

# Comparison of numerical predictions with CO<sub>2</sub> pipeline release datasets of relevance to CCS applications

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## Introduction

- Carbon dioxide (CO<sub>2</sub>) transportation in CCS scenarios can be achieved in different ways, but it is commonly acknowledged that high pressure pipelines carrying dense phase CO<sub>2</sub> will be the most reliable and cost effective choice.
- Their safe operation is of paramount importance as the inventory would likely be several thousand tonnes and CO<sub>2</sub> poses a number of dangers upon release due to its physical properties; it is a colourless, odourless asphyxiant which sinks in air and has a tendency to solid formation upon release from high pressure, with subsequent sublimation.
- A number of projects have included experiments investigating the behaviour of high pressure CO<sub>2</sub> releases simulating accidental or operational CCS scenarios. Typically these are dense phase pure CO<sub>2</sub> releases into air with varying liquid fractions and varying atmospheric conditions. Data is available in the public domain, either published or freely downloadable, from the CO2PIPETRANS and CO2PIPEHAZ European-funded projects, from the industry-funded COOLTRANS research programme and from laboratory scale experiments e.g. [1].
- In this presentation, we perform the first overall comparison between the available datasets by employing our state-of-the-art multi-phase heterogeneous discharge and dispersion model.

## Numerical Modelling Technique

- Calculations employed an adaptive finite-volume grid algorithm which uses a rectangular mesh with adaptive grid refinement [2]. These calculations use an axisymmetric cylindrical coordinate system. A compressibility-corrected  $k-\epsilon$  model is used to represent the turbulent Reynolds stresses.
- Time-averaged, density-weighted forms of the transport equations are integrated using a shock-capturing conservative, upwind, second-order accurate Godunov numerical scheme.
- An efficient thermodynamic method employs a composite equation of state (EoS) with the Peng-Robinson EoS [3] in the gas phase and look-up tables from the Span and Wagner EoS [4] in the liquid phase.
- This composite approach has now been validated for CO<sub>2</sub> releases into air [5, 6], as well as punctures [7] and ruptures [8] of buried CO<sub>2</sub> pipelines.
- The composite method now employs look up tables from the superior Jager and Span [9] EoS for solid CO<sub>2</sub>, instead of data from the DIPPR database.

