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## NON-CLASSICAL REGRESSION LAWS FOR DROPLET VAPORIZATION.

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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<sup>2</sup> 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  $k/\rho D c_p$   
 $\ell$ : 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  
 $\beta$ : coefficient of the supercritical droplet regression law  
 $\mu$ : chemical potential  
 $\rho$ : