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Numerical Modelling of Particle-Laden Sonic CO_2 Jets with Experimental Validation

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Abstract. The characteristics of the particle distribution, evolution and movement in a sonic jet release of carbon dioxide (CO_2) from a high pressure reservoir are investigated. The motivation is to numerically model the sonic jet with particles,using the hitherto unknown initial particle distribution measured herein,and hence understand and numerically reproduce the experimentally observedparticle behaviour downstream of the Mach shock, including turbulence characteristics and level of agglomeration. We employ a Reynolds-averaged Navier-Stokes scheme with adaptive mesh refinement (AMR), combined with a Lagrangian particle tracker and particle distribution function. The model is seeded at the nozzle with the experimentally measured particle distribution and exploited to reproduce the observed characteristics of the jet. These releases are designed to be representative of a sonic CO_2release into the atmosphere and so provide data to help interpret how accidental or operational releases from the transport aspect of a carbon capture and storage chain might behave.

Keywords: CCS, CO_2, multi-phase flow, experimental measurement, mathematical modelling, pipeline depressurization
PACS: 02.60.-x, 47.11.-j,47.11.Df, 47.40.Ki, 47.40.-x, 47.55.-t 47.85.Dh

INTRODUCTION

Predicting the correct fluid phase and solid particle behaviour during the discharge process in the near-field of sonic carbon dioxide (CO2) jets is of particular importance in assessing the behaviour associated with the transport aspects of carbon capture and storage (CCS) schemes, given the very different physical hazardprofiles of CO2 in the gaseous and solid states. Recent work [1] has shown high pressure releases of supercritical CO2result in an initial condensation-formed particle diameter distribution centred around 0.1 micrometers. Agglomeration also occurs along the sonic jet. Recent work by our group has investigated high pressure liquid phase releases of CO2, measuring liquid-breakup particle size distributions along the jet, in order to quantify particle evolution. In the work presented here, we take the measured initial particle size distribution and numerically model the particle behaviour with appropriate evolutionary models in order to reproduce the observed behaviour.

NUMERICAL TECHNIQUE

The numerical technique fully described in [2] was used to predict the flow.Predictions were based on the solutions of the density-weighted time-averaged (Favre) forms of the transport equations for mass, momentum and total energy, with closure of this equation set achieved using a compressibility-corrected k-ε turbulence model. Solutions were obtained of the time-dependent, axisymmetric forms of the descriptive equations and the integration of the equations performed by a shock-capturing conservative, upwind second-order accurate Godunov numerical scheme. The fully-explicit, time-accurate, cell-centered finite-volume Godunov method was a predictor-corrector procedure, where the predictor stage is spatially first-order, and used to provide an intermediate solution at the half time-step. This solution is then subsequently used at the corrector stage for the calculation of second-order accurate fluxes that lead to a second-order accurate cell-centered solution. A Harten, Lax, van Leer Riemann solver was employed to calculate fluxes at cell boundaries. The numerical scheme employs an unstructured AMR techniquewhich automatically allows for fine resolution in the regions of strong gradients and lower resolution elsewhere, as shown in Figure 1. The grid is also defragmented in hardware memory on every timestep, increasing efficiency further.In order to fully model the range of temperatures and pressures in releases of pressurised CO_2, the scheme employs a new composite numerical three-phase equation of state method. This efficient method employs

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the two-phase Peng-Robinson[3] equation of state in the gas phase, look-up tables from the two-phase Span & Wagner[4] equation of state in the liquid phase, and Design Institute for Physical Properties(DIPPR®) 801 database[5] to correctly model the latent heat of fusion and the solid phase.This novel development is necessary as temperatures drop below the triple point, which other methods [3,4] do not account for. The scheme was employed in combination with a particle distribution function with logarithmic mass bins and Lagrangian particle tracker. A turbulent shear agglomeration modeldependent on the square root of ε[6] has been employed to model agglomeration along the jet.

