Sub- or supercritical? A flamelet analysis for high-pressure rocket propellant injection

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It remains an open problem as to whether droplets exist during the injection of liquid oxygen in a rocket combustion chamber at pressures higher than the oxygen critical pressure. While surface tension and thus droplets vanish in a pure fluid, a mixture state may exhibit a higher critical pressure, possibly reintroducing surface tension. In this paper, we address this problem by analyzing the non-premixed flamelet representation of combustion under liquid propellant rocket engine (LRE) conditions. The turbulent flames in a LRE can be thought of as being composed of elementary 1D laminar counterflow diffusion flames. The physically possible configurations for a given rocket operating condition, corresponding to the boundary conditions of the 1D flamelet problem, are captured by variation of the strain rate. For an exemplary supercritical operating condition ($p = 7$ MPa, $T_{\text{in,LOX}} = 120$ K, $T_{\text{in,H2}} = 295$ K) we show that, despite local mixing, the fluid never reaches a multiphase state from equilibrium combustion to quenching. The transition from supercritical liquid oxygen to an ideal gas state is found to occur in what is essentially a pure fluid process; real fluid mixing only occurs among LOX and water with a water mass fraction < 3% before the ideal gas transition. Representing the mixing trajectories of each flamelet in a reduced pressure – reduced temperature diagram allows to capture all physical mixture states of a configuration in a single plot. This approach furthermore allows to intuitively assess changes in operating conditions with respect to critical-state conditions.

I. Introduction

Unlike subcritical injection, injection at supercritical pressures is presently considered not well understood (Oefelein, Gautam and Gupta). Bellan asked in 2000: “Does a supercritical spray exist, and if so, what is it?” Nevertheless, high pressure liquid propellant rocket engines are technically relevant and are operated successfully.

The topic has received much attention over the last 15 years; experimental results have completely altered the view on the physical phenomena (Oschwald et al., Candel et al., Zong and Yang, Oefelein, Bellan, Habiballah et al.), and researchers largely agree on the observed phenomena. The shadowgraphs in Fig. 1a show that no droplets or ligaments are visible at supercritical pressure. However, at these conditions the interface appears diffuse (Habiballah et al.), elongated features separate from the core, and the interface dissolves (Oschwald et al.). In fact, the process is described as resembling turbulent mixing rather than subcritical liquid jet break-up shown in Fig. 1b (Newman and Brzustowski, Habiballah et al., Candel et al., Oschwald et al., Bellan). The time scales of the mixing process also form the rate determining
step of flame spreading, the momentum flux ratio of aerodynamic break-up loses its significance (Candel et al.\textsuperscript{6}). Comparisons with numerical simulations suggest that observed length scales are related to the turbulent Taylor scale (Oschwald et al.\textsuperscript{38}). For common LOX post thicknesses, the flame is anchored in a small recirculation zone behind it, see Fig. 2. This has been observed experimentally (Mayer and Tamura,\textsuperscript{31} Ivancic,\textsuperscript{21} Candel et al.\textsuperscript{5,6}) and numerically (Oefelein and Yang\textsuperscript{37}). In typical hydrogen-rich combustion, the flame encloses the oxygen stream. Experiments (Mayer et al.,\textsuperscript{30,31} Candel et al.\textsuperscript{6}) and simulations (Yang,\textsuperscript{45} Oefelein and Yang\textsuperscript{35,37}) show that the flame effectively separates oxygen from hydrogen, and that combustion takes place in the hot mixing layer (Oefelein\textsuperscript{30}). Juniper et al.\textsuperscript{22} point out that a strain rate required to quench a flame in LOX-GH2 combustion exceeds the strain rates found in rocket engines by an order of magnitude. Thus, after ignition, the flame is attached to the LOX post and will remain so; inert mixing of hydrogen and oxygen does not occur.

