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Comparison of Numerical Predictions with CO_2 pipeline release datasets of relevance to carbon capture and storage applications

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International Symposium on Fluid Dynamics
ICCMSE 2015, 20-23 March 2015, Athens, Greece

Overview

- Brief introduction to Carbon Capture and Storage
- Near-field sonic dispersion of carbon dioxide (CO_2) from high pressure pipelines
  - Thermodynamic model
  - Numerical method
  - Validation
    - Free releases into air
    - Punctures of buried pipelines
    - Ruptures of buried pipelines
- Comparison to available experimental datasets
- Conclusions

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.

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

Near-field dispersion model

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- Thermodynamic model: *(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;
    - Originally NIST/DIPPR data for the solid phase and latent heat of fusion now improved with 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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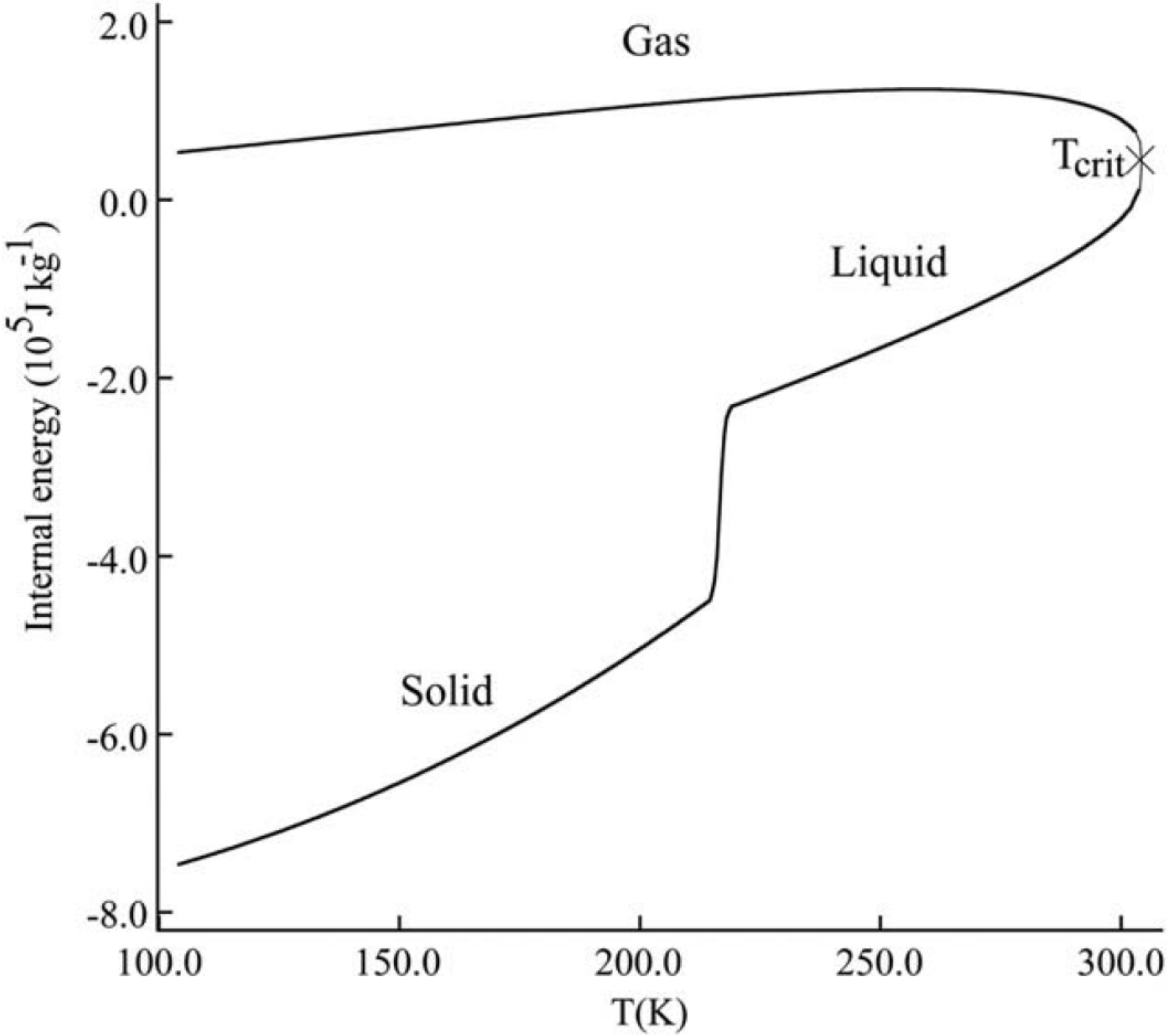
- Thermodynamic model (continued):



- Internal energy on the saturation line.

- T_{crit} marks the critical temperature.

- The triple point can be identified by the steep connection between the liquid and solid phases – the latent heat of fusion.

Near-field dispersion model

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

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

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

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

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

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

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

where S is the entropy per unit mass.

