Towards a multiscale strategy for modeling high-pressure flow of carbon dioxide for sequestration

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Abstract

The flow patterns formed in a pipe carrying two or more immiscible fluids are among the most subtle, scientifically challenging emergent phenomena of classical physics. They are challenging computationally as well theoretically due to their sensitivity to small scale phase dispersion and resegregation. They are technologically important due to their effects on transport of materials of economic and societal importance, such as oil, gas, coal slurry, and carbon dioxide. For underground sequestration, carbon dioxide is transported at pressures at which several phases can coexist. To maximize the likelihood of successful predictive simulation of such flows, three requirements must be met, (i) the simulation must be three-dimensional (3D), (ii) the largest possible range of scales must be resolved, and (iii) the parameterization of unresolved scales must be accurate. The effort proposed here will focus on the use of a novel modeling approach designed to meet the first two requirements, including consideration of accurate subgrid parameterization within that approach. The ansatz we propose is based on a strategy called Autonomous Microscale Evolution (AME) [13], in which the flow is advanced on space-filling arrays of linear structures that are coupled in a manner that yields 3D flow advancement at large scales and 1D resolution of small scales on individual structures. The key idea is the 1D model representation of turbulent flow interaction with microphysical evolution. The AME modeling strategy is motivated by considering the relevant physics at various scales. At large scales, the flow is sensitive to vessel geometry (e.g., pipe diameter and inclination) and to forcing mechanisms, which are pressure drop and gravity in the present situation. These controlling factors are inherently 3D in character. All of these factors contribute to anisotropy at smaller scales, but their role at these scales is to modify the dominant smaller-scale tendency, which is the turbulent cascading that generates and sustains the smaller-scale activity. At still smaller scales, viscosity, interfacial surface tension and density variations play increasingly important roles in modulating the turbulent cascade, the net tendency being to inhibit or counteract inter-phase dispersion. Despite the complications, the dominance of turbulent cascading in the intermediate ('inertial') range of scales suggests the possibility that some reduced form of modeling might adequately capture the relevant phenomenology. The key modeling approach, termed One-Dimensional Turbulence (ODT) [1] in which turbulent flow evolution along a notional 1D line of sight is emulated by applying instantaneous maps to sub-intervals of the line to represent the effect of individual turbulent eddies on property profiles along the line. Velocity profiles evolve on the line, controlling map occurrences and affected by those occurrences, resulting in self-contained flow evolution that obeys applicable conservation laws. The original formulation of ODT (Kerstein 1999) was extended and applied to geophysical flows, e.g. Rayleigh-Bénard convection [2], buoyancy

reversal [3], layering in stably stratified flows [4], the nocturnal atmospheric boundary layer [5], and double diffusive convection [6]. Similar methodologies have been applied to turbulent jet flames [7], premixed turbulent flames [8], and autoignition [9]. It has been used as sub-grid closure for LES [10,11,12]. A summary of recent applications in combustion is found in [14]. Though ODT is predictive in many respects, it lacks the capability to generate 3D large-scale flow structure in response to large-scale forcing reinforced by feedback from dynamically active microphysics. This limitation has been addressed by coupling arrays of ODT instantiations (objects) in a manner that yields coarse-grained 3D evolution consistent with the governing equations. A low-Mach-number constant-property implementation of this strategy denoted ODTLES has been developed and demonstrated [11]. Compared to a resolution of a Direct Numerical Simulation (DNS) which is N cube for N points in one direction, AME only needs 3*N points thus allowing for larger ranges in scale for a given amount of computational power. Here we propose the development of a variant of AME suitable for multiphase pipe flow simulation, and use of this formulation to attain the capability to predict various flow patterns, which appear due to the complex interaction of turbulence, buoyancy, and multiphase dynamics. One local ODT substructure will be a line of sight through a multiphase flow. On this line a sequence of phase intervals are represented using level sets, see e.g. [15]. The surface tension at interfaces stores potential energy and the ODT processes can create, move, and annihilate interfaces.

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Contribution type: Poster

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