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LOX DROPLET VAPORIZATION IN A SUPERCRITICAL FORCED CONVECTIVE ENVIRONMENT

Chia-chun Hsiao and Vigor Yang
Propulsion Engineering Research Center
Department of Mechanical Engineering
The Pennsylvania State University
University Park, PA 16802

SUMMARY:

Modern liquid rocket engines often use liquid oxygen (LOX) and liquid hydrogen (LH_2) as propellants to achieve high performance, with the engine operational conditions in the supercritcal regimes of the propellants. Once the propellant exceeds its critical state, it essentially becomes a puff of dense fluid. The entire field becomes a continuous medium, and no distinct interfacial boundary between the liquid and gas exists. Although several studies have been undertaken to investigate the supercritical droplet behavior at quiescent conditions, very little effort has been made to address the fundamental mechanisms associated with LOX droplet vaporization in a supercritical, forced convective environment. The purpose of this work is to establish a theoretical framework within which supercritical droplet dynamics and vaporization can be studied systematically by means of an efficient and robust numerical algorithm.

TECHNICAL DISCUSSION:

Several analyses based on the model of a spherical droplet in a quiescent environment were recently developed to address the characteristics of supercritical droplet vaporization([1][2][3][4]). The model is adequate only for small droplets which become equilibrium with the ambient flow. Contrarily, convective effect is clearly observed for large droplets as a result of high momentum inertia of the liquid phase. Figure 1 depicts the situation examined here, showing an isolated vaporizing LOX droplet in a convective hydrogen environment. The initial temperature of the droplet is subcritical, but the ambient temperature and pressure are in the supercritical regime of oxygen. As a result of heat transfer from the surrounding gases, the droplet surface temperature increases rapidly and reaches its critical mixing point. Under this condition, the sharp distinction between gas and liquid phases disappears. The droplet regression can be best characterized by tracing the location of the critical temperature.

Governing Equation

The analytical model is based on the complete time-dependent conservation equations of mass, momentum, energy and species concentration for a multicomponent system with variable properties. If body forces, viscous dissipation, radiation, and chemical reaction are ignored, these equation can be written in the following vector form.

Mass:

$$\frac{\partial}{\partial t}\iiint \rho dV + \iint \rho u_j dA_j = 0. \tag{1}$$

Momentum:

$$\frac{\partial}{\partial t}\iiint \rho u_i dV + \iint \rho u_i u_j dA_j = \iint \tau_{ij} dA_j. \tag{2}$$

Energy:

$$\frac{\partial}{\partial t}\iiint \rho e dV + \iint \rho e u_j dA_j = \iint \tau_{ij} u_i dA_j - \iint (q_T)_j dA_j. \tag{3}$$

Species Concentration:

$$\frac{\partial}{\partial t}\iiint \rho Y_l dV + \iint \rho Y_l u_j dA_j = -\iint (q_{M,l})_j dA_j . \tag{4}$$

where

$$\tau_{ij} = -p\delta_{ij} + 2\mu e_{ij} - \frac{2}{3}\mu(\nabla \cdot u)\delta_{ij} .$$

Standard notations in fluid mechanics and thermodynamics are used in (1)-(4). The specific total energy e is defined as

$$e = \sum_{i=1}^{l} Y_l \int_{T_{ref}}^{T} C_{p,l} dT - \frac{p}{\rho} + \frac{u_i u_i}{2},$$

where the index l represents the number of species considered, Y_l the mass fraction of species l, and T_{ref} the reference temperature for energy. Fick's and Fourier's laws are used to approximate the species and thermal diffusion in (3) and (4), respectively.

Property Evaluation

Thermophysical properties, including both thermodynamic and transport properties, play a decisive role in determining droplet vaporization behavior. It is generally accepted that thermal conductivities and heat capacities of pure fluids and fluid mixtures can be divided into three contributions, and correlated in terms of density and temperature. For example, the thermal conductivity of fluid oxygen can be expressed as [5]

$$\lambda(\rho, T) = \lambda_o(T) + \Delta\lambda_{exc}(\rho, T) + \Delta\lambda_{crit}(\rho, T). \tag{5}$$

The first term on the right-hand side represents the value in the dilute-gas or zero-density limit, which is independent of density and can be accurately predicted by kinetic-theory equations and an m-6-8 model potential. The second is the excess thermal conductivity which, with the exclusion of unusual variations near the critical point, characterizes the deviation from λ_o for a dense fluid. The sum of λ_o and $\Delta\lambda_{exc}$ is sometimes called the "background" thermal conductivity. The third term refers to the critical enhancement which accounts for the anomalous increase above the background thermal conductivity as the critical point is approached. There are two separate regions where the critical enhancement of thermal properties is important. The first region is located in the close vicinity of the critical point, and is the region where a scaled equation of state must be used, as defined by Sengers et al[6]. For oxygen with T_c = 154.581 K and ρ_c = 0.436 g/cm^3, this region is bounded approximately by $150 \leq T \leq 160$ K and $0.32 \leq \rho \leq 0.544$ g/cm^3. The second region, designated as the extended critical region, covers the ρ-T domain in which critical enhancement is significant, but the fluid behavior can be described by an analytical equation of state such as a modified Benedict-Webb-Rubin (BWR) type. This region can extend to quite high temperatures, up to approximately $2T_c$. The critical enhancement along various isotherms can be centered on a density, ρ_{center}, which deviates slightly from the critical density and decreases with increasing temperature. More detail description can be found in [4].