Near-field dispersion model

- Numerical 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 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

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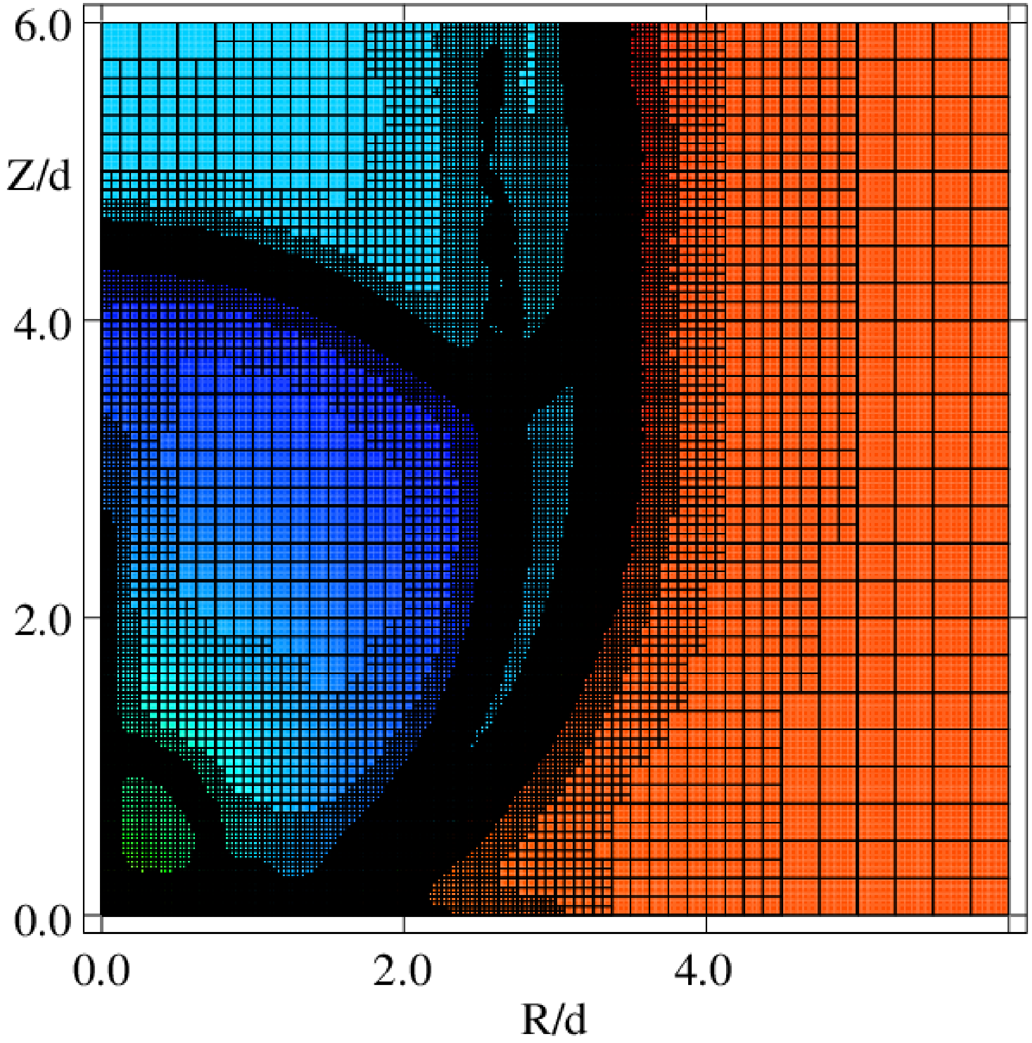
- Numerical method (continued):