There is still debate as to whether the oxygen break-up occurs at supercritical or subcritical conditions. While the critical pressure of pure oxygen is exceeded, this might not be true for the local mixture critical pressure when oxygen comes into contact with other species: In a binary mixture, the critical temperature will lie between the individual critical temperatures while the mixture critical pressure can exceed the pure fluids critical pressure significantly (Reid et al.\textsuperscript{41}). This may cause the emergence of residual surface tension at supercritical pressures with respect to the pure fluid values, and has been demonstrated experimentally: Figure 3 from Mayer et al.\textsuperscript{29} shows the transition from diffusion- to surface-tension-dominated break up at twice the critical pressure of the injected nitrogen when the environment is mixed with helium.

There are essentially two established approaches for analyzing the thermodynamic states expected in a liquid propellant rocket engine: The first approach seeks to analyze a certain spatial profile through a flame.
This profile may be taken from a multidimensional computation, e.g. Oefelein,\cite{Oefelein2015} or from a 1D counterflow diffusion flame, e.g. Lacaze and Oefelein\cite{Lacaze2016} or Ribert et al.\cite{Ribert2017} The profile may be extracted in physical or mixture-fraction space. Lacaze and Oefelein\cite{Lacaze2016} studied the shift of the mixture-critical point in a counterflow diffusion flame. For the operation condition investigated (\(p = 7\) MPa, \(T_{\text{in,LOX}} = 120\) K, \(T_{\text{in,H2}} = 295\) K), they showed that the mixture critical pressure in the reaction zone exceeds the chamber pressure. However, being far away from the coexistence line, they concluded that a two-phase flow does not occur. In contrast to the studies which focused on H2-LOX mixing, Lacaze and Oefelein pointed out that water diffusion towards the LOX core has a stronger effect and thus needs to receive more attention. However, a profile extracted from an unsteady simulation necessarily represents a single point in time along an arbitrary line in space. In particular, at a different moment or at a different position, the thermodynamic situation may be completely changed. Similarly, a 1D counterflow diffusion flame profile corresponds to a single strain rate, while strain rates in a 3D flame vary spatially and temporally.

The second approach analyzes the inert mixing of the propellants in a 0D approach, see e.g. Mayer et al.,\cite{Mayer2019} Kuo,\cite{Kuo2020} Yang et al.,\cite{Yang2021} Oschwald et al.,\cite{Oschwald2022} Dahms and Oefelein.\cite{Dahms2023} Assuming an adiabatic inert mixing process between LOX and GH2, an equilibrium temperature for a given mixture fraction is determined. Then, calculation of vapor-liquid-equilibrium properties are carried out. Recently, Dahms and Oefelein extended this analysis by introducing a Knudsen number based evaluation of the interfacial thickness to determine the existence of residual surface tension under LRE conditions. They found that formation of droplets and ligaments may occur at supercritical pressure in inert LOX-GH2 mixtures. The approach is general in the sense that it can be evaluated for all mixture fractions. However, as discussed above, a pure mixture of oxygen and hydrogen cannot be expected in a liquid propellant rocket engine after ignition. Second, reaction products that are present in the flow are not accounted for. Finally, the assumption of adiabatic mixing is strictly only valid in the limit of unity Lewis number, as molecular and thermal transport determine local composition and temperature during the physical injection process.

So far, a systematic investigation of the thermodynamic structure of supercritical non-premixed flames has not been carried out. Following the flamelet arguments of Peters,\cite{Peters2014} a flame can be represented in composition space by a local 1D problem where the physical injection conditions form the numerical boundary conditions and the structure is given in terms of the mixture fraction. A variation of strain rate then yields the physically possible flow states for a given operation condition.

In the present paper we use this flamelet approach to study the general structure of cryogenic H2-LOX diffusion flames at supercritical pressure and address the question as to whether subcritical mixture states are attained in a H2-LOX coaxial injection problem for given engine operating conditions.

