RANS Modelling of Sonic CO_2 Jets

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Introduction

- Considerable cross-disciplinary efforts are addressing the fundamentally important and urgent issue of understanding the consequences of accidental releases from pressurised CO_2 pipelines for carbon capture and storage applications.
- The modelling of CO_2 fluid dynamics poses a unique set of problems due to its unusual phase transition behaviour and physical properties. This work addresses issues concerning the accurate modelling of accidental releases due to pipeline puncture or rupture.

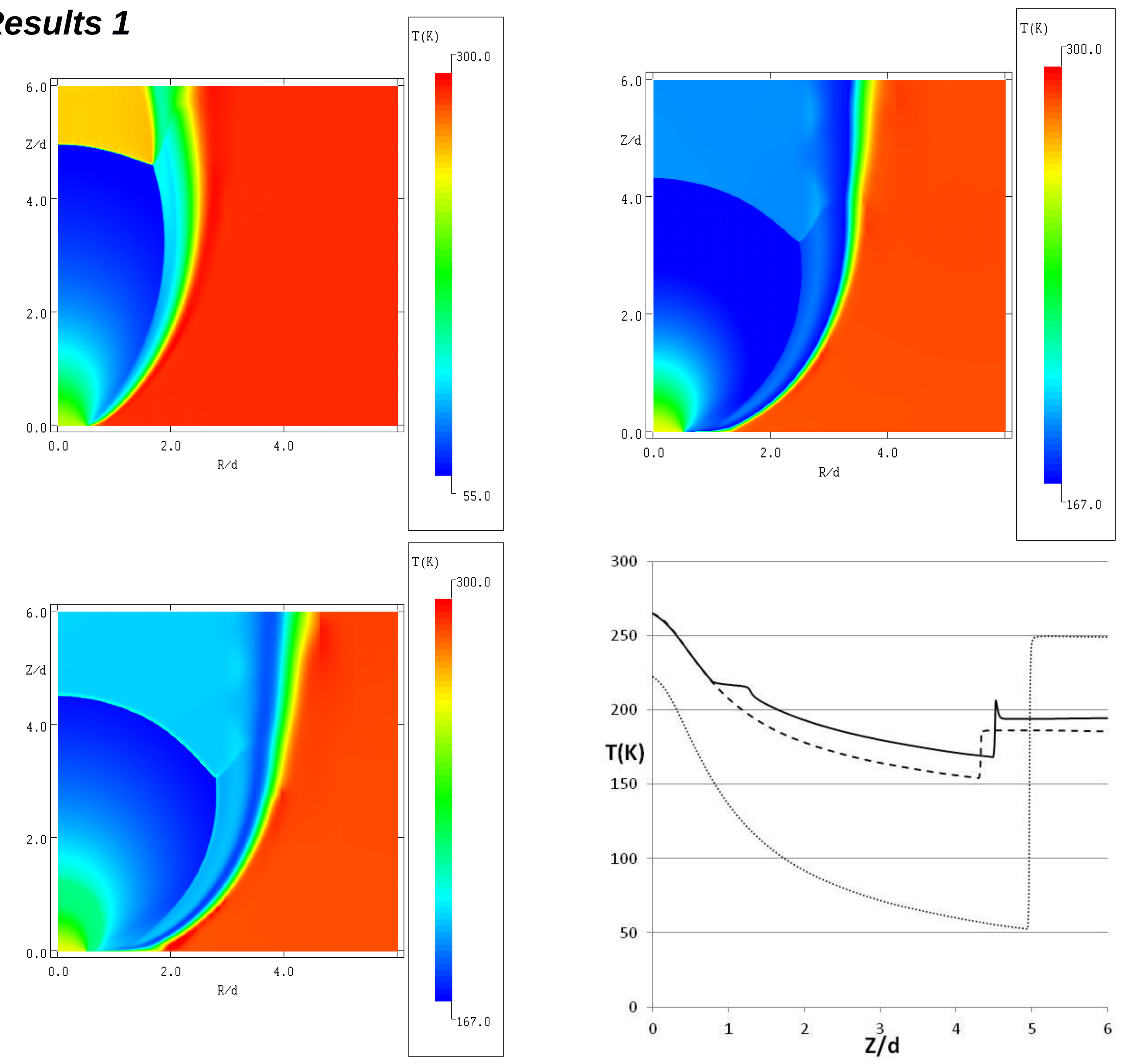
Composite Non-Ideal Equation of State

- A composite equation of state has been constructed in which the gas phase is computed from the Peng-Robinson equation of state [1] and the liquid and condensed phases, including the latent heat of fusion, from tabulated data generated with the Span and Wagner equation of state [2] and the DIPPR Project 801 database [3].
- Saturation pressure, gas and condensed phase densities, sound speed and internal energy have all been tabulated against temperature, providing the basis for a fully functional form for differentiation, interpolation and extrapolation in numerical simulations.
- No discontinuity or loss of accuracy at the critical point or anywhere along the saturation curve has been encountered by using this composite approach with different equations of state as the composition has ensured that the Helmholtz free energy has continuous first derivatives.

Turbulent Compressible Flow Mathematical Modelling

- Calculations employed an adaptive finite-volume grid algorithm which uses a two-dimensional rectangular mesh with adaptive grid refinement [4].
- A k-ε model is used to represent the turbulent Reynolds stresses. The model proposed by Sarkar et al. [5] has been implemented to account for compressibility effects.
- Time-dependent, density-weighted forms of the descriptive equations are integrated using a shock-capturing conservative, upwind second-order accurate Godunov numerical scheme [6]. A Harten, Lax and van Leer Riemann solver was employed to calculate fluxes at cell boundaries [7].

