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Thermodynamic structure of supercritical LOX–GH2 diffusion flames

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ABSTRACT

In this study, we evaluate the thermodynamic structure of laminar hydrogen/oxygen flames at supercritical pressures using 1D flame calculations and large-eddy simulation (LES) results. We find that the real fluid mixing behavior differs between inert (cold flow) and reactive (hot flow) conditions. Specifically, we show that combustion under transcritical conditions is not dominated by large-scale homogeneous real-fluid mixing: similar to subcritical atomization, the supercritical pure oxygen stream undergoes a distinct transition from liquid-like to gas-like conditions; significant mixing and combustion occurs primarily after this transition under ideal gas conditions. The joint study of 1D flame computations and LES demonstrates that real-fluid behavior is chiefly confined to the bulk LOX stream; real fluid mixing occurs but in a thin layer surrounding the LOX core, characterized by water mass fractions limited to 3%. A parameter study of 1D flame solutions shows that this structure holds for a wide range of relevant injection temperatures and chamber pressures. To analyze the mixing-induced shift of the local fluid critical point, we introduce a state-space representation of the flame trajectories in the reduced temperature and reduced pressure plane which allows for a direct assessment of the local thermodynamic state. In the flame, water increases the local mixture critical pressures, so that subcritical conditions are reached. This view of limited mixing under supercritical conditions may yield more efficient models and an improved understanding of the disintegration modes of supercritical flows.

1. Introduction

Injection at supercritical pressures is a technology ubiquitous in transportation; it is used in Diesel engines, gas turbines, and rocket engines [1,2]. At these conditions, subcritical break-up into ligaments and droplets, Fig. 1a, is replaced by a turbulent mixing process, Fig. 1b, when the surface tension vanishes under supercritical conditions [2–5].

However, a categorization based on the pure propellant critical pressures has been shown to be too simplistic: the critical pressure of a mixture may significantly exceed the critical pressures of the components [6], thus an injection process that is supercritical with respect to the injected fluid and the background gas, henceforth referred to as ‘nominally supercritical’, may still exhibit subcritical break-up characteristics. This has been demonstrated experimentally [7,8] and numerically [9–11].

The view of Fig. 1 has also informed the development of the respective numerical models: the sharp interfaces in subcritical injection typically lead to an approach in which interfaces are tracked, whereas the diffuse mixing in supercritical injection is treated as a problem of accurately modeling the thermodynamics of the real fluid-state behavior and mixing. A ‘real fluid’ in this context is characterized by significant intermolecular forces that render the ideal gas equation of state inapplicable, consistent with the view in physical chemistry [12]. The canonical model was introduced by Oefelein and Yang [13].

This approach has been used extensively to study nominally supercritical combustion of liquid oxygen (LOX) with gaseous hydrogen (GH2), representative of liquid rocket engines. In such engines, the flame is anchored in a recirculation zone behind the LOX post of a coaxial injector [3,4,13]. Juniper et al. [14] noted that the quenching strain rate of a GH2/LOX flame exceeds the maximum values found in rocket engines by an order of magnitude. Indeed, it can be assumed in numerical modeling of rocket engines that the reactions reach a chemical equilibrium [15,16]. Experiments [3,4] and simulations [13,17,18] show that the flame effectively separates oxygen from hydrogen; the flame encloses the oxygen stream due to hydrogen-rich operating conditions. For specific flow conditions, combustion and mixing may take place in the ideal gas limit [19,20]. Thus, liquid propellant rocket engines

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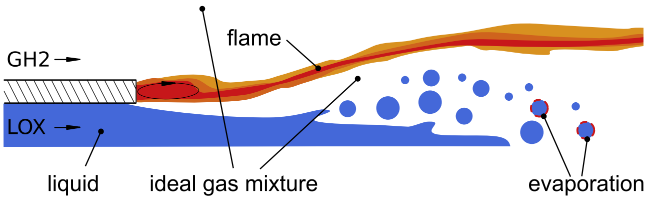
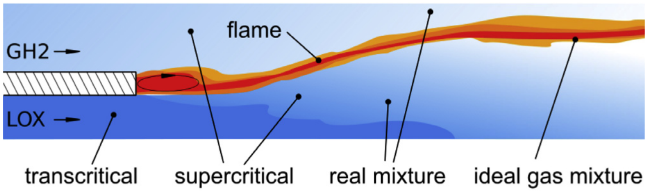


(a) Subcritical atomization.



(b) Supercritical jet disintegration.

Fig. 1. Characterization of subcritical and supercritical injection.

exhibit combustion conditions that closely resemble idealized diffusion flames. Ribert et al. [21] and Pons et al. [22] used this insight to address counterflow diffusion flames under trans- and supercritical conditions, an approach that has since been adopted by other groups [23–25]. Since, large-eddy simulations (LES) of supercritical injection have become state-of-the-art [26,27], with fundamentals still being investigated [28,29].