Figure 3: Injection of cryogenic nitrogen into nitrogen environment at a) 2.8 MPa (\(p_r = 0.83\)); b) 3.5 MPa (\(p_r = 1.03\)); c) 6.9 MPa (\(p_r = 2.03\)). d) Injection into mixture of N\(_2\) and He at 6.9 MPa. From Mayer et al.\cite{Mayer2021}
II. Numerical Method

Following the flamelet assumptions (Peters\textsuperscript{40}) a profile through a diffusion flame can be represented by a 1D-counterflow diffusion flame, depending only on the boundary conditions and the strain rate. The mathematical boundary conditions are determined by the physical engine inflow conditions. For a given operating point, the problem is thus reduced to a single variable - the strain rate (in physical space) or scalar dissipation rate (in mixture fraction space). Furthermore, the possible values of the strain rate are limited: in the lower limit the flame approaches equilibrium conditions, in the higher limit, the flame is quenched. Thus by analyzing the 1D configuration of a counterflow diffusion flame with a strain rate between equilibrium and quenching for the boundary conditions of the engine propellant injection conditions, every physical elementary flame is covered.

A. Governing equations

The axisymmetric, laminar counterflow diffusion flame admits a self-similar solution and can be simplified to a one-dimensional problem.\textsuperscript{20, 23} The governing equations including continuity, radial momentum, species and temperature equations can be written as

\[
\frac{d}{dx}(\rho u) + 2\rho V = 0, \\
\rho u \frac{dV}{dx} + \rho V^2 = \frac{d}{dx}(\mu \frac{dV}{dx}) - \Lambda, \\
\rho u \frac{dY_k}{dx} + \frac{dJ_k}{dx} = \dot{\omega}_k, \\
\rho u c_p \frac{dT}{dx} = \frac{d}{dx}(\lambda \frac{dT}{dx}) - \sum_k J_k \frac{dh_k}{dx} - \sum_k \dot{\omega}_k h_k,
\]

where conventional notations are used, \( V = v/r \), \( \Lambda = (\partial p/\partial r)/r \), \( h_k \) is the partial enthalpy of species \( k \), and \( J_k = \rho Y_k V_k \) is the diffusion flux for species \( k \). The governing equations are closed with an equation of state which will be introduced in the next subsection.

The governing equations and the equation of state are implemented in the Cantera package.\textsuperscript{15} Special care has been taken to fully resolve the thermodynamic nonlinearities near the pseudo-boiling region by modifying the grid adaptation strategy. As noted by Ribert et al.,\textsuperscript{42} Soret and Dufour effects in high-pressure combustion are negligible since the pressure enhances the chemical reactions, thus, their relative importance is diminished; the influence of the Soret effect will be evaluated in the following. A high-pressure chemical kinetic mechanism from Burke et al.\textsuperscript{32} is used for the H\(_2\)/O\(_2\) combustion accounting for 8 species and 27 reactions.

B. Thermodynamic relations

The Peng-Robinson equation of state (PR EoS)\textsuperscript{39} is used in this study for the evaluation of thermodynamic quantities. Real-fluid effects are accounted for by departure functions that are derived from the chosen state equation to ensure thermodynamical consistency of the governing equations. The state equation is expressed as

\[
p = \frac{RT}{v - b} - \frac{a}{v^2 + 2bv - b^2}
\]

where \( R \) is the gas constant, \( v \) is the specific volume, and the coefficients \( a \) and \( b \) are dependent on temperature and composition to account for effects of intermolecular forces. For mixtures, the coefficients \( a \) and \( b \) in Eq. (2) are evaluated as:

\[
a = \sum_{\alpha=1}^{N_S} \sum_{\beta=1}^{N_S} X_\alpha X_\beta a_{\alpha\beta}, \\
b = \sum_{\alpha=1}^{N_S} X_\alpha b_\alpha,
\]

where

\[
A.1
\]
where \( X_\alpha \) is the mole fraction of species \( \alpha \). The coefficients \( a_{\alpha\beta} \) and \( b_\alpha \) are evaluated using the recommended mixing rules by Harstad et al.\(^\text{17} \):

