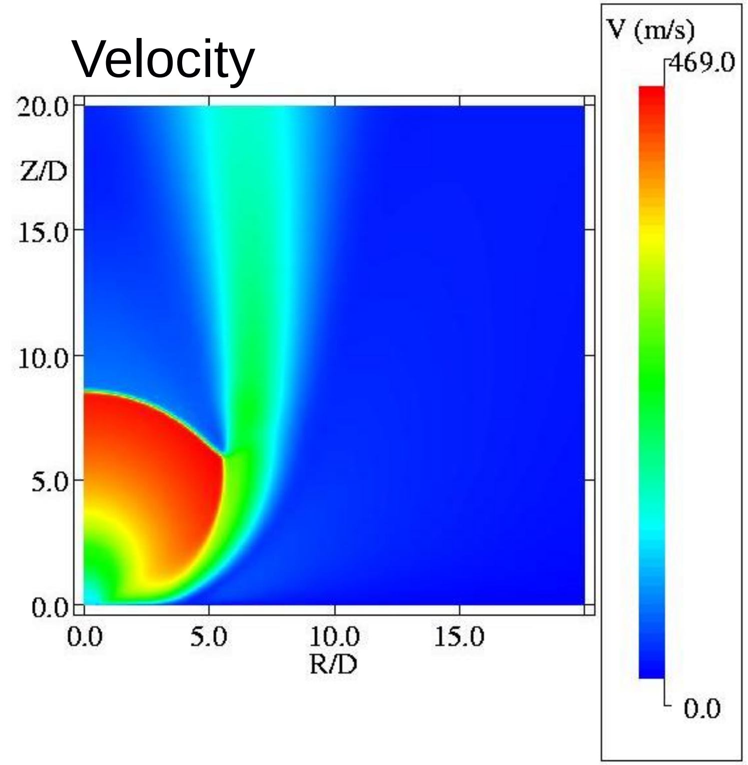
- Dense phase release from a 150bar reservoir through 25mm (D) vent pipe.
- Steady state release conditions achieved by supplying a driving pressure

Temperature



Velocity



Near-field shock containing region: 20D x 20D (0.5m x 0.5m)

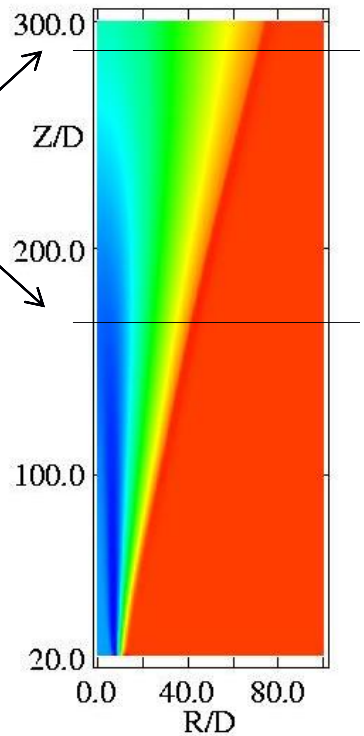
*Wareing et al., Int. J. Greenhouse Gas Control, **20**, 254-271 (2014)*

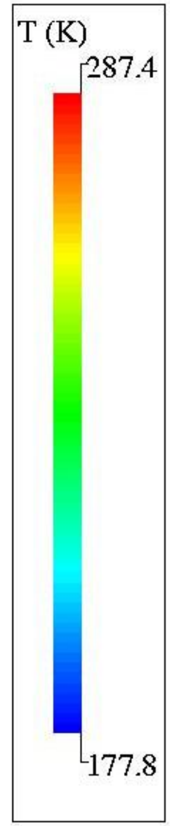
Venting: free liquid phase

Measuring planes at:

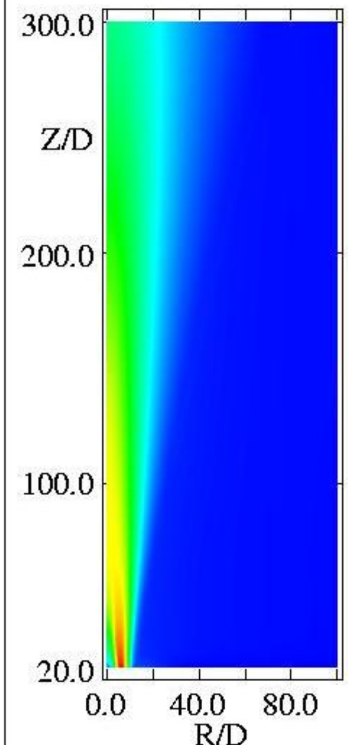
- 4m (165D)
- 7m (288D)