Numerical Algorithm

The model considered here is characterized by strong couplings among heat transfer, transient diffusion, and phase transition, etc.. Because various time and length scales are involved in the entire process, the numerical scheme for solving this serious stiffness problem becomes a challenge. Moreover, the singular behavior of momentum balance in the limit of diffusion-dominant process adds further complications. In view of these difficulties, a numerical algorithm capable of treating time-accurate low Mach-number compressible flow has been developed. The scheme is constructed in two steps. First, a rescaled pressure term is used in the momentum equation to circumvent the pressure singularity at very low Mach number.

$$p(x, y, t) = p_0 + \bar{p}(x, y, t)$$

The second step is based on the establishment of a dual time-stepping integration procedure. With the addition of a set of well-conditioned artificial time derivatives to the conservation laws, a new system of governing equations is obtained whose converged solution in pseudo-time corresponds to a time-accurate solution in the physical-time domain.

$$\Gamma\frac{\partial Z}{\partial \tau} + \frac{\partial Q}{\partial t} + \frac{\partial (E - E_v)}{\partial x} + \frac{\partial (F - F_v)}{\partial y} = S$$

where τ presents pseudo time, and $Z = (p', u, v, h, Y_i)$.

RESULTS:

As a first study of supercritical droplet behavior, A spherical droplet with an introductory temperature of 300 K is first placed in a supercritical, forced convective environment($T_\infty = 1000K$). The droplet Reynolds number based on the relative velocity is 60. The droplet is 100 μm in diameter and contains 100% oxygen initially. As a result of large temperature gradient between gas and liquid phases, surface temperature raises and reaches critical condition shortly. Due to the dimishment of surface tension, droplet deformation and shattering can be clearly observed. Figure 2 shows the density contours, streamlines, and velocity vectors at $t = 0.02ms$ in a supercritical environment with H_2 as the ambient gas. Figure 3 shows the oxygen concentration contours. Results indicate that the ambient gas mass diffusivity plays an important role in determining the droplet behavior. A high mass diffusivity causes rapid penetration of the ambient gas into the droplet, and consequently modifies the droplet dynamics (e.g., deformation, shattering, etc.) caused by the density difference between the droplet and the gas.

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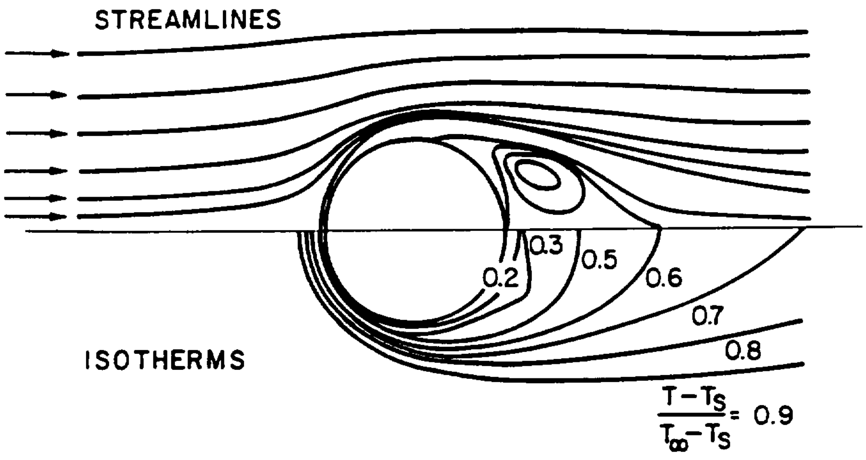

Figure 1: Schematic of a vaporizing LOX droplet in hydrogen stream.

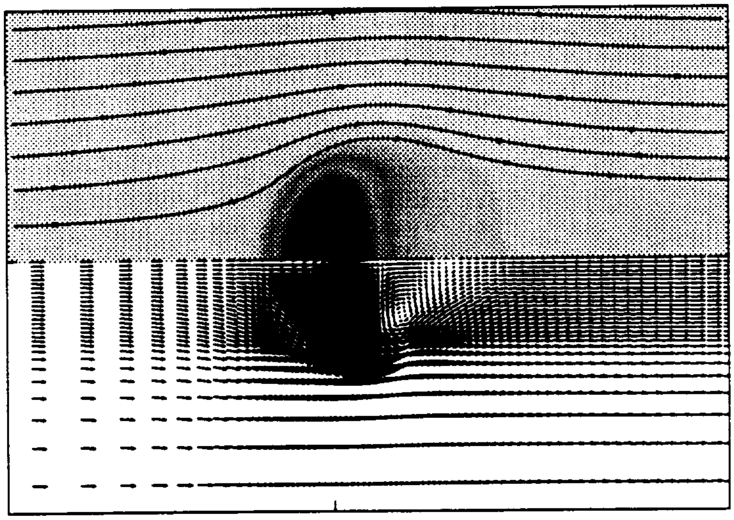

Figure 2: Density contours, streamlines and velocity vectors of LOX droplet vaporizing in a hydrogen environment. $Re = 60, t = 0.02ms$.

