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Transcritical Vaporization of Liquid Fuels and Propellants

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An overview is provided of some challenges associated with predicting spray combustion processes in propulsion systems operating at pressures and temperatures that are above the critical values of the pure fuel or propellant injected in the liquid phase (e.g., diesel engines and cryogenic liquid rocket engines). The issues determining high-pressure phase equilibria are outlined first. Then, the case of the gasification of a liquid fuel (propellant) droplet in a quiescent environment is considered. The reviewed literature shows that the more advanced models now provide consistent predictions regarding, for instance, the variation of droplet lifetime with pressure. The droplet gasification process at these conditions is essentially unsteady. Recent studies using molecular dynamics simulations to investigate transcritical droplet vaporization are briefly discussed. Next, the effects of convection, secondary atomization, and the proximity of neighbors on supercritical droplet combustion are considered. Published results indicate that the latter tends to preclude droplets in clouds from reaching the critical mixing state. Forced convective effects on the behavior of a droplet at supercritical conditions are considerable because they couple with a significantly reduced surface tension coefficient to produce secondary atomization and a one order of magnitude reduction in the droplet lifetime. Finally, a specific example is given of how supercriticality influences the overall performance of propulsion systems.

Nomenclature

B_T = heat transfer number
C_p = specific heat
D = droplet diameter
$\mathcal{E}_{\text{mist}}$ = correction to B_T due to the mist
$\dot{m}$ = vaporization rate
$\dot{m}_{\text{BLS}}$ = boundary-layer stripping rate
Nu = Nusselt number
P = pressure
Q_ℓ = heat conducted into the droplet
R = droplet radius
R^0 = gas constant
Sh = Sherwood number
T = temperature
t = time
u = radial velocity
v = molar volume
$\dot{\mathcal{W}}$ = gasification rate
Y = mass fraction
α = thermal diffusivity
γ = specific heat ratio
ΔH = enthalpy of vaporization
ΔU_∞ = droplet/gas relative velocity
ρ = density
σ = surface tension coefficient

Subscripts

c = critical
g = gas
H_2 = hydrogen
ℓ = liquid phase
r = reduced: normalized by the critical value
S = surface
0 = initial
∞ = at infinity

Superscripts

$\widehat{\ }$ = average in the boundary layer
$\sim$ = modified to include heat transfer effect of stripping
$'$ = fluctuation

Introduction

THE prevalence of high-pressures and supercritical conditions (above the critical values of the pure liquid fuel or propellant injected) in liquid-fueled jet engines and liquid rocket engines is a prominent challenge to the modeling and the fundamental understanding of the mechanisms controlling combustion. Accordingly, the past decade has seen a reemergence of investigations aimed at providing a detailed description of the phenomena inherent to these conditions. Topics of interest include prediction of phase equilibria at high and supercritical pressures[1–8] (choice of a proper equation of state, definition of the critical interface, importance of liquid diffusion), significance of transport property singularities in the neighborhood of the critical mixing conditions, influence of convection (including secondary atomization), D^2-law behavior at supercritical conditions,[9] droplet lifetime predictions,[5–8,10,11] dense spray behavior,[12–15] combustion product condensation (LOX/H_2),[2,9,10,16,17] and flame structure at high and supercritical pressures.[9] Many of these issues are still controversial or unresolved and are reviewed in this paper.

The actual process is characterized by the supercritical combustion of relatively dense sprays in a highly convective environment. However, most research studies considered decoupled problems to isolate a limited set of issues. Consequently, the bulk of the results obtained so far was derived in the case of an isolated droplet gasifying (no reaction) in a quiescent environment, whereas other aspects such as convective effects, influence of neighboring droplets, detailed chemical kinetics, or product condensation have received scarcer and more recent attention.

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There are key challenges associated with operation at near-critical and supercritical conditions to increase efficiency and combustion rate processes. The distinction between liquids and gases disappears at high pressures above the thermodynamic critical point, which has a very strong nonlinear dependence on the composition. This introduces some crucial phenomena that were neglected decades ago, when the compositional distinction between the original liquid and its surrounding gases in the combustor were neglected. Also, the reduced surface tension can cause a new mechanism to be the rate controlling factor for energy conversion. Our discussion will focus on some work that addresses those challenges; a broad review of those challenges is not attempted here.