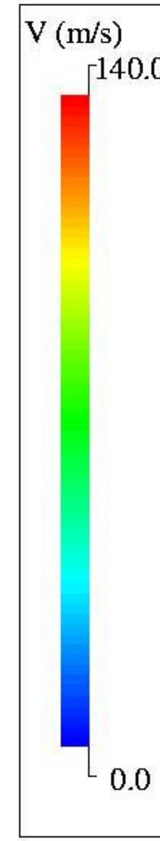
Temperature





Velocity





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

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

Venting: free liquid release

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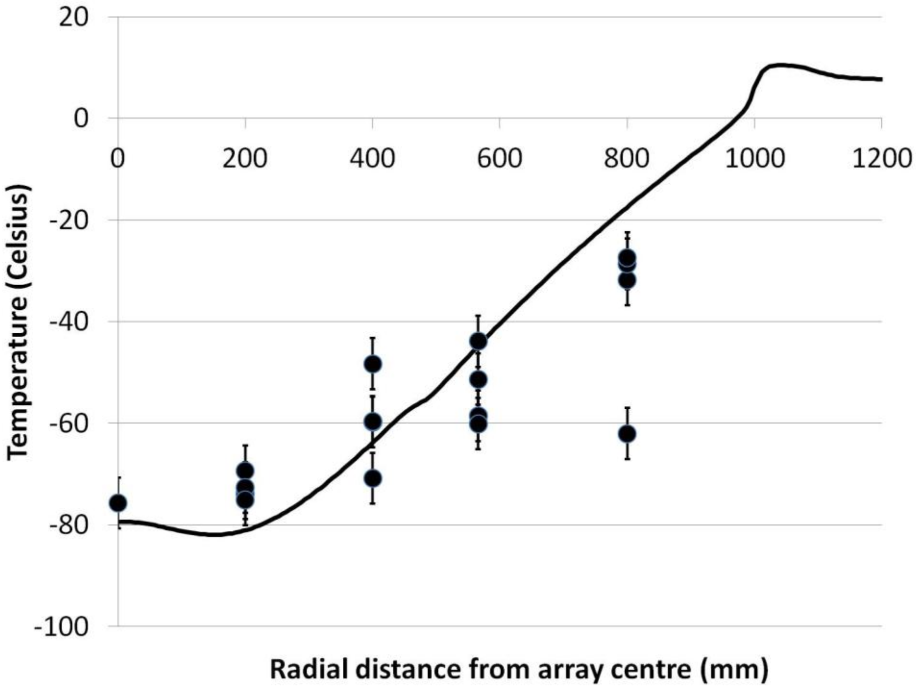
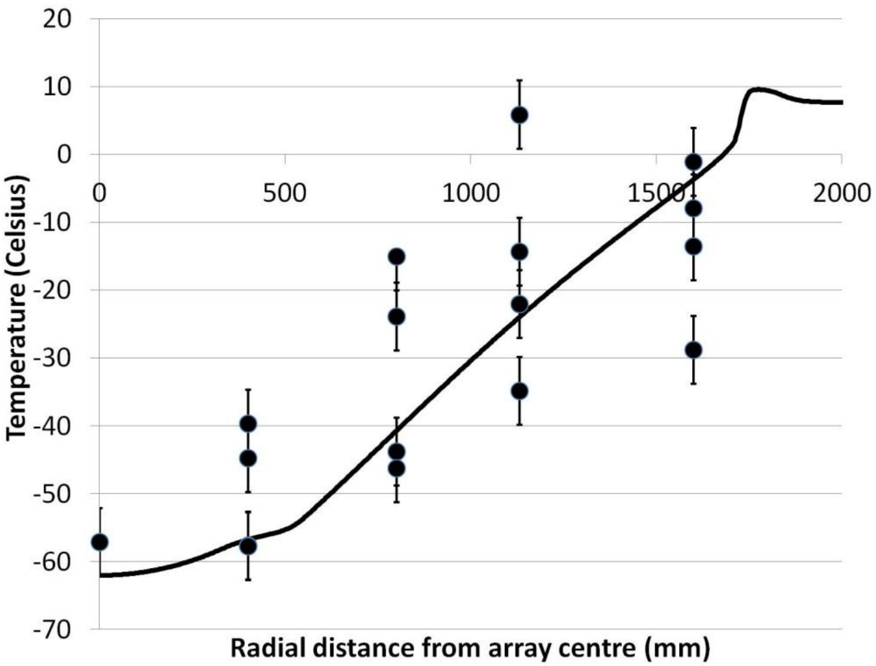
(a) 4m above the vent



(b) 7m above the vent



- **Core temperature prediction in good agreement** with data at 4m and 7m.
- **Predicted jet widths also in good agreement with data.**
- A cross-wind of 2.5 m/s has led to some spread in the data at 7m.

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

Venting: free gas phase

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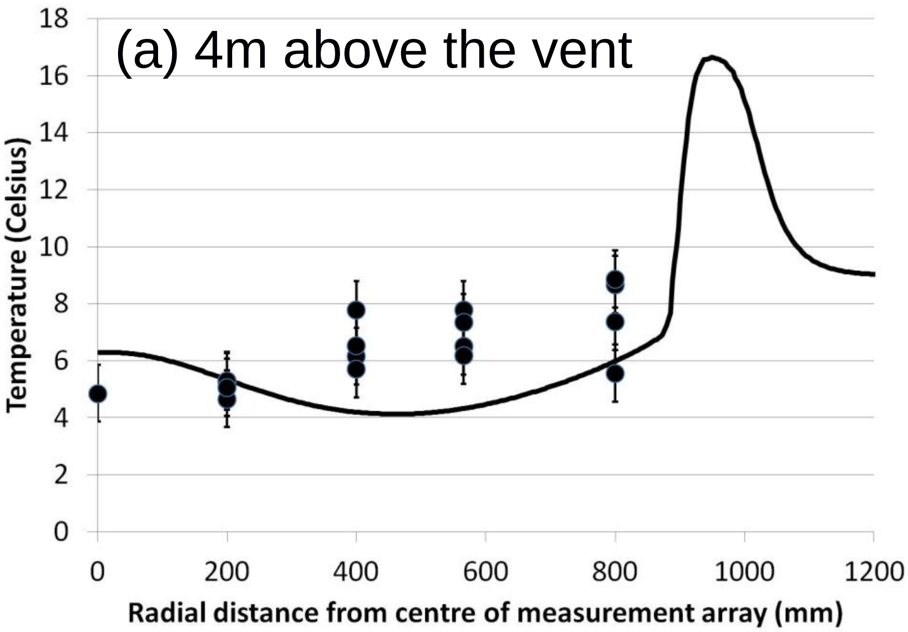
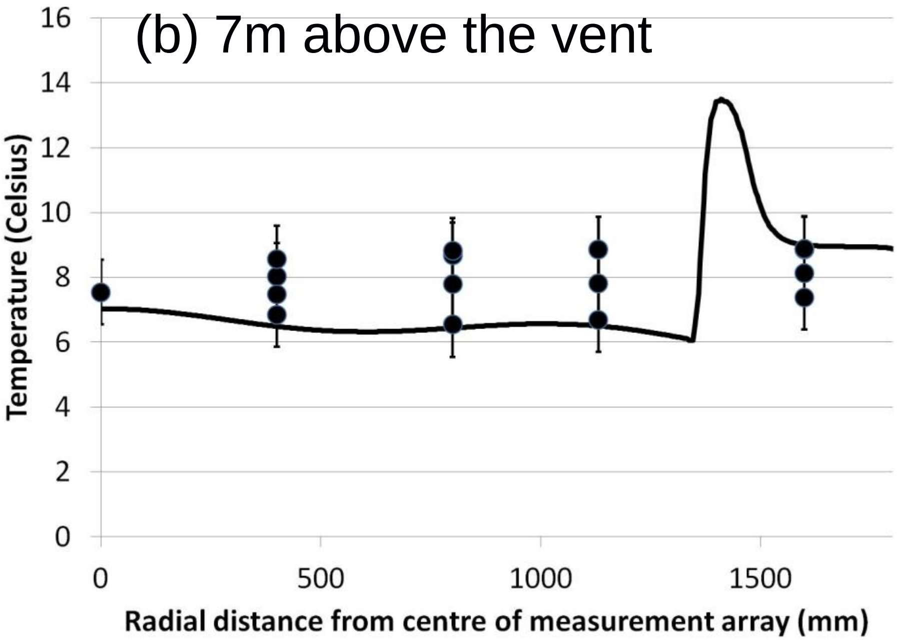
- Gas phase release from a 35bar reservoir through a 25mm vent pipe.
- Steady state release conditions achieved by supplying a driving pressure





Despite the considerably different temperature range observed as compared to the dense phase release, predicted core jet temperatures and widths are again in good agreement with the data on both planes

