Particle-laden Sonic CO_2 Jets

Investigation of initial particle distribution and turbulent shear agglomeration

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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 and particle 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 particle-laden sonic CO_2 jets formed as a result of pipeline puncture or rupture.

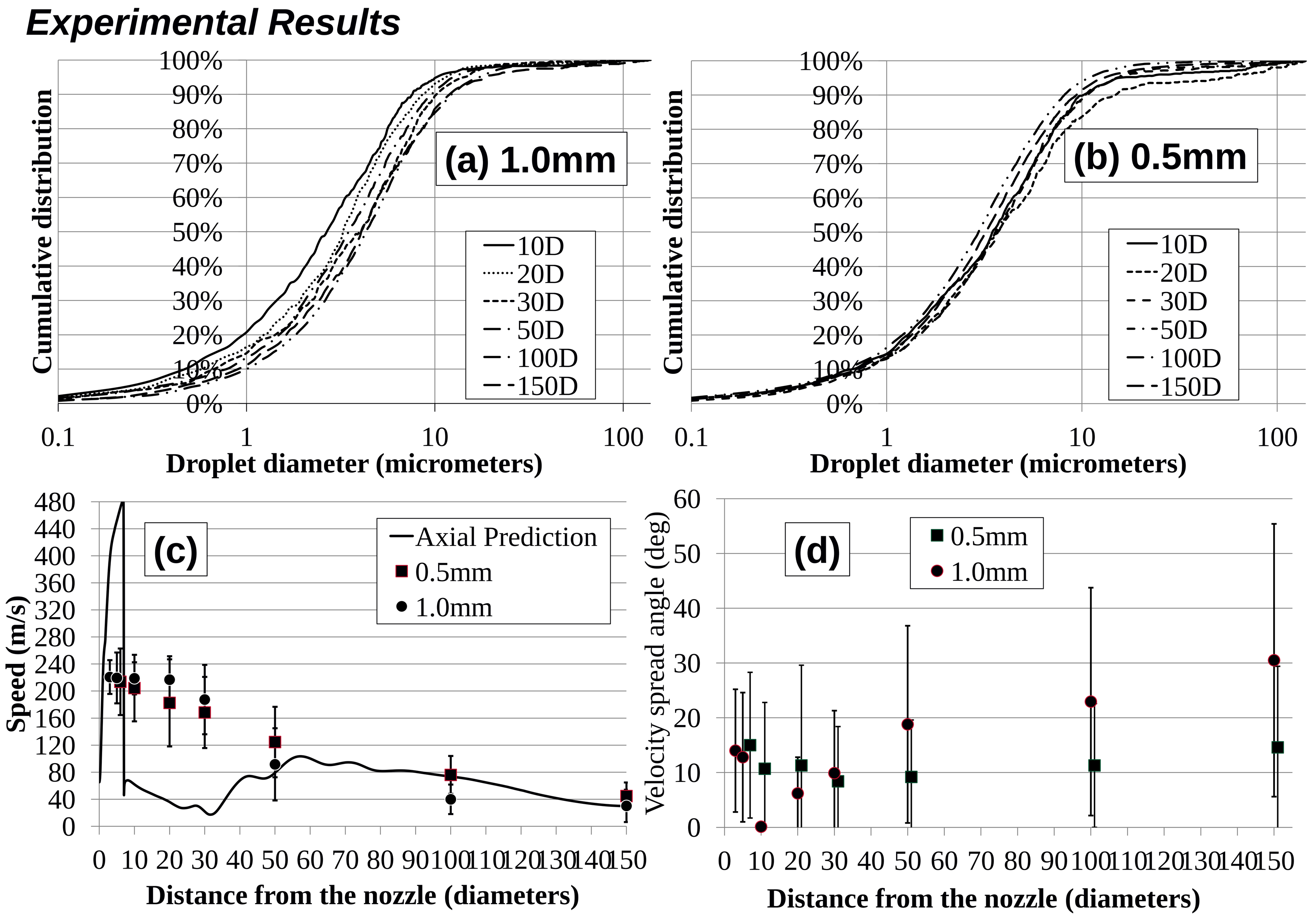
Composite Non-Ideal Equation of State

- A composite equation of state has been constructed for CO_2 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

- Numerical calculations employed an adaptive finite-volume grid algorithm which uses a two-dimensional rectangular mesh with adaptive grid refinement.
- A k-ε model is used to represent the turbulent Reynolds stresses. The model proposed by Sarkar et al. [4] 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 [5]. A Harten, Lax and van Leer Riemann solver was employed to calculate fluxes at cell boundaries [6].

