

Pressure-coupled vaporization response of *n*-pentane fuel droplet at subcritical and supercritical conditions

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Abstract

The dynamic response of a liquid fuel droplet to externally impressed pressure oscillations is studied comprehensively over a wide range of mean pressures. Both subcritical and supercritical conditions are considered. The formulation treats a complete set of conservation equations and incorporates real fluid thermodynamics and transport theories. As a specific example, the situation with isolated *n*-pentane droplets in nitrogen is studied at various forcing frequencies. Results are correlated with the liquid thermal inertial time, instantaneous droplet radius, and oscillation frequency. The magnitude of the vaporization response increases with increasing pressure, mainly due to the decreased enthalpy of vaporization at high pressures. The increased sensitivity of droplet thermophysical properties to ambient flow variations at high pressures also plays a role. The phase angle of the vaporization response function, however, appears to be independent of the ambient pressure. An abrupt increase in the response function takes place when the droplet surface reaches its critical mixing state. A major factor contributing to this phenomenon is the abnormal variations of fluid thermophysical properties near the critical mixing point.

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1. Introduction

Combustion instability has haunted the development of high-performance combustors since the 1940s. The problem severely impairs engine operation and often leads to catastrophic consequences [1,2]. For most liquid-fueled systems, pro-

pellants are delivered into a combustion chamber as a spray of droplets. Since droplet vaporization represents a rate-controlling process in the system, the dynamic behavior of spray combustion is essentially a statistical consequence of the vaporization characteristics of each individual droplet. An understanding of droplet response to ambient flow oscillations is thus a prerequisite in treating combustion instability.

Systematic investigation of the dynamic responses of droplet vaporization and combustion to ambient flow fluctuations commenced in the sixties. Strahle [3] examined droplet-burning responses in a forced convective field in which a small-amplitude sound wave is introduced into the free stream. Since the exact solution for his formulation could only be found near the forward stagnation point, emphasis was focused on the

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local (stagnation point) vaporization responses. He examined the boundary layer surrounding the droplet and showed that the amplitude of the vaporization response increases with increasing frequency. His model erroneously predicted that the vaporization response to pressure oscillation is unbounded, approaching infinity as the square root of frequency goes to infinity. Heidmann and Wieber [4] studied the vaporization processes of *n*-heptane droplets to traveling transverse oscillations in combustors over a fairly wide range of flow conditions. The data were correlated with a dimensionless parameter – the frequency normalized by one half of the droplet lifetime. In their study, the peak response was found to occur when the droplet life time is approximately equal to the oscillation period. Negative gains may happen when the vaporization time is greater than about three times the oscillation period. Allison and Faeth [5] studied the response function of a burning liquid monopropellant (hydrazine) strand to imposed pressure oscillations. It was found that the combustion response tends to peak in two frequency ranges: one corresponding to interaction with liquid phase transient effects, which could be verified both theoretically and experimentally; and the other corresponding to gas phase transient effects, which could only be examined theoretically. Tong and Sirignano [6] implemented transient heating and mass diffusion models for the liquid phase and proposed that the unsteady droplet vaporization is a potential mechanism for driving combustion instabilities. Recently, Masoudi and Sirignano [7] studied the droplet vaporization response in a vertical flow environment.

Although the preceding studies have provided significant information about the underlying mechanisms involved in droplet vaporization response, the majority of them were conducted at low pressures. A number of fundamental issues remain unresolved for high-pressure conditions. In the present work, a comprehensive study is conducted to investigate droplet vaporization in a forced-oscillatory environment over a broad range of ambient pressures and forcing frequencies. Both subcritical and supercritical conditions are considered. The theoretical formulation is based on a complete set of conservation equations of mass, momentum, energy, and species concentrations, incorporating a self-consistent method for evaluating transport and thermodynamic properties. Emphasis is placed on the underlying mechanisms that dictate the dynamic response of droplet vaporization. Results are correlated in terms of droplet diameter, lifetime, and thermophysical properties, as well as oscillation frequency.

2. Theoretical formulation

The problem of concern is an *n*-pentane droplet evaporating in a quiescent nitrogen

environment with a periodic pressure oscillation, as shown schematically in Fig. 1. Forced convection and buoyancy effect are neglected. The problem is thus governed by a set of conservation equations in a spherically symmetric coordinate system. Details about these equations and relevant interfacial boundary conditions can be found in Refs. [8–12]. In addition, a self-consistent and efficient method for evaluating fluid thermophysical properties is described in Ref. [13].

The theoretical formulation is solved using an implicit finite-volume numerical scheme detailed in Refs. [14,15]. The overall treatment has been numerically verified and experimentally validated against several test problems involving isolated *n*-heptane droplet vaporization in quiescent nitrogen environments [14], liquid oxygen (LOX) droplet vaporization in quiescent hydrogen and water environments under both sub- and supercritical conditions [11], LOX droplet vaporization in supercritical hydrogen streams [12], supercritical nitrogen jet dynamics [16,17], supercritical combustion of LOX and methane [18], and high-pressure counterflow diffusion flames of LOX and hydrogen [19].

3. Results and discussion

The present study focuses on the vaporization response of an isolated *n*-pentane droplet in nitrogen at elevated pressures. The critical temperature and pressure of *n*-pentane are 470 K and 33.7 atm, respectively. The initial droplet temperature is 300 K, and the ambient nitrogen temperature is 1500 K. The mean pressure is either in the subcritical (10 and 20 atm) or the supercritical (50 and 80 atm) regime of the fuel. Early in the droplet lifetime, a large temperature gradient exists across the liquid/gas interface, rendering a strong heat flux which is transferred into the droplet interior. Part of the energy is thus used to vaporize the liquid droplet, while the remainder goes to heat-up the droplet interior. As a consequence, the droplet surface temperature increases, and either of two different scenarios, subcritical and supercritical, may occur [13]. If the ambient pressure is much less than the critical value of the fuel,

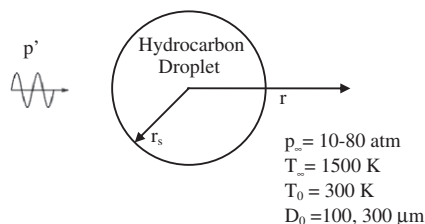


Fig. 1. Schematic of an isolated droplet vaporizing in a forced-oscillatory environment.

the surface temperature increases and eventually approaches the pseudo wet-bulb state. The droplet surface provides a well-defined boundary to separate the liquid from the ambient gas. The droplet vaporization rate can be easily quantified by evaluating the mass flux through the surface. On the other hand, if the ambient temperature and pressure are both in the supercritical regime of the fuel, with the increase in the droplet surface temperature, the characteristic times of the transport processes in both the liquid and gas phases approach the same order of magnitude. At some point during the droplet lifetime, the distinction between these two phases disappears, rendering a continuous fluid medium in the entire domain. Under this condition, the transport processes inside the droplet become as important as those outside. The vaporization response is expected to exhibit phenomena different from the low pressure cases. The droplet vaporization rate can be obtained by tracking the time variation of the droplet residue mass confined by the critical mixing temperature. It is noteworthy that the critical mixing properties vary with the pressure oscillation. To avoid unnecessary confusion, the interface defining supercritical vaporization is selected based on the critical mixing value at the mean pressure.

Figure 2 shows the temporal evolution of the droplet surface temperature at various mean pressures. The rapid heat-up immediately after $t = 0$ results from the steep temperature gradient near the droplet surface. At pressures below 20 atm, the droplet surface temperature levels off at the pseudo wet-bulb state after a short transient period. As the pressure increases to 50 atm, the surface temperature increases continuously throughout the entire droplet lifetime. Once the pressure increases to 80 atm, the droplet surface temperature can achieve its critical mixing state at 8.3 ms. Afterwards, the entire flowfield becomes a continuous supercritical fluid mixture.

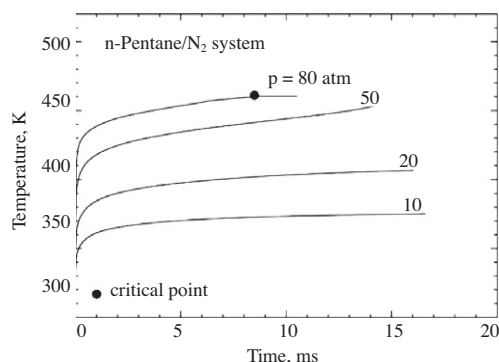


Fig. 2. Temporal evolution of droplet surface temperature at various pressures; $D_0 = 100 \mu\text{m}$, $T_\infty = 1500 \text{ K}$, $T_0 = 300 \text{ K}$.

Figure 3 shows the droplet diameter squared versus time at various mean pressures. The droplet vaporization rate increases persistently with increasing pressure, mainly due to the reduced enthalpy of vaporization at elevated pressures. At low pressures, once the droplet surface reaches its pseudo wet-bulb state, the classical d^2 -law can be used to describe the vaporization process. The situation, however, becomes quite different at high pressures. The continuous variations of the droplet interior and surface properties prohibit the use of the d^2 -law in predicting the droplet vaporization rate.

Figure 4 shows the time histories of the droplet vaporization rate and pressure oscillations for a mean pressure of 50 atm. The amplitude of pressure fluctuation is 5% of the mean value. The vaporization rate does not respond instantaneously to the pressure variation; rather, there is a time lag between the two processes. The amplitude of the induced vaporization fluctuation varies throughout the droplet lifetime. To clarify the physical mechanisms involved in the transient response of droplet vaporization to ambient pressure oscillation, it is useful to define the various characteristic time scales: droplet residue time τ_1 , liquid thermal inertial time τ_2 , liquid thermal diffusion time τ_3 , and gas phase thermal diffusion time τ_4 , as listed in Table 1. The variable τ_v denotes the droplet vaporization (life) time, R the instantaneous droplet radius, ρ the fluid density, C_p the constant-pressure heat capacity, λ the thermal conductivity; the subscript s denotes droplet surface, and l the liquid phase.

Figure 5 shows the temporal evolution of these time scales at 10 atm. The droplet residue time τ_1 decreases persistently, while the other parameters first increase in the early stage and then drop to zero at the end of the droplet lifetime. During the initial heat-up period, the predominant factor is the increase of the surface temperature caused by the energy transfer from the ambient gas,

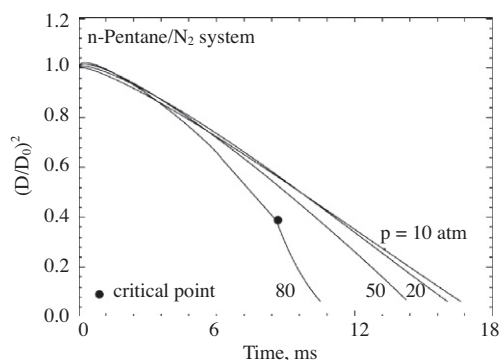


Fig. 3. Time histories of droplet diameter squared at various pressures; $D_0 = 100 \mu\text{m}$, $T_\infty = 1500 \text{ K}$, $T_0 = 300 \text{ K}$.

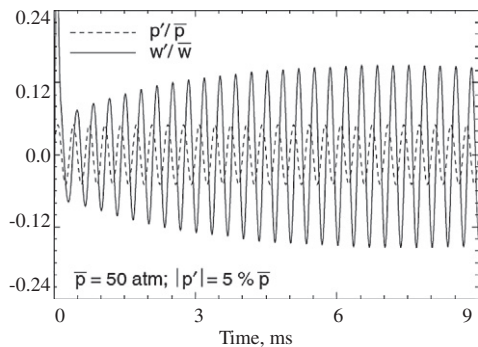


Fig. 4. Temporal variations of pressure and droplet vaporization rate fluctuations ($p = 50$ atm).

Table 1
Characteristic time scales involved in droplet vaporization.