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

Punctures: validation overview

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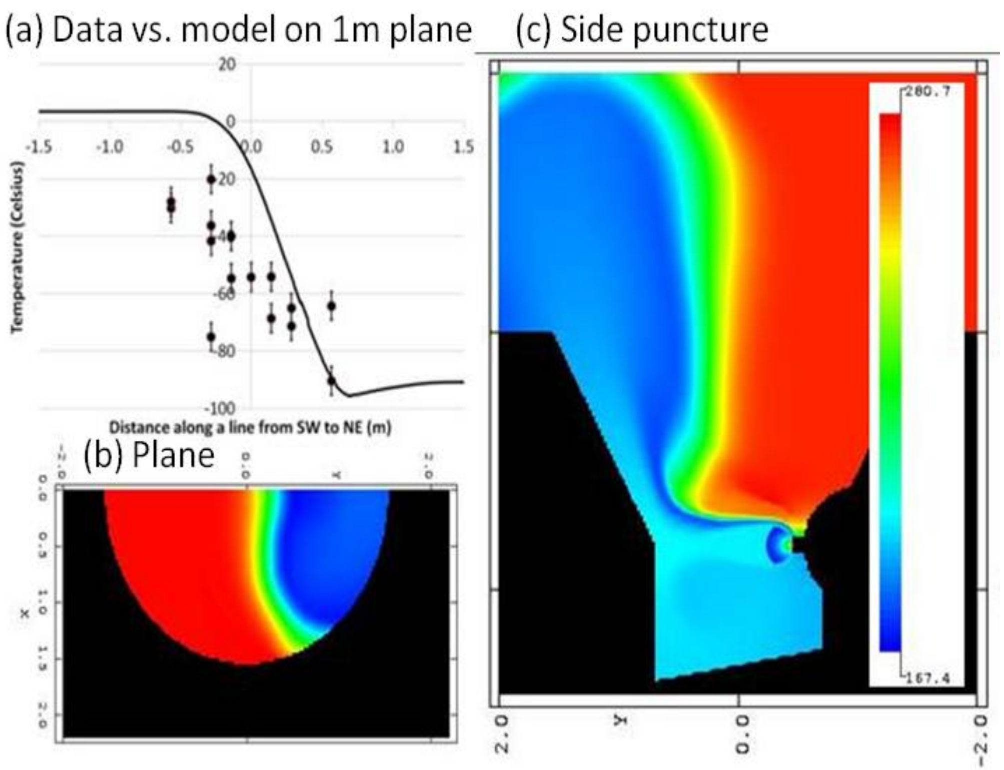