High-Pressure and Supercritical Droplet Combustion

High-pressure and supercritical ambient conditions have a considerable influence on the mechanisms controlling engine behavior and performance. Most of these effects are related to droplet behavior. When liquid propellant is injected in a combustion chamber where the thermodynamic conditions are supercritical, all aspects of the combustion process from atomization to chemical reaction can be expected to depart significantly from the better known subcritical patterns. In the past two decades, numerous studies have investigated how and to what extent supercritical conditions may affect these various aspects of isolated droplet combustion in a quiescent environment. A detailed review of these investigations was recently contributed by Givler and Abraham.[18]

Typical models[3,5,8] include a detailed computation of the high-pressure phase equilibria based on a cubic equation of state. A prevalent cubic equation of state used in this range of pressures and temperatures by the spray combustion community[1,3,5,8,19–21] has been the Redlich–Kwong equation of state derived in 1949 (Ref. 22):

$$P = R^0T/(v - b) - a/[T^{0.5}v(v + b)] \qquad (1)$$

This empirical cubic equation has only two parameters, a and b. This equation was then modified by Chueh and Prausnitz[23] to include the dependence of a and b on composition and temperature. Although derived for pure components, these equations are often used for mixtures by means of mixing rules. Note that, when hydrogen is involved [liquid oxygen (LOX)/H_2 system, for instance], its quantum nature must be taken into account in the definition of the mixture rules. Phase equilibrium is expressed in terms of mechanical, thermal, and chemical equilibrium. The equation of state is used in the computation of the fugacity of each component in each phase required to express the chemical equilibrium. The resulting equation system is solved iteratively to yield the equilibrium composition in each phase at the given pressure and temperature. Note that the numerical solution of the equation system defining phase equilibrium is not trivial and requires a carefully designed iteration scheme.[24] The computed equilibrium compositions are generally in good agreement (see Fig. 1) with the scarce experimental data.[25]

More recently variations of the Redlich–Kwong[22] equation, such as the Soave–Redlich–Kwong equation that allows a to be a function of temperature (see Refs. 4–6), have been employed because of their better accuracy in predicting phase equilibria for particular mixtures. There is no evidence however, that these improvements affect significantly the predicted overall droplet behavior.

Another challenging inherent issue in simulating transcritical phase processes is evaluating transport properties. Some transport properties, for example, thermal conductivity, are expected to diverge at the critical transition. To quantify this singular behavior, a given transport property is considered to be the sum of a low-density value, an excess value due to high-pressure effects, and a critical enhancement including the singular effects at the critical transition. Many authors duly note this issue, but in general actual models rarely include critical enhancement corrections because the data are still scarce and our understanding in this area limited. More details about this issue can be found in the works of Sengers and Sengers[26] and Sengers et al.[27] Indeed, this issue is still the topic of active fundamental research.[28–30] Finally, as important and fundamental as these transport property singularities are to our understanding of critical phenomena, it is likely that their macroscopic effects on droplet behavior in conditions relevant to actual processes, for example, convective droplet heating and vaporization, are negligible (cf. the following sections).

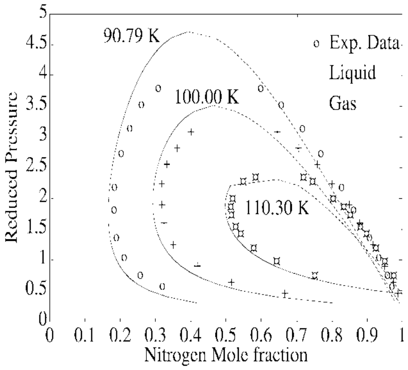


Fig. 1 Comparison of the predicted high-pressure phase equilibrium for the nitrogen/hydrogen system to the experimental data of Streett and Calado[25] (taken from Ref. 5).

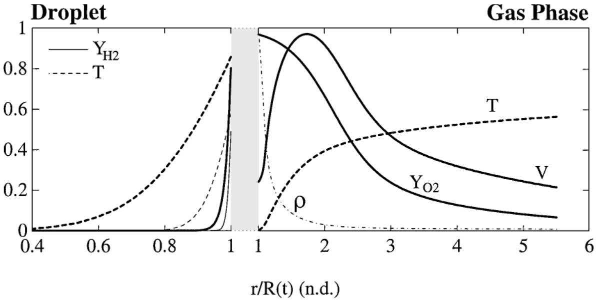


Fig. 2 LOX droplet (100 K) vaporizing in hydrogen (1500 K and 100 atm) (taken from Ref. 5).