\[
a_{\alpha\beta} = 0.457236 \left( \frac{RT_{c,\alpha\beta}}{p_{c,\alpha\beta}} \right)^2 \left( 1 + c_{\alpha\beta} \left( 1 - \sqrt{\frac{T}{T_{c,\alpha\beta}}} \right) \right)^2, \tag{4a}
\]

\[
b_\alpha = 0.077796 \frac{RT_{c,\alpha}}{p_{c,\alpha}}, \tag{4b}
\]

\[
c_{\alpha\beta} = 0.37464 + 1.54226\omega_{\alpha\beta} - 0.26992\omega_{\alpha\beta}^2. \tag{4c}
\]

The critical mixture conditions for temperature, pressure, molar volume, compressibility, and acentric factor are determined using the corresponding state principles as:

\[
T_{\text{cr},\alpha\beta} = \sqrt{T_{\text{cr},\alpha}T_{\text{cr},\beta}(1 - k_{\alpha\beta})}, \tag{5a}
\]

\[
p_{\text{cr},\alpha\beta} = \frac{RT_{\text{cr},\alpha\beta}}{v_{\text{cr},\alpha\beta}}, \tag{5b}
\]

\[
v_{\text{cr},\alpha\beta} = \frac{1}{8} \left( v_{\text{cr},\alpha}^{1/3} + v_{\text{cr},\beta}^{1/3} \right)^3, \tag{5c}
\]

\[
Z_{\text{cr},\alpha\beta} = \frac{1}{2} \left( Z_{\text{cr},\alpha} + Z_{\text{cr},\beta} \right), \tag{5d}
\]

\[
\omega_{\alpha\beta} = \frac{1}{2} (\omega_\alpha + \omega_\beta). \tag{5e}
\]

where \( R \) is the universal gas constant, \( T_{\text{cr}} \) is the critical temperature, \( p_{\text{cr}} \) is the critical pressure, \( v_{\text{cr}} \) is the critical molar volume, \( Z_{\text{cr}} \) is the critical compressibility factor, \( k_{\alpha\beta} \) is the binary interaction parameter, and \( \omega \) is the acentric factor. The critical properties of the major species are taken from the NIST database.\(^\text{26} \) For the intermediate species, the critical properties are determined based on the Lennard-Jones potential.\(^\text{14} \) Critical values for all the species considered in this study are listed in Table 1. Details of the evaluation of partial derivatives and departure functions for all other thermodynamic quantities can be found in.\(^\text{18, 19, 27} \) Transport quantities are evaluated from Chung’s methods\(^\text{7, 8} \) for viscosity and thermal conductivity; Takahashi’s correction\(^\text{43} \) is used for the binary diffusion coefficients.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>( \text{H}_2 )</th>
<th>( \text{O}_2 )</th>
<th>( \text{H}_2\text{O} )</th>
<th>( \text{O} )</th>
<th>( \text{H} )</th>
<th>( \text{OH} )</th>
<th>( \text{H}_2\text{O}_2 )</th>
<th>( \text{HO}_2 )</th>
<th>( \text{N}_2 )</th>
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<td>( T_{\text{cr}} ) [K]</td>
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<td>190.82</td>
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<td>( p_{\text{cr}} ) [MPa]</td>
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<td>22.064</td>
<td>7.088</td>
<td>31.013</td>
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<td>4.786</td>
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<tr>
<td>( v_{\text{cr}} ) [cm(^3)/mol]</td>
<td>64.28</td>
<td>73.37</td>
<td>55.95</td>
<td>41.21</td>
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<td>41.21</td>
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<td>( \omega )</td>
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<td>0.022</td>
<td>0.344</td>
<td>0.0</td>
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<td>0.0</td>
<td>0.0372</td>
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</tr>
</tbody>
</table>

Table 1: Critical properties of species in \( \text{H}_2/\text{O}_2 \) combustion, where \( T_{\text{cr}} \), \( p_{\text{cr}} \), \( v_{\text{cr}} \) and \( \omega \) represent, respectively, the critical temperature, critical pressure, critical molar volume and acentric factor of the species.

C. Mixture critical point

It is not necessary to explicitly calculate the mixture critical pressure and temperature to solve the system of equations outlined above. For an a posteriori analysis, we use the pseudocritical method described by Reid et al.\(^\text{41} \) The mixture critical temperature is determined from

\[
T_{\text{mix,cr}} = \sum_{\alpha=1}^{N_S} X_\alpha T_{\alpha,\text{cr}}, \tag{6}
\]

the mixture critical pressure can be computed from

\[
p_{\text{mix,cr}} = \frac{RT_{\text{mix,cr}} \sum_{\alpha=1}^{N_S} X_\alpha Z_{\alpha,\text{cr}}}{\sum_{\alpha=1}^{N_S} X_\alpha v_{\alpha,\text{cr}}}. \tag{7}
\]
D. Mixture fraction

It is convenient to analyse the structure of non-premixed flames in compositional space by means of the mixture fraction $Z$ (see e.g. Peters\textsuperscript{40}). Here, we use a formulation based on the hydrogen atom also used by Lacaze and Oefelein:\textsuperscript{25}

$$Z_H = W_H \left( 2 \frac{Y_{H_2}}{W_{H_2}} + \frac{Y_H}{W_H} + 2 \frac{Y_{H_2O}}{W_{H_2O}} + \frac{Y_{OH}}{W_{OH}} + \frac{Y_{HO_2}}{W_{HO_2}} + 2 \frac{Y_{H_2O_2}}{W_{H_2O_2}} \right),$$

(8)

where $Y_\alpha$ and $W_\alpha$ are mass fraction and molecular weight, respectively.

E. Verification of the numerical method

A comparison of the results with the direct numerical simulation (DNS) of a two-dimensional counterflow diffusion flame in the transcritical regime by Lacaze and Oefelein\textsuperscript{25} was undertaken. The pure oxygen/hydrogen streams are injected at $T_{LOX} = 120$ K and $T_{GH_2} = 295$ K, respectively, at a base pressure of 7.0 MPa. This DNS was conducted using the PR EoS, an O’Conaire mechanism,\textsuperscript{34} and transport properties due to Ely and Hanley.\textsuperscript{11, 12} This benchmark case allows to assess the validity of our flamelet assumptions by investigating all parameters of interest. This case is close to the equilibrium condition, corresponding to conditions of low Damkohler number. The strain rate, calculated as the velocity difference of the injectors divided by the stream separation (Lacaze and Oefelein\textsuperscript{25}), for the problem is set to $10^5$ s$^{-1}$, This corresponds to a scalar dissipation rate of about $10^4$ s$^{-1}$, following the classical relationship between the strain and the scalar dissipation rate in laminar flamelets derived by Peters.\textsuperscript{40}

Figure 4 shows the comparison of temperature, compositions, density and specific heat capacity between current simulation and the DNS results. Mesh adaptation was employed to fully resolve the pseudo-boiling region, and mesh convergence studies were performed to ensure that the solution is mesh independent. Both results with and without the Soret effect are presented. It can be seen that the Soret effect has a small but noticeable influence on all major flame properties; including it improves agreement with the reference solution, all of the results presented in the following are simulated with Soret effect taken into account. The real-fluid effects, near the oxidizer injector plane, are evidenced in Figs. 4c and 4d. The local peak in the specific heat and the drop in density are well captured by the current model, with an absolute difference of $\Delta Z_H = O(10^{-4})$ in the location of the peak of the specific heat capacity. It should be noted that these figures are presented in a logarithmic scale. All other flame properties are very well captured by the current computational approach.