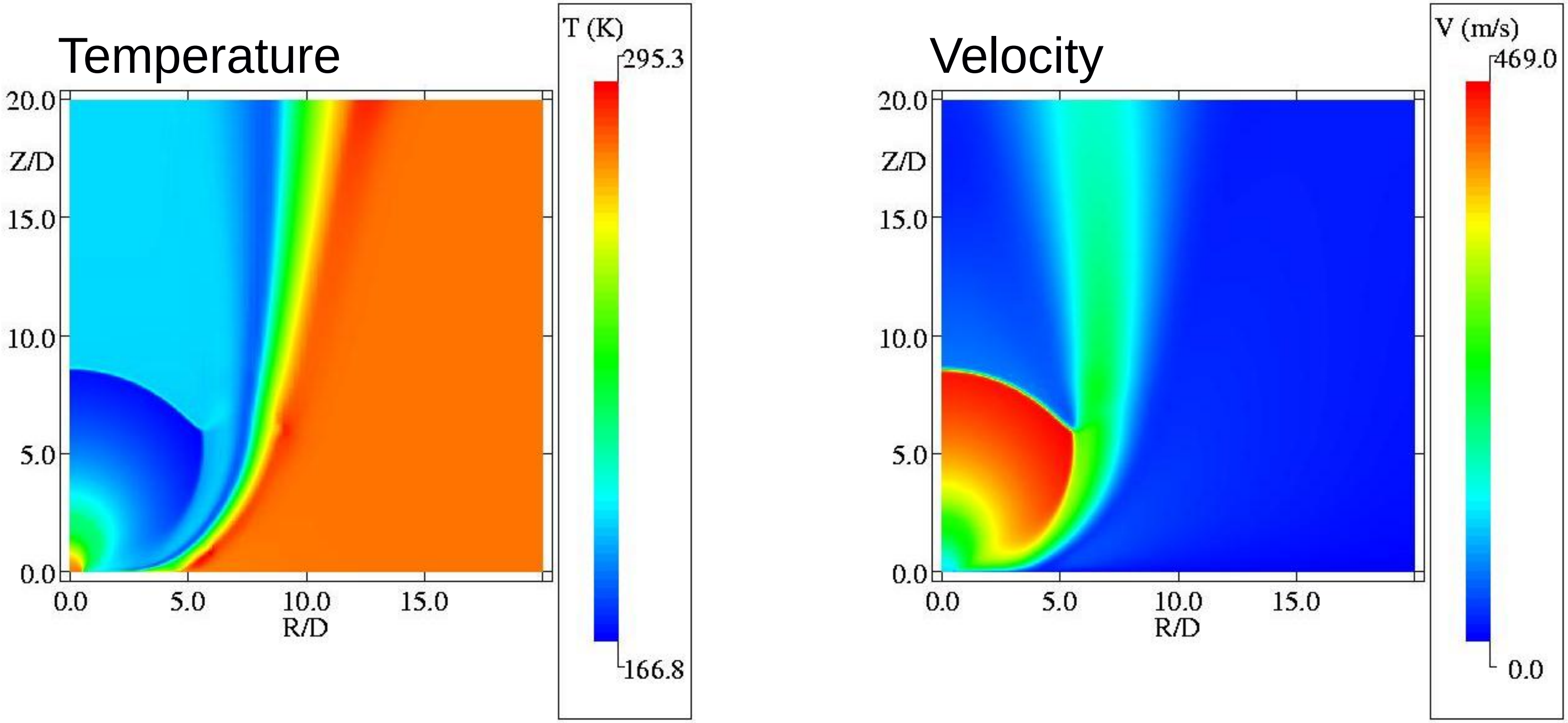


• Adaptive meshing around the Mach shock in a dense high pressure release of CO_2.

Note the axis units are in release diameters.

Validation: dense phase free release

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



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

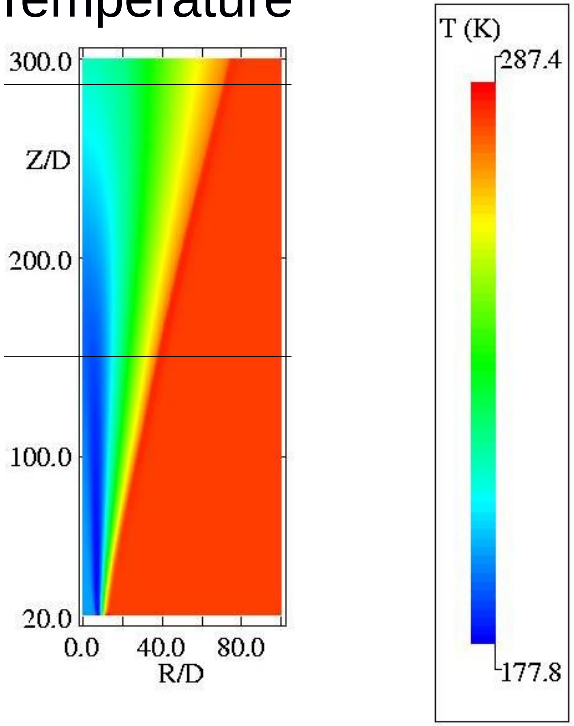
Wareing et al., Int. J. Greenhouse Gas Control, ***20****, 254-271 (2014)*

Validation: dense phase release

Measuring planes at:

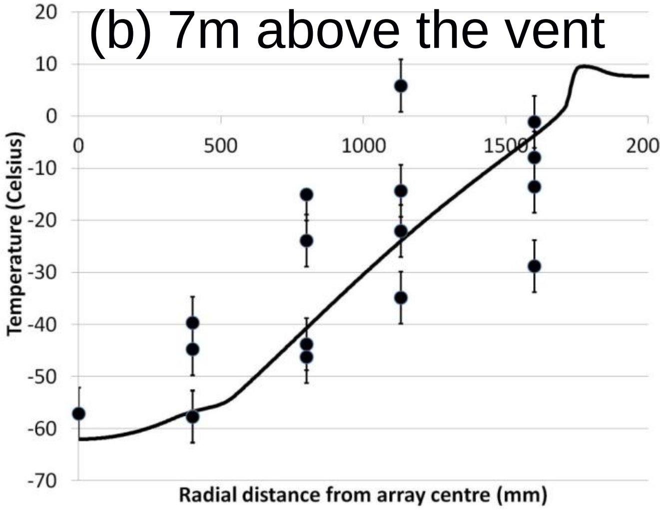
- 4m (165D)
- 7m (288D)