The predictions of current models[4–6,8] are qualitatively consistent. Consider a liquid droplet just after introduction into a hot, supercritical, quiescent environment. The droplet is heated by conduction, and its diameter increases because the liquid density decreases as the temperature rises. Yang et al.[31] note that, because the density inside the droplet is nonuniform, liquid convection inside the droplet should be considered. The droplet surface temperature rises until the surface temperature reaches the computed critical mixture value. During this phase the mixture composition on either side of the liquid/gas interface is imposed by the chemical equilibrium, and mass diffusion occurs in the droplet. For example, Fig. 2 (from Ref. 5) shows the predicted behavior of a LOX droplet (100 K) vaporizing in hydrogen (1500 K, 100 atm). The temperature $[(T - T_0)/(T_{\text{ref}} - T_0),\ T_{\text{ref}} = 150\,\text{K}]$ and hydrogen mass fraction $(Y_{\text{H}_2}/Y_{\text{H}_2,\text{ref}}, /Y_{\text{H}_2,\text{ref}} = 0.02)$ profiles at $t = 0.1$ ms (thin lines) and 0.9 ms (thicker lines) within the droplet are plotted on the left side of Fig. 2. The temperature $[(T - T_S)/(T_\infty - T_S)]$, mass fraction, velocity $(u/u_{ref},\ u_{\text{ref}} = 5\,\text{cm/s})$, and density $(\rho/\rho_{\max},\ \rho_{\max} = 323\,\text{kg/m}^3)$ profiles in the gas phase are plotted on the right side.

Note that the number of degrees of freedom of the corresponding thermodynamic system, as given by the Gibbs phase rule, is two (two components minus two phases plus two). The case considered here is that of a mixture for which the pressure P is prescribed. Hence, only one degree of freedom is left. In the subcritical case, the interface temperature is the last degree of freedom. Once it is known, the phase equilibrium conditions yield the mixture's composition.

Alternatively, requiring that the mixture be critical adds one condition to the system that is then completely defined; that is, the corresponding values of temperature and composition, Y_c and T_c, are fully determined, (see Fig. 3 or Fig. 2 in Ref. 6 and Fig. 1 in

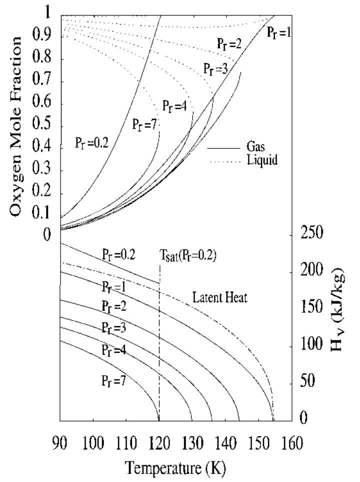


Fig. 3 Computed phase equilibrium of the oxygen/hydrogen system (taken from Ref. 5).

Ref. 8). In Fig. 3, the variation of the latent heat of oxygen (energy required to vaporize 1 kg of pure LOX at saturation conditions in its own vapor) with temperature is also plotted (mixed lines) for comparison with the variation of the enthalpy of vaporization.

In general, Y_c and T_c do not coexist at the same point in space; they only coexist when the critical mixing condition is reached at the interface. However, when this happens the concept of an interface ceases to be relevant. If a droplet lifetime is to be determined, the part of the computation domain constituting the supercritical droplet must be defined. Two definitions have been chosen in the literature and neither really corresponds to the critical mixing conditions. Yang et al. choose the isotherm at the critical mixing temperature as the supercritical droplet boundary,[31] whereas Haldenwang et al. choose the composition isopleth at the critical mass fraction.[8]

Consider a droplet of liquid component A in gaseous component B at pressure P_a. The liquid initial temperature is T_ℓ and the initial ambient temperature is $T_a > T_\ell$. For conditions well below the critical conditions, temperature varies continuously throughout the surrounding gas and liquid interior and is continuous across the liquid/gas interface. A negligible amount of the ambient gas dissolves in the liquid; composition and densities are discontinuous across the interface but piecewise continuous in the gas and in the liquid.