III. Results

A. Limiting cases

Figure 4 represents an exemplary solution for a counterflow diffusion flame, in terms of mass fraction and temperature distribution. In the limit of low scalar dissipation rates, the flames will reach an equilibrium structure. An increase in scalar dissipation rate causes heat to be transported by diffusion faster than liberated by reaction, reducing the maximum flame temperature. If the scalar dissipation rate exceeds a threshold, the flame will quench. Figure 5 (left) shows a plot of the attained maximum flame temperature for the same boundary conditions as a function of the scalar dissipation rate, corresponding to the stable branches of the classical S-curve (e.g. Peters\textsuperscript{40}).

Figure 5 (right) compares the structure of an equilibrium flame on the burning branch to the structure of a flame close to quenching, corresponding to the respectively marked points of the S-curve. In the equilibrium case, hydrogen and oxygen mix only in a small region around $Z_H \approx 0.13$. The maximum flame temperature exceeds 3500 K. The quenching flame behaves very differently: oxygen and hydrogen are present throughout the whole mixture fraction space, the maximum temperature is reduced by more than 1000 K.

Juniper et al.\textsuperscript{22} note that the quenching strain rate of a GH2-LOX flame lies an order of magnitude above the maximum values found in rocket engines. Indeed, it can be assumed in numerical modeling of rocket engines that the reaction can be assumed to reach a chemical equilibrium (e.g. Urbano et al.\textsuperscript{44}). Thus, all flamelets in a rocket engines can be expected to share the structure of the equilibrium flame.
Figure 4: Validation of the equilibrium flame (lines) with the numerical simulation by Lacaze and Oefelein (symbols).

Figure 5: Influence of strain rate / scalar dissipation rate on flamelet structure.
Figure 6: Pseudoboiling transition of cryogenic oxygen for various inlet temperatures; shown are density (left) and isobaric specific heat capacity (right). The transition from a liquid-like to a gas-like supercritical fluid is characterized by maxima in heat capacity $c_p$ and the density gradient.

B. The pseudoboiling transition

We have seen that mixing among oxygen and hydrogen exclusively occurs in the hot reaction zone in the equilibrium flame, Fig. 5 right. However, the transition to the cryogenic oxygen $Z_H \rightarrow 0$ needs to be evaluated in more detail.

Figure 6 shows profiles of heat capacity and density for various inlet temperatures. The pseudoboiling transition (Banuti,\textsuperscript{1} Oschwald et al.,\textsuperscript{38} Hickey et al.\textsuperscript{18}) is the transition from a liquid-like to a gas-like supercritical fluid. While continuous, this transition resembles subcritical vaporization; the main difference is that pseudoboiling occurs over a finite temperature range rather than at a specific saturation temperature. Lacaze and Oefelein\textsuperscript{25} emphasized a thermal barrier effect associated with the peak in heat capacity which limits heating of the liquid-like cryogenic fluid. In composition space, pseudoboiling is characterized by the maximum heat capacity, which approximately coincides with the steepest density gradient,

$$\left(\frac{\partial c_p}{\partial Z}\right)_{PB} = 0, \quad \left(\frac{\partial^2 \rho}{\partial Z^2}\right)_{PB} = 0.$$ (9)

We see that the pseudoboiling transition occurs at $Z_H \approx 1.3 \times 10^{-3}$ for an oxidizer temperature of 90 K, i.e. in almost pure oxygen. An increase in temperature moves the transition to lower mixture fractions, and reduces its width $\Delta Z_H$ (note the logarithmic scaling).

C. The ideal gas transition

We have seen that cryogenic oxygen undergoes its liquid-like to gas-like transition before significant mixing occurs. But does the mixing, that eventually takes place, happen under ideal or real fluid conditions? The compressibility factor $Z$ is a measure of deviation from ideal gas behavior. It is defined as

$$Z = \frac{p \rho}{RT},$$ (10)

and can be understood as a nondimensional parameter relating the real pressure to the pressure an ideal gas with the same density and temperature would exert. Thus, in an ideal gas, $Z \equiv 1$.

