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Computation of three-dimensional three-phase flow of carbon dioxide using a high-order WENO scheme

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ABSTRACT

We have developed a high-order numerical method for the 3D simulation of viscous and inviscid multiphase flow described by a homogeneous equilibrium model and a general equation of state. Here we focus on single-phase, two-phase (gas–liquid or gas–solid) and three-phase (gas–liquid–solid) flow of CO_2 whose thermodynamic properties are calculated using the Span–Wagner reference equation of state. The governing equations are spatially discretized on a uniform Cartesian grid using the finite-volume method with a fifth-order weighted essentially non-oscillatory (WENO) scheme and the robust first-order centered (FORCE) flux. The solution is integrated in time using a third-order strong-stability-preserving Runge–Kutta method. We demonstrate close to fifth-order convergence for advection–diffusion and for smooth single- and two-phase flows. Quantitative agreement with experimental data is obtained for a direct numerical simulation of an air jet flowing from a rectangular nozzle. Quantitative agreement is also obtained for the shape and dimensions of the barrel shock in two highly underexpanded CO_2 jets.

1. Introduction

The deployment of CO_2 capture and storage (CCS) is regarded as a key strategy to mitigate global warming [1]. To design and operate CCS systems in a safe and cost-effective way, accurate data and models are needed [2]. This includes models and methods to simulate the near field of a CO_2 jet resulting from the decompression of equipment containing high-pressure CO_2. The data from these near-field simulations are e.g. used as input for less resolved simulations of the dispersion of CO_2 in the terrain [3–5].

This type of scenario puts some requirements on the models and numerical methods to be used. Depressurization of CO_2 from supercritical pressures typically involves complex three-phase (gas–liquid–solid) flow. Describing this kind of flow necessitates a multiphase flow model and an equation of state (EOS) that is accurate and capable of capturing the three-phase behavior [6,7]. For high vessel pressures, the CO_2 jet resulting from a leak will form a shock, which the numerical method must be able to capture. In addition, we would like the numerical method to maintain discrete conservation of mass, momentum and energy and, due to computational efficiency, to be of high order in smooth regions of the computational domain, without producing spurious oscillations in the solution near discontinuities.

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Wareing et al. [7,8] and Woolley et al. [9] studied CO_2 jets using a Reynolds-averaged Navier–Stokes model. The flow model was combined with a composite EOS [7] to describe three-phase CO_2 flow. The flow model was solved using a conservative, shock-capturing second-order scheme, as described by Falle [10].

However, advances have been made in constructing and implementing finite-volume, shock capturing and conservative numerical methods of higher order. Titarev and Toro [11] presented a procedure relying on weighted essentially non-oscillatory (WENO) interpolation [12] and achieved fifth-order convergence for their smooth and inviscid two-dimensional isentropic vortex problem. Their scheme was extended to include interpolation of velocity derivatives and computation of viscous transport of momentum and dissipation of kinetic energy by Coralic and Colonius [13]. Such a numerical scheme is suitable for execution on parallel computers by domain decomposition [14].

In research on numerical methods for compressible multiphase flow, the ideal-gas and stiffened-gas EOS [15,16] are commonly employed, due to their simplicity and relatively large number of applications. This is true both for 1D [17–19] and 3D models, e.g. [13]. The stiffened-gas EOS can be regarded as a linearization about a reference state. In many cases, however, it is necessary to consider more adapted EOSs in order to achieve the necessary accuracy. This often entails a significantly higher computational complexity. As an example, Dumbser et al. [20] presented an unstructured WENO scheme employing a real EOS for water.

For CCS applications, it is often necessary to describe a large thermodynamic property space, involving multiple phases, for instance for the depressurization from a transport pipeline operated at a supercritical pressure around 100 bar down to atmospheric conditions. In these cases, an accurate EOS is required [6], such as the one by Span and Wagner [21] (SW). Therefore, in order to perform high-fidelity near-field studies of CO_2 jets, we need to combine a high-order numerical scheme with a general EOS.

This combination would also benefit the development of predictive fluid–structure models aiding in the design of CO_2-transport pipelines against running fractures [22,23]. For practical and computational reasons, the CO_2 flow is commonly described using a 1D model, which implies a simplified description of the pressure forces on the opening pipe flanks [22]. A full 3D description of the flow might provide more accurate predictions.

In the present work we want to study complex CO_2 flows which may be single phase, two-phase (gas–liquid or gas–solid) or three-phase (gas–liquid–solid). In doing so, we extend the high-order scheme of Titarev and Toro [11] and Coralic and Colonius [13], applying it to the homogeneous equilibrium multiphase flow model and a formulation allowing the use of a general EOS. Since the applications we are interested in typically involve sharp temperature gradients, we include heat conduction in our model and in the numerical treatment of diffusive fluxes, as well as a temperature-dependent viscosity.

We validate the implementation of the model and numerical methods through several test cases, including a turbulent air jet from a rectangular nozzle. We also demonstrate that the numerical methods exhibit high-order convergence when dealing with diffusive fluxes and two-phase flows. Finally, we perform detailed simulations of CO_2 jets, employing the SW EOS.

The rest of this paper is organized as follows. Section 2 reviews the governing equations, while the treatment of inflow and open boundary conditions is briefly described in Section 3. Section 4 deals with the numerical methods. Section 5 demonstrates the accuracy and robustness of the scheme, including the direct numerical simulation of an air jet, while Section 6 discusses the simulation of a CO_2 jet. Section 7 concludes the study.

2. Models

2.1. Fluid dynamics

We consider a three-dimensional flow of a fluid that may consist of multiple phases. The different phases are assumed to be in local equilibrium and to move with the same velocity. The flow may then be described by a homogeneous equilibrium model (HEM), which can be formulated as a system of balance equations,

$$\partial_t \boldsymbol{Q} + \partial_x \boldsymbol{F} + \partial_y \boldsymbol{G} + \partial_z \boldsymbol{H} = \boldsymbol{S}(\boldsymbol{Q}). \tag{1}$$

Here $\boldsymbol{F}$, $\boldsymbol{G}$ and $\boldsymbol{H}$ are the fluxes in the x-, y- and z-direction, respectively, and $\boldsymbol{S}(\boldsymbol{Q})$ is the vector of source terms. The vector $\boldsymbol{Q}$ contains the state variables,

$$\boldsymbol{Q} = \left[\rho, \rho u_x, \rho u_y, \rho u_z, E\right]^{\mathrm{T}}, \tag{2}$$

where ρ is the fluid density, u_x, u_y and u_z are the flow velocities and E is the total energy density. Thus the system (1) describes conservation of mass and balance of momentum and energy of the fluid. The total energy is

$$E = \rho e + \frac{1}{2}\rho\left(u_x^2 + u_y^2 + u_z^2\right), \tag{3}$$

where e is the specific internal energy of the fluid. The total energy is thus the sum of internal and kinetic energy.