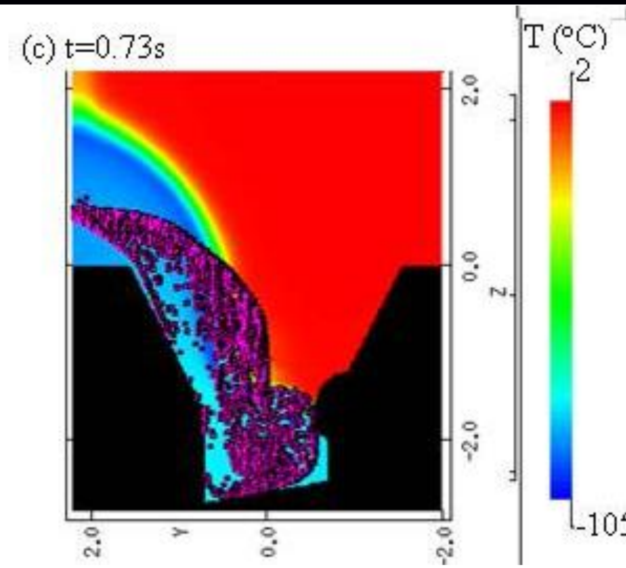

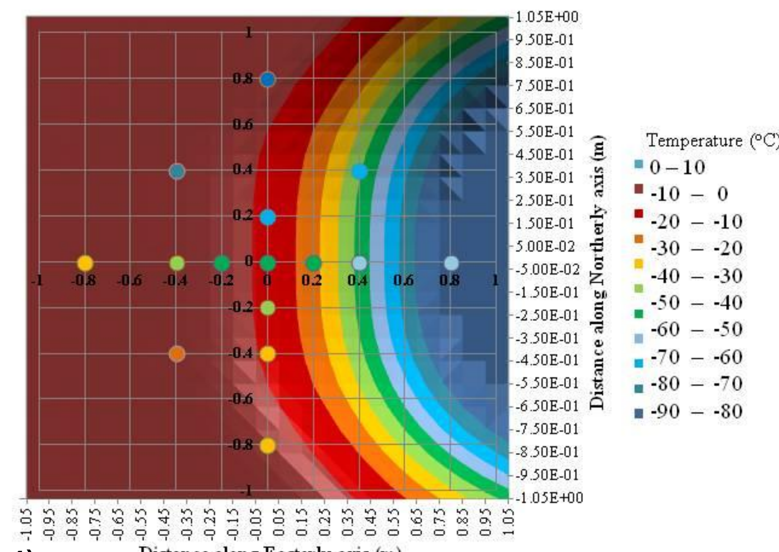

*Wareing et al., Int. J. Greenhouse Gas Control, **29**, 231-247 (2014)*

Ruptures: validation at ¼ scale

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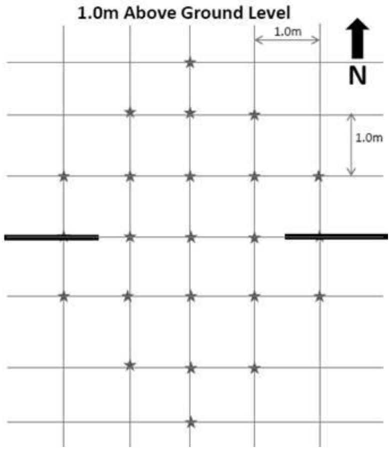
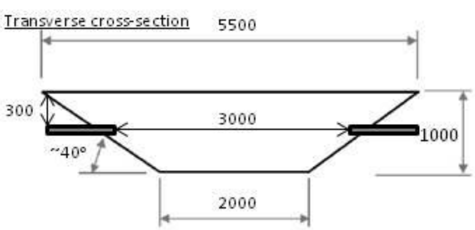
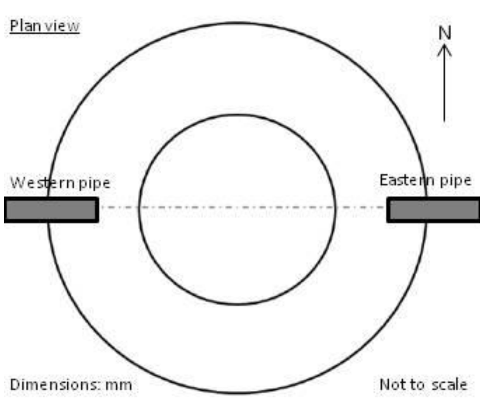
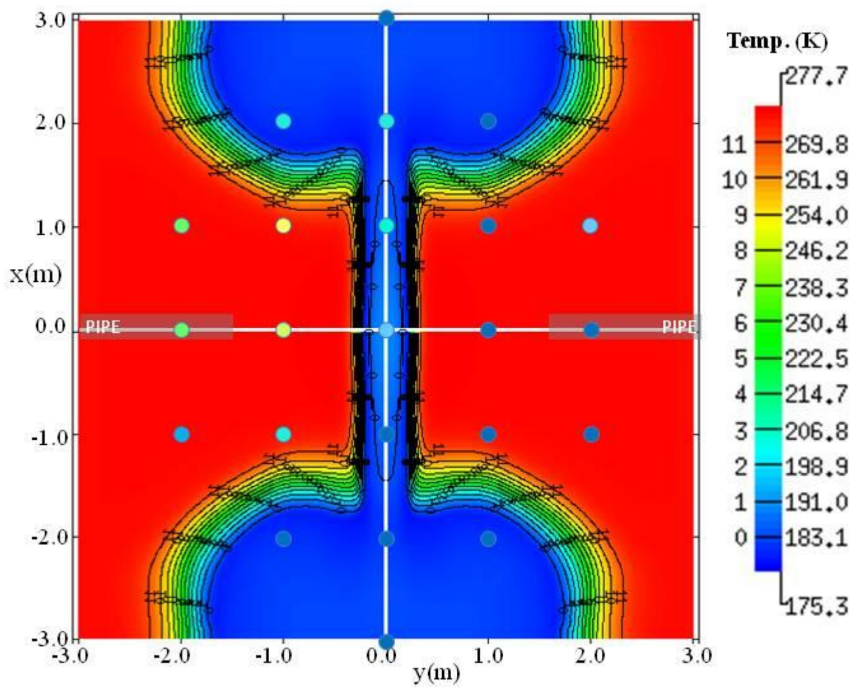


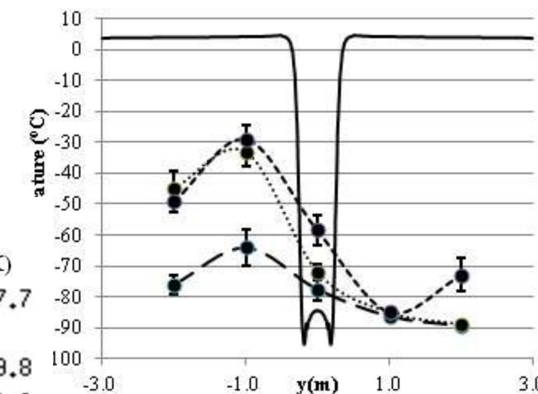




Pipeline diameter D=0.15m

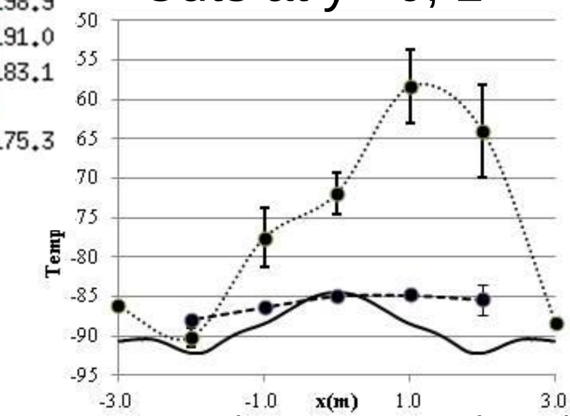
1m above crater





Cuts at x= -1, 0, 1

Cuts at y= 0, 1



*Wareing et al., Int. J. Greenhouse Gas Control, **42**, 701-711 (2015)*

Comparison to other datasets

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- Temperature data regarding near-field releases of high pressure liquid CO_2 has been obtained from a number of sources.

- From each test, consistent, averaged temperature measurements for comparison to the RANS predictions have been used.

- Each measurement has a variance of a degree or two over this averaging period and the thermocouples are ±5K accurate, hence an error of 5K should be assumed throughout.

- The plotted temperature is the simple average for that particular sensor in that particular test during a steady-state averaging period.

- The tests are either free releases from an isolated depressurising reservoir, or buffered with a driving pressure to maintain the reservoir pressure.

Comparison to experimental datasets

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TABLE (1). Experimental data regarding near-field releases of high pressure liquid phase CO_2.

Name	**Release diam. (D) (mm)**	**Horiz./ Vert.**	**Reservoir pressure (barg)**	**Estimated liquid frac. at nozzle (%)**	**Buffer/ free**	**Source**
BP Test 2	11.94	H	155	-	Buffer	CO2PIPETRANS
BP Test 5	25.62	H	157	-	Buffer	CO2PIPETRANS
BP Test 11	11.94	V	82	-	Buffer	CO2PIPETRANS
Shell Test 3	12.7	H	150	-	Buffer	CO2PIPETRANS
Shell Test 5	25.4	H	150	-	Buffer	CO2PIPETRANS
Shell Test 11	12.7	H	80	-	Buffer	CO2PIPETRANS
HSL Test C	2.0	H	54	84%	Free	Purcell et al.
HSL Test D	4.0	H	49	86%	Free	Purcell et al.
CLTRNS T7	24.3	V	150	100%	Buffer	COOLTRANS
INERIS T6	9.0	H	95	~100%	Free	CO2PIPEHAZ
INERIS T7	12.0	H	85	~100%	Free	CO2PIPEHAZ
INERIS T8	25.0	H	77	~100%	Free	CO2PIPEHAZ
INERIS T11	12.0	H	83	~100%	Free	CO2PIPEHAZ
INERIS T12	25.0	H	77	~100%	Free	CO2PIPEHAZ
INERIS T13	50.0	H	69	80-90%	Free	CO2PIPEHAZ