If $P_a > P_c$ and $T_a > T_c$, the temperature is at the critical value, T_c, at some point, but not necessarily at the interface. However, the gaseous mass fraction of A is smaller than the critical value, Y_c, whereas the liquid mass fraction of A is larger than the critical value. Hence, whereas an isotherm with the critical value immediately appears, a mass fraction isopleth with the critical value appears only when the interface discontinuities disappear, as shown in Figs. 4 and 5. In Fig. 4, t_c is the time at which the droplet surface reaches the critical mixing conditions, and $t_1 < t_c < t_3$. R_1 and R_c are the droplet radii at t_1 and t_c, respectively. R_3 denotes the location of the critical interface at $t = t_3$. Figure 5 shows a sketch of the trajectories that a fluid element in the droplet that is initially liquid can follow through a T/Y plot of the binary phase equilibrium. Here, t_1 corresponds to the vaporization behavior of a fluid element that is initially closer to the interface and thus vaporizes before the interface reaches the critical mixing conditions, and t_c corresponds to the vaporization behavior of a fluid element that is initially closer to the droplet center such that it crosses the interface just when it is at the critical mixing conditions. As the droplet heats, its surface temperature increases toward the critical mixture value, T_c, and as dictated by phase equilibrium, ambient gas dissolves in the liquid, and the magnitude of the interface density and composition discontinuities decrease. Still, the critical temperature and the critical composition do not occur at the same point in space and time. When and where the discontinuity first disappears, the temperature, composition, and density assume their critical values simultaneously. After that time, the critical isotherm and the critical mass fraction isopleth will regress as further heating and mixture occur, until they reach the droplet center (cf. Figs. 4 and 5).

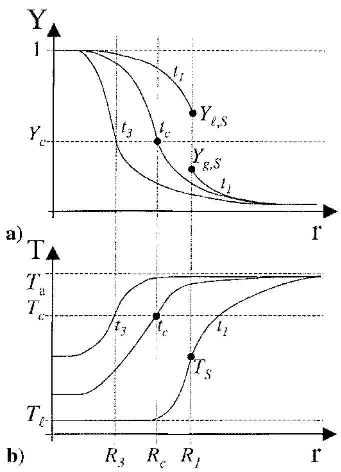
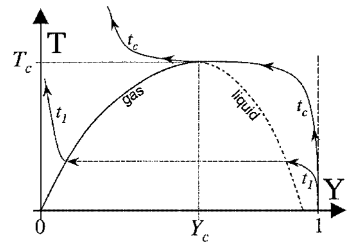


Fig. 4 Transcritical behavior of the a) mass fraction isopleths and b) isotherms.

Fig. 5 Trajectories that a fluid element in the droplet that is initially liquid can follow through a *T*/*Y* plot of the binary phase equilibrium.



The scarce experimental data show that the droplet lifetime exhibits a transcritical minimum.[8] That droplet lifetime is predicted to decrease as the subcritical pressure is increased is attributed to the liquid/gas density ratio decreasing to one.[8,32] For supercritical pressures, the supercritical droplet boundary regression rate is controlled by mass diffusion, and thus the droplet lifetime increases with pressure. Yang et al. have shown that, in vaporization only cases (no combustion), the quasi-steady state is never reached.[31] However, the work of Daou et al.[9] on supercritical combustion of a LOX droplet using a detailed reaction mechanism indicates that, after an initial transient corresponding to the ignition phase characterized by the fast propagation of a premixed flame, a diffusion flame is established, and combustion proceeds in a quasi-steady manner. Daou et al. found that during this latter stage the D^2 law is approximately valid. Note that these conclusions cannot be directly compared to the classical model for particle combustion at high pressure proposed by Spalding[33] in 1959 because Spalding's model really dealt with a different problem, that of the combustion of a gas puff. This model did not include a high-pressure phase-equilibrium model and considered infinite reaction rate. A complete discussion of the validity of the D^2 law for supercritical droplet combustion is provided in Ref. 18.

MD Simulation of Transcritical Droplet Vaporization

Clearly, some of the crucial problems that have to be faced at the critical point, such as the singularity of some transport coefficients, would benefit from a microscopic approach. As such an approach, molecular dynamics (MD) has been the subject of increasing interest over the past decade. This interest has also been driven by the availability of ever-increasing computing power.

It is not within the scope of this paper to provide a detailed description of the MD approach. Instead, our goal is to emphasize the significant progress that has recently been made toward the use of MD to elucidate some of the issues relevant to the prediction of droplet vaporization at supercritical conditions. An excellent introduction to this method is provided by Rapaport.[34]

The MD approach simulates the behavior of matter by computing the behavior of the molecules. This requires extremely large resources of computational power. The simplest models are based on spherical particles, but more complex configurations can be considered.[34] Typically, the particle interaction potential used is the Lennard–Jones 6–12 potential. MD simulations have been attempted since the early 1950s. However, only small numbers of particles could be considered at that time (less than 100).

