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ABSTRACT
Droplet vaporization or combustion is usually studied assuming quasi-steady hypotheses for the vapor and a constant and uniform temperature for the liquid. A "D^2 law" is then obtained for the diameter evolution.
This is not the case for near-critical droplets in the general case, and also for sub-critical droplets in transient heat-up regime. We present here these two situations: near-critical vaporization in a pure fluid, and pure liquid vaporization in a gaseous mixture.

NOMENCLATURE

A:	diluent
B_M , B_T	Spalding parameters for mass, for heat transfer respectively
$c_{L,}$ c_p:	specific heat per unit mass of the liquid, of the gas at p=cte
D:	droplet diameter : D=2 r_S
$\mathcal{D}$	diffusion coefficient
D_m :	diameter of the sphere of maximum unit mass flow rate
F:	liquid or gaseous fuel
k:	thermal conductivity
Le:	Lewis number $k/\rho D c_p$
ℓ :	latent heat of evaporation per unit mass
M:	mass of the droplet
$\dot{m}$:	unit mass flow rate
$\dot{M}$:	droplet evaporation rate
p:	pressure
p_{sat}:	saturated vapor pressure
Q_L:	heat rate brought to the drop minus the latent heat of evaporation.
r:	radius
r_S:	droplet radius
T :	temperature
t:	time
v:	radial velocity
x, y:	abscissa, ordinate
X_j,Y_j	mole fraction, mass fraction respectively
β :	coefficient of the supercritical droplet regression law
μ :	chemical potential
ρ :	density
σ :	surface tension
τ :	non-dimensional time
τ_T :	heat transfer time in the droplet
τ_v :	life time of the droplet

Subscripts and superscripts

C:	critical point
i:	initial
i, j:	chemical species
L, l:	in the liquid phase
m:	position where the unit mass flow rate is maximum
QS:	quasi-Steady
S:	at the droplet surface
Sat:	saturated vapor
T:	relative to the heat exchanges
0:	relative to supercritical "droplet" diameter
∞ :	at infinite

INTRODUCTION

Droplet evaporation and combustion are basic phenomena for liquid propellant rocket engines. The combustion process depends on the chemical composition of the injected propellants, on the injector design, and on the injection conditions. The initial diameter distribution of droplets is an important parameter of the problem. Interactions between droplets play a role [1], [2], [3], [4] and may not be neglected for dense clouds. Droplets are often considered as spherical. But this hypothesis becomes no more valid, in particular for a small gas-liquid surface tension in the presence of a non zero relative velocity.

The droplet life time, and also the droplet diameter regression law, are important to know for the modeling of combustion processes and then for performance calculations of combustion devices.

Liquid droplets are generally injected in a gaseous environment with different temperature, pressure and velocity. A relaxation time is then necessary for a droplet to reach the stabilized values. At the end of this relaxation period, the velocities of gas and liquid are equal, and droplet temperature reaches a uniform temperature equal to the temperature of saturated vapor at the liquid surface.

Sometimes, the droplet life time short for reaching these equilibrium conditions. It is then possible to be always in a transient situation for temperature or/and for velocity. In the opposite case, equilibrium temperature and velocity are reached during the droplet life time.

VAPORIZATION OF A "DROPLET" UNDER SUPERCRITICAL PRESSURE

At supercritical pressures, in the pure body case, there is not distinct liquid and vapor phases: the whole domain is monophasic. The density relaxation of a dense fluid pocket in a hotter and isobaric atmosphere is nevertheless similar to the vaporization process of a subcritical liquid droplet provided that the thermal diffusivity of the fluid pocket is much lower than the surrounding atmosphere. An area where density and diffusion time gradients are important insulates the dense pocket from the surrounding atmosphere [5], [6]. The dense pocket is thus named supercritical "droplet" and the strong density gradient is compared to a thick "interface".

For a critical fluid pocket (critical density, critical temperature) introduced in an (hotter) atmosphere at the critical pressure, the diffusivity condition previously mentioned is valid for all atmosphere temperatures because of the critical vanishing of the diffusivity in the critical pocket. At clearly supercritical pressures, this diffusivity condition is more restrictive and needs, in ideal fluid condition, $T_\infty >> T_i$, with T_∞, the atmosphere temperature and T_i the initial temperature of the dense fluid pocket. The "interface" being thick, two choices can be made for the definition of the reference border of the supercritical "droplet": the first one consists in choosing an isochore ρ_m located at the end of the strong density gradient area that follows the fluid pocket. It can be shown that this area located at the end of the strong density gradient is the place where the unit mass flow rate is maximum. The second one consists in choosing a reference isochore ρ_0 at the beginning of the strong density gradient area..