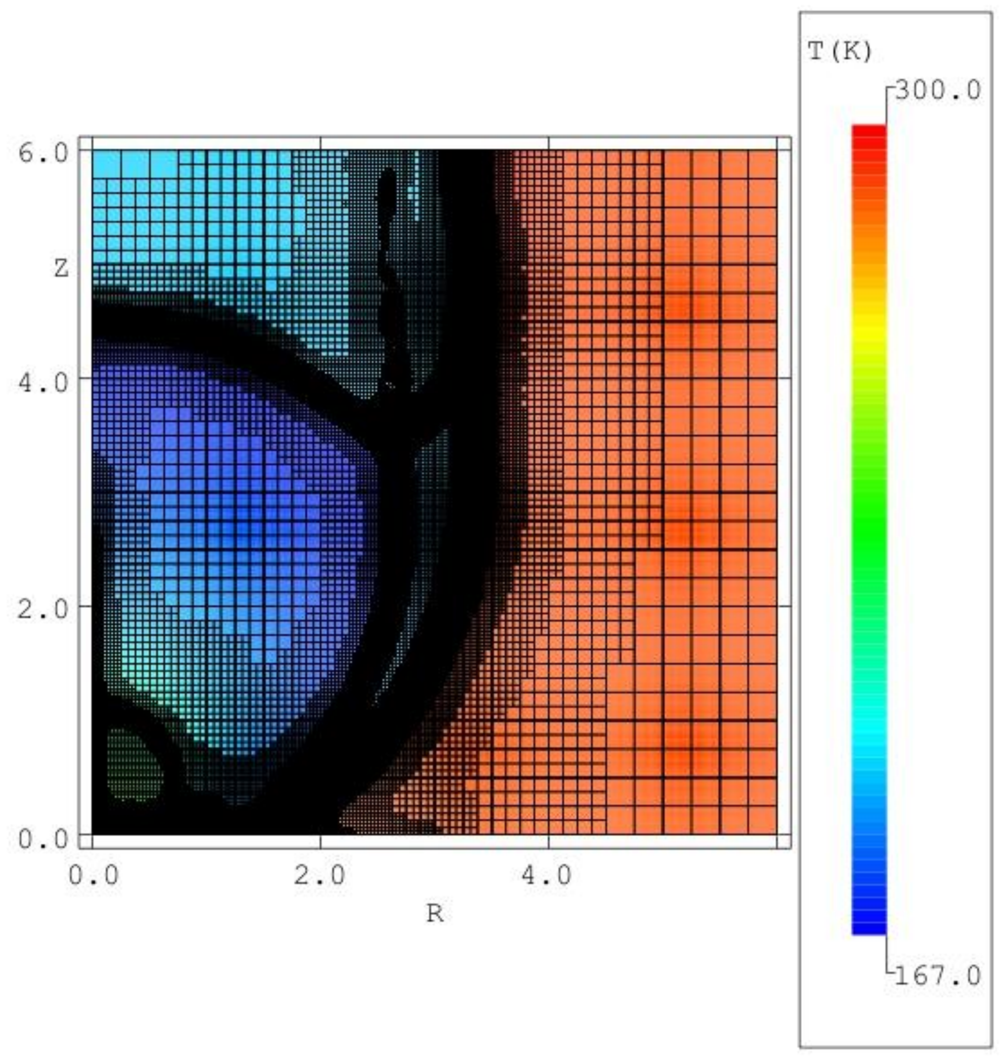
Results 1



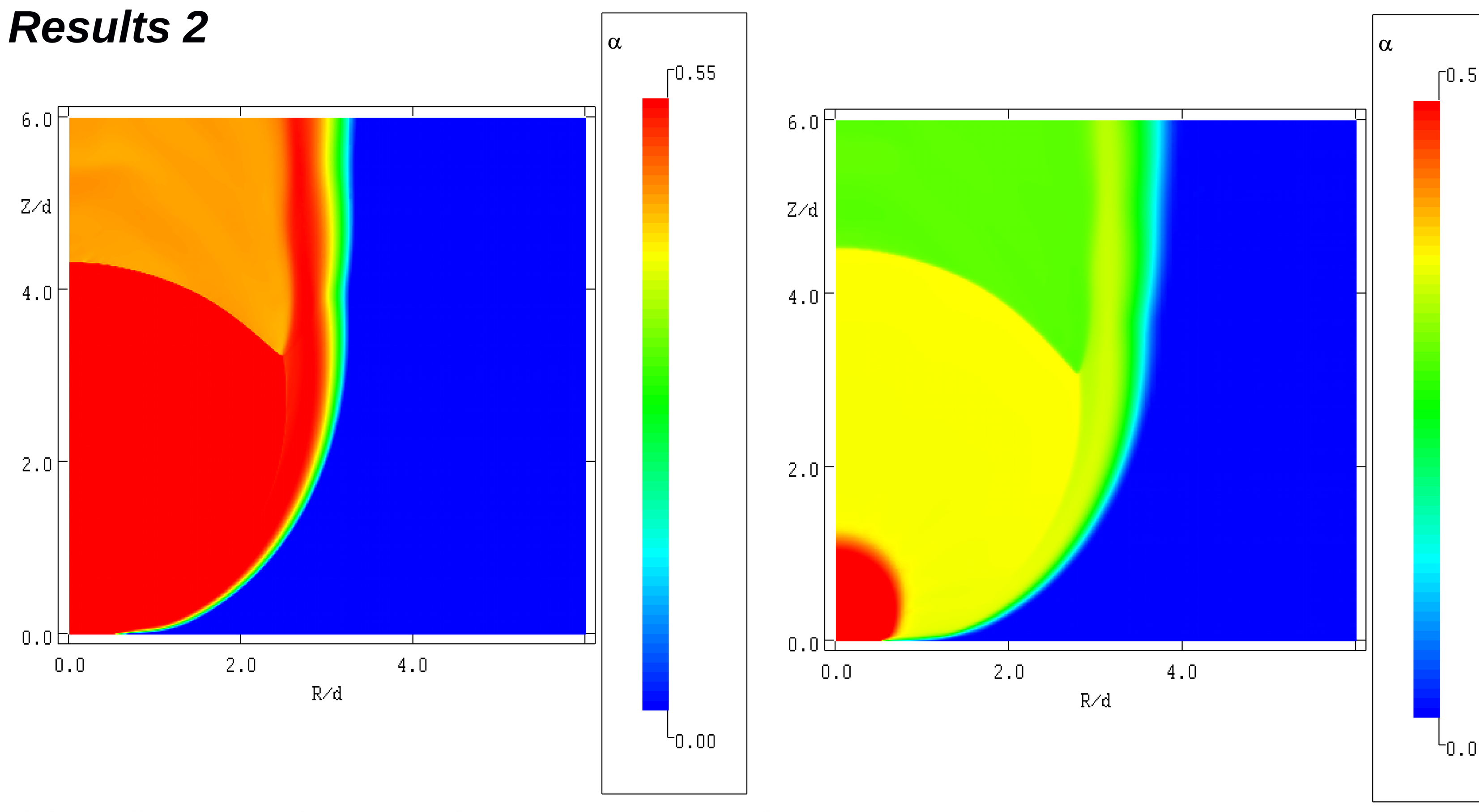
This figure shows the temperature structure of the jet produced by the ideal equation of state (top left), the Peng-Robinson equation of state (top right) and the new composite method (bottom left). In the lower right panel, we show a comparison along the centreline axis between the three models – ideal (dotted line), Peng-Robinson (dashed line) and composite (solid line). Employing the three-phase accurate composite method changes the Mach shock structure, widens the jet and leads to higher temperatures post-Mach shock.