Figure 7 shows the evolution of $Z$ and hydrogen, oxygen, and water mass fraction for the equilibrium condition and the near quenching flame. Real fluid behavior occurs only on the oxidizer side. In the equilibrium case, $Z \approx 1$ for $Z_H < 3.0 \times 10^{-3}$, while $Y_{O_2}$ has only marginally reduced from 1. Figure 7 shows that this dilution can be attributed to water diffusing into the oxygen-stream. Following the definition of the mixture fraction $Z_H$ in Eq. (8), we obtain a water mass fraction of 0.027 at the transition to an ideal gas.

We can conclude that the transition from cryogenic oxygen to an ideal gas occurs under almost pure conditions. This is consistent with the results of Banuti et al.\textsuperscript{2}
Figure 7: Compressibility $Z$ for equilibrium (solid) and near quenching (dashed) flame. Real fluid behavior occurs only on the oxidizer side. In the equilibrium case, $Z \approx 1$ for $Z_H < 2.0 \times 10^{-3}$, for near quenching at $Z_H < 1.0 \times 10^{-2}$.

**D. Thermodynamic profiles**

Evaluation of the real gas $Z$ shows deviation from an ideal gas state, but does not provide information about a possible multiphase nature of the flow. A multiphase state, i.e. coexistence of liquid and vapor, only occurs along the vapor pressure curve of a fluid. This curve terminates with the critical point; processes passing the critical point at supercritical pressures only exhibit single phase behavior.

The critical point of a mixture may deviate substantially from the critical point of its constituents, it can be calculated using the mixing rules Eqs. (6) – (7). In order to evaluate the profile of the thermodynamic state, Lacaze and Oefelein\textsuperscript{25} introduced plots of reduced temperature and pressure versus the mixture fraction for their burning branch profile. Only when reduced pressure and reduced temperature are simultaneously smaller than unity, subcritical multiphase behavior is possible. We combine the pressure and temperature plot in a single graph to facilitate direct evaluation.

Exemplarily, a structure plot for the equilibrium, the quenching, and the mixing case from Fig. 5 left, is shown in Fig. 8. We do not observe subcritical multiphase behavior for any of the cases.

**E. The ‘ribbon plot’ as system representation**

Interpretation of Fig. 8 is not straightforward even though each graph represents but a single scalar dissipation rate. In order to extend this analysis for system evaluation, all physically different values need to be assessed, causing a large number of necessary plots. In addition, it is somewhat involved to deduce the thermodynamic profile from these plots, even when pressure and temperature are combined – let alone anticipating the effect of changes in operating conditions.

There is a more intuitive way of representing the data by eliminating the mixture fraction and combining the $p,T$ information in a single plot for every scalar dissipation rate. The resulting map is shown in Fig. 9. Every trajectory connecting O$_2$ and H$_2$ represents a flamelet solution for a single strain rate. Inert mixing yields the blue monotonically rising line at purely supercritical pressures, reactive flamelet solutions form a loop extending into subcritical pressures at supercritical temperature. The red and green lines are the equilibrium and quenching flamelet, respectively.

Crossing the pseudoboiling point causes a change in slope of the flamelet trajectories; this is much more pronounced in the inert case than in the reacting cases.

For the given operating conditions ($p = 7$ MPa, $T_{in,LOX} = 120$ K, $T_{in,H2} = 295$ K), it is apparent that multiphase states do not occur anywhere in the flame as no trajectory passes the critical point at subcritical pressure and would thus cross the coexistence line.
Figure 8: Defining the local composition in the flamelet in the pure mixing, the unstable and in the burning branch. The reduced pressure is shown along with the local temperature divided by the pseudo-boiling point temperature of the mixture. The shaded region marks subcritical temperatures.

