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ACCURATE CALCULATION OF GAS-LIQUID-SOLID FLOW OF CO_2 USING A WENO METHOD

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The present work [1] is concerned with the development of an accurate 3D computational fluid dynamics (CFD) model able to handle complex three-phase (gas-liquid-solid) flow. Such a model has applications within CO_2 transport and injection, process equipment, safety systems and dispersion into the atmosphere, which are key topics within CO_2 capture and storage (CCS). CCS is regarded as a key method to mitigate global warming.

The flow model is a homogeneous equilibrium model, in which kinetic, mechanical, thermal and chemical equilibrium is assumed. The effect of viscosity and thermal conduction is included. Since the flow can contain shocks and discontinuities, a robust and shock-capturing numerical method is employed. The spatial discretization is based on the finite-volume method with a fifth-order weighted essentially non-oscillatory (WENO) scheme using the robust first-order centred (FORCE) flux as approximate Riemann solver. The solution is integrated in time by a third-order strong-stability-preserving Runge–Kutta method.

Studies on numerical methods for compressible multiphase flow often employ simple equations of state (EOS) like the stiffened-gas EOS. This is not possible here, among other things, because it is necessary to accurately describe the CO_2 properties across the wide range of states encountered by decompression from a supercritical pressure of about 100 bar down to atmospheric pressure. We therefore employ the Span–Wagner multiparameter reference EOS, which can describe the gas and liquid phases, including, with an adaptation, the solid phase.

Numerical benchmark cases are calculated, demonstrating close to fifth-order convergence for smooth single- and two-phase flows. We then study the case of a highly underexpanded CO_2 jet, and we compare the computational results to the experimental observations of Pursell [2] and obtain good agreement for the shape and dimensions of the barrel shock.

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References

[1] Gjennestad MA, Gruber A, Lervåg KY, Johansen Ø, Ervik Å, Hammer M, Munkejord ST. Computation of three-dimensional three-phase flow of carbon dioxide using a high-order WENO scheme. *J Comput Phys* 2017; 348:1–22. doi:10.1016/j.jcp.2017.07.016.

[2] Pursell M. Experimental investigation of high pressure liquid CO_2 release behaviour. In: *Hazards XXIII – Institution of Chemical Engineers Symposium Series*, vol. 158. Southport, UK, 2012; pp. 164–171.