Progress in transcritical combustion : experimentation, modeling and simulation

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Transcritical conditions correspond to situations where the operating pressure exceeds the critical pressure but the injection temperature is below the critical value. Such extreme conditions, which are encountered for example in high performance rocket engines, introduce fundamental scientific challenges with many technological implications. Advances on these issues are reviewed in this article. It is shown that progress has been substantial on the experimental level and that this has provided an important data base for parametric analysis and model development. Improved real gas thermodynamics and transport models have allowed investigations of geometrically simple problems such as combustion of spherical pockets or in strained flames formed by the counterflow of transcritical and supercritical streams. Calculations of complex flames formed by transcritical injection of reactants have also been carried out using RANS models, but much of the recent effort has been focused on the adaptation of computational tools for large eddy simulation of transcritical flows. Recent calculations of typical transcritical injection configurations indicate that simulations can suitably retrieve flame structures and trends observed experimentally. It is concluded that progressively more complex configurations will become tractable with advanced transcritical LES tools and that this should help improve current understanding of fundamental processes and advance design methods.

1 Introduction

Combustion is often carried out at high pressure giving rise to many difficult issues. This is the case for example in engines and propulsion systems where compression is essential to work extraction from the thermodynamic cycle. The pressure level has been continuously brought to higher values in gas turbines to increase the thermal efficiency. Higher pressures in liquid rocket engines (LRE) thrust chambers have provided augmented specific impulses. In modern LREs the pressure often exceeds the critical value of one of the reactants and the system operates under supercritical conditions. In gas generators the pressure is often above the critical values of the two propellants and the injection temperatures are below the critical temperatures. Conditions of this type prevail in most high performance LREs where pressure is typically above 10 MPa and reaches levels as high as 40 MPa well over the critical value of oxygen $p_c(O_2) = 5.04$ MPa. In LREs propellants are stored in cryogenic form and the injection temperature of the oxidizer is usually below the critical value of this substance. This type of injection is then generally designated as "transcritical". Under such unusual conditions the density of the oxygen stream is quite high and takes liquid-like values in excess of 1000 kg m^{-3}. The evolution in the chamber is nearly isobaric and the mixing and conversion of reactants yields high temperature gases at very low densities. In the supercritical range, surface tension and latent heat of vaporization have vanished and the change in density takes place in the absence of a liquid/gas interface. There is however a large density contrast between the injected stream and the supercritical (gaseous)environment. Combustion under such extreme conditions introduces important design issues and engineering trade-offs. There are many technical questions are linked to the definition of injection elements for ensuring the flame stability during all phases of operation. One of the current issues is to reduce the number of elements using larger mass flow rate injection systems. This change must be done without increasing the flame length and size of the reaction zone. The engine ignition sequence must be defined with great care to avoid a violent initiation accompanied by a pressure wave that can defuse the turbo. Dimensions of the thrust chamber should take into account the length of the reaction zone formed by the injection devices. In the gas generator design, the temperature stratification of burnt gases from combustion must be reduced to avoid hot spots at the turbine and allow optimum operation of this machine very busy on the thermal. An important issue is that of high frequency combustion instabilities whose effects on the motor can be disastrous. Instabilities result from coupling between combustion and acoustic mode of the chamber. The induced oscillations can reach considerable magnitudes of about 20 % of the pressure intensifying chamber heat flux to the walls and the injection plane with the result of rapid degradation of the chamber and the spectacular destruction of the system. This situation is inherently unsteady and understanding of combustion dynamics phenomena constitutes a key challenge for the field (a collective book on the problem of LRE combustion instabilities is due to Yang and Anderson [1]).

The previous issues have led to a wide range of investigations during the recent period which are the subject of the present review.

It is worth noting at this point that much of the information on transcritical injection, mixing and combustion was not available during the early stages of the development of rocket engines and that the technology put into flight systems was most often designed without the fundamental basis generated more recently. Progress in liquid rocket propulsion technology during the second half of the 20th century has led to commercial utilization of space and a continuous growth of space applications to telecommunications, earth observation and global positioning. Propulsion system design has relied during this early period on accumulated experiences from full scale testing, engineering analysis and application of basic combustion principles. The situation has evolved in the last period where research has brought informations on the processes controlling combustion under transcritical conditions. This has provided new insights into a complex process and new tools for improving gas generator, injection elements and thrust chamber design.

Experiments have provided a large amount of data on the structure of transcritical mixing and combustion. This has been made possible by exploiting new model scale cryogenic combustion facilities in combination with modern optical and laser diagnostics and computerized data acquisition and processing. Selected results of experimental investigations are reviewed in section 2. Much effort has been expanded in parallel to examine central issues in the analysis of supercritical fluids and devise tools for the description of thermodynamics and transport properties in this range. Advances in this area are reviewed in section 3. Progress has also been made in the numerical modeling of transcritical mass transfer and combustion. Calculations have concerned problems in which the geometry is simplified (spherical inclusions, counterflow strained flames). In addition some direct simulations have also been carried out in the supercritical range. These advances are described in section 4. Progress in large eddy simulation (LES) is probably the most visible with developments of transcritical combustion LES tools with calculations of the injector nearfield and more recently with computations of full scale transcritical flames. Data gathered on cryogenic flames at high pressure have been used to assist these modeling efforts and support the development of numerical simulation tools. This research has been made possible by the remarkable evolution in computational ressources including massively parallel technologies. Progress in transcritical LES is described in section 5.

2 Selected experimental results

Combustion under extreme conditions corresponding to the transcritical range has been investigated in model scale experiments simulating gas generator or thrust chamber conditions. Most of the available data correspond to flames formed by shear coaxial injectors in which liquid oxygen is injected by a central post surrounded by an annular stream of hydrogen. Some experiments carried out on the Mascotte test bench also concern flames formed by liquid oxygen and supercritical or liquid methane. Other experiments have also been carried out in the absence of combustion. These cold flow tests provide informations on the mixing processes at supercritical pressure, a key element towards the study of reactive systems.

2.1 Mixing under transcritical conditions

Because surface tension and latent heat of vaporization vanish at supercritical pressure [2], the break-up mechanism which prevails under subcritical pressure conditions is no longer observable. This has been examined for example by Mayer, Oschwald and their groups at DLR [3–5] and by Chehroudi *el al.* [6] and more recently by Segal and Polokov [7]. This is illustrated in Figure 1.