τ_1	Droplet residue time	$\frac{\tau_v - \ell}{\rho_l C_{p,l} R^2}$
τ_2	Liquid thermal inertial	$\frac{\rho_l C_{p,l} R^2}{k_l}$
τ_3	Liquid thermal diffusion	$\frac{\rho_l C_{p,l} R^2}{k_l}$
τ_4	Gas phase diffusion	$\frac{\rho_g C_{p,g} R^2}{k_g}$

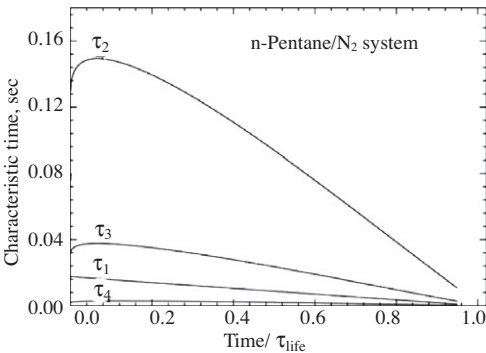


Fig. 5. Temporal evolution of characteristic times involved in droplet vaporization ($p = 10$ atm).

which consequently modifies the thermophysical properties (i.e., density, specific heat, and thermal conductivity) on the droplet surface, leading to increased characteristic times. After the surface has reached the thermodynamic wet-bulb state, the characteristic times decrease with decreasing droplet diameter.

To quantify the dynamic behavior of droplet vaporization, a pressure-coupled response function is defined as follows.

$$R_p = \frac{(\bar{w} - \tilde{w})/\bar{w}}{|(\bar{p} - \tilde{p})/\bar{p}|} \tag{1}$$

where the parameter R_p denotes the droplet response function, $\tilde{w}$ the instantaneous droplet

vaporization rate under an oscillating condition, $\bar{w}$ that in a quiescent environment, and p the pressure. Figure 6 shows the effect of frequency on the vaporization response. The initial droplet temperature and diameter are 300 K and 100 μm , respectively. The ambient mean pressure is 50 atm. Three different frequencies, i.e., 500, 2000, and 6000 Hz, are considered. Since the physical processes associated with droplet vaporization are intrinsically transient in time, the impressed pressure oscillation can easily exert significant influences on these processes and subsequently modify the vaporization behavior. The magnitude of the vaporization response increases with frequency. In the high frequency regime, the time period for the pressure oscillation is much smaller than the liquid thermal inertial time in the droplet interior. The variation of the surface temperature is too slow to keep in pace with the ambient pressure variation. Since the phase-equilibrium condition is enforced at the droplet surface, the pressure-induced variation in the surface composition becomes a dominant factor, showing an amplitude enhancement. At low and moderate frequencies, heat transfer from the ambient gas is used either to vaporize the liquid fuel and/or to heat-up the droplet interior. The droplet surface temperature fluctuates as a result of the unsteady heat transfer into the droplet. Since the thermal diffusion and relaxation processes in the droplet interior are inherently transient and characterized by their respective time scales, a time delay is present for the surface temperature to respond to the ambient pressure oscillation. Consequently, the surface properties, including species concentrations and enthalpy of vaporization, which depend strongly on the surface temperature, vary accordingly. This changes the driving mechanism for the vaporization process, and as such affects the dynamic behavior of the droplet vaporization response. Figure 6 also indicates that the magnitude of the response function first increases, due to the rapid heat-up in the early stage of the vaporization process, and then reaches a maximum and finally decreases. This phenomenon can be attributed to the decrease of

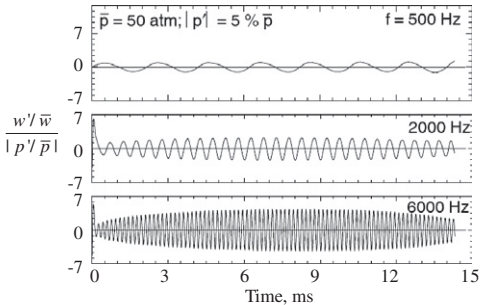


Fig. 6. Effect of frequency of pressure oscillation on droplet vaporization rate fluctuation.

the characteristic time with decreasing droplet size.