Furthermore, ample evidence for a structure of the supercritical state space has been collected. Specifically, experimental [30,31] and theoretical [32,33] results indicate that distinct liquid-like and gas-like supercritical states can be distinguished. These states are separated by the Widom line, an extension to the coexistence line characterized by peaks in the isobaric specific heat capacity. The Widom line is a general fluid property [34] and can even be identified in mixtures [35]. The relevance of the Widom line for injection lies in pseudoboiling [2], the transition from liquid-like to gas-like supercritical states across the Widom line. Pseudoboiling resembles subcritical boiling, where a peak in the thermal expansivity causes a sudden drop in density, and a peak in isobaric specific heat capacity acts as an energy sink akin to the latent heat of vaporization [36]. Pseudoboiling has been identified as an important process in injection and combustion [23,37].

So far, a systematic investigation of the thermodynamic structure of supercritical non-premixed flames with respect to mixtures and transitions has not been carried out. Therefore, we address three questions in the present work: (1) In which part of the flame are real-fluid effects (pure fluid and mixing) relevant? (2) How does the local thermodynamic state and the critical point change throughout the flame? 3) How sensitive are these results with respect to changes in the injection conditions? To address these questions, we compute LES and 1D flame structures of the cryogenic LOX/GH2 diffusion-flame at nominally supercritical pressure, covering inert and reactive cases. Variation of the 1D conditions over a range of strain rates from near-equilibrium to quenching conditions, pressures, injection temperatures, and dilution, are evaluated to assess the generality of the initial results. The spatial distribution of real fluid thermodynamics is demonstrated using LES results.

2. Numerical methods

This section discusses the numerical methods used for the present study. First, the thermodynamic model used for real fluid mixtures is introduced. The discussions of the 1D flame solver and the LES solver, which use this thermodynamic model, follow. The section concludes with relations used in the analysis of the results.

2.1. Thermodynamic relations

The Peng–Robinson equation of state (PR EoS) [38] is used in this study for the evaluation of thermodynamic quantities. A cubic EoS has been chosen for its computational efficiency and readily available mixing rules; PR has been chosen for its accuracy especially for supercritical fluids [13]. Real-fluid effects are accounted for by departure functions that are derived from the state equation to ensure thermodynamic consistency of the governing equations. The PR state equation is expressed as

$$p = \frac{RT}{v-b} - \frac{a}{v^2+2bv-b^2}, \tag{1}$$

where R is the gas constant, v is the specific volume, and the coefficients a and b are functions of temperature and composition, accounting for effects of intermolecular attractive forces and volume displacement. For mixtures of N_S species, the coefficients a and b in Eq. (1) are evaluated as [6]

$$a = \sum_{\alpha=1}^{N_S}\sum_{\beta=1}^{N_S} X_\alpha X_\beta a_{\alpha\beta}\,, \tag{2a}$$

$$b = \sum_{\alpha=1}^{N_S} X_\alpha b_\alpha\,, \tag{2b}$$

where X_α is the mole fraction of species α. The coefficients $a_{\alpha\beta}$ and b_α are calculated using the mixing rules recommended by Harstad et al. [39], with

$$a_{\alpha\beta} = 0.457236\frac{(RT_{cr,\alpha\beta})^2}{p_{cr,\alpha\beta}}\left[1+c_{\alpha\beta}\left(1-\sqrt{T/T_{cr,\alpha\beta}}\right)\right]^2, \tag{3a}$$

$$b_\alpha = 0.077796\frac{RT_{cr,\alpha}}{p_{cr,\alpha}}\,, \tag{3b}$$

$$c_{\alpha\beta} = 0.37464 + 1.54226\omega_{\alpha\beta} - 0.26992\omega_{\alpha\beta}^2\,. \tag{3c}$$

The critical properties of the major species are taken from the NIST database [40], the critical properties of the intermediate species are determined based on their Lennard–Jones potentials and their acentric factor is set to zero, following Giovangigli et al. [41]. The critical properties for all species considered in this study are compiled in Table 1.

In mixtures, the local critical pressure and temperature vary with composition. While the mixture critical temperature lies between the component pure fluid values, the mixture critical pressure may significantly exceed the pure fluid values. Both can be determined using the pseudocritical method described by Reid et al. [6], where

$$T_{\mathrm{cr,mix}} = \sum_{\alpha=1}^{N_S} X_\alpha T_{\mathrm{cr},\alpha}, \tag{4a}$$

$$p_{\mathrm{cr,mix}} = RT_{\mathrm{cr,mix}}\frac{\sum_{\alpha=1}^{N_S} X_\alpha \mathcal{Z}_{\mathrm{cr},\alpha}}{\sum_{\alpha=1}^{N_S} X_\alpha v_{\mathrm{cr},\alpha}}. \tag{4b}$$

The compressibility factor $\mathcal{Z}$ [6] is an important nondimensional parameter in real fluid thermodynamics, quantifying the deviation from ideal gas behavior. It is defined as

$$\mathcal{Z} = \frac{pv}{RT}. \tag{5}$$

The critical compressibility factor $\mathcal{Z}_{\mathrm{cr}}$ [6] corresponds to the compressibility factor evaluated for T_{cr}, p_{cr}, and v_{cr}. Previous results