Figure 9 is useful for a number of reasons. First, it allows for the direct assessment as to whether the coexistence line is crossed or not instead of inferring this from two graphs as in Fig. 8. Second, it can combine the complete set of data from the stable branches of the S-curve (Fig. 5). This means that it does not only highlight a singular condition, but instead may contain every physically possible trajectory in the $p_r-T_r$ phase space. It thus allows a complete representation of a combustion chamber operating condition as determined by the chamber pressure and the inflow boundary conditions for GH2 and LOX. Third, the plot allows to develop intuition as to what effect a change in operating conditions has: Increasing or decreasing the chamber pressure leads to an upward and a downward translation of the ribbon plot, respectively. Changing the inflow temperatures will lead to a lateral translation of the $O_2$ and $H_2$ point in the plot; the closed loop reaction zone will approximately retain its position, as heat release in the flame dominates the enthalpy change by a marginally different inflow temperature. Changing the propellant will alter the positions of the end points and possibly shape of the trajectories.

IV. Discussion

We identified several phases in cryogenic, supercritical diffusion flames, as depicted in Fig. 10: First, The oxygen is injected in as supercritical liquid-like fluid and transitions to a gas-like vapor state (pseudoboiling); second, the supercritical gas-like vapor transitions to an ideal gas; third, as an ideal gas, oxygen mixes and reacts in the hot flame.

Figure 11 shows the flame structure in physical space, highlighting the two thermodynamic transitions that the oxygen has to undergo before entering the reaction zone.
Figure 9: Plot of all flame structure trajectories between pure oxygen and pure hydrogen in terms of the local reduced pressure and temperature. Since the critical point is not passed at subcritical pressures by any trajectory, the flow consists of a single phase at every point.

This isolation of real fluid behavior in the oxygen phase can be used to interpret the transitions from a pure fluid perspective in a phase diagram. Figure 12 shows the injection process in the $p_T$ diagram of oxygen, data are retrieved from the NIST database.\(^{26}\) The arrow traces the transition of pure oxygen across the pseudoboiling line into the ideal gas region.

V. Conclusion

The present paper seeks to address the question as to whether injection of LOX/GH2 into rocket engines at operating conditions exceeding the critical pressure of oxygen can be considered sub- or supercritical when mixing and combustion are taken into account. For the investigated steady-state operating condition ($p = 7$ MPa, $T_{\text{in,LOX}} = 120$ K, $T_{\text{in,H2}} = 295$ K), we found that the flow consists of a single phase.

Our approach evaluates 1D flamelet solutions for the whole burning branch between equilibrium combustion and quenching. A new representation of the local thermodynamic state in terms of reduced temperature and pressure tracks each flame trajectory along the mixture fraction from hydrogen to oxygen, allowing for a

Figure 10: Schematic of a flame anchored behind the LOX post in GH2/LOX injection. The flame separates oxygen and hydrogen flow and is anchored behind the LOX post. LOX transitions into an ideal gas state before significant mixing occurs.
Figure 11: Schematic view of the counterflow diffusion flame in physical space. The flame location, pseudo-boiling point and stagnation point are defined on the flame for a typical hydrogen/oxygen flame. The normalized distribution of the specific heat, temperature and density as well as the compositional structure of the flame is presented. The oxygen undergoes two thermodynamic transitions – pseudoboiling and to an ideal gas – before entering the flame.

Figure 12: Pure fluid phase diagram, showing the positions of the thermodynamic transitions and the injection process. The pseudoboiling line is an extension of the coexistence line up to $p_r = 3$. The shaded region marks ideal gas behavior, i.e. $0.95 < Z < 1.05$. The arrow traces the pure fluid injection process; mixing occurs where the shaft is shown as dashed and the pure fluid view no longer applies.
clear interpretation and an intuitive assessment of the influence of changing operating conditions (injection conditions, chamber pressure, propellants).

We found that the injected oxygen undergoes two thermodynamic transitions before entering the reaction zone: LOX transitions from a liquid-like, to a gas-like state, and finally to an ideal gas state before water diffuses in from the reaction zone. Thus, mixing in an attached LOX/GH2 flame occurs essentially under ideal gas conditions. The effect of real fluid mixing rules on flame structure solutions can thus be expected to be small.

The real fluid thermodynamic transitions in supercritical cryogenic injection are pure fluid phenomena, a physical understanding of these phenomena is thus mandatory to understand high pressure injection.

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References