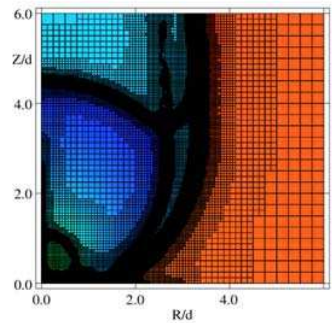

FIGURE 1. The adaptive grid. The automatic mesh refinement around gradients at a Mach shock from a nozzle at z=0, r<0.5.

EXPERIMENTAL MEASUREMENTS

The experimental work was conducted in a laboratory setting in a large container with a separate vent system fitted to ensure safe handling of the CO_2. A 20millilitre (ml)capacity canister of liquid CO_2 was pressurised to 68.9bar and allowed to equilibrate to ambient temperature for one hour. The canister was then clamped into a frame with the nozzle protruding into a custom-made Perspex box (dimensions 50 mm ×50 mm × 500 mm), flush with the internal surface of the box. Two custom-made nozzles were used with diameters of 0.5mm and 1.0mm - the largest usable for the experimental rig. The instrument used for measurement was a Dantec fiberflow laser Doppler anemometer (LDA), with a Dantec classic phase Doppler anemometer (PDA) module. The data were processed using a Dantec burst spectrum analyser and Dantec BSA flow software. The illumination was provided by a Spectra-Physics Stabilite 2017 multi-spectral argon-ion continuous wave laser. The LDA was initiated and the measurement volume was located on the centerline of the jet, at a range of distances from the nozzle. Data collection was commenced and 10 seconds later a 1/4 turn gas valve was opened to release the CO_2 from the canister into the Perspex box. Each experiment was released into the atmosphere in the container, mimicking a discharge from saturated conditions into a regular atmosphere, although the Perspex box is rapidly filled with CO_2. Measurements were obtained at 3 (1.0 mm only), 5 (0.5 mm only), 6 (1.0mm only), 10, 20, 30, 50, 100 and 150 nozzle diameters (D) downstream.

RESULTS AND DISCUSSION

The experiments have directly measured the initial particle distribution post Mach shock and shown it to be nozzle size independent and centred on a diameter of 1 to 2 micrometres (Figure 2), in agreement with Weber number predictions. Whilst 80% of the particles have a diameter of 10 micrometres or less, there is an extended population of particles at larger diameters, indicating a large-diameter-skewed log-normal distribution in the initial expansion from the nozzle. This scale-independence would indicate the distribution can be directly applied in safety studies at all scales, for example in simulations of accidental dense phase CO_2full-bore releases from high pressure pipelines.

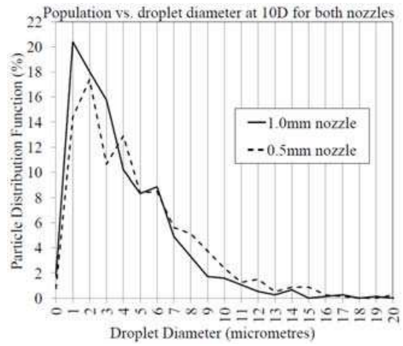

FIGURE 2. Experimental results. The post Mach shock particle distribution at 10D along the jet from the release point for the 0.5 mm and 1.0mm diameter nozzles.

The experiments have shown no change in particle distribution along the jet in the 0.5mm diameter nozzle case (Figure 3a). In the 1mm diameter nozzle case (Figure 3b), the shift rightwards of the cumulative distribution is evidence for net agglomeration between 10D and 50D.Between 100D and 150D, the distribution moves left, indicating net evaporation.As part of the technique, the velocity of each particle was measured in terms of stream-aligned and transverse components. In Figure 4a, we show the average magnitude of velocity for both cases, along with the numerical prediction of centerline fluid velocity. The experimentally measured velocities are reasonably similar, but are not in total agreement with the prediction until 50D from the nozzle. We also show the angle of the velocity vector to the centerline (Figure 4b). The angles derived from the experimental measurements are similar initially (up to 30D) but then the average angles are greater, with a wider distribution in the 1.0mm diameter nozzle case. This also corresponds to slightly lower average velocities.

If you impose the measured initial particle distribution at the nozzle in the numerical model, ashear agglomeration model [6] is able to reproduce the observed agglomeration along the jet in the 1.0mm diameter nozzle case (Figure 5). To understand the results in the 0.5mm diameter nozzle case, and the particle velocity measurements, other influences need to be considered in order to estimate how the flow affects the particles. From the DIPPR database, the dynamic viscosity of CO2 is given by μ = a1 + a2T + a3T2, where a1 = 1.12×10-6, a2 = 4.98×10-8 and a3 = -1.09×10-11. From this and [4],at 280K, μ = 1.43×10-5 kg m-1 s-1 and ρparticle = 0.883×103 kg m-3. At 200K, ρparticle = 0.883×103 kg m-3and ρparticle = 1.546×103 kg m-3.For particles with radius r = 10-6 m and a relative velocity of 1 m s-1, this gives a Reynolds number Re < 0.1, which means that we can use the low Reynolds number limit for the viscous drag. It can be shown that the particle relaxation time is 3×10-5 seconds (s) at 200 K and 1.4×10-5 s at 280 K. At the nozzle exit T~280K and the velocity is approximately 100 m s-1, so the stopping distance due to viscous drag is 1.4mm. This is not a negligible distance as the shock is at 3mm for the 0.5mm case and 6mm for the 1.0mm case. The flow accelerates from 100 m s-1 at the nozzle to around 450 m s-1 at the Mach shock (~6D), hence considerably extending the stopping distance (i.e. the distance at which the particles reach dynamic equilibrium with the fluid. For the size of nozzles under consideration here, it is clear that we cannot assume that the particle inertia is negligible. This is in agreement with the experimental particle velocities that do not follow the fluid velocity (see Figure 4a).

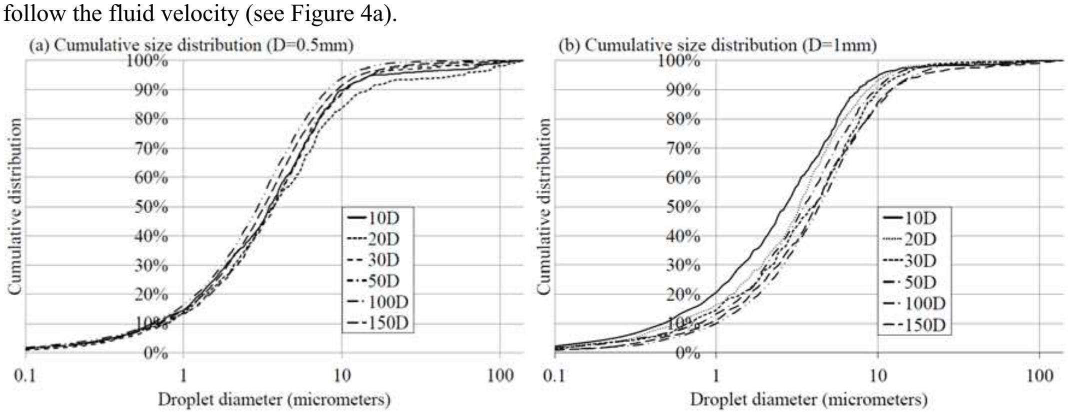

FIGURE 3. Experimental results. The particle distribution at various distances downstream for both cases.