The dense jet dissolves in the ambient gas with no evidence of droplet generation. For a reduced pressure ($\pi_r = p/p_c$ *i.e.* the ratio between the pressure and the critical value) slightly larger than unity, "finger-like" structures appear on the jet edge, a feature which is not observed at low pressures [6]. As pressure is further increased, the flow resembles that of a variable density turbulent gas flow. This behavior is quantitatively confirmed by experimental measurements of initial spreading rates deduced from backlighting visualizations. Analysis of the fractal dimension of the jet mixing layer boundary also indicates that the value obtained for transcritical stream is similar to that found for classical turbulent free jets [6,8]. Quantitative measurements of density [3,4,9], density spreading rate and density decay coefficients obtained by [5,10] using spontaneous Raman scattering indicate that the general trends can be deduced from studies of variable density flows. It is also found that the high density contrast in the injector nearfield stabilizes the initial mixing layer, leading to a strong anisotropy of the turbulent structures and to a much longer potential core than what is observed in constant or weakly variable jets [5].

The case of a coaxial injection is studied by Davis and Chehroudi [11–13], who considered injection of a single species in an ambient gas formed by that same species. In another set of experiments, Mayer et al. [4] and Mayer and Smith [14] use a dense nitrogen jet surrounded by a high velocity coaxial stream of helium. Again, there are no droplets [14] and the fluid density evolves continously between the high density value in the central core and the surrounding gas. Analytical developments carried out by Lasheras *et al* [15], Rehab *et al.* [16] and Villermaux [17] and pursued by Villermaux and Rehab [18] indicate that coaxial mixing is essentially governed by the momentum flux ratio between the outer gaseous stream and the central liquid stream ($J = (\rho_g v_g^2)/(\rho_l v_l^2)$). According to these authors, the intact length of the central core is inversely

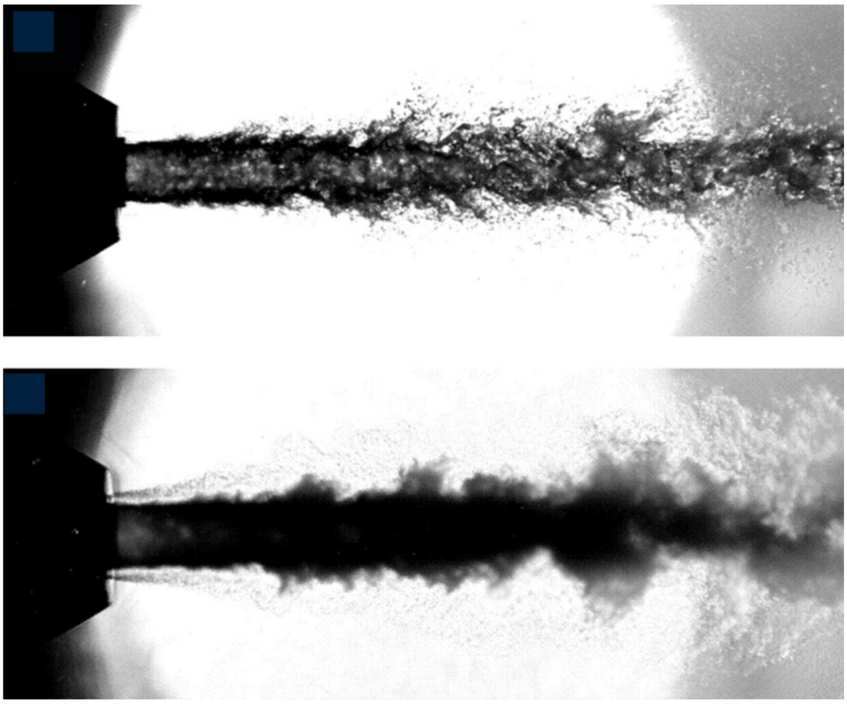


Figure 1: *Backlighting images of coaxial injection of nitrogen surrounded by an annular jet of helium. Top: subcritical injection at a pressure of 1 MPa. Bottom : transcritical injection of nitrogen at a pressure of 6 MPa. From [4].*

proportional to the square root of this momentum flux ratio ($l_c \simeq J^{-1/2}$). The more recent studies carried out by Cherhoudi tend to indicate that the exponent of the momentum flux ratio changes with the pressure. Under subcritical conditions this exponent is closer to 0.2 while at near or supercritical conditions, this exponent is closer to 0.5. This is illustrated in Figure 2.

When compared with the round jet configuration, a strong reduction of the jet core intact length is observed when the central jet is surrounded by a high speed supercritical stream as explained by Oschwald et al. [5]. This reduction is more pronounced as the ratio between the outer and the inner jets momentum fluxes is increased [19]. The dark-core length of the coaxial jet at near- and supercritical pressure follows a similar momentum flux ratio dependency reported for the single-phase shear-coaxial jets.

A remarkable conclusion of cold flow investigations is that transcritical jets or coaxial jets formed by a transcritical stream surrounded by a supercritical flow share many common features with variable density turbulent jets and that mixing takes place in a manner which is qualitatively similar to that prevailing in variable-density turbulent jets.

2.2 Flame structures

Liquid oxygen / supercritical hydrogen flame structures at high pressure are considered in experiments carried out by Mayer et al. [20] and by Juniper et al. [21] (see also Candel et al. [22] for a review). Most of the analysis is based on backlighting and OH* emission imaging which are both integrated over the line of sight. Typical emission images corresponding to

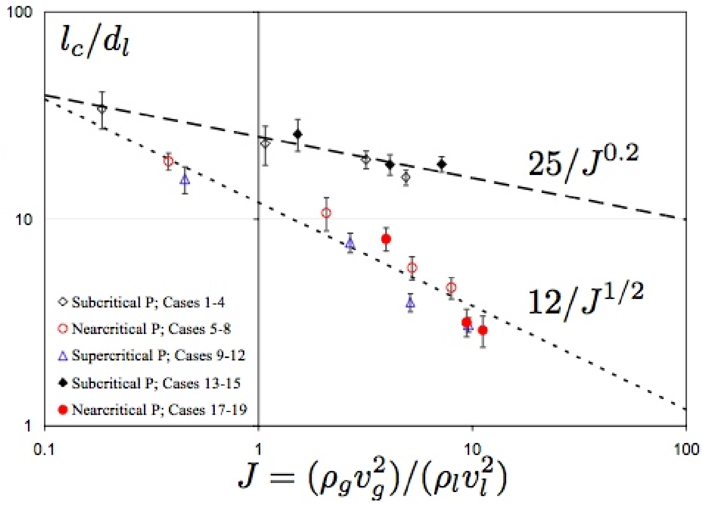


Figure 2: *Reduced dark core length (l_c/d_l) as a function of the momentum flux ratio. Subcritical conditions are represented by diamond symbols. Near critical and supercritical conditions are represented by circle and triangle symbols. The open symbols correspond to higher outer-jet injection temperatures ($T_g \simeq 190$ K). Adapted from [11].*

LOx/GH2 flames at a pressure of 6.3 MPa are shown in Figure 3. Emission of OH* radicals is seen to begin in the near vicinity of the LOx injection channel lip.