Figure 7 shows the effect of the mean pressure on the droplet vaporization response. The vaporization response increases with increasing pressure. The dominant factor contributing to this phenomenon is the pressure dependence of enthalpy of vaporization, which decreases with increasing pressure. As a result, a large amplification gain is observed at a high pressure. At the supercritical pressure ($p = 80$ atm), the vaporization rate fluctuates with an increasing amplitude in the early stage of the droplet lifetime. Once the droplet surface reaches the critical mixing condition, an abrupt growth of the response function occurs, due to rapid variations of droplet thermophysical properties across the critical mixing state. To help understand this intriguing phenomenon, the enthalpies of vaporization at three different pressures around the mean pressure of 80 atm are calculated, as shown in Fig. 8. If the ambient pressure experiences an isothermal oscillation with a 10% decrease in amplitude, i.e., from point A to B, the enthalpy of vaporization increases by 50 KJ/kg. The ensuing influence on the vaporization rate

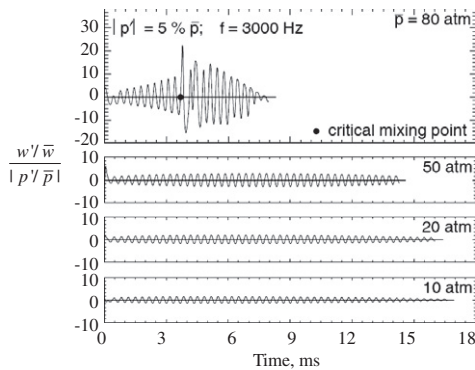


Fig. 7. Effect of mean pressure on droplet vaporization rate fluctuation.

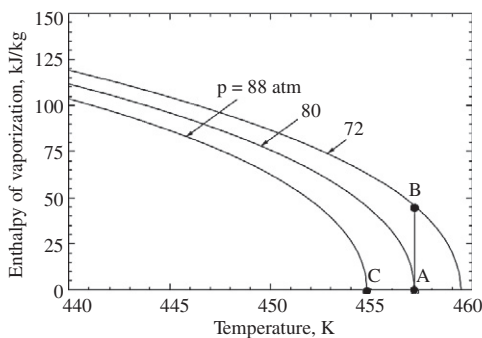


Fig. 8. Temperature dependence of enthalpy of vaporization at three different pressures.

is profound. On the other hand, if the ambient pressure increases by 10% in amplitude, i.e., from point A to C, the droplet surface remains at the critical mixing state. The changes in the thermo-physical properties with increasing pressure, however, strongly influence the heat transfer and mass diffusion processes near the droplet surface, and thus the vaporization behavior.

Figure 9 shows the magnitude of the instantaneous droplet vaporization response $|R_p|$ as a function of the normalized liquid thermal inertial at various pressures. In Figs. 9–12, the liquid thermal inertial is normalized with the pressure oscillation frequency f . It should also be noted that the droplet vaporization response function does not correlate well at 80 atm (not shown) since it corresponds strongly to pressure oscillations and ensuing sharp property variations at the critical mixing point. This case has not been analyzed in the present study and should be further investigated. In Fig. 9, curves a and b, plotted in solid lines, are the instantaneous magnitudes of the response function with an initial droplet diameter of 100 μm and over a broad range

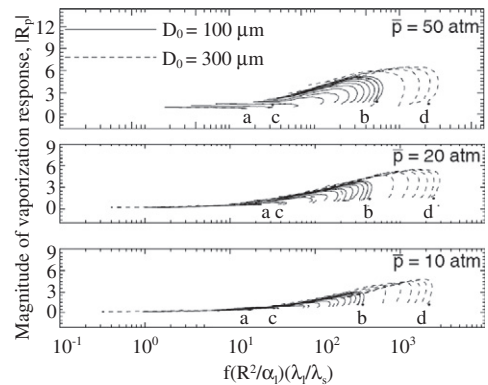


Fig. 9. Instantaneous magnitudes of droplet vaporization responses at various mean pressures.