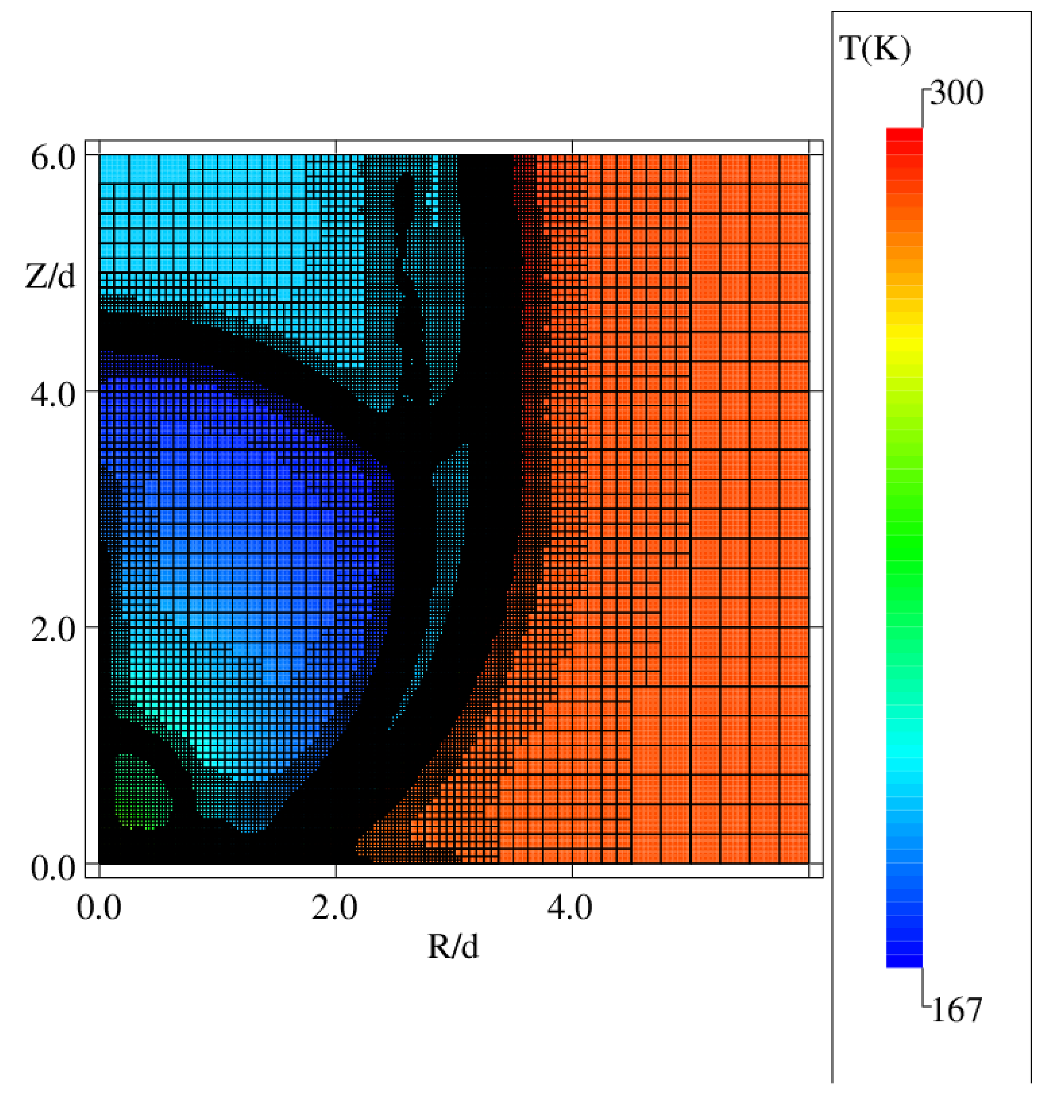
Experimental Results



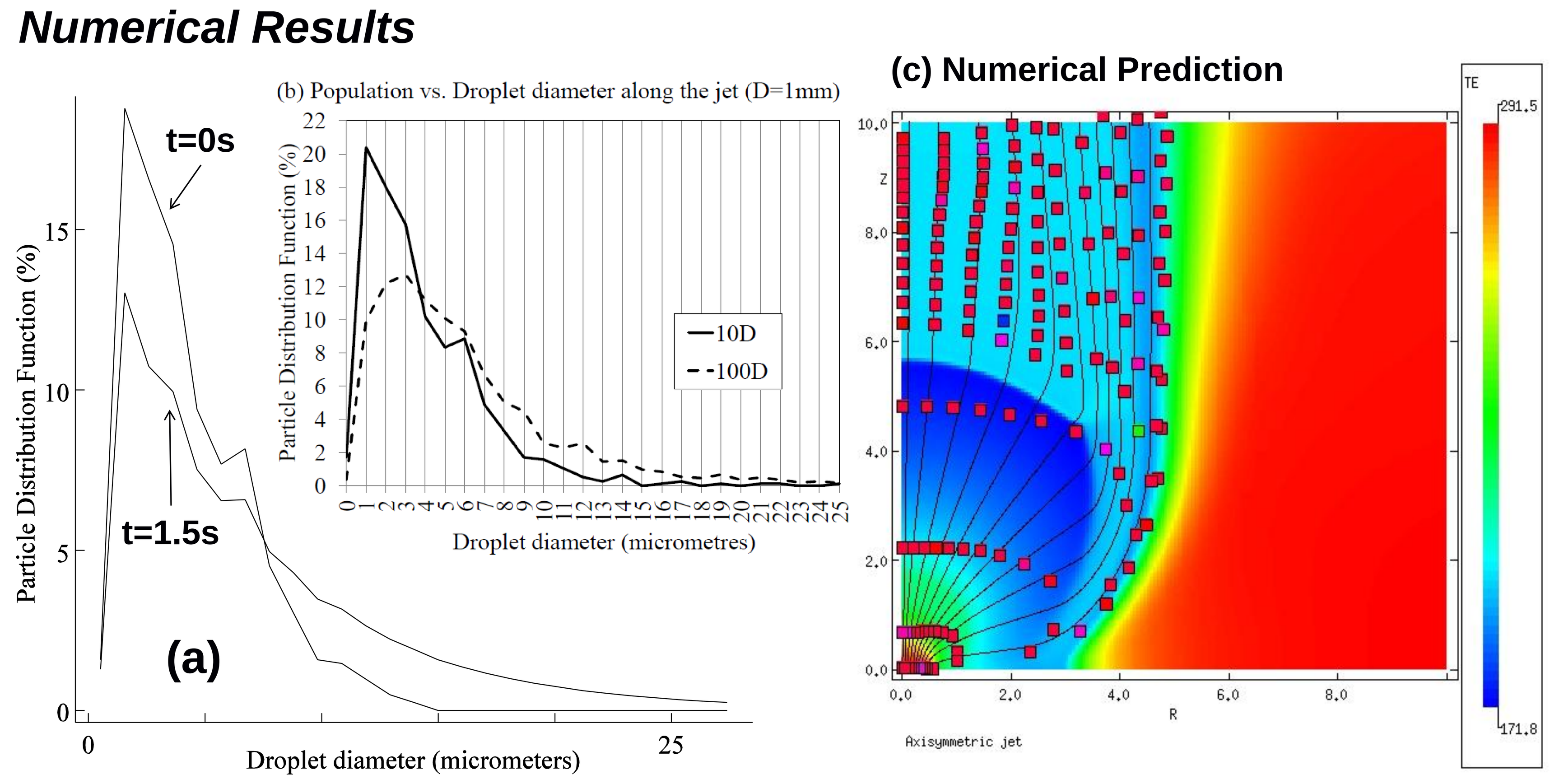
- The experimental work was carried out in a laboratory setting. A 20ml canister of liquid CO_2 at 68.9 bar and room temperature was released through either a 0.5mm or 1.0mm diameter (D) nozzle into a Perspex box (50×50×500 mm).
- A Dantec laser Doppler anemometer with a phase Doppler anemometer module was used to measure particle sizes and velocities at various distances from the nozzle along the centreline of the resulting sonic jet.
- The experiments have shown that the initial particle distribution post Mach shock is nozzle size independent, with a distribution centred on a diameter of 1 to 2 μm, in agreement with Weber number predictions (Figures a and b).
- Agglomeration along the jet occurs only in the D=1.0mm case (Figure a).
- Average velocity magnitudes are very similar in both cases (Figure c).
- The average velocity vector angle from the centreline is greater in the D=1.0mm case, corresponding to slightly lower velocity magnitudes (Figure d).

Adaptive Grid

The Adaptive Mesh Refinement (AMR) 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, refining the grid only in areas of strong gradients, employs an unstructured grid approach, requiring an order of magnitude less memory. The grid is also defragmented in hardware memory on every timestep, overall giving an order of magnitude faster computation times than structured grid AMR.



Numerical Results



- The numerical scheme described above was used in combination with a particle distribution function with logarithmic mass bins and a Lagrangian particle tracker.
- A turbulent shear agglomeration model dependent on the square root of ε [7] has been initially employed in order to model agglomeration along the jet.
- Numerical predictions employing this turbulent shear agglomeration model (a) are able to reproduce the experimental observations (b) at an equivalent distance downstream. The Lagrangian particle tracker is able to track the particles through the Mach shock.
- However, there are indications from the experimental velocity data that the particles are not in equilibrium with the flow.

Conclusions

- The initial particle distribution is nozzle size independent and hence can be directly imposed at a puncture or rupture in safety studies regarding the transport of liquid CO_2 in high pressure pipelines.
- For small nozzles, such as those studied here, the particle inertia is not negligible and hence the particles are neither in thermal or dynamical equilibrium.
- By 50 nozzle diameters downstream, experimental results indicate the particles have reached dynamic equilibrium with the fluid. The spread of velocity vectors would indicate larger nozzle releases are more turbulent and hence the experimentally observed agglomeration can be numerically modelled in terms of simple turbulent shear agglomeration.
- Future work will examine the effects of turbulence on the particles through further experimental work and three-dimensional LES modelling and RANS modelling with an improved turbulence closure of the equation set.

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