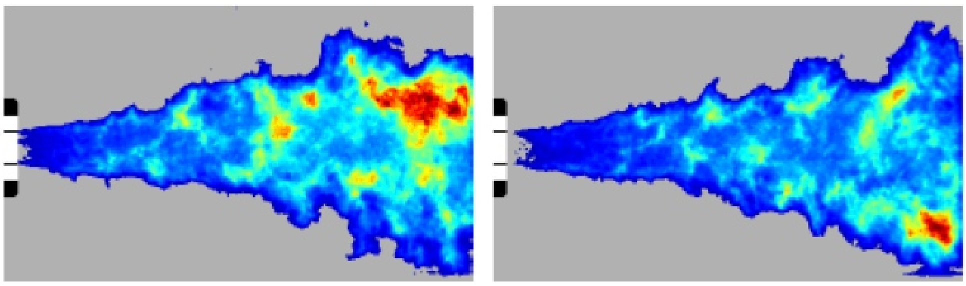


Figure 3: *Instantaneous images of OH* emission from a LOx/GH2 flame. Pressure p = 6.3 MPa, J=9, mixture ratio E =2. [23].*

There is one set of data where the flame instantaneous structure is obtained from laser induced fluorescence (Figure 4). Structure of flames formed by injection of transcritical oxygen surrounded by a high speed supercritical methane stream are reported by Singla et al. [24]. As for pure mixing cases, experimental observations Habiballah et al. [25] suggest that the central oxygen stream gives rise to large density gradients. No drops or ligaments are created and small highly wrinkled structures which "dissolve" in the ambient gases are also noticed [20, 25]. The flame structure at supercritical pressure differs from that observed under subcritical conditions. The flame expansion angle is smaller than that observed at subcritical pressure. At subcritical pressure the liquid oxygen jet is broken down and atomized into a spray of droplets which vaporize. The reactive region surrounding the droplet spray is formed by the gaseous oxygen encountering the stream of hydrogen or methane. At supercritical pressure, mass transfer from the high density oxygen stream to the surrounding flow is dominated by turbulent mixing and heating processes and is governed by the amount of surface area and by the local strain rates and heat fluxes acting in this region. As a consequence, coaxial flames in the transcritical regime are thinner than at subcritical pressure and spread closer to the cold and dense oxygen jet. These flames do not however penetrate into the central core occupied by the dense oxygen stream [22].

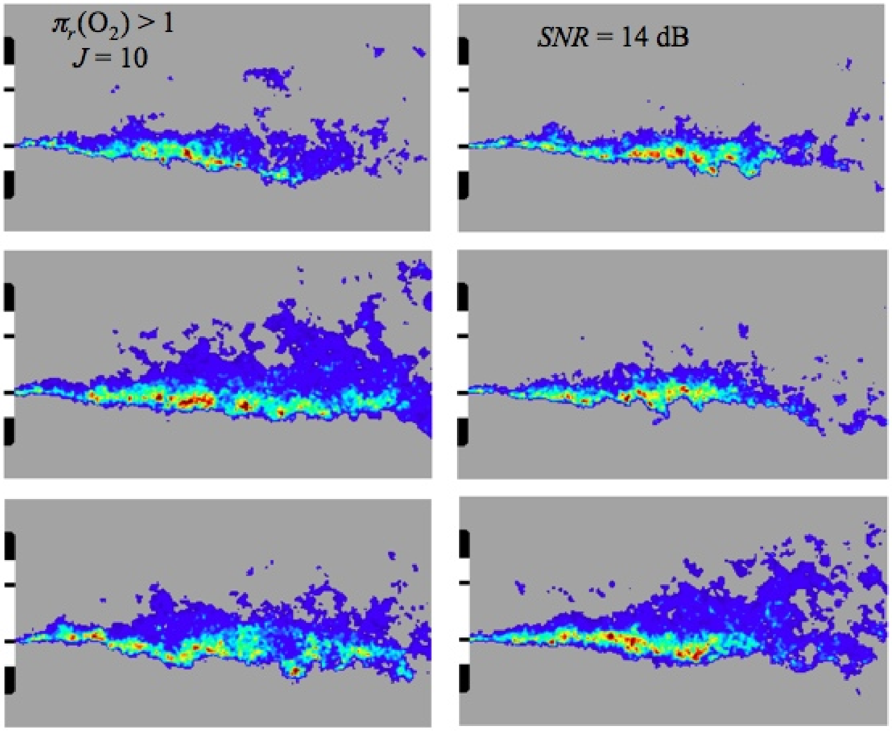


Figure 4: *OH PLIF images in the injector nearfield for a LOx/GH2 flame at transcritical injection conditions.* $p = 6.3$ *MPa, J=9, E =2,* $\Delta t_{exp} = 50ns$. *The image ends at 8*d_L*Ox from the injection plane. The cryogenic flame is thin, well established, and anchored to the oxygen injector lip. At a distance from the injector the flame sheet is wrinkled by turbulent fluctuations [23].*

Singla et al. [24] also describe flames formed under doubly transcritical injection conditions in which transcritical oxygen is surrounded by a coaxial stream of transcritical methane. This gives rise to an unusual flame pattern characterized by two embedded conical layers of light emission indicating that chemical conversion takes place in two distinct concentric more or less conical regions (Figure 5(b)). The inner layer established in the vicinity of the oxygen jet boundary resembles a standard turbulent diffusion flame while the outer reactive layer is established near the boundary of the dense methane stream which takes the form of a fairly open conical surface.