Temperature

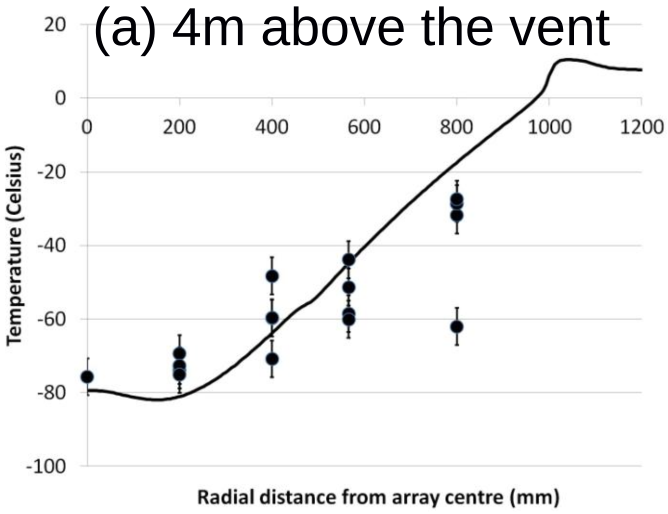


<u>Predictions</u>

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



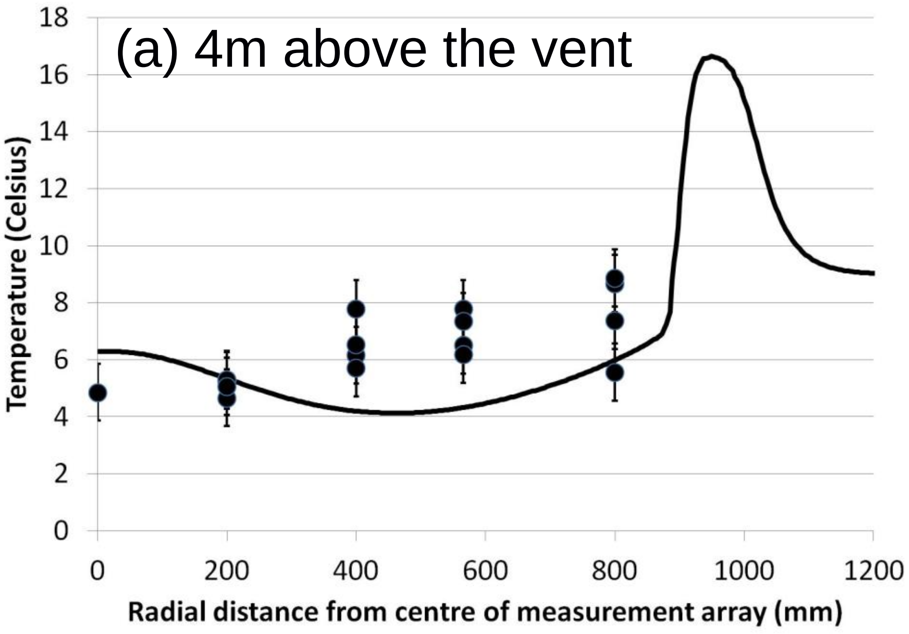
(b) 7m above the vent



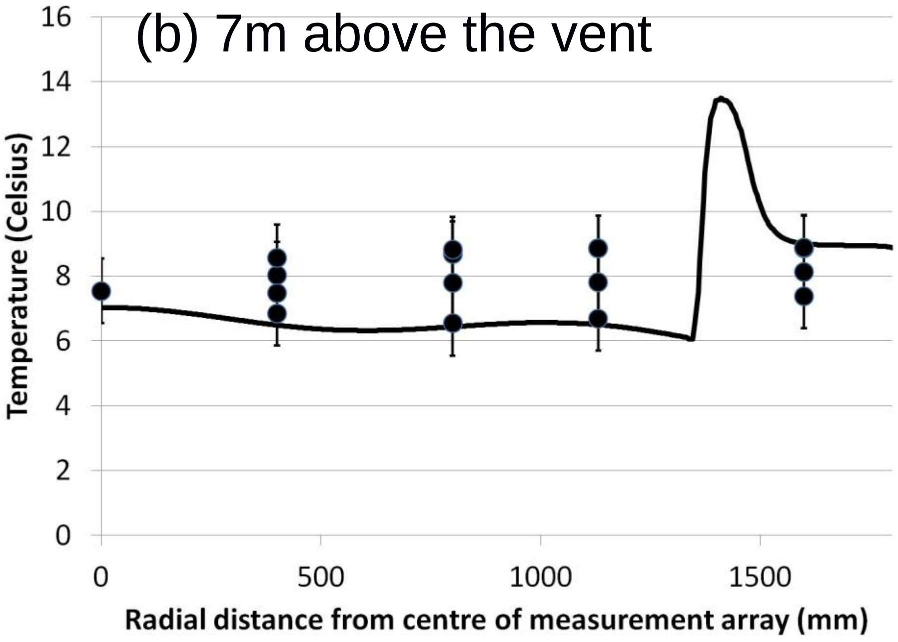
(a) 4m above the vent

Validation: gas phase free release

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



(a) 4m above the vent



(b) 7m above the vent

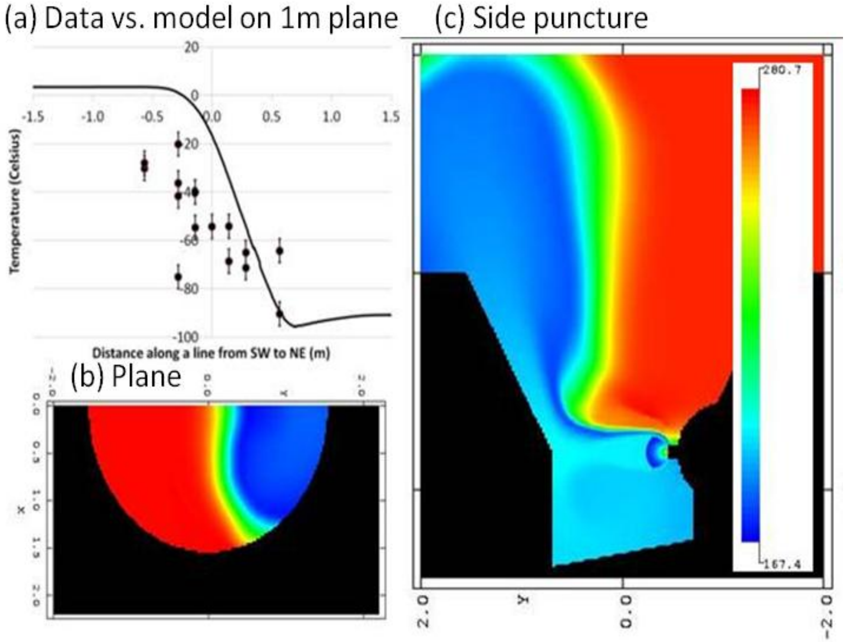
- Despite the considerably different temperature range observed as compared to the dense phase release, predicted