Overall comparison

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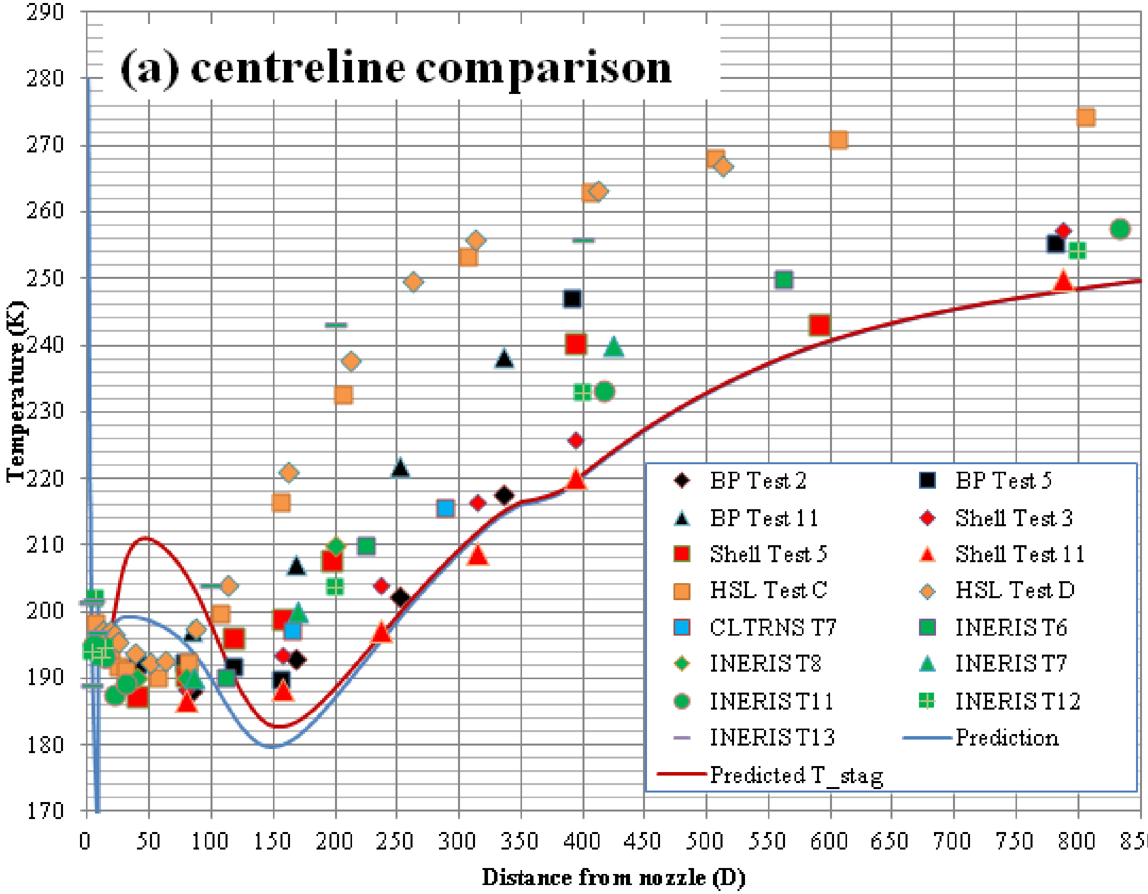
• A comparison between experimental data and numerical prediction along the centreline of the jet.



• Experimental errors of ±5K throughout; error bars omitted for clarity.

Radial comparison at 80D

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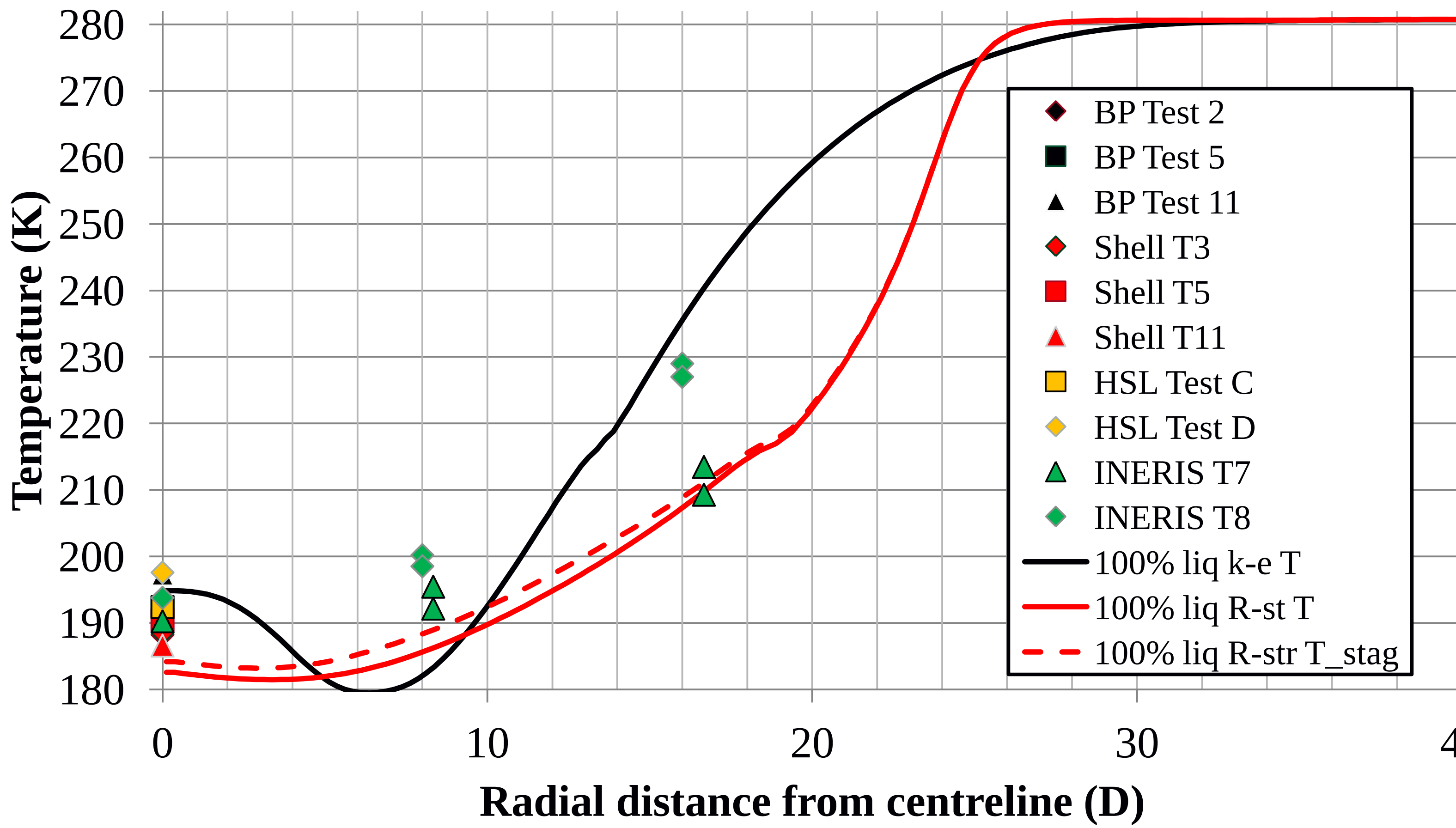
- A comparison between experimental data and numerical prediction radially at various points along the centreline.