Mass Diffusion Exerts Strong Influence on Droplet Behavior in a Supercritical, Forced-Convective Environment

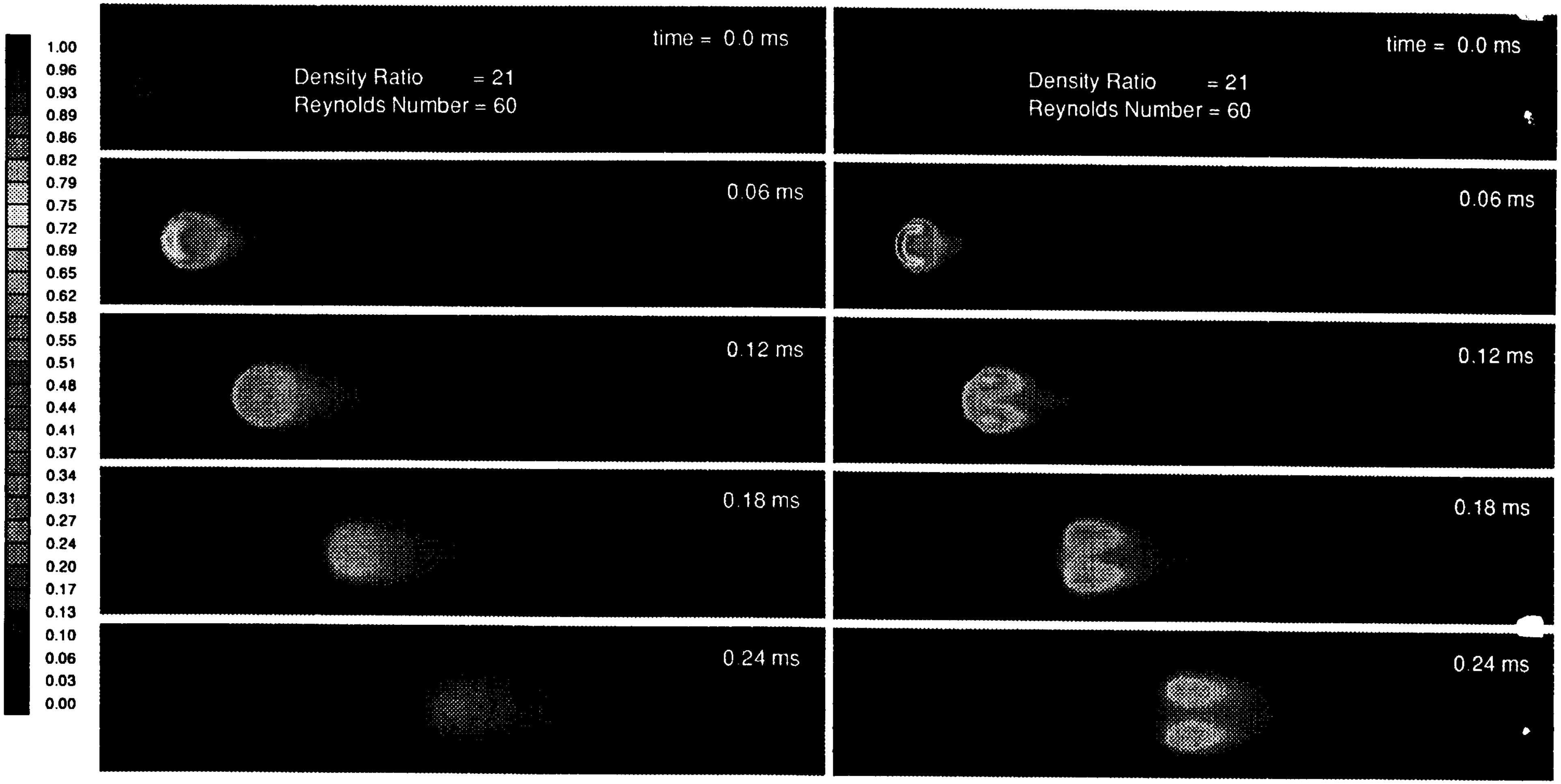
- High Mass Diffusivity
- Low Mass Diffusivity

Figure 3: Time history of mass fraction of a vaporizing droplet at supercritical condition.