core jet temperatures and widths are again in good agreement with the data on both planes

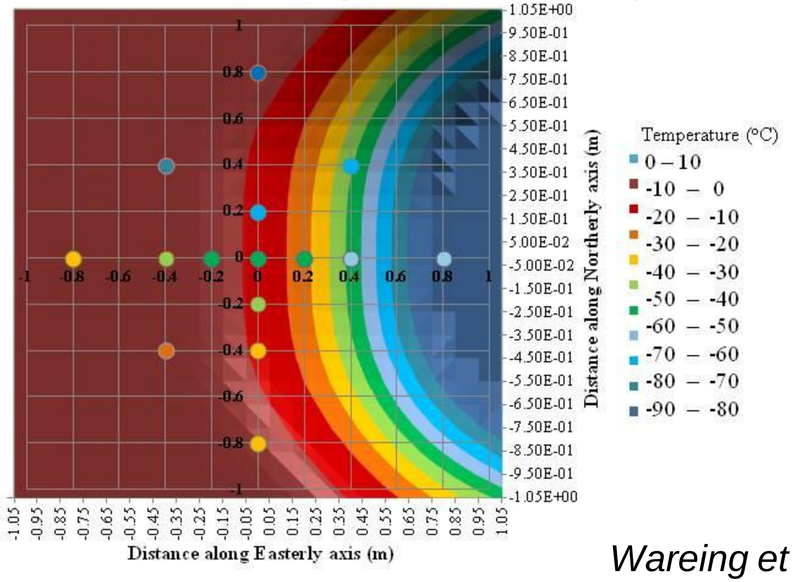
*Wareing et al., Int. J. Greenhouse Gas Control, **20**, 254-271 (2014)*

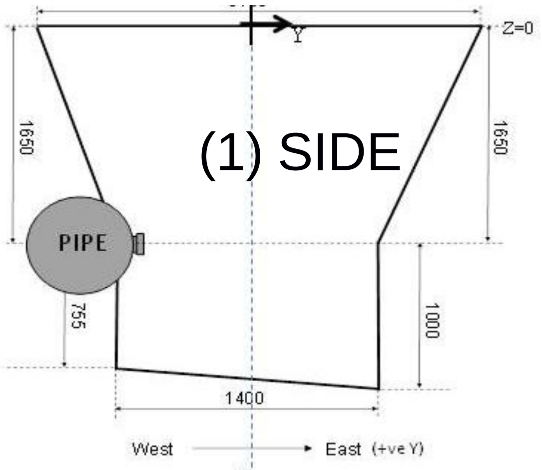
Validation: punctured pipeline

Experimental setup

- 0.9m diameter pipeline.
- Pipeline pressurised to 150bar.
- 25mm diameter circular puncture.
- Preformed craters based on observations of real craters.
- Experimental measurements taken on arrays 1m and 2m above ground level for the side puncture only.