Let us name D_m the diameter of the domain bordered by the isochore ρ_m and D_0 the diameter of the domain bordered by the isochore ρ_0. It was shown [6], [7] that the diameter D_m satisfies the "D²" law : $D_m^2 = 1 - \tau$, with, τ the non-dimensional time, ratio between the time and the life time of the « droplet ». The diameter D_0 satisfies (see *figure 1*):

$$D_o^\beta - \beta D_o = (1-\beta)\sqrt{1-\tau} \qquad (1)$$

The parameter β is of order one at slightly sub or supercritical pressures : the D^2 law is not satisfied for D_0 at such pressures according to the previous relation. As the pressure is becoming clearly subcritical, β is becoming greater. Given that the diameter D_o is made non-dimensional with the initial diameter of the "droplet", $D_0(\tau) \leq 1$ and, for great values of β, the previous equation becomes at first order :

$D_o^2 = 1 - \tau$. The D² law is thus recovered in clearly subcritical conditions.

Remarks :

- It would be interesting to define an effective surface tension in supercritical conditions. Indeed, phenomena analogous to those observed in miscible fluids leading to effective superficial tension, also appears in pure fluids when high temperature gradients occur [7], [8], [9]. This is illustrated in the case of a cold drop falling into the hotter same fluid [11].
- A slightly different problem is in particular involved in the injection zone of cryogenic engines. One has to consider the isobaric vaporization at supercritical pressure of a cold «droplet » in a hot ambience. The droplet is initially at subcritical temperature. Out of the near-critical zone there is no singularity of the heat conductivity, and therefore it appears a heat-up period, as in the following section but with a real gas state equation.

EVAPORATION WITH HEAT-UP OF A LIQUID DROPLET IN A GASEOUS MIXTURE

In the classical quasi-steady theory [12],[13] there is no heat-up of the droplet, and the heat coming from the gas is entirely used to evaporate the liquid surface (QS regime). In the present theory, there is heat exchange between gas and liquid bulk of the droplet (heat-up regime). We consider a spherical drop of pure liquid, vaporizing in an ideal gaseous mixture. A quasi-steady hypothesis is supposed for the gaseous phase but not for the liquid droplet which is supposed to have a uniform temperature varying with time. The equations of the quasi-steady gas flow are $\dot{M} = 4\pi r^2 \dot{m},\ \dot{m} = \rho u$,

$$\dot{M}\frac{dY_j}{dr} - 4\pi\rho D r \frac{d^2(rY_j)}{dr^2} = 0,$$

$$\dot{M} c_p \frac{dT}{dr} - 4\pi k r \frac{d^2(rT)}{dr^2} = 0,$$ with the boundary conditions: at infinity ($r = \infty$): $Y_j = Y_{j\infty}$, $T = T_\infty$, and at the droplet surface ($r_S = D/2$):

$$Y_{jS}, T_S, 4\pi\rho D r_S^2 \left.\frac{dY_j}{dr}\right|_S = -\dot{M}\left(Y_{jL} - Y_{jS}\right) \quad ,$$

$$4\pi \frac{k}{c_p} r_S^2 \left.\frac{dT}{dr}\right|_S = \dot{M}\frac{\ell}{c_p}.$$

Then, solution of the diffusion equation writes $\dot{M} = 4\pi\rho D r_S \ln(1 + B_M)$, with $B_M = (Y_{FS} - Y_{F\infty})/(1 - Y_{FS})$.

On the other hand, solution of the conduction equation is modified because of the change of the condition at the droplet surface. One introduces the heat flux Q_L which characterizes the heat brought to the drop in addition to that necessary for evaporation. The mass flow rate becomes $\dot{M} = 4\pi(k/c_p) r_S \ln(1 + B_T)$, with $B_T = c_p(T_\infty - T_S)/(\ell + Q_L/\dot{M})$. To continue the resolution, it is also necessary to have an expression for Q_L. For that we need to study heat exchanges inside the droplet. For example, if they are infinitely fast, droplet temperature remains uniform at any moment but varies with time; thus we have $M c_L \frac{dT_S}{dt} = Q_L$, where c_L is the specific heat of the liquid. Temperature of the droplet surface is no more fixed, contrarily to the classical theory. It varies during the heating period. There is always evaporation at equilibrium at the surface, but the temperature being variable, the partial pressure of species F varies with time and thus the concentration Y_{FS} adapts itself to temperature variations.