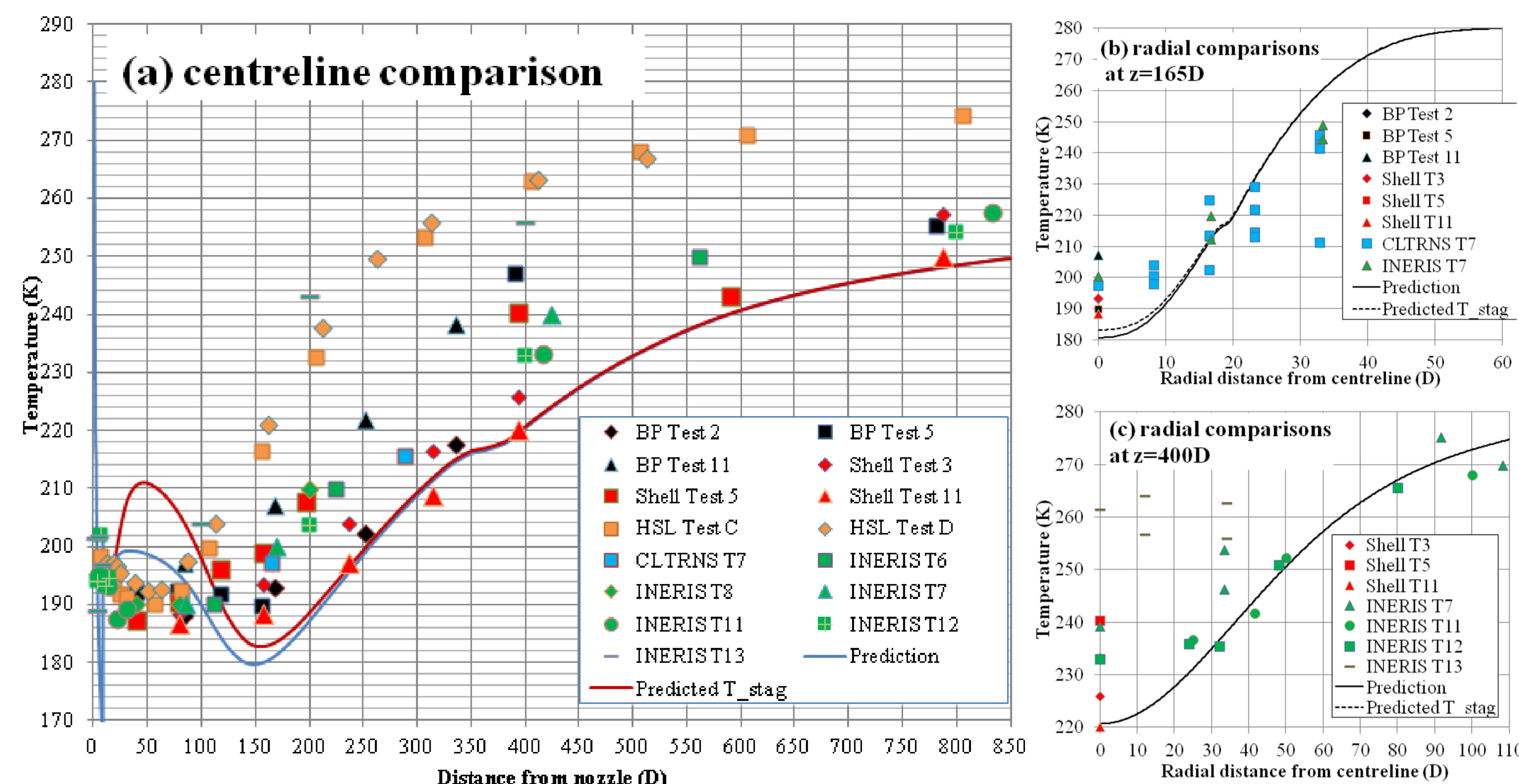
## Experimental Datasets

- We have obtained experimental temperature data regarding near-field releases of high pressure liquid CO<sub>2</sub> from a number of sources. These are detailed in Table 1, with differences between the tests highlighted.
- From each test, we have used consistent, averaged temperature measurements for comparison to the RANS predictions. Each measurement has a variance of a degree or two over this averaging period and the thermocouples are  $\pm 5K$  accurate, hence we have assumed an error of 5K.
- 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.