- Improved fit with Reynolds stress turbulence model

Radial comparison at 100D

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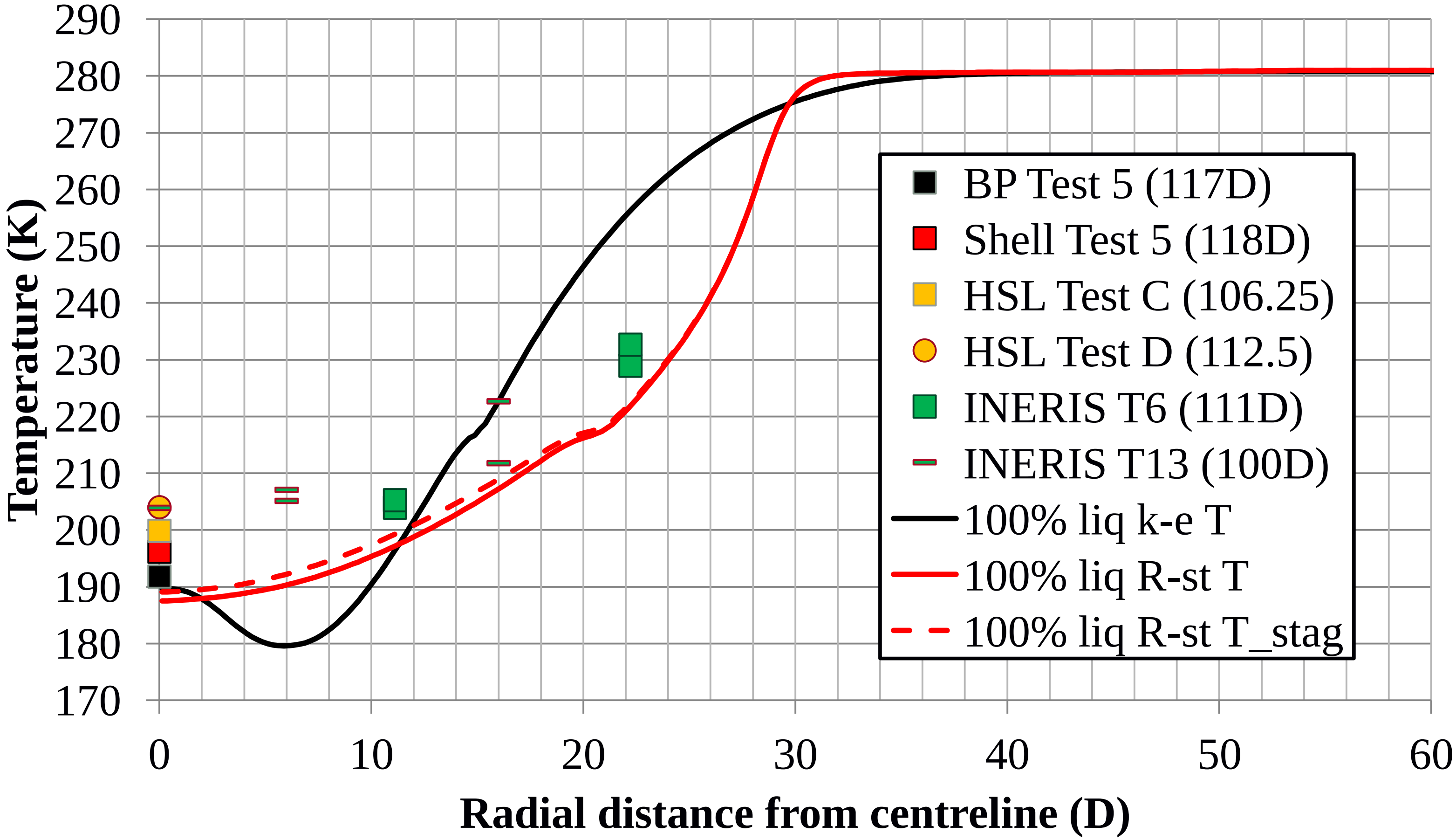
• A comparison between experimental data and numerical prediction radially at various points along the centreline.