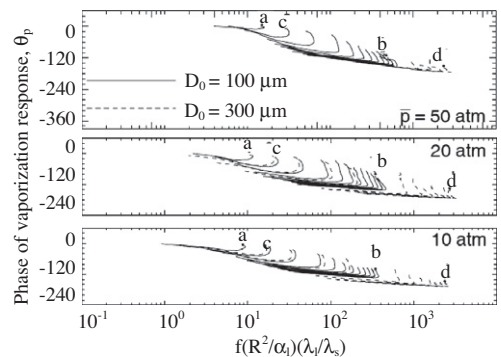


Fig. 10. Instantaneous phases of droplet vaporization response at various pressures.

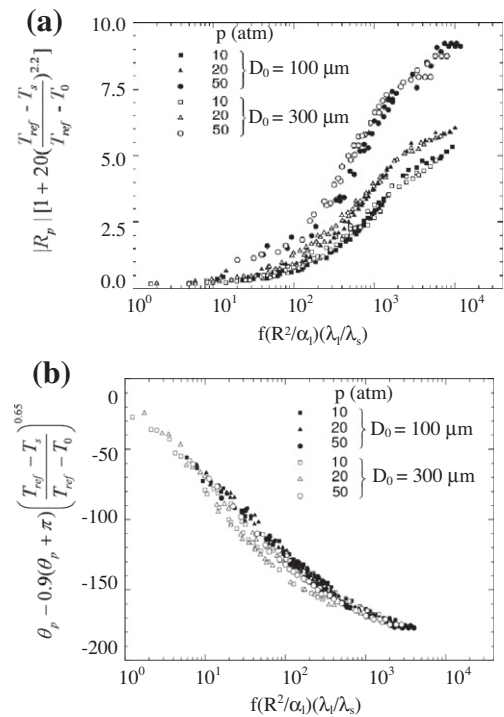


Fig. 11. Correlations of droplet vaporization response; (a) magnitude, and (b) phase angle.

of frequencies, i.e., 250, 500, 1000, 2000, ..., 9000 Hz. Curves c and d, plotted in dashed lines, are for an initial droplet diameter of 300 μm over a frequency range of 10, 50, 100, 250, 500, 1000, 2000, ..., 7000 Hz. For all the cases considered here, the amplitude of the pressure oscillation remains at 5% of the mean pressure. Results indicate that the droplet heat-up process, which occurs in the early stage of the vaporization, produces a strong influence on the magnitude of the droplet vaporization response. When the droplet surface temperature levels off and approaches a quasi-steady state, all the lines in the figure merge for both large (300 μm) and small (100 μm) droplets.

Figure 10 shows the phase of the instantaneous droplet vaporization response function θ_p . During the initial heat-up period, the droplet liquid thermal inertial and transient diffusion strongly affect the vaporization rate, showing an increase of the phase angle as the surface temperature increases. The phase lag increases from 0° toward 180° as the frequency increases, due to the large deviation of the characteristic time between the pressure oscillation and vaporization rate in the high frequency range. It is worth noting that all droplets essentially follow the same trend.

Figure 11 shows the dependence of the magnitude and phase angle of the droplet vaporization response on the mean pressure. The data points