**TABLE (1).** Experimental data regarding near-field releases of high pressure liquid phase CO<sub>2</sub>.

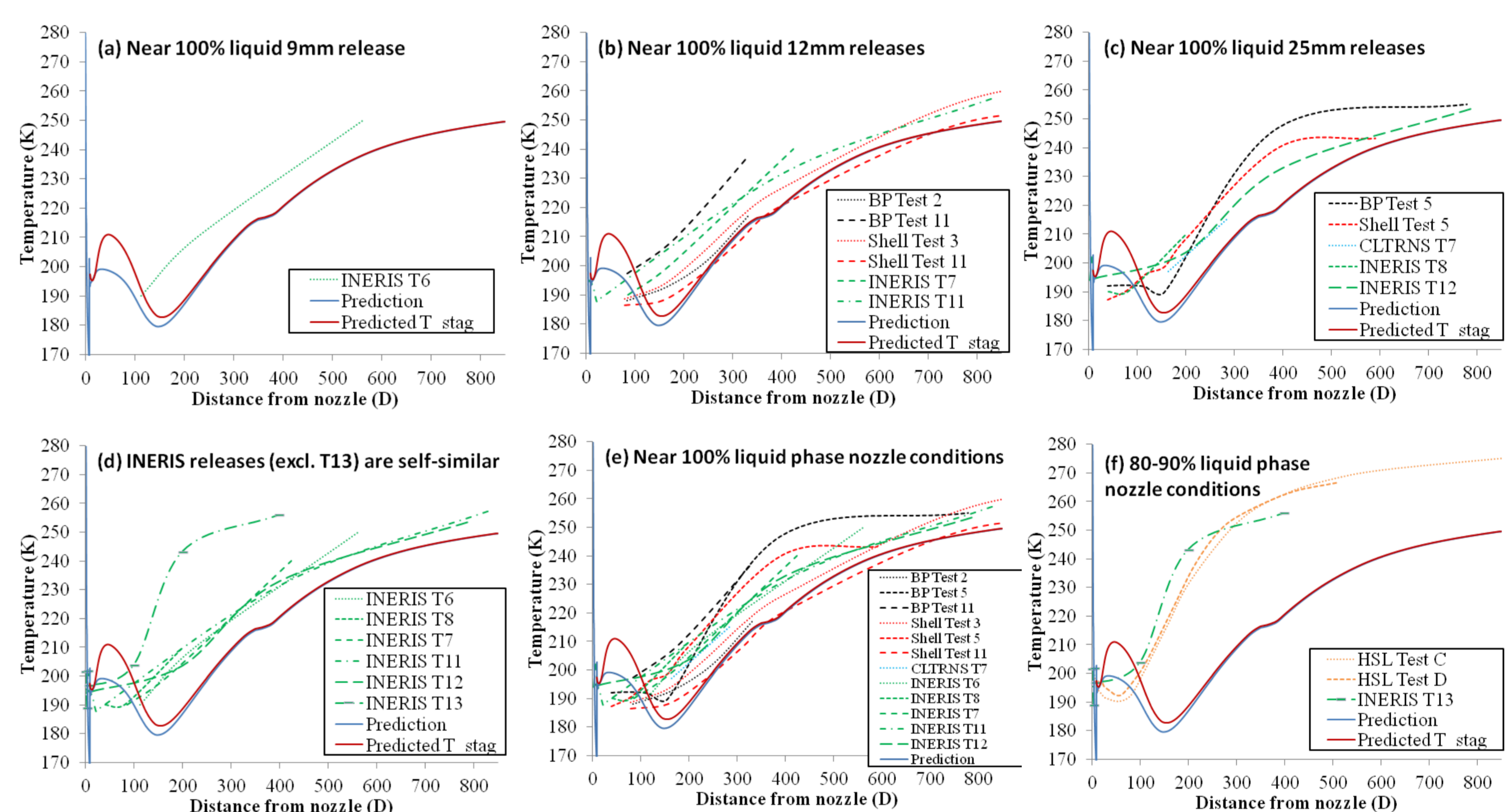
Name	Release diam. (D) (mm)	Horiz./Vert.	Reservoir Pressure (barg)	Estimated liq. fraction at nozzle	Buffer/free	Source
BP Test 2	11.94	H	155	Unknown	Buffer	CO2PIPETRANS
BP Test 5	25.62	H	157	Unknown	Buffer	CO2PIPETRANS
BP Test 11	11.94	V	82	Unknown	Buffer	CO2PIPETRANS
Shell Test 3	12.7	H	150	Unknown	Buffer	CO2PIPETRANS
Shell Test 5	25.4	H	150	Unknown	Buffer	CO2PIPETRANS
Shell Test 11	12.7	H	80	Unknown	Buffer	CO2PIPETRANS
HSL Test C	2.0	H	54	84%	Free	[1]
HSL Test D	4.0	H	49	86%	Free	[1]
CLTRNS T7	24.3	V	150	100%	Buffer	COOLTRANS [6]
INERIS T6	9.0	H	95	100%	Free	CO2PIPEHAZ [5]
INERIS T7	12.0	H	85	100%	Free	CO2PIPEHAZ [5]
INERIS T8	25.0	H	77	100%	Free	CO2PIPEHAZ [5]
INERIS T11	12.0	H	83	100%	Free	CO2PIPEHAZ [10]
INERIS T12	25.0	H	77	100%	Free	CO2PIPEHAZ [10]
INERIS T13	50.0	H	69	80-90%	Free	CO2PIPEHAZ [10]

## Results 1



- A comparison between experimental data and numerical prediction along the centreline of the jet (a) and radially at 165D (b) and 400D (c) along the centreline. The experimental data has an error of  $\pm 5K$  throughout; error bars are omitted in the figure for clarity.

## Results 2



- A comparison of different subsets of the data. Varying nozzle diameters  $D=9mm$  (a),  $D=12mm$  (b) and  $D=25mm$  (c). INERIS tests (d). Release point phase conditions 100% liquid in (e) and 80-90% liquid in (f). Dashed lines connect experimental data points, solid lines the same numerical predictions.

## Discussion and Conclusions

- In 'Results 1' we show for the first time all the available datasets on the centreline of the jet, dimensionalised according to the release diameter (D), predicted centreline fluid and stagnation temperatures stitched together from the numerical simulations. The numerical prediction agrees well, but is at the colder limit of the available experimental data.
- We also demonstrate in 'Results 1' agreement between numerical predictions and experimental data of the radial temperature distribution from multiple sources at 165D and 400D along the centreline.
- In 'Results 2' we have split the representation of the data according to nozzle diameter with 100% liquid fraction (2(a)-2(c)), INERIS data (2(d)) and liquid phase fraction 100% liquid in (e) and 80-90% liquid in (f). For  $\sim 100%$  liquid releases, the centreline temperatures are self-consistent when dimensionalised according to nozzle diameter. The releases with liquid fraction known to be in the range 80-90% are reasonably closely grouped together (2(f)).
- Liquid fraction at the release point is therefore a key parameter for differentiating between these datasets.**
- In conclusion, we have shown here for the first time that our method, with an improved equation of state, is able to model multiple datasets for sonic CO<sub>2</sub> decompressions from high pressure pipelines.
- A number of simulations are now planned to explore this further, with an improved second-moment Reynolds stress turbulence model.

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