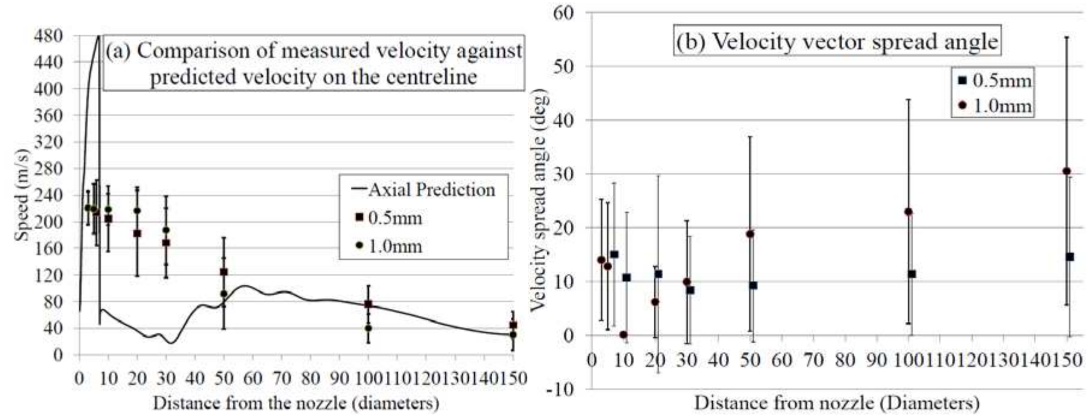

FIGURE 4. Experimental results and numerical predictions. Measurements of velocity (circles and squares) and the predicted velocity along the centerline. Error bars indicate 1σ of theparticular nozzle distribution at the specific distance downstream.

Thermal relaxations times can be estimated in a similar way, using [7]. It can be shown that the thermal relaxation distance is 6.0 mm at 280K at the nozzle for a velocity of 100 m s^{-1}, and 100 times longer at 200K. For small nozzles, such as those considered here, the particles do not reach thermal equilibrium with the flow.

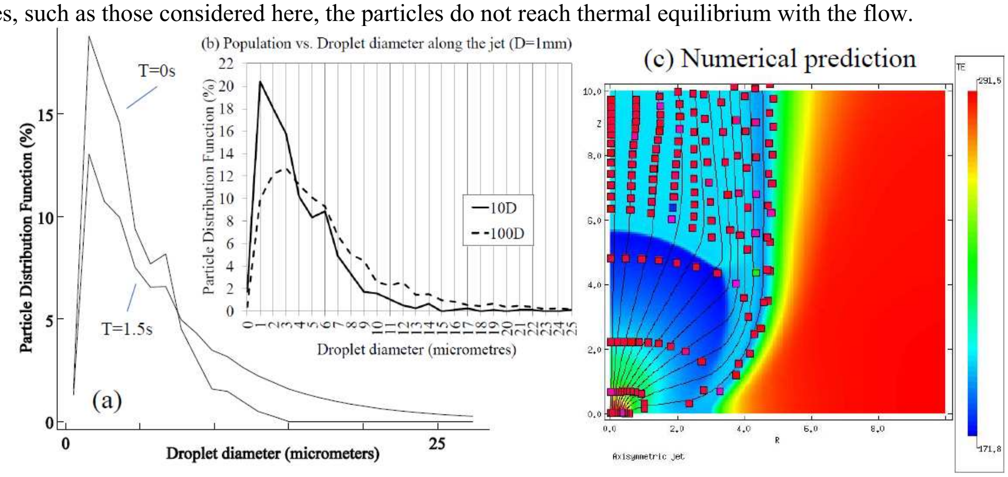

FIGURE 5. Numerical predictions. (a) Predicted turbulent shear agglomeration according to Saffman [8] used to model (b) the experimental results for the 1.0 mm diameter nozzle case reproduced with linear mass bins and (c) axisymmetric temperature predictions of the near-field Mach shock structure with stream lines and particles positions (squares).

CONCLUDING REMARKS

CO2particles from a high pressure liquid release through the small nozzle diameters considered here (0.5mm and 1.0mm) are neither in dynamical equilibrium nor thermal equilibrium with the sonic flow. As such then, the particles obtain their velocity through the force of the release. By 50mm or so along the jet, the experiments indicate they are in equilibrium with the fluid. In the 1.0mm diameter nozzle case, the particles are more likely to see turbulent structures and we are able to numerically model the net agglomeration observed along the jet through a turbulent shear agglomeration model [6]. The experimental velocity variation reflects the turbulence in the jet which we intend to fully model in future simulations. These equilibrium issues have less of a bearing for CCS schemes where the release diameter could be up to the pipeline diameter (~1m) in the case of a full bore rupture, much larger than the relaxation distances discussed above.

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