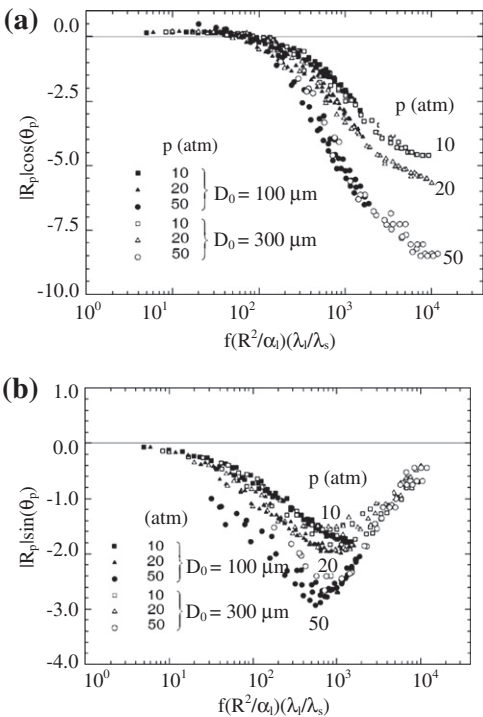


Fig. 12. Correlations of droplet vaporization response function; (a) real part, and (b) imaginary part.

are sampled sequentially throughout the droplet lifetime ($t/\tau_v = 0.1, 0.3, 0.5, 0.7, 0.9$). The filled and hollow symbols represent the data for droplets with an initial diameter of 100 and 300 μm , respectively. The effect of the initial heat-up on the droplet response is compensated using the following correction:

$$|R_p|^* = |R_p| \left[1 + 20 \left(\frac{T_{ref} - T_s}{T_{ref} - T_0} \right)^{2.2} \right] \quad (2a)$$

$$\theta_p^* = \theta_p - 0.9(\theta_p + \pi) \left(\frac{T_{ref} - T_s}{T_{ref} - T_0} \right)^{0.65} \quad (2b)$$

where T_0 is the spatially averaged droplet temperature, and T_s the droplet surface temperature. The parameter T_{ref} is defined as

$$T_{ref} = \begin{cases} \text{pseudo wet-bulb temperature} & p \leq p_c \\ \text{critical mixing temperature} & \text{otherwise} \end{cases} \quad (3)$$

where the pseudo wet-bulb and critical mixing temperatures are listed in Table 2. Results obtained for different initial droplet diameters scatter along the same curve at a given pressure. The amplitude of the response function increases with increasing pressure, due to the susceptibility of the enthalpy of vaporization to pressure oscillation at high pressures. On the other hand, the effect of the

Table 2
Pseudo wet-bulb and critical mixing temperatures.

Pressure (atm)	Pseudo wet-bulb temp. (K)	Critical mixing temp. (K)
10	376.1	–
20	409.0	–
50	–	466.3
80	–	460.3

mean pressure on the phase angle appears quite limited. It decreases from 0° in the low frequency limit to -180° at high frequencies, as shown in Fig. 11b.

In order to determine whether the droplet vaporization process is a driving or damping mechanism in a pressure oscillation environment, the real and imaginary parts of the response function are evaluated. Figure 12 shows the results. Based on dynamics theory, a positive real part represents a driving mechanism for combustion instability, while a negative value represents a damping effect [20]. The peak response occurs when the normalized liquid thermal inertial time reaches a value of around 20, suggesting a strong coupling between the pressure oscillation and vaporization response. A cut-off frequency exists when the normalized time reaches around 200. The droplet vaporization response then switches from a positive to a negative value, thereby changing from a driving to a damping effect on combustion instability. The imaginary part of the response function in Fig. 12b accounts for the phase angle variation of the resultant combustion oscillation.

4. Conclusions

A comprehensive analysis has been conducted to study the dynamic response of droplet vaporization to externally impressed pressure oscillations in a quiescent environment. The work considered a wide range of mean pressures, including both subcritical and supercritical conditions.

The theoretical formulation is based on a complete set of conservation equations and accommodates a self-consistent method for evaluating transport and thermodynamic properties. As a specific example, isolated *n*-pentane droplets in nitrogen were investigated systematically. The ambient mean pressure was found to exert significant influence on the magnitude of the droplet vaporization response. It increases with increasing pressure, due to the decreasing effect of pressure

on the enthalpy of vaporization. The phase angle of the response function, however, remains insensitive to the mean pressure, and can be correlated well with the normalized liquid thermal inertial time. Once the droplet surface reaches the critical mixing point, the droplet vaporization response experiences an abrupt change, a phenomenon that can be attributed to the rapid variations of fluid thermophysical properties across the critical mixing state.

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