• Improved fit with Reynolds stress turbulence model

Radial comparison at 165D

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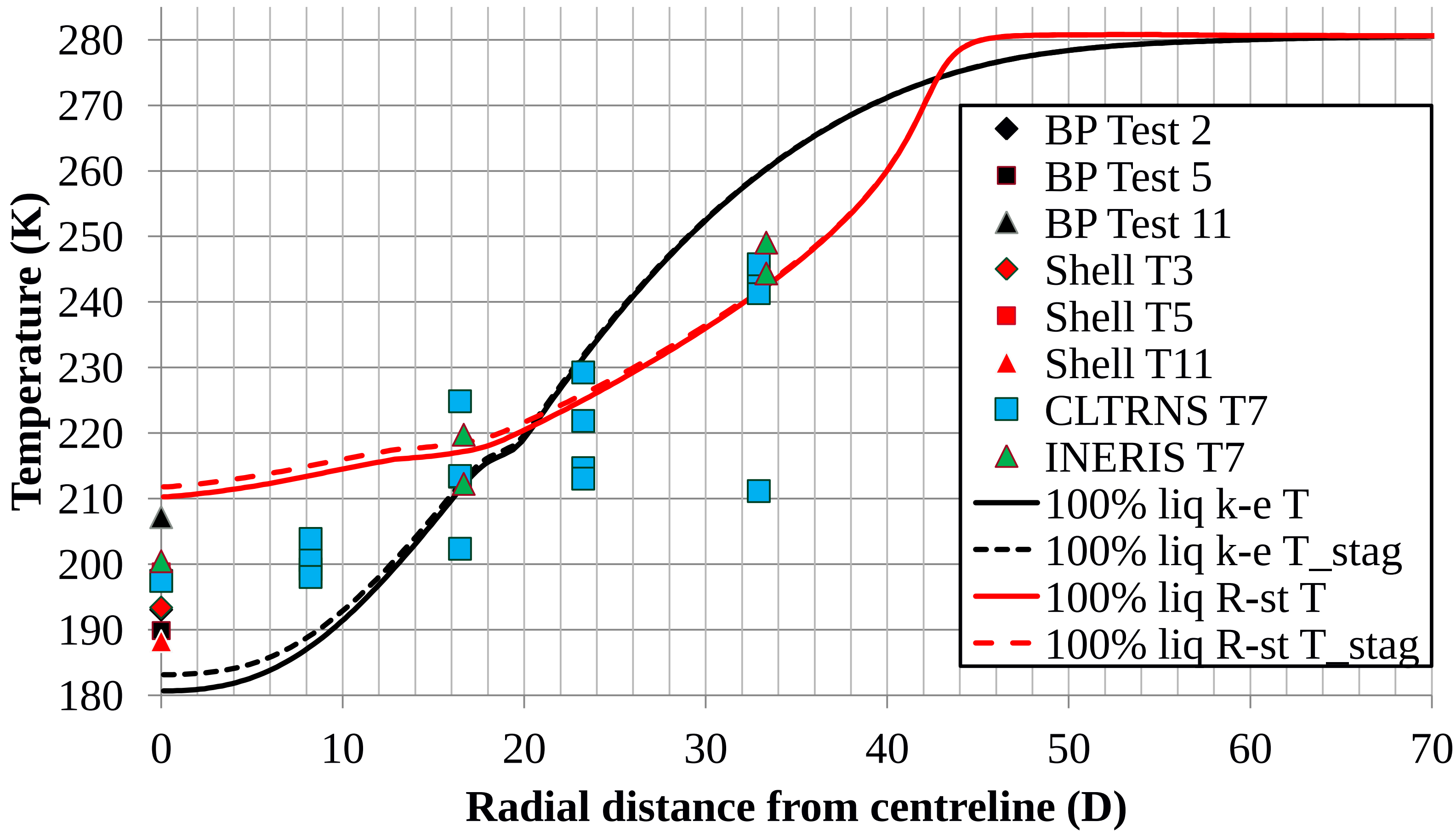
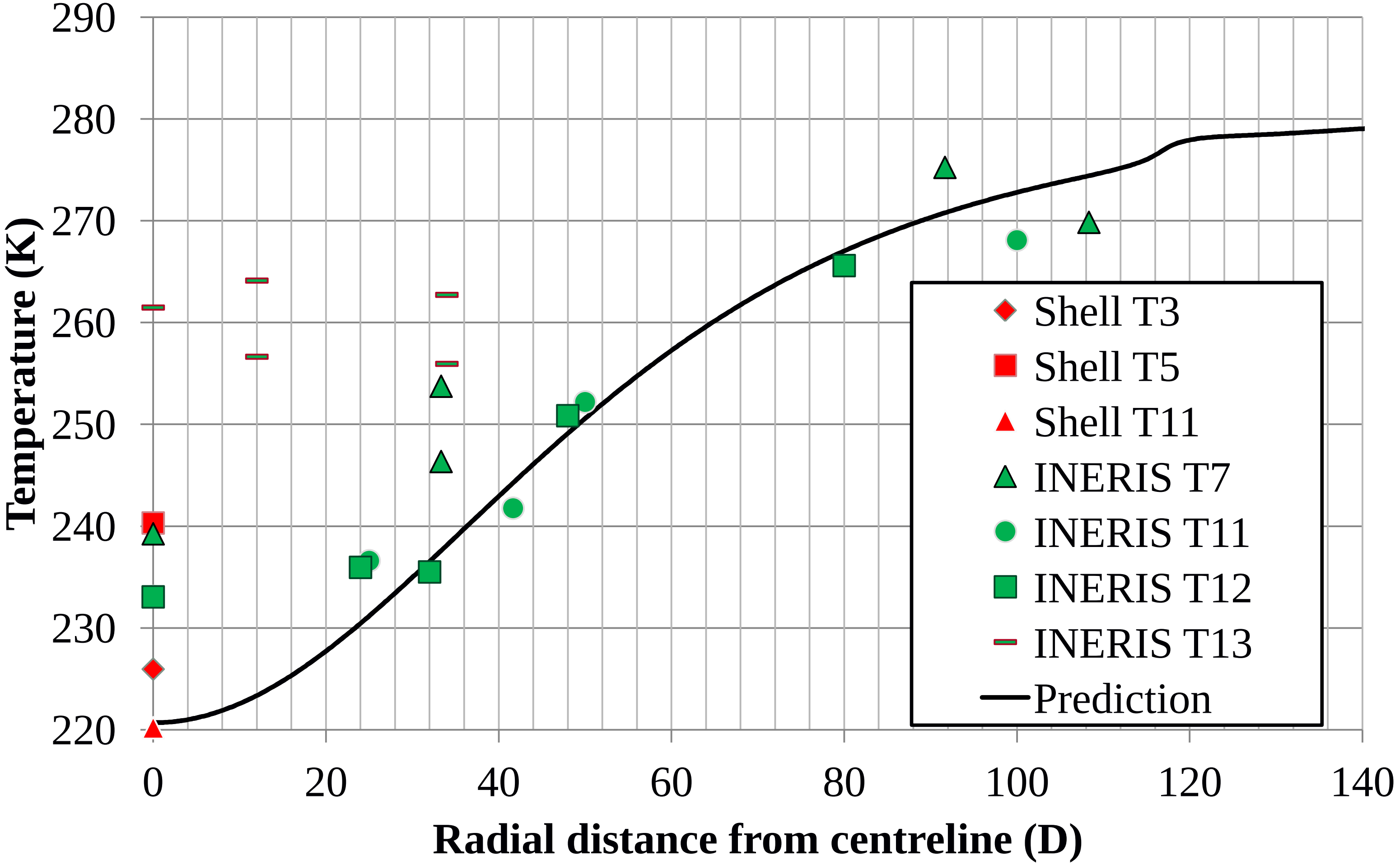
- A comparison between experimental data and numerical prediction radially at various points along the centreline.



- Further turbulence model tuning required

Radial comparison at 400D

• A comparison between experimental data and numerical prediction radially at various points along the centreline.