In non-stabilized regimes, characteristic time for liquid heating tends to be higher than the time for boundary-layer heating. Heating time Δt_{hu}, and droplet lifetime Δt_{ex} are of the same order of magnitude for kerosene droplets, but for LOX droplets $\Delta t_{hu} \rangle \Delta t_{ex}$.

In the case of infinitely fast heat exchanges in the liquid phase, we need to solve the following system: $$\frac{dT_S}{dt} = \frac{12k\ell}{\rho_L c_L c_p D^2}\left(\frac{B'_T}{B_T} - 1\right)\ln(1 + B_T),$$

$$D\frac{dD}{dt} = \frac{4k}{\rho_L c_p}\ln(1 + B_T) \qquad (2)$$

where B_T was defined foregoing and where $B'_T = c_p(T_\infty - T_S)/\ell$.

Note that in QS regime, $B'_T = B_T$. The Spalding parameter B'_T depends on the droplet temperature T_S. The Spalding parameter for heat exchange B_T is connected to the Spalding parameter for mass exchange B_M by the equation $\dot{M} = 2\pi \frac{k}{c_p} D \ln(1+B_T) = 2\pi\rho \mathcal{D} D \ln(1+B_M)$.

So B_T is a function of B_M, which depends on gaseous fuel mass fraction at the droplet surface (if the Lewis number Le is equal to unity, we have $B_T = B_M$). This mass fraction is connected to temperature T_S by the equilibrium relation $\mu_L = \mu_F$. When μ_L is function of T only, and for an ideal gas mixture, this lead to $p\, X_{FS} = p_{sat}(T_S)$. The equilibrium law writes for instance [14] $p_{sat}(T_S) = exp(a - b/(T_S - c))$, where *a*, *b* and *c* are constant coefficients.

Then, we can relate Y_{FS} to the surface molar fraction X_{FS} and the surface mass fraction Y_{FS} appears as a function of surface temperature T_S and total pressure p, which is assumed uniform and constant: $Y_{FS} = f(T_S, p)$. Thus B_T and B'_T are functions of T_S only.

The latent heat itself is function of temperature and concentration at the surface. Indeed, from the relation of Clapeyron, one has per mole of pure substance: $L = (RT^2/p)(dp/dT)_{sat}$. This relation, applied here to unit mass, by replacing the pressure by the partial pressure becomes $\ell = \frac{(M_A - M_F)Y_{FS} + M_F}{M_A M_F} \quad \frac{b R T_S^2}{(T_S - c)^2}$. As temperature and concentrations are not constant in the droplet surrounding, the averaged properties c_p, k are evaluated at the reference temperature and composition $\overline{T} = T_S + A_r(T_\infty - T_S)$, $\overline{Y}_F = Y_{FS} + A_r(Y_{F\infty} - Y_{FS})$. $A_r = 1/3$ is generally chosen.

Thus the coefficients appearing in (2) are functions of D and T_S only. They form a non linear system of two differential equations. Solution of this system gives both functions $T_S(t), r_S(t)$ and consequently $Y_{FS}(t)$.Simplified hypotheses are used by Chin & Lefebvre [14], [15] to solve system (2). Two D^2 laws can be considered, one for the heat-up period Δt_{hu}, the other for the steady-state phase Δt_{QS}. The used relations result in particular from approximations of time derivatives. We present here a new method.

Equations of system (2) can be written in the form $D^2 \frac{dT_S}{dt} = F(T_S)$, $\frac{dD^2}{dt} = G(T_S)$. We make the two following assumptions: 1) We suppose that the droplet temperature is of the form: $T_S = T_{QS} + (T_i - T_{QS})e^{-t/\tau_T}$ where τ_T is a thermal relaxation time and T_i, T_{QS} the droplet temperature, respectively in initial conditions and in stabilized regime. 2) In the stabilized regime, the droplet square radius is a linear function of time, then: $G(T_S) \to K_{QS}$ *for* $T_S \to T_{QS}$. We suppose a linear law for $G(T_S)$: $G(T_S) = -K_{QS} + h(T_S - T_{QS})$ for all the regimes.