Two types of MD studies are relevant to the topic of droplet vaporization at supercritical conditions: MD simulation of supercritical fluids[35,36] and MD simulation of droplet behavior.[37–39] It is only very recently that MD has been successfully applied to the problem of droplet behavior at supercritical conditions.[40]

There is a growing interest in using MD simulations to investigate supercritical fluids both from the chemistry (e.g., physical chemistry of supercritical fluids, structure and dynamics of clusters[41]) and chemical engineering (e.g., hazardous waste conversion using oxidation in supercritical water[42]) points of view. Whereas most of the literature on this topic focuses on simulating the behavior of supercritical fluids, such simulations can also be a powerful tool in the study of singular transport behavior near the critical point.[35] Luo et al.[35] have successfully used two-dimensional MD simulations to predict the unusual behavior of highly compressible fluids in the near-critical region, where the hydrodynamic theory is still valid. Their analysis of the temperature–temperature and density–density time-correlation functions showed that, in this region, the temperature relaxation is acoustically driven and the density behavior is mostly diffusive. In their investigation, Luo et al. elected to limit themselves to a two-dimensional fluid system to be able to consider larger wavelengths than a three-dimensional system would allow for a given number of particles. They note that, closer to the critical point, the correlation length becomes comparable to the system size and that the density fluctuations are so large that the computational requirements become unrealistic.

In 1977, Rusanov and Brodskaya,[37] used a method developed by Alder and Wainwright[43] to investigate the dependence of the surface tension coefficient on the surface tension radius. The surface tension coefficient increases when the droplet size decreases. Furthermore, the omission of nonadditive interactions that are important in real liquids may lead to significant errors in the prediction of macroscopic quantities such as the phase transition temperature. Rusanov and Brodskaya's[37] simulations were limited by the computational power available in the mid-1970s to 500 molecules. In the mid-1980s, Thompson et al. were able to perform MD simulations with up to 2004 molecules to study the same problem.[38] Their results, although more detailed, are qualitatively similar to Rusanov and Brodskaya's.[37]

More recently, Long et al.[39] and Kaltz et al.[40] have used MD to simulate the vaporization of submicrometer droplets at subcritical and supercritical conditions, respectively. Their configuration is actually a droplet vaporizing in a field of vaporizing droplets inasmuchas periodic boundary conditions are used. In the subcritical regime, their results are in good agreement with the Knudsen theory of aerosols for example, vaporization rate. These simulations have been extended to consider the vaporization of three-dimensional submicrometer LOX drops at pressures from 2 to 20 MPa and temperatures from 200 to 300 K. These simulations have confirmed that the validity of assumptions typically used in the subcritical regime, for example, quasi-steady approximation, holds at much higher pressures (Fig. 6).

In Ref. 40 it is also noted that, because the cases considered typically have high Knudsen numbers, the results of MD simulations are not suitable for comparison with the classical results of the D^2 law. Furthermore, other important phenomena such as convection have yet to be included in MD simulations. Finally, and more important, the simulation of the behavior of three-dimensional fluids in the near-critical region where the hydrodynamic theory is not valid presents theoretical and computational challenges that have yet to be tackled.

Convective Effects and Secondary Atomization in Supercritical Spray Combustion

Practical environments such as those found in jet and rocket engines are characterized by strong convection. Convection affects droplet behavior in two ways. First, heat transfer and mass transfer are enhanced by convection. Furthermore, in supercritical environments, the surface tension coefficient of a droplet decreases to zero as the interface temperature approaches the critical conditions. Hence droplet deformation and secondary atomization can be initiated by smaller values of the droplet/gas relative velocity.

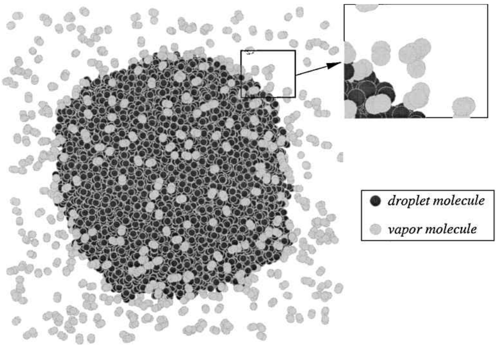


Fig. 6 Molecular dynamics simulation of a saturated LOX droplet at 100 K; droplet contains roughly 9300 molecules (reproduced from Ref. 40 with permission).