Other studies also provide indications on effects of flow parameters and on the influence of a recess. When the LOx post exit section is recessed with respect to the hydrogen exhaust section, it is found by Juniper [26] that the dense oxygen jet features long wave instabilities which augment the spreading rate. The large amplitude unstable motion of the central core is analyzed by Juniper and Candel [27] who show that the flow behaves like a confined wake and that the dense inner jet surrounded by a high speed lighter outer stream promotes a wake-like global instability in the central stream. This unstable behavior of the central core has also been

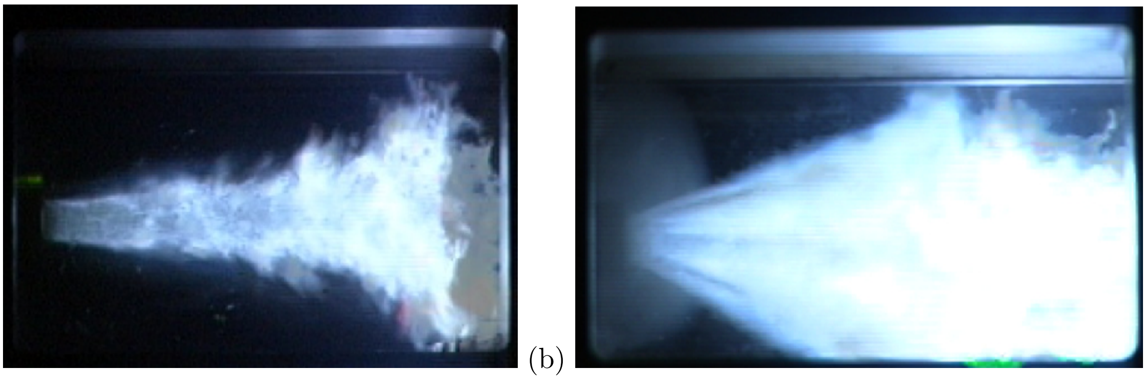


Figure 5: *Direct images of flames formed by coaxial injection of liquid oxygen and methane. (a) The methane stream is supercritical.* $p = 5.6$ *MPa,* $T_{LOx} = 85$ *K,* $T_{CH4} = 288$ *K (b)* $p = 5.4$ *MPa,* $T_{LOx} = 85$ *K,* $T_{CH4} = 120$ *K.*

observed more recently by Lux and Haidn for a coaxial injection of methane and oxygen [28].

2.3 Flame stabilization

Stabilization is a central issue in the design of injection systems. Experiments on coaxial cryogenic injectors fed with liquid oxygen and supercritical hydrogen gas, indicate that the flame is anchored in the near vicinity of the LOx post injector lip. Transcritical oxygen / supercritical hydrogen (see Figure 6) or methane coaxial jet flames stabilize at a small distance behind the inner lip.

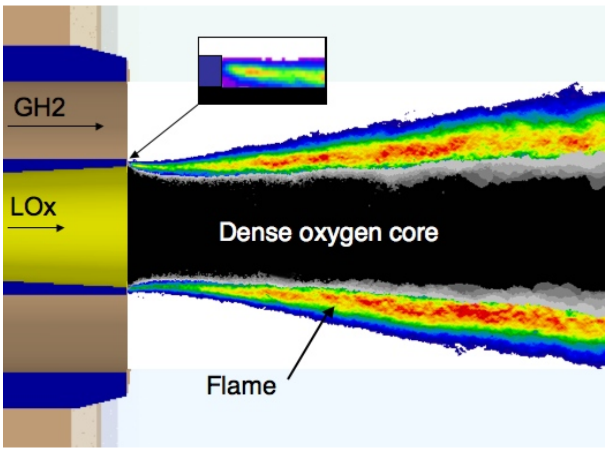


Figure 6: *Image of the transcritical flame formed between liquid oxygen and supercritical hydrogen. A slice of the average emission intensity is shown in color. The average oxygen jet position is shown in grayscale. The near-injector region is also shown in an is expanded form. From Juniper et al. From Juniper et al. [29].*

This distance is less than the lip thickness for oxygen /hydrogen flames as can be seen in Figure 7. The anchor point is less close to the injector lip in the oxygen / methane flame. These features are revealed by Juniper *et al.* [21] on the basis of Abel transformed average emission images and by Singla *et al.* [23] using laser induced fluorescence images. It is interesting and astonishing to note that the flame is adjacent to a high speed stream but remains anchored near the LOx post. To understand how this can be so, it is first observed that oxygen / hydrogen and oxygen /methane flames are quite resistant to strain rates imposed by the flow. It can be shown that extinction of oxygen / hydrogen or oxygen / methane counterflow diffusion flames requires very high strain rates and that the values needed are generally not reached under typical combustion chamber conditions [29–31]. Extinction of the flame even when it is pinched against the condensed oxygen is under such circumstances quite improbable. Extinction by strain may be possible at pressures well below 1 bar, where the flame is thicker and less intense. It is considered, however, that the flame tip would blow out of the zone behind the lip before such conditions could be reached indicating that if the flame is stabilized near the injector lip, the flame will spread therefrom and that extinction will be improbable.

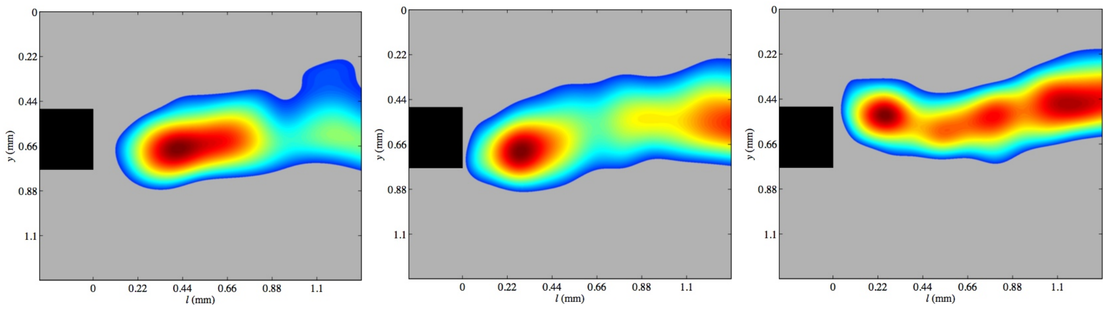


Figure 7: *OH-PLIF images of the flame holding region. Liquid oxygen and supercritical hydrogen are injected above and below the step respectively. The OH distribution in the flame edge is shown on the standard color scale.* $p = 6.3\,MPa$*. From Singla et al. [23].*

In another numerical investigation of the reactive region established behind the lip, it is shown that flame anchoring is essentially determined by a single parameter formed by the ratio Ψ of the lip height to the flame thickness . This quantity is by far the most important parameter defining the stability of the reactive layer as shown by Juniper and Candel [32]. When $\Psi > 1$ the flame edge is tucked behind the lip and the flame is stable (Figure 8(a)). When $\Psi < 1$ the flame is thicker than the lip, it becomes sensitive to the high speed flow and can be blown away from the lip (Figure 8(b)). This analysis is confirmed by laser induced visualizations of OH in the initial region which indicate that when the reactive layer is thinner or of the same order as the lip thickness the flame anchor point remains in the near vicinity of the lip. When this layer is thicker than the lip, the flame is sensitive to the high speed flow and its edge moves around. Stabilization is only dynamically achieved under these conditions [33].