Then, we obtain the result: $F(T_S) \approx \frac{T_{QS} - T_S}{\tau_T}\left(D_i^2 - \frac{h}{\tau_T}(T_S - T_i) + \tau_T K_{QS} \ln\left(\frac{T_{QS} - T_S}{T_{QS} - T_i}\right)\right)$ and for the diameter :

(3) $D^2 \approx D_i^2 - \frac{h}{\tau_T}(T_{QS} - T_i) - K_{QS}\, t + \frac{h}{\tau_T}(T_{QS} - T_i)e^{-t/\tau_T}$

T_{QS} is such that $F(T_{QS}) = 0$, K_{QS} is such that $K_{QS} = -G(T_{QS})$, τ_T is equal to $\tau_T = (T_{QS} - T_i)D_i^2/F(T_i)$, and we have $h = (G(T_S) - G(T_i))/(T_{QS} - T_i)$. The profiles of $(D/D_i)^2$ as a function of time are given in *figure 2* for particular values of the coefficients.

CONCLUSIONS

Two cases of droplet regression have been examined:

- A near critical droplet in its pure vapor has been studied in section 1, which gives well a D^2 law but not for the droplet diameter D_0 as usually defined, but for a particular diameter D_m. On the contrary a non linear law was found for D_0 as a function of time. An approximate law was given, depending on a coefficient β.

- A subcritical vaporizing droplet in a hotter gaseous mixture. A simplifying assumption was that the droplet temperature keeps its uniformity. This corresponds to an infinite conductivity for the liquid. We have summarized the theory of Chin and Lefebvre who consider two successive D^2 law, one for the heat up regime and the other for the following QS regime. In this section, we proposed an alternative method with simple hypotheses. A continuous profile is obtained.
- The D^2 law is not valid too in other cases of heat-up regime, when the droplet is not assumed to have a uniform temperature, without or with an external flow, as it was supposed in section 2. Law & Sirignano [16] studied the case of a purely conducting droplet numerically and using series expansions. To simplify the continuous conduction problem, it is possible to consider a two-layer model or a n-layer model [17]. For not purely conductive droplets, Abramson & Sirignano [18] proposed to assimilate the heat transfer inside the droplet to a purely conductive problem, and doing that they introduce an effective conduction coefficient.

KEYWORDS
Droplet regression; vaporization; combustion; transitory regime; heat-up; supercritical; subcritical

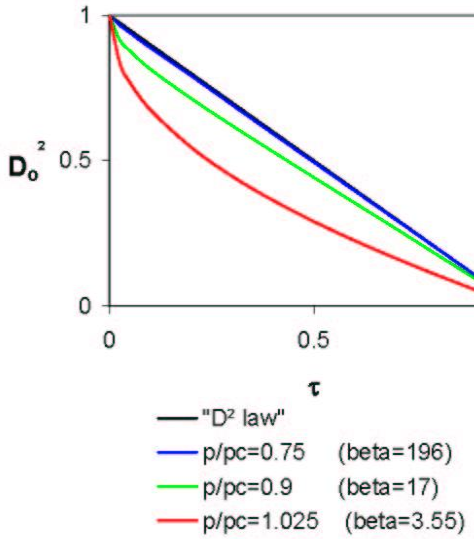

Figure 1. Square of the droplet diameter as a function of the reduced time τ for different pressures. Pc is the critical pressure.

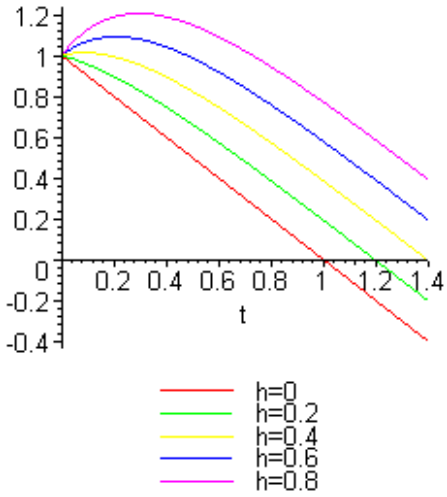

Figure 2. $\left(D/D_i\right)^2$ as a function of reduced time $\tau = K_{QS} t / D_i$, for $\tau_T = 0.3$, for a subcritical droplet.

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