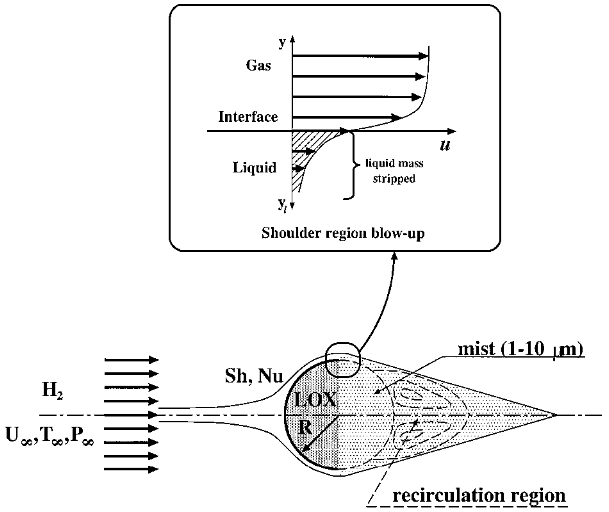


Fig. 7 Droplet undergoing boundary-layer stripping; liquid stripped from the parent drop surface is atomized in a mist of small (1–10 μm) droplets (taken from Ref. 10).

Convective effects on the behavior of a droplet in a supercritical environment have often been limited to heat and mass transfer effect or droplet deformation without breakup.[44] Litchford and Jeng[2] included the effect of convection on heat and mass transfer rates in their model for a LOX droplet vaporization at supercritical conditions using the film model for droplet vaporization. However, the validity of their results is somewhat undermined by their neglecting the difference between the liquid propellant and the surrounding gas specific heats that reaches one order of magnitude in the LOX/H_2 case.[5] Litchford and Jeng did note that stripping was likely to occur in environments typical of cryogenic rocket engines, and they performed an order of magnitude analysis to evaluate the stripping rate; they concluded that stripping would be important only after the droplet interface reached the critical mixing conditions.[2]

Delplanque and Sirignano[5] followed a similar path. Their model for droplet vaporization in a supercritical convective environment (without secondary atomization), based on Abramzom and Sirignano's film model,[45] showed that a LOX droplet injected in a rocket engine is likely to reach the critical state before it disappears, much sooner than in a quiescent atmosphere.

However, Delplanque and Sirignano showed that, because of the behavior of the surface tension coefficient at near-critical conditions, a LOX droplet in a rocket engine is likely to undergo secondary atomization in the stripping regime [mass removal from its surface by aerodynamic shearing (Fig. 7)] before the droplet

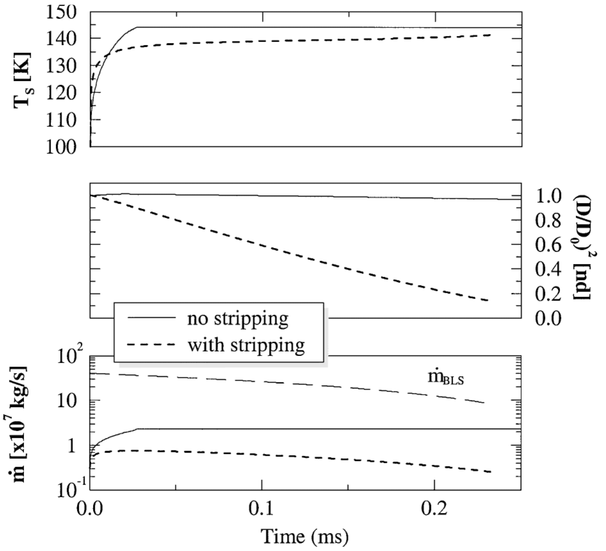


Fig. 8 Influence of boundary-layer stripping on predicted droplet behavior at supercritical conditions (taken from Ref. 10).

interface reaches the critical mixing conditions and, thus, for most of its lifetime.[5]

Prior analyses[2,46,47] of the magnitude of the stripping rate had indicated that the stripping rate might be much larger than the convective vaporization rate with an obvious consequence on the droplet lifetime. Delplanque and Sirignano[10] expanded on the work of Ranger and Nicholls[46,47] to develop an integral analysis of the coupled gas–liquid boundary layers at the droplet interface and obtained an expression for the mass removal rate including blowing effects:

$$\dot m_{\rm BLS} = \pi D\left(\int_0^\infty \rho_\ell u_\ell \, \mathrm{d}y\right) = 3\pi R\widehat{\rho_\ell}\Delta U_\infty A\alpha_\ell\sqrt{\frac{\pi R}{2}} \qquad (2)$$

where A (the nondimensional interfacial velocity) and α_ℓ (a liquid boundary-layer velocity profile parameter) are functions of the droplet size, its velocity relative to the gas, and gas and liquid properties.[10] Their modified film model uses a corrected heat transfer number to include the effect of stripping on the heat transfer into the droplet,

$$\tilde B_T \equiv \frac{\widehat{Cp}_{g,\mathrm{O}_2}(T_\infty - T_S) + \mathcal{E}_{\rm mist}/\dot m}{\overline{\Delta H}_v(T_S) + Q_\ell/\dot m} \qquad (3)$$

where $\mathcal{E}_{\rm mist}$ is a correction to the driving potential due to the presence of the mist.