Adaptive Grid

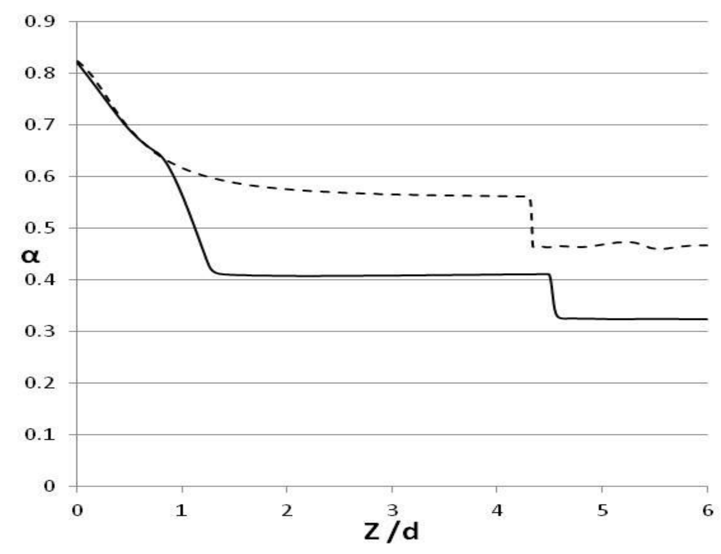
The Adaptive Mesh Refinement grid when simulating a CO_2 release is shown on the right. Levels 1 to 5 of the grid are shown. Level 0 is only present outside this subset of the domain. The AMR method employs an unstructured grid approach, requiring an order of magnitude less memory and giving an order of magnitude faster computation times than structured grid AMR.



Results 2



This figure shows the amount of condensed phase CO_2 as a fraction of the total CO_2 in the jet predicted by the Peng-Robinson equation of state (left) and the composite equation of state (right). On the right, we show a comparison along the jet axis between the two models – Peng-Robinson (dashed line) and composite (solid line). Including latent heat considerably changes the condensed phase fraction.



Conclusions

- We have developed a new composite equation of state capable of predicting the thermophysical properties of CO_2 for the range of temperatures and pressures of interest to the carbon capture and storage industry and in other applications.
- A comparison of predictions of sonic CO_2 jets has been performed employing an ideal equation of state, the Peng-Robinson equation of state [1] and the new composite method.
- Unlike the other approaches, the composite method accounts for the solid phase and the latent heat of fusion and as a result, correctly predicts the pure CO_2 mixture of solid and gas at atmospheric pressure to be at the sublimation temperature.
- These simulations have demonstrated it is crucial to employ a three-phase accurate equation of state accounting for the latent heat of fusion to model atmospheric dispersion from high pressure CO_2 pipelines.

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