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A systematic approach to high-fidelity modeling and efficient simulation of supercritical fluid mixing and combustion

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ABSTRACT

Advances in fluid-flow modeling and simulation techniques over the past two decades have improved understanding of the intricate flow physics and combustion dynamics in the supercritical regime. However, there remain many numerical issues to be addressed, including turbulence closure modeling, combustion modeling, and the evaluation of real-fluid thermodynamic and transport properties. The challenges can be broadly categorized into two areas: (1) achieving highly accurate simulation through inclusion of all the necessary physics and (2) developing a computationally efficient framework to achieve simulation results in a reasonable turnaround time. This paper investigates these challenges and presents a systematic approach to achieve high-fidelity and efficient simulation of supercritical fluid mixing and combustion using large-eddy simulation (LES) techniques. The unresolved subgrid-scale (SGS) term in the filtered equation of state (EOS), which is generally neglected for ideal gases, becomes significant for real fluids, especially in regions of strong property gradients at supercritical conditions. The relative error for the filtered density can reach up to 40%, and this uncertainty can propagate and contaminate calculations of the conservation equations. Two closure models for the SGS term in the EOS are proposed: a gradient-based and a mixing-based approach. Both approaches reduce the modeling error considerably. Flamelet-based combustion models are also examined at supercritical conditions. The probability density functions (PDFs) for mixture fraction and scalar dissipation rate are evaluated using a data-driven approach. The presumed beta-function distribution accurately describes the PDF of the mixture fraction at low mixture fraction variance, but deviates at high variance (>0.01). The lognormal distribution can capture the shape of the extracted PDF of the scalar dissipation rate but underestimates the peak value. An alternative combustion model using finite-rate chemistry integrated with dynamic adaptive chemistry and correlated transport is developed, rendering a computationally efficient and affordable framework. The efficiency of evaluating real-fluid thermodynamic and transport properties, a computationally expensive procedure, is dramatically enhanced using tabulation and correlated dynamic evaluation techniques. Finally, suggestions are provided regarding opportunities for future research.

1. Introduction

Supercritical mixing and combustion have received significant attention over the past two decades, mainly because of increasing demand for higher thermal efficiency in propulsion and power-generation systems. The operating pressures in these systems often exceed the thermodynamic critical points of the fluids involved. Liquids initially injected at a subcritical temperature may heat up and experience a thermodynamic phase transition into the supercritical regime. Many distinctive behaviors occur during the transition and differ from the phenomena encountered at subcritical conditions, such as diminishing of surface tension and absence of droplet formation and a two-phase interface. As a result, single-phase-like, diffusion-dominated mixing takes place between dense and light fluids in the presence of large property gradients [1–4].

Extensive experimental studies have led to improved qualitative understanding of the fundamental physics involved in supercritical fluid flows [5–13]. However, such measurements are limited by the extreme operating conditions and by the currently available experimental techniques. Computational techniques serve as a powerful tool to provide more detailed information about the flow structures and dynamics at supercritical conditions, and many numerical modeling and simulation studies have been carried out in this area. Computational modeling, however, poses a variety of challenges, including the classical closure issues associated with turbulent combustion and a unique set of problems introduced by thermodynamic non-idealities and transport anomalies [1]. Several

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numerical solvers have been developed to tackle these challenges [14–21]. Collaborative efforts have also been made to assess the accuracy of different research codes using canonical subscale rocket combustors, such as the gaseous O_2 (GOX) /gaseous H_2 test rig [22] and the GOX/gaseous CH_4 test rig [23]. Similar predictions by different numerical solvers have been examined using a two-dimensional mixing layer configuration [24].

An important challenge for numerical solvers is the ability to achieve accuracy and stability in regions of steep gradients, which are manifested by sharp variations of thermodynamic and transport properties across the pseudo-boiling line, also known as the Widom line [25]. In this region, directly solving the full conservation equations of mass, momentum, species, and energy in a coupled manner can cause erroneous pressure fluctuations because of insufficient grid resolution [26]. Wang et al. [27] defined a fluid transition layer where the density gradient exceeds the 90% of its maximum value. The transition layer connects the compressed liquid regime to the supercritical regime, and it must be carefully treated to resolve the property gradients and prevent abnormal fluctuations of these variables. To mitigate spurious pressure oscillations, Terashima and Koshi [28] introduced a pressure evolution equation to replace the energy conservation equation and solved pressure along with other independent variables simultaneously. Ma et al. [20] applied an extended double-flux method to transcritical flows to overcome the same issue. These methods, however, cannot ensure energy conservation. Another approach is dual time-stepping integration with a preconditioning scheme [29,30], in which pressure is considered as one of the primitive variables and solved in every pseudo-time iteration. The pseudo-time convergence gives the pressure without unphysical oscillations, and it substitutes back to the original conservation equations to obtain a time-accurate solution. This methodology is implemented in the studies described here.