Results obtained with this model confirmed that the stripping rate is much larger than the gasification rate. Figure 8 (from Ref. 10) shows that the predicted lifetime of a 100-μm LOX droplet injected at 100 K in gaseous hydrogen at 1000 K, 100 atm, with a relative velocity of 20 m/s is reduced by at least one order of magnitude when stripping occurs. An important consequence is that, in most cases, the droplet disappears before the interface reaches the critical mixing conditions.[5]

Influence of Neighbors on Droplet Combustion at High and Supercritical Pressure in Dense Sprays

Models attempting to capture the neighboring effects on the vaporization and combustion behavior of droplets are not novel. A detailed review may be found in Ref. 48. The approaches used may be classified based on the spatial distribution of droplets considered, from streams to clouds.

The so-called group combustion model provides a phenomenological description of the combustion modes of dense droplet clouds using a continuum approach, where the droplets are idealized as point sources of mass and point sinks of energy (see, for instance, Refs. 49 and 50). The droplet array method allows a more detailed description of the interdroplet region because idealized droplet arrangements are considered (cf. Refs. 48 and 51). However, the total number of droplets that can be considered is limited by the computational time and memory required.[48]

These models typically provide an evaluation of the corrections that must be made to the magnitude of the energy sink and mass source terms to account for proximity effects. Ryan et al.[52] have shown in the subcritical case that the corrections yielded by the group combustion approach and by the droplet array approach do not differ significantly.

Because flames in jet and rocket engines are usually anchored in a region of high spray density, the influence of neighboring droplets on high-pressure and supercritical droplet combustion behavior needs to be evaluated.

Jiang and Chiang[13–15] have recently contributed an approach based on the model developed by Bellan and Cuffel.[53] Jiang and Chiang consider a cloud of droplets surrounded by a hotter homogeneous gas region. Their droplet model is similar to those discussed earlier.[13] Convective effects are neglected (except for Stefan flow). Multiple droplet interactions are modeled using the sphere of influence concept. The simulations of Jiang and Chiang[15] indicate that a droplet is less likely to reach the critical mixing conditions when it is in a cloud than when it is isolated. Furthermore, they found that such droplet clouds do not follow the D^2 law at any pressure.

An analysis of the effect of species and temperature nonuniformities induced by neighboring droplets on the transcritical combustion behavior of LOX droplets in a convective environment was contributed by Delplanque and Sirignano.[12] This study used the droplet array approach (parallel streams), where the droplets are followed in a Lagrangian manner. The model used to predict the droplet behavior is that described in the preceding section and allowed secondary atomization in the stripping mode. This analysis showed that despite the hindering effects of droplet drag and accelerating gas flow due to the contribution of the vaporizing droplets to the overall mass flux, the gasification rate in this configuration is still controlled by secondary atomization with a characteristic time one order of magnitude smaller than that associated with primary vaporization. However, the presence of a reaction zone created by the combustion of preceding droplets enables the droplet surface to reach the critical mixing conditions.[12]

Supercritical Droplet Combustion Behavior Influence on Propulsion Systems Overall Performance Example: Liquid Rocket Combustion Instability

The preceding section indicates that supercritical ambient conditions and their influence on physical properties such as surface tension significantly affects droplet lifetime. The goal of this section is to show how this result may affect the predicted overall performance of propulsion systems using the example of one of the most challenging research problems in rocket engine technology: combustion instability.

The open-loop response of LOX droplets to prescribed oscillatory ambient conditions consistent with liquid-rocket engines was investigated by Delplanque and Sirignano[54] using the supercritical droplet combustion models described in the preceding sections both for isolated droplets and droplet arrays. This study evaluated the combustion stability assuming concentrated combustion at the injector end, short nozzle, and isentropic flow downstream of the combustion zone.[55] A response factor $\mathcal{G}$ was computed[54]:

$$\mathcal{G} = \frac{\iint \dot{\mathcal{W}}' p' \, \mathrm{d}t \, \mathrm{d}z}{\iint p'^2 \, \mathrm{d}t \, \mathrm{d}z} \qquad (4)$$