Comparison: variation of liquid fraction

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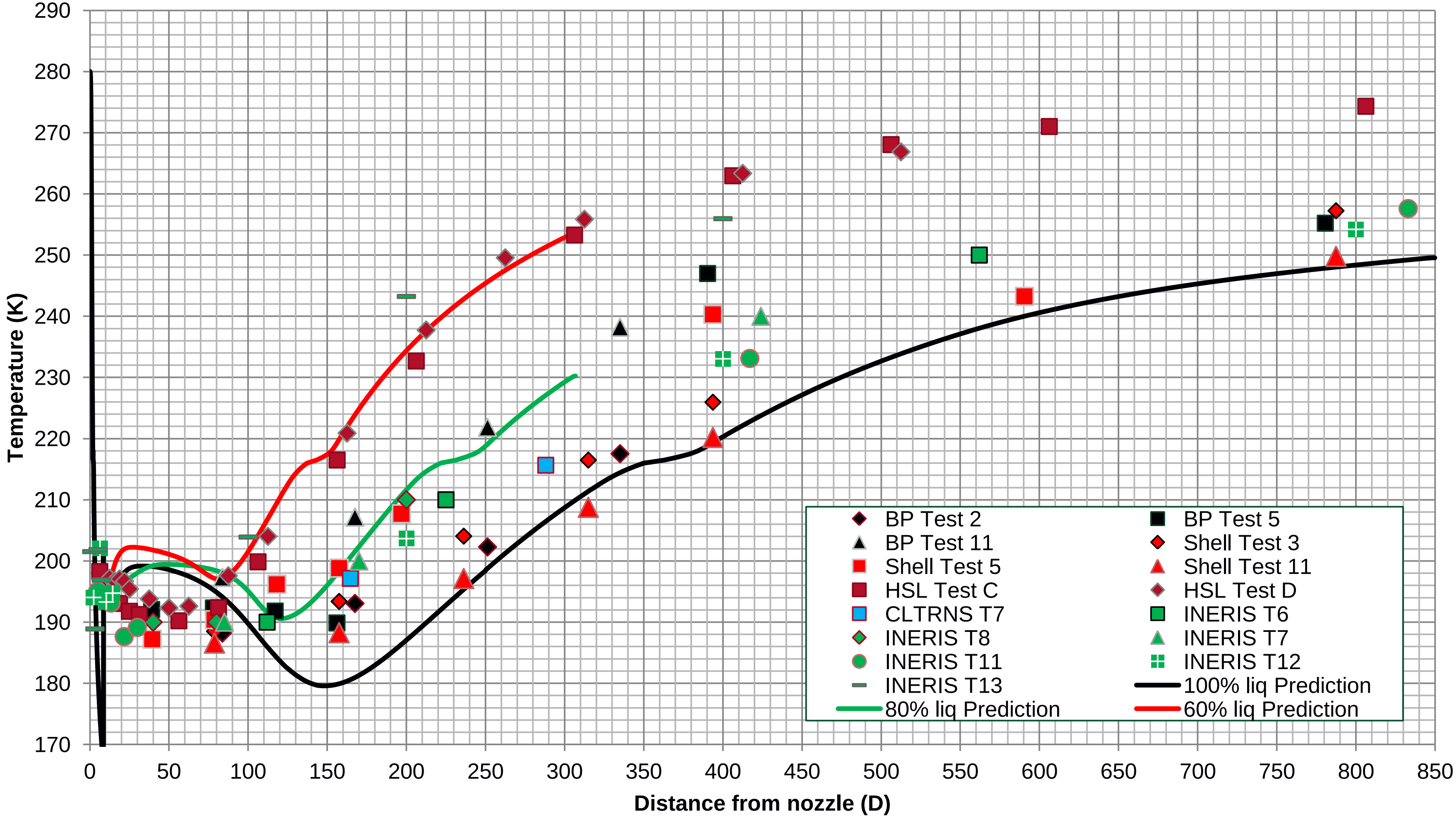

- Prediction: **100% liquid CO_2**, **80% liquid CO_2**, **60% liquid CO_2**
- HSL tests: <85% CO_2

Comparison: recent data on impurities

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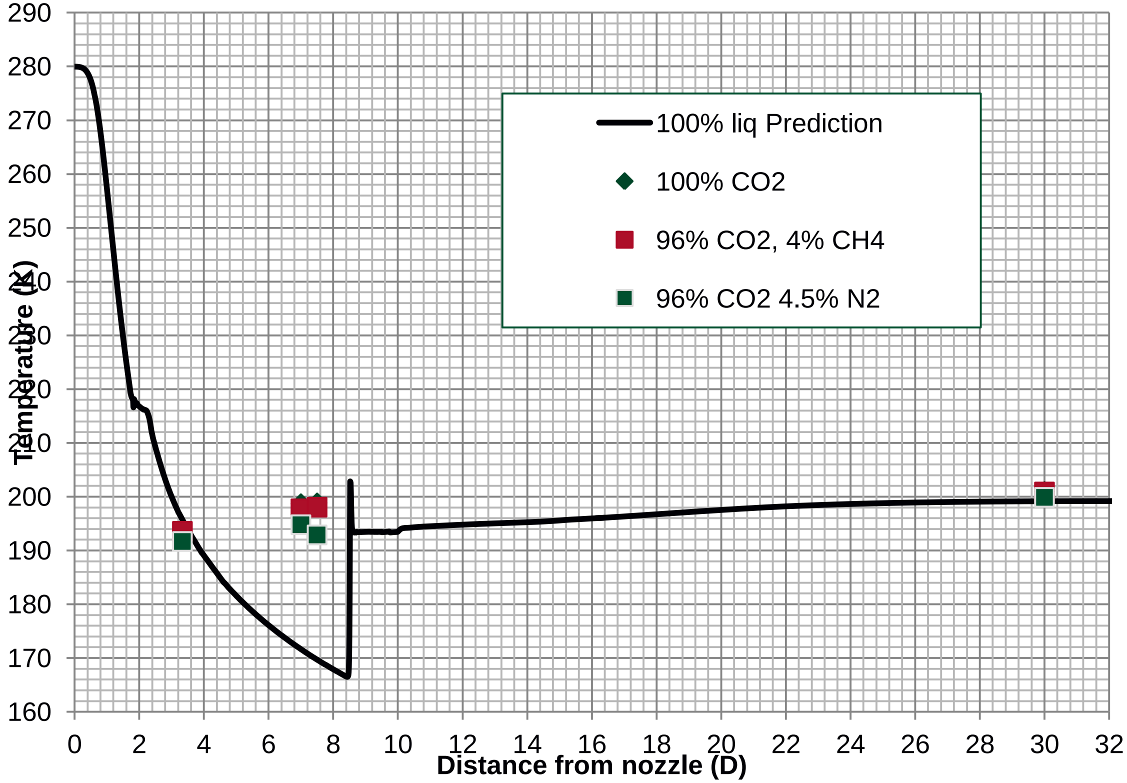
- 3 recent **impurity** tests, all liquid phase high pressure releases



- No meaningful difference in this data between the pure CO_2 release, 4% methane release and 4.5% nitrogen release.

Experimental data: INERIS; CO2QUEST

Discussion and Conclusions

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- All the available datasets are shown together on the centreline of the jet, non-dimensionalised according to the release diameter (D).
- Predicted centreline fluid and stagnation temperatures stitched together from the numerical simulations are also shown.
- **The numerical prediction agrees well on the centreline**, bounding the colder limit of the available experimental data as it is 100% liquid CO_2.
- **Agreement is demonstrated between numerical predictions and experimental data of the radial temperature distribution** from multiple sources at various distances along the centreline.
- **Liquid fraction at the release point is a key parameter for differentiating between the datasets,** improving fit to the data**.**
- **Low levels of impurity would appear to have no effect on near-field temperatures in the dispersion plume –** more work required**.**
- **The numerical method, with an improved equation of state, is able to model multiple datasets** for sonic CO_2 decompressions.

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Thank you for listening

Any questions or comments?

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References

Equation of state: Wareing et al., AIChE Journal, **59**, 3928-3942 (2013)
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Particle-laden CO_2 jets: Wareing et al., AIP Conference Proceedings, **1558**, 98 (2013)