Large-eddy simulations of transcritical and doubly-transcritical LOx-methane flames

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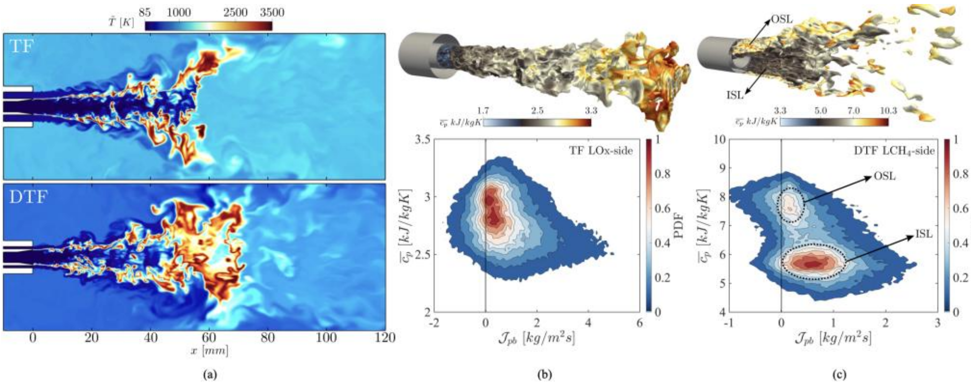
Abstract
This study presents a comprehensive numerical investigation of oxygen-methane flames operating under transcritical and doubly-transcritical conditions. Using high-fidelity large-eddy simulations (LES), the work focuses on characterizing the turbulent pseudo-boiling, a critical phenomenon in high-pressure rocket engine combustors where fluids exhibit a pseudo-phase transition. Two different flame configurations are studied and compared: a transcritical regime, where only the oxygen is injected in a liquid-like state, and a double-transcritical regime, where both propellants experience transcritical conditions. A dedicated strategy is developed to define the turbulent pseudo-boiling rate within a combustion LES framework. Statistical analyses reveal that pseudo-boiling is not only governed by local thermodynamic states but also by complex interactions with turbulent flows. The results emphasize that turbulence acts as both a driver and a modulator of pseudo-boiling. These findings provide important insights into the role of thermophysical property modeling in combustion simulations and its interplay with turbulent motions, demonstrating the need for robust LES methods in design-oriented campaigns of next-generation LRE propulsion systems.

Introduction
In recent years, the oxygen-methane propellant combination has gained attention as a promising option for space propulsion, offering several advantages over more traditional mixtures such as oxygen-kerosene and oxygen-hydrogen. In addition to its higher specific impulse, superior cooling capabilities and lower likelihood of coking and soot formation make methane a competitive alternative to heavier hydrocarbons such as RP-1, especially in sustainable propulsion technologies such as reusable liquid rocket engines (LRE). Although oxygen-methane combustion provides a lower specific impulse than the oxygen-hydrogen combination, methane offers important practical advantages such as higher liquid storage density and a higher boiling point - properties that enable lighter, smaller, and simpler cryogenic storage and thermal management systems. While oxygen-methane combustion has attracted growing attention for space propulsion, most high-fidelity simulations have focused on non-reacting cryogenic mixing, especially to study pseudo-boiling phenomena [1]. Direct Numerical Simulations (DNS) studies involving reacting oxygen-methane mixtures remain limited due to their extreme computational cost

and often rely on simplified two-dimensional configurations. Prior work has explored flame stabilization and propagation mechanisms under doubly-transcritical conditions [2, 3], yet a detailed analysis of pseudo-boiling in reacting flow conditions remains scarce. In this context, large-eddy simulations (LES) offer a practical alternative, balancing computational cost and physical fidelity. In recent years, LES has been used to model transcritical flames, mainly focusing on numerical stability and avoiding spurious pressure oscillations under stratified real-fluid conditions. While substantial progress has been made in understanding transcritical combustion, LES studies addressing the pseudo-boiling mechanism are still lacking, further motivating the present work.

Methods and results

This study employs high-fidelity LES to simulate transcritical and doubly-transcritical flames using an in-house finite-volume tabulated chemistry solver based on the OpenFOAM suite [4, 5]. The combustion model relies on a real-fluid flamelet-based approach, which comprises a detailed high-pressure thermodynamic and transport properties estimation and a consistent modeling of the turbulence-chemistry interactions using a presumed-PDF approach. A dedicated strategy is developed to identify the effective pseudo-boiling state when using turbulent combustion models. To characterize the interplay between the pseudo-boiling mechanism in a turbulent flow, we propose the concept of the mixture fraction's displacement speed [1]. The turbulent pseudo-boiling rate is analyzed by adapting two reference thermodynamic injection states from the experimental tests described in Singla et al. [6]. The comparison reported in Fig.1 between the transcritical (TF) and doubly-transcritical flames (DTF) reveals distinct features in terms of flame



morphology and turbulent structures. In the transcritical case, the flame

Figure 1. Comparison of the instantaneous temperature field (a) between transcritical and doubly-transcritical flames. JPDF between J_{pb} and c_p for TF LOx-side (b) and DTF LCH4-side (c).

appears narrow and elongated, with steep thermal gradients and a clearly defined flame front. In contrast, the DTF shows more intense wrinkling and a broader high-temperature region, especially near the injector. The flame is slightly longer and more spatially dispersed. Leveraging bi-variate statistics analysis, for the LOx jet of the TF, the joint-PDF between the isobaric speific heat c_p and the pseudo-boiling rate J_{pb} exhibits unimodal behavior with the most probable events clustered around the effective turbulent pseudo-boiling state, and a gradual probability decay as c_p varies. In contrast, the coaxial liquid methane (LCH4) jet of the DTF exhibits two distinct peaks. In particular, since LCH4 is a coaxial jet, it pseudo-boils across a surface with two sides, an inner and an outer side. This bimodal behavior reflects the different thermodynamic conditions in the inner (ISL) and outer (OSL) shear layers. Specifically, the ISL, located between the flame and the methane jet, is characterized by low and uniform values of c_p. This leads to a broad region of statistically significant high mass flux events. Conversely, the OSL, located between the outer methane jet and the recirculation zone, has higher c_p values, resulting in a second, narrower cluster associated with lower mass flux.

Conclusions

This study explored turbulent pseudo-boiling phenomena in transcritical and doubly-transcritical oxygen-methane flames using a high-fidelity, flamelet-based LES framework. The results indicated that pseudo-boiling is diffusion-limited and primarily driven by normal mass fluxes, especially in the oxidizer-rich region. While both configurations exhibit similar pseudo-boiling rates for the LOx stream, the doubly-transcritical condition shows significantly lower rates on the fuel-rich side due to methane's higher specific heat and complex interaction with the turbulent flowfield. The joint statistics between thermal inertia and mass fluxes indicate that intense strain is required at pseudo-vaporization zones to overcome their insulating nature and support an efficient mixing in cryogenic injection scenarios.

References

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