2.4 Interaction with acoustic modulations

The interaction of acoustic waves with transcritical flows is of interest for the study of combustion instability. This interaction may influence the mixing efficiency and this can in turn change the combustion efficiency. Effects of an acoustic modulation on a single round jet at sub- and supercritical pressure is investigated by Chehroudi and Talley [34] who find that the acoustic modulation have a limited impact at supercritical pressure when compared to subcritical-pressure cases. The impact of the modulation reduces as the inlet mass flow rate is increased. It has then been extended to coaxial injectors by [19, 35, 36]. A strong reduction of

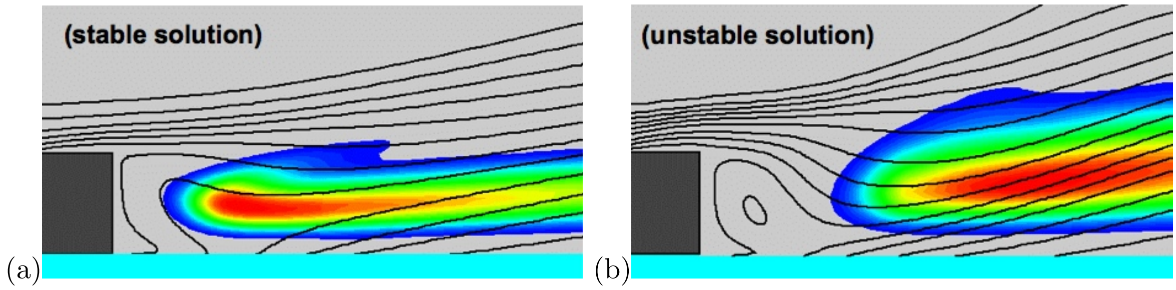


Figure 8: *Flow configurations at different values of* Ψ*, which is the ratio of the step height,* h_s*, to the flame thickness,* δ_f*. For* $\Psi > 1$ *the flame edge is tucked into a slow-moving region behind the step. For* $\Psi < 1$ *the flame cannot support itself in this region. It becomes exposed to the free stream and blows off. (a) "Tucked flame",* h_s *= 0.2 mm,* δ_f *= 0.16 mm,* $\Psi = 1.25$*. (c) "Exposed flame",* h_s *= 0.2mm,* δ_f *= 0.28 mm,* $\Psi = 0.71$*.* U_{H_2} *= 150 ms*$^{-1}$*,* T_{H_2} *= 350 K. From Juniper et al. [32].*

the jet length penetration is reported, even for a moderate amplitude of acoustic modulation. Rodriguez *et al* [37, 38] also observed a strong effect of the phase of the acoustic modulation on the jet penetration length and dark core instability. Rocket engines are nevertheless characterized by very high pressure fluctuations, which reach 20 % of the chamber pressure. Such extreme amplitude values have been recently reached by [39, 40]. This experiment mounted on the Mascotte test rig of Onera, is carried out on a multiple injector combustor featuring five coaxial injection elements. An actuator generates transverse acoustic modes. The most recent version of this device designated as the Very High Amplitude Modulator (VHAM) operates under subcritical and transcritical conditions. Studies involving non-reactive and reactive cases clearly highlight a strong reduction of the jet and flame length. This is a sign that the transverse acoustic modulation interacts strongly with the rate of heat release rate and that this markedly changes the flowfield.

3 Thermodynamics and transport properties of transcritical fluids

Propulsion system operation at high pressure over a wide range of temperatures introduces many new modeling issues, because the working fluid evolves from a liquid-like to a gaseous-like state. One has to replace the perfect gas equation of state and the corresponding thermodynamic functions by a consistent description of the real gas behavior in the high pressure range.

3.1 Equation of state and thermodynamics

To account for density changes at subcritical temperature, molecular interaction forces can no longer be neglected and the perfect gas equation of state (EOS) has to be replaced by more elaborate equations of state, a problem considered most notably by Bellan and Yang and their groups (see for example Harstad et al. [41] and Yang [42]). At supercritical pressure but at low temperature, fluids exhibit properties which are similar to those of a liquid. As temperature is increased above the critical value, the evolution approaches that of a perfect gas. In addition to the important variation in density, rapid changes of the fluid thermodynamic properties characterize the near-critical region, and this notably differs from a perfect gas. As an example, the fluid compressibility decreases as density is increased and this gives rise to a significant increase in the speed sound. The specific impedance of the fluid is also enhanced, a fact which is of prime importance in the analysis of acoustic interactions.

The change in thermodynamic properties theoretically modifies the reactivity since chemical potentials are modified. Such effects of the non-ideality are nevertheless limited, except in the very high pressure range, at pressures in excess of 40 MPa (see for example Giovangigli et al. [43]).

3.2 Transport properties

A second issue is concerned with the evaluation of transport properties. Reliable methods exist for the estimation of viscosity and thermal conductivity as discussed for example in [2], [44] or [42]. The estimation of the mass diffusion coefficients is more difficult, mainly because of the lack of experimental data available in the low temperature, high pressure range. Methods generally rely on correlations obtained over large sets of data. The methods generally make use of the corresponding state principle. Complete formalisms derived from gas kinetic theory are also available. A discussion of these questions is offered in [45] or [43]. Practical methods and a consistent set of rules are discussed in [46]. A set of computational routines which extends the Chemkin package [47] to the transcritical domain is also described in the latter reference. Calculated values of viscosity and heat conductivity are in good agreement with data from NIST (see Figures 9).