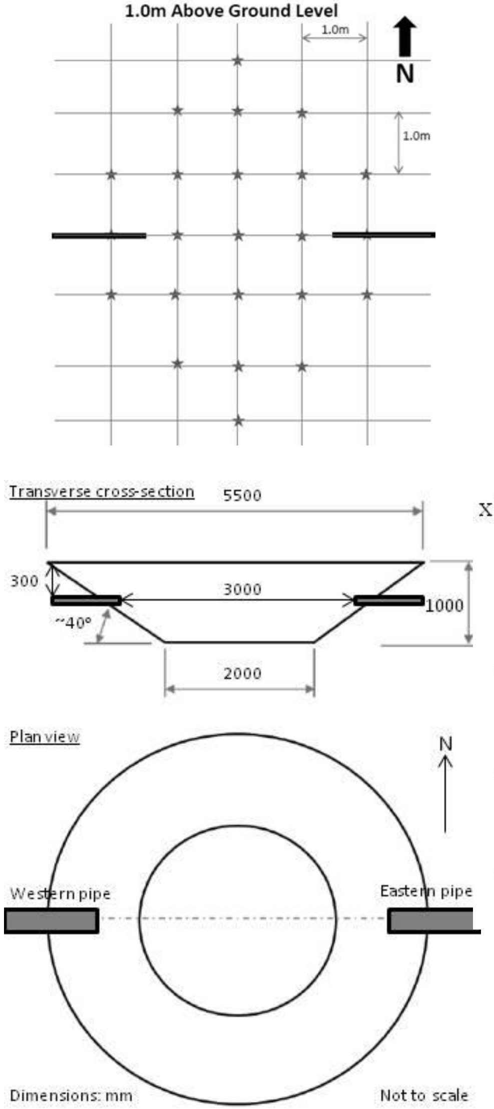




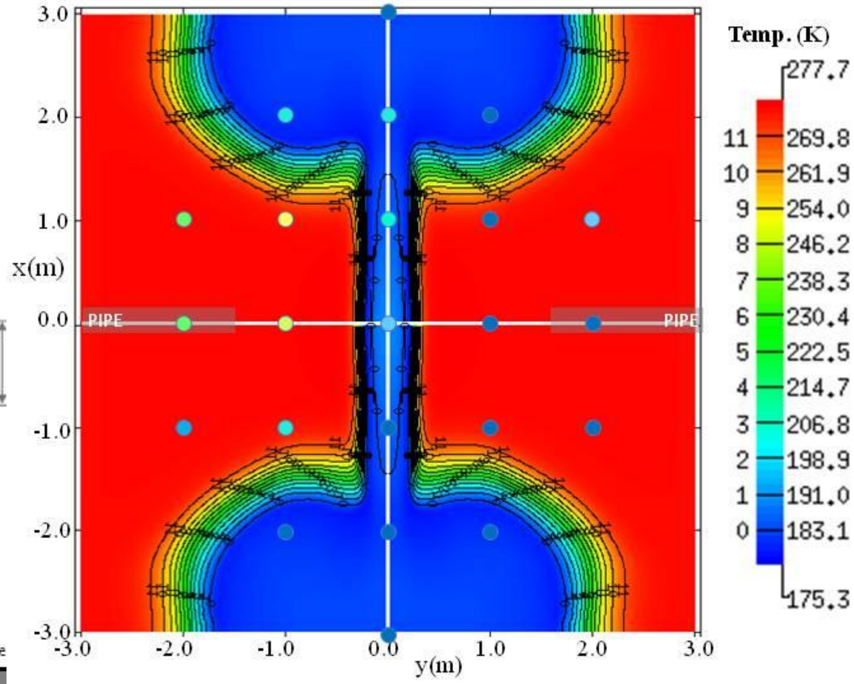
(1) SIDE

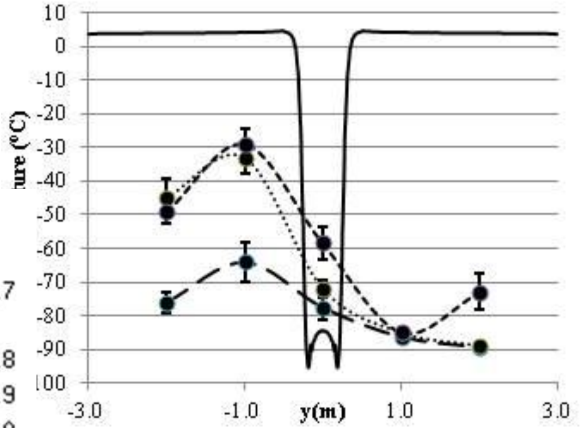
Wareing et al., Int. J. Greenhouse Gas Control, ***29****, 231-247 (2014)*