(where the primes denote fluctuations with respect to the nonoscillatory values) to quantify the Rayleigh criterion that states that an initially small pressure perturbation will grow if the considered process adds energy in phase (or with a small enough phase lag) with pressure. Delplanque and Sirignano[54] (see also Ref. 56) note that an underlying assumption to this definition of $\mathcal{G}$ is that the gasification rate provides a good approximation of the energy release rate. $\mathcal{G} > 0$

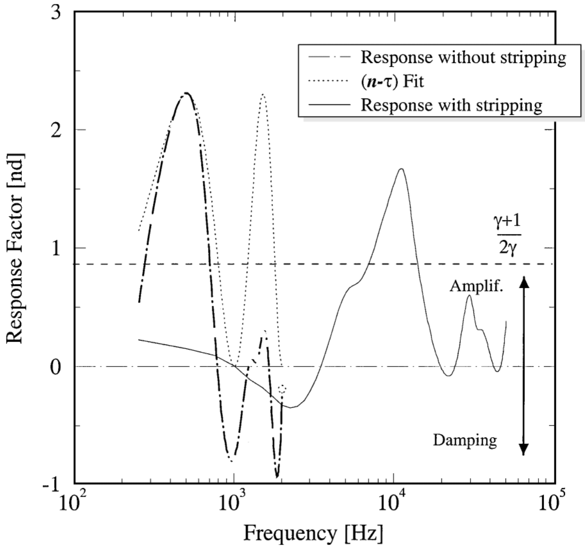


Fig. 9 Response factor for an isolated LOX droplet with and without stripping: T_∞ = 1000 K, P_∞ = 100 atm, and ΔU = 20 m/s (taken from Ref. 54).

($\mathcal{G} < 0$) indicates that the gasification process has a destabilizing (stabilizing) effect. When $\mathcal{G} > 0$, the destabilizing effect must also overcome the potential acoustic losses from the exhaust nozzle for the gasification process to drive the instability. The corresponding threshold value for $\mathcal{G}$ is $(\gamma + 1)/(2\gamma)$. It can be estimated assuming concentrated combustion at the injector end, short nozzle, and isentropic flow downstream of the combustion zone.[55]

This model showed that the frequency at which the peak response factor occurs is mainly correlated to the droplet lifetime. Therefore, because secondary atomization in the stripping mode results in a one order of magnitude reduction in droplet lifetime, it causes a corresponding shift in the peak frequency (Fig. 9). Consequently, when stripping occurs, the peak frequency is significantly larger than the acoustic frequencies of the common modes for standard cryogenic rocket engine chambers. Delplanque and Sirignano[54] argued that, because in these engines droplets are likely to undergo secondary atomization in the stripping regime for most of their lifetime, this phenomenon could explain the observed better stability of such engines compared to storable propellant engines.[57] Furthermore, the computations also demonstrated that, under the modeling assumptions, there exists a finite frequency range over which the response factor of the droplet gasification process exceeds the threshold value with or without stripping. Hence, this process can drive combustion instabilities for the longitudinal mode with or without stripping.

Qualitative estimates of the influence of neighboring droplets on the droplet response to an oscillatory field obtained using the droplet stream model described earlier[12,32] showed that the isolated droplet configuration underestimates the driving potential of the gasification process.

Conclusions

Over the past 20 years investigations, both theoretical and experimental, of spray combustion at supercritical conditions have largely focused on the case of one or a few droplets in a quiescent gas. The more advanced models now provide consistent predictions. The droplet gasification process at these conditions is essentially unsteady.[4,31] The interface regression does not follow the D^2 law at these conditions, but the D^2 law does provide an order of magnitude approximation.[8] In cases with combustion, the D^2-law approximation was found to be acceptable for most of the droplet lifetime.[9]

Because conditions of practical interest generally involve numerous droplets in a convective environment, more recent studies have been focusing on these aspects. The results obtained so far indicate that the presence of neighbors tends to preclude droplets in clouds from reaching the critical mixing state.[15] Furthermore, the D^2 law was found to be invalid at any pressures for droplets in clouds.[15] The effect of forced convection on the behavior of a droplet at supercritical conditions is considerable because it is coupled with the effects of a significantly reduced surface tension coefficient. When this phenomenon is taken into account, the droplet lifetime is found to be controlled by secondary atomization in the stripping regime, yielding droplet lifetimes one order of magnitude smaller than those predicted in the absence of stripping.[10,12] Furthermore, the occurrence of stripping minimizes the importance of transcritical phenomena such as the expected singularity of some transport properties so that good predictions can be obtained even with a rather crude modeling of these singularities.

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