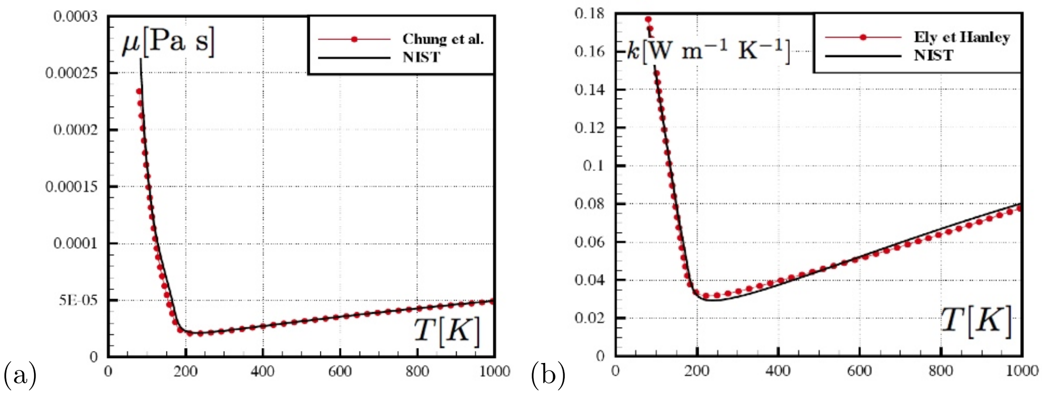


Figure 9: *Transport coefficients of oxygen. (a) Viscosity, (b) Heat conductivity. $p = 7$ MPa. From Pons et al. [46].*

4 Detailed modeling and simulations of transcritical mixing and combustion

4.1 Transitional mixing layer

The mixing layer established between two fluids flowing at different velocities constitutes a generic configuration which has often served in modeling studies. Mixing layers at high pressure have been considered more recently by [48] [49] and [50]. These simulations correspond to moderate temperatures of the working fluids which do not feature the large density contrast found under transcritical injection conditions. Results of this series of calculations are reviewed by [51]. When temperature exceeds the critical value, flows of reactants in a supercritical state are less difficult to handle numerically than those corresponding to a transcritical state but the mixing layer simulations highlight the effect of non-ideality on mixing and stability. Due to the presence of density gradients, anisotropy is shown to play an important role leading to modifications of the mixing layer structure.

4.2 Isolated pockets of dense fluid ("droplets")

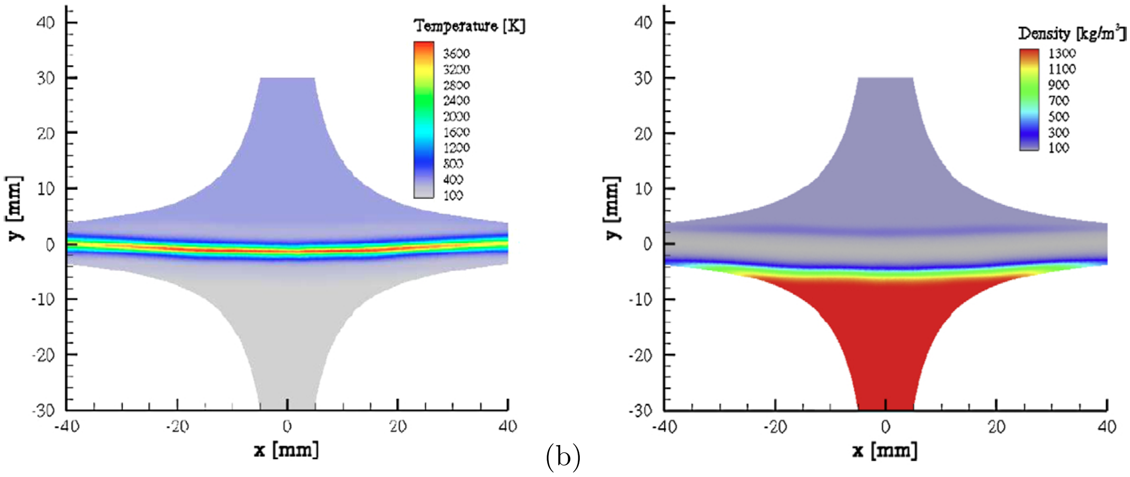
Modeling studies in the transcritical range have initially concerned mass transfer and combustion in the simplified spherical geometry. Spherical pockets of transcritical fluids placed in a supercritical environment are considered in a group of studies carried out by Delplanque and Sirignano [52], Daou *et al* [53], Oefelein and Yang [54], Oefelein and Aggarwal [55], Harstad and Bellan [56], Okong'o *et al* [49], Okong'o and Bellan [57]. This effort has also been reviewed by Yang [1,42], Sirignano [58] and Harstad and Bellan [44]. In the spherical geometry the problem is reduced to a single spatial dimension. These calculations are theoretically useful but have limited practical importance since spherical inclusions are not produced by coaxial injectors of the type discussed in section 2. Indeed, the standard process of atomization, governing subcritical liquid injection and giving rise to droplet sprays, does not prevail in the transcritical range. There are no droplets in that range because surface tension has vanished. One observes instead a highly wrinkled surface which separates the dense transcritical propellant from the surrounding lighter fluid. Mass transfer from the dense stream is then controlled by the available exchange surface area and by the local strain rates or scalar dissipation associated with turbulent fluctuations and by the local heat fluxes. These characteristics are exploited in a physical model derived by Jay et al. [59] where the rate of mass transfer is deduced from the local strain rate level and from the amount of exchange surface area between the dense oxygen stream and the surrounding flow.

4.3 Transcritical strained flames

Under transcritical conditions, the local flame layer can be described in terms of strained flames and the turbulent flame can be modeled as a collection of strained reactive elements convected and distorted by the flow but keeping an identifiable structure. It is then more adequate to consider the structure of transcritical strained flames, a problem envisaged more recently [31, 46]. A complete set of computational routines which extends the Chemkin package to the transcritical domain, designated as Transchem, is also described by Pons et al. [46]. These simulations indicates that under typical conditions prevailing in rocket engines, a fast chemistry assumption is reasonable. In addition, it is shown that real-gas features have a negligible influence inside the reaction-layer, and it is suggested that the changes in the flame pattern observed experimentally (Sec. 2) are essentially due to the presence of the high-density central jet, which plays a key role in the mass and heat transfer to the surrounding stream and feeds the flame with oxidizer, the latter spreading close to the cold and dense oxygen jet [22]. Most of these studies are carried out in a one-dimensional framework but there is also a case where the strained flame is treated as a multidimensional problem [60]. This is illustrated in Figure 10.