Validation: ruptured pipeline



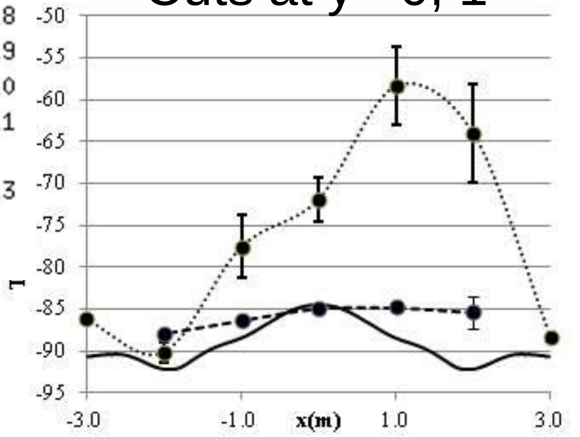
1m above crater





Cuts at x= -1, 0, 1

Cuts at y= 0, 1



Wareing et al., Int. J. Greenhouse Gas Control, doi: 10.1016/j.ijggc.2015.01.020 (2015).

Comparison to experimental datasets

- 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 the averaging period.

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

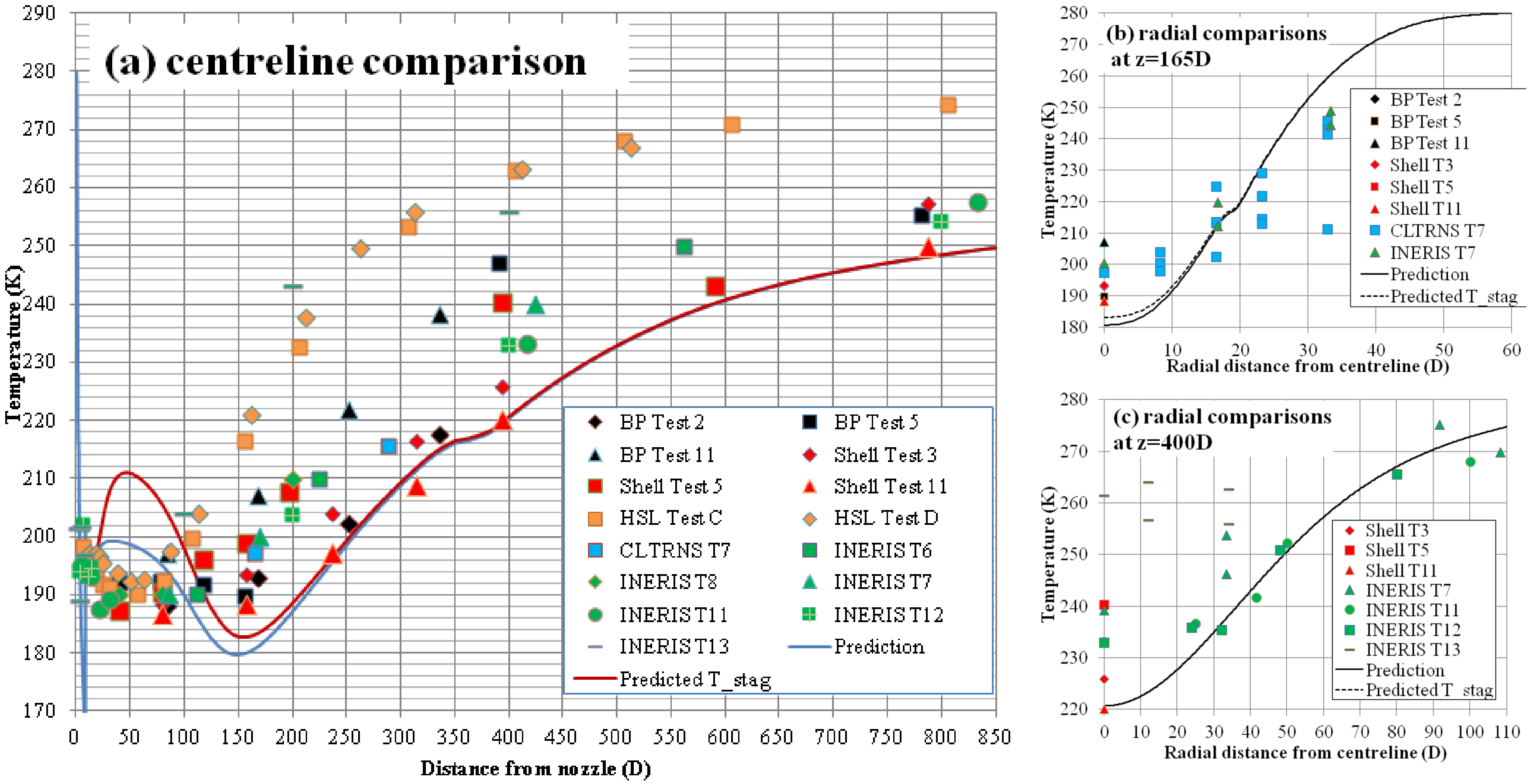
Comparison to experimental datasets

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

Comparison to experimental datasets

- A comparison between experimental data and numerical prediction along the centreline of the jet and radially at 165D and 400D along the centreline.