Turbulence closure remains a challenge for modeling supercritical flows. Although direct numerical simulations (DNS) resolve all the turbulent scales and steep gradients of fluid properties, they are constrained to simple flows with low Reynolds numbers and low density ratios [15,31–35]. DNS is computationally prohibitive for problems with practical configurations, which include complex geometries and high Reynolds numbers. The large-eddy-simulation (LES) technique has been widely employed to simulate operational systems at elevated pressures [19,36–42]. In LES, the unclosed subgrid scale (SGS) terms must be carefully modeled. In most studies, however, the SGS models developed for low-pressure turbulent flows have been directly applied to supercritical regimes without appropriate justification. The traditional Smagorinsky model leads to unsatisfactory results in the transcritical and supercritical regimes [43]. Furthermore, flow properties, such as compressibility factor and specific heat, are generally calculated from the LES-resolved variables, without considering the effect of the corresponding SGS fluctuations. These SGS terms, which are negligible at low pressures may become significant and even comparable to the leading-order terms (such as the convection terms) at high pressures [33,43,44]. In particular, the SGS term in the filtered equation of state (EOS) plays an essential role in obtaining filtered pressure (or density) accurately [45]. Proper modeling of the SGS term in the filtered EOS at supercritical pressures is one of the focal points in the current study of supercritical fluid flows and combustion.

Modeling turbulence/chemistry interactions (TCI) is another challenging task. For non-premixed systems, chemical reactions can only take place when fuel and oxidizer are mixed at a molecular level. Molecular mixing of scalar quantities and subsequent chemical reactions in turbulent flows occur at the smallest scales and are characterized by the scalar dissipation rate. This implies that chemical source terms typically cannot be resolved in LES and must be modeled. There are a variety of turbulent-combustion models available, such as flamelet-based models [46–49], the conditional moment closure model (CMC) [50], the eddy-dissipation-concept (EDC) model [51], the thickened-flame model [52], the linear-eddy mixing (LEM) model [53], and the transported probability density function (TPDF) [54], among others. The advantages and challenges of these models have recently been reviewed for aero-propulsion applications [55,56] and high-speed propulsion systems [57]. In most of these models, the probability density function (PDF) plays a crucial role. For conserved scalar models, a beta-function distribution is pressumed for the marginal filter PDF of the mixture fraction. Its validity has been successfully assessed against experimental and DNS data for various flows at low pressures [58,59]. However, it has been directly applied to high-pressure simulations [42,45,60], without validation. The applicability of the beta-function PDF for the filtered mixture fraction in supercritical flows is examined in the present work. On the other hand, the finite chemistry model does not make inherent assumptions about the PDF of flow quantities, and instead directly solves the chemical kinetics based on the instantaneous thermodynamic state of the mixture. The challenge is to model the subgrid turbulence-chemistry interactions, given the prohibitively large computational cost associated with detailed chemistry mechanisms.

Supercritical flows typically include dense fluids with high Reynolds (Re) numbers, and hence cover a broad range of turbulent length and time scales. In the transcritical flow regime for a typical rocket combustor, the density ratio can be as high as 100, and the transition region is on the order of 10 μm. Extremely fine grid distribution is required to resolve the density stratification. This in turn dramatically increases the computational cost. The situation becomes even more severe when real-fluid property evaluation is involved. The time required for the computation of thermodynamic and transport properties can be about 50% of the total CPU time. To alleviate the situation, acceleration techniques such as GPU acceleration [61] and tabulation [62,63], have been explored. Two techniques, a tabulation-based method and a correlated dynamic evaluation method, are explored in the present work for time-efficient real-fluid property evaluation.

The purpose of this paper is to report the authors' efforts to systematically investigate and address the key modeling and simulation challenges associated with supercritical fluid mixing and combustion. Several important aspects, including SGS closure, turbulence/chemistry interactions, and real-fluid property evaluation, are discussed. The rest of the paper is organized as follows: Section 2 presents the theoretical framework, and Section 3 demonstrates the state-of-the-art simulations using this framework. Section 4 then discusses the details of issues and strategies for high-fidelity modeling and efficient simulation, in terms of developing SGS models for EOS, examining combustion models, and accelerating evaluation of real-fluid thermodynamics and transport properties. Finally, key conclusions of the work and future directions are summarized in Section 5.

2. Theoretical framework

2.1. Conservation equations

The underlying physiochemical processes of supercritical combustion involve real-fluid behaviors, multi-species transport, chemical reactions, and turbulent mixing, as well as turbulence/chemistry interactions over a wide range of time and length scales. The governing equations for modeling such intricate phenomena must be addressed carefully. In this section, the full conservation equations of mass, momentum, energy, and conserved scalars are first presented, and then the Favre-filtered conservation

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