5 Numerical simulations at supercritical pressure

RANS approach



(a) (b)

Figure 10: *Map of temperature (a), density (b) of a strained flame formed by a transcritical stream of oxygen injected at 80 K and 1 m s^{-1} impinging on a supercritical methane stream at 300 K and 5 m s^{-1} in a 7 MPa environment. From Pons et al. [60].*

The general trend in engineering has been to develop computational tools to replace costly experimentation and time-consuming testing. Simulations are also welcomed because they provide information which are otherwise inaccessible experimentally. In complex situations like those considered in the present article, simulations used in combination with experiments provide essential insights in the process. Substantial efforts have been made in recent years to develop numerical methods for reactive flows. To deal with turbulent flames, this effort has initially relied on Reynolds Average Navier-Stokes (RANS) equations. It is known however, that the Reynolds average framework introduces difficult turbulence closure issues. One central problem is to define a suitable model for of the average volumetric rate of reaction. The treatment of transcritical injection and combustion gives rise to additional difficulties. One has in particular to use adequate equations of state and make sure that mass transfer from the dense core to the surroundings is well represented. Demoulin *et al.* [61] propose a model which takes into account the large density variation between the two streams. Suitable representation of the mean flame brush has been obtained. RANS or unsteady-RANS simulations have also been achieved by Cheng and Farmer [62], Tucker [63], Merkle [63], Benarous and Liazid [64], Cutrone *et al* [65] or Poschner and Pfitzner [66]. An alternative model proposed by Jay et al. [59] relies on surface density concepts to deal with transcritical injection conditions. A balance of surface density is used to represent the mass transfer process which takes place between the dense (low-temperature) oxygen stream and the lighter (higher-temperature) oxygen surrounding flow. This is combined with a local model of the mass transfer rate and with a combustion model based on a balance equation for the flame surface density. It is shown that the combined flame and interface model (CFIM) developed on this basis provides flame structures and distributions of mean reaction rate which suitably retrieve experimental data.

Reynolds average models are however limited to the analysis of essentially steady flows and cannot be used to examine many questions of interest like those related to combustion / acoustic coupling and instabilities. Closure schemes also have a moderate degree of generality. This is why much of the current effort in the numerical modeling of practical systems is focused on Large Eddy Simulations (LES). It is however important to note that practical thrust chamber configurations of interest in rocket propulsion involve a large number of injectors and cannot be treated in the LES framework. Such configurations are still calculated with RANS flow solvers. A number of problems are however accessible to LES as will be seen in what follows. The review is focused on LES of transcritical injection and combustion. This has required the development of solvers which can be used in the transcritical regime. In addition to the description of the fluid properties (Sec. 3), numerical simulation of transcritical jet flames leads to modeling issues. Methods that are currently employed to represent the chemical conversion in the LES framework are reviewed below and selected results are described.

LES numerical issues

In the LES framework the balance equations of fluid mechanics are spatially filtered. The large scales are resolved while effects of small scales are treated with subgrid-scale models. The application of LES to fluid dynamics problems is now widespread. In addition to the fluid properties computation for high pressure conditions, LES of transcritical flows requires special care to account for the large density gradients existing in the flow. It is also necessary to reconsider the subgrid-scale model and the description of the spatially filtered reaction rates.

First, the solver has to be fully consistent with the real-gas thermodynamics. This in particular leads to generalized expressions for the boundary conditions [67, 68]. Depending on the solver, numerical methods also have to be expressed in terms of generalized thermodynamics [68–71]. Subgrid scale models which are currently used in large eddy simulations of transcritical flows are mostly inherited from perfect gas formulations. Their adequacy needs to be checked, an issue which has been of concern and is currently being investigated. Some preliminary results suggest that subgrid -models derived for perfect gases provide suitable results under supercritical conditions (at least when the flow involves a single species) as indicated by Selle and Schmitt [72]. Moreover, several non-reacting and reacting LES [73, 74] have already been performed with a reasonable degree of agreement with experiments. Nevertheless, it should be pointed out that the nonlinear nature of the state equation, thermodynamics and transport properties at supercritical pressures introduces unclosed terms which arise from the filtering of the conservation equation. These terms which are generally neglected in the simulations might have to be included in future calculations. Selle *et al.* [50] show that terms arising from the filtering of pressure and, to a lesser extent, of transport terms, are no longer negligible (many of these terms are classically neglected in perfect gas large eddy simulations). A sub-grid scale model is proposed *a priori* and and *a posteriori* study has been carried out more recently by Taskinoglu and Bellan [75].

LES of non-reactive flows

LES has first been used to simulate a few non-reactive flows, which have been the subject of experimental studies (Sec. 2). Three-dimensional transcritical round jets have been simulated by Zong [76], Zong et al. [77], Schmitt et al. [78] and [72]. The large density-contrast has a stabilizing effect on the initial mixing layer as evidenced for example by Zong *et al.* [73]. Overall agreement is obtained with the available experimental data.In the case of coxial jets, effects of momentum flux ratio J are well retrieved in the simulations. It is found for example that high values of this parameter lead to the formation of an inner recirculation region and that the central dense jet is terminated in the near vicinity of the injection exhaust section [79]. The impact of an acoustic perturbation on coaxial jets is also considered by [80] and more recently by [79]. A strong reduction of the intact core length is obtained, even with low amplitude transverse acoustic waves. In particular, Schmitt *et al* [79] notice that the high density inner jet features a reduced response to the acoustic perturbation when compared with the outer gaseous jet, a result which suggests a modification of the coupling mechanism between the imposed acoustic modulation and the flow. This uncoupling between the dense core and incident acoustic waves is probably caused by real gas effects which lead to large values of the specific impedance of the dense stream inducing a large contrast in the specific impedance of the flow. It is also worth noting that more complex flows like those characterizing pressure swirl injection have been simulated by [81].

LES of reactive flows

Developments in transcritical combustion have been made more recently. One difficult issue in combustion LES is to devise suitable descriptions of the flame on the relatively coarse grid used in this type of calculation. This central point is the subject of some recent effort. From experimental observations, it is clear that combustion takes place in a purely non-premixed regime (as can be deduced from experimental images of the instantaneous flame, see Sec. 2). This regime prevails except for the doubly transcritical case where a premixed flame is also formed. A number of methods are now available for the large eddy simulation of gaseous flames [82]. One of these methods based on a flame thickening technique has been widely used to deal with gas turbine combustion ([83] for example). This model leads to a reasonable agreement for coaxial injection [84]. Other descriptions of LES combustion models reviewed in [63] describe methods developed at Sandia National Laboratories, Georgia Institute of Technology and Pennsylvania State University.

Simulations of jet flames have been carried out in the transcritical range most notably by [69], [85], [86] and [74]. These calculations correspond to a flame formed by the coaxial injection of transcritical oxygen surrounded by an annular flow of supecritical hydrogen but the computational domain only covers the near vicinity of the coaxial injector in the case of transcritical oxygen / supercritical hydrogen combustion. The calculated flame is stabilized in the wake region behind the LOx post and spreads near the LOx jet boundary. More recent efforts [84,87,88] deal with similar coaxial cases but the computational domain is extends over a much larger domain with the aim of calculating the complete flame from the injection element to the tip and obtaining instantaneous flame structures and an estimate of the axial spread of the mean flame. Calculations in [84] are based on the flame thickening method. More recent work [78] concerned with the case of transcritical oxygen supercritical methane shear coaxial injection introduces a combustion model inspired by developments in the RANS framework and based on an infinitely-fast reaction assumption is explored to describe the chemical conversion process. It is found that the flame structure determined numerically resembles that investigated experimentally [24]. Results are quite encouraging as can be seen in Fig. 11.

This shows examples of LES results of coaxial flames operating in the transcritical range. The same model applied to transcritical oxyxgen surrounded by a supercritical stream of hydrogen provide flame structures which are qualitatively close to those observed experimentally (Figure 12).

There are also simulations of some multiple jets configurations but these are carried out with an axisymmetric formulation (Masquelet *et al.* [89], see also [90] and [91]). The objective was to compute the heat flux at the chamber wall. Results show limited success but show that the heat flux is naturally unsteady and that this can be linked to motion of the jet flame.

6 Conclusion

This article reviews some advances in transcritical injection and combustion. On the experimental level, the data accumulated during the recent period provide information on flames formed

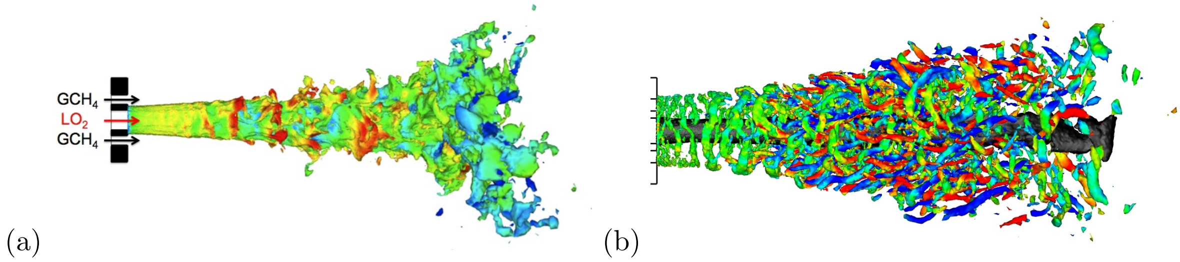


Figure 11: *Results of LES results obtained with a transcritical version of the AVBP flow solver (a) Iso-surface of temperature (1750 K) of a transcritical oxygen / supercritical methane coaxial flame colored by axial velocity (dark blue: -10 m s^{-1} ; red: 90 m s^{-1}). (b) Turbulent fluctuations in the methane stream reprsented by Q-criterion isocontours colored by the axial velocity. (case G2 of [24]). Figures from [87].*

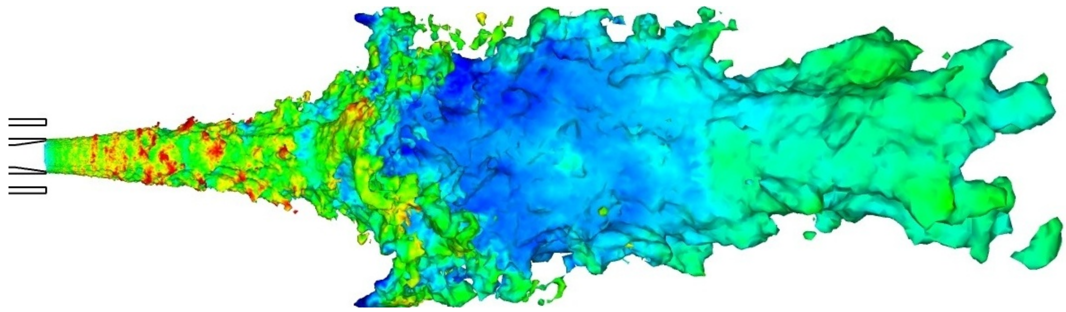


Figure 12: *LES results obtained at the EM2C lab using the AVBP solver from Cerfacs. Iso-surface of temperature (2000 K) of a transcritical oxygen / supercritical hydrogen coaxial flame (case A60 of [21]) colored by axial velocity (dark blue: -50 m s^{-1} ; red: 150 m s^{-1}).*

by LOx and supercritical hydrogen or methane gases and by doubly-transcritical injection of LOx and liquid methane. Experimental results indicate that the flame remains attached to the lip of the oxygen injector over the complete range of pressures, inlet velocity and hydrogen temperatures investigated. The stabilization mechanism has been elucidated by combining experimental PLIF and emission imaging information and detailed calculations of this limited but important region of the flow. Data obtained by applying PLIF has also provided instantaneous slices across the flame at a pressure as high as 6.3 MPa. Progress has also been made on the modeling level. Unified descriptions of thermodynamics and transport properties of transcritical fluids have been developed. These elements have been used to examine mass transfer and combustion issues in simplified geometries leading to a one dimensional treatment (spherical pockets of liquid oxygen surrounded by hydrogen, strained flames formed by a counterflow of transcritical and supercritical reactants...). Important advances have been made in the large eddy simulation of transcritical combustion. This has been made possible by taking into account the special behavior of fluids injected at high pressure (above critical) but below critical temperature. A specific treatment is required in this range to account for the large density contrast associated with the passage from dense low temperature fluid to the light high temperature environment. Combustion models have been derived to represent the chemical conversion process and obtain suitable descriptions of nonpremixed flames. Calculations of transcritical liquid oxygen/ supercritical methane configurations yield flame structure which are close to those investigated experimentally. The flame length is approximately retrieved. The calculation also provides detailed distributions of the main variables controlling this problem, some of which are not accessible in the experiment. Other calculations of transcritical oxygen/ supercritical hydrogen provide spatial distributions of heat release which qualitatively agree with those deduced experimentally from OH* emission maps. Much of the future work will focus on further developments of simulation tools for transcritical combustion. The objective will be to include improved descriptions of complex kinetics and multi-species transport. One of the challenges in this field will be to deal with the doubly transcritical configurations where the two propellants are injected at a temperature below critical. Efforts will also be directed at the simulation of multiple flame configurations corresponding to the highly packed arrangements found in liquid rocket engines. With the continuous increase of computational resources it appears that such more complex problems will become tractable. Another area where transcritical simulations could be informative is that of combustion dynamics. It is already possible to deal with cold injection streams and turbulent flames modulated by external acoustic perturbations. Future simulations will be address problems of acoustic / combustion interactions in simple and more complex configurations.

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