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

Comparison to experimental datasets

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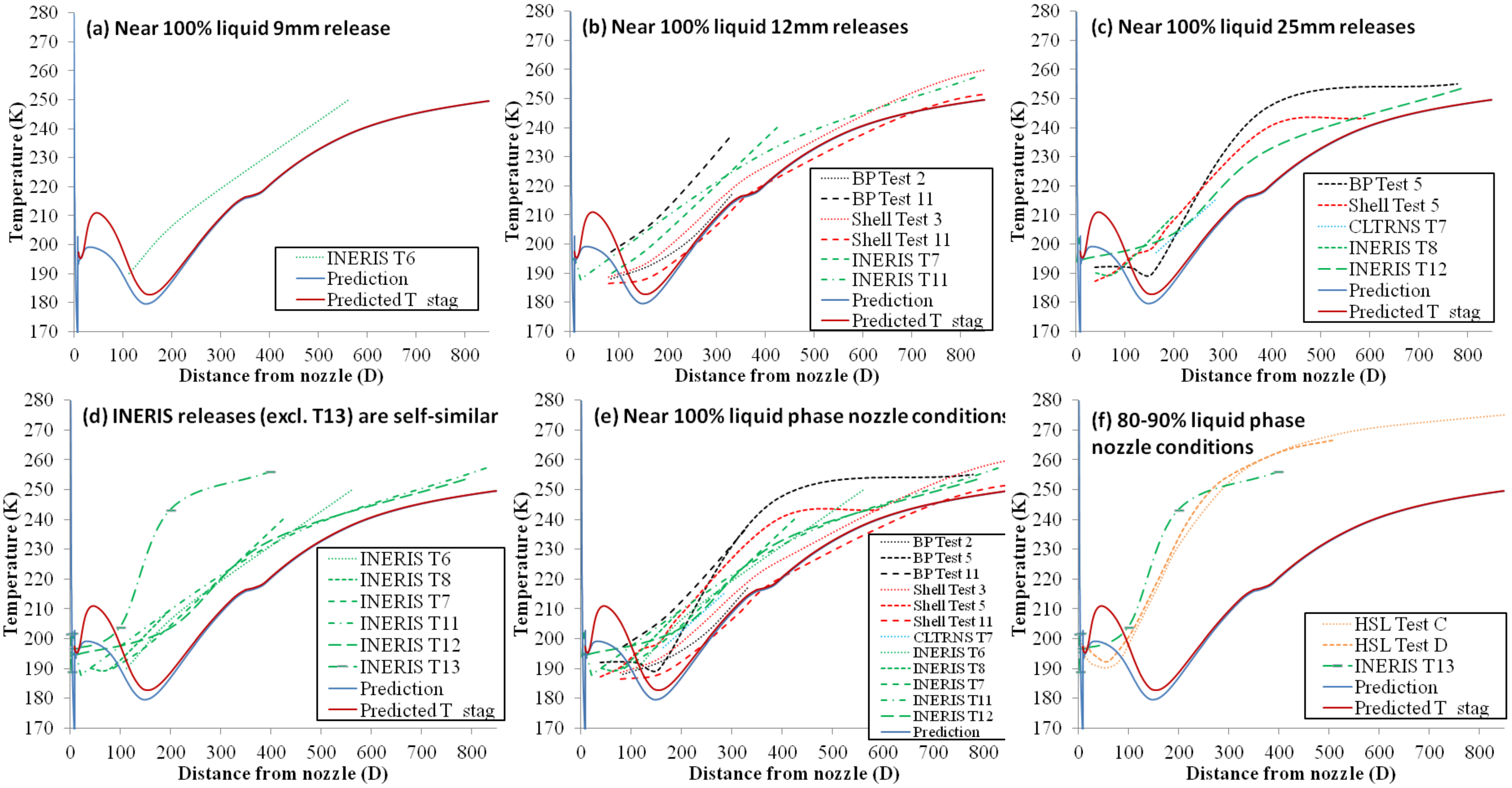

- Subsets of the data: D=9mm (a), D=12mm (b) and D=25mm (c). INERIS tests (d). 100% liquid (e) and 80-90% liquid (f).

Discussion and Conclusions

- All the available datasets are shown together on the centreline of the jet for the first time, 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**, but is at the colder limit of the available experimental data.
- **Agreement is demonstrated between numerical predictions and experimental data of the radial temperature distribution** from multiple sources at 165D and 400D along the centreline.
- By separating the datasets**, liquid fraction at the release point has been shown to be a key parameter for differentiating between the datasets.**
- **The numerical method, with an improved equation of state, is able to model multiple datasets** for sonic CO_2 decompressions.
- A number of simulations are now planned to explore this further, with an improved second-moment Reynolds stress turbulence model.

Thank you for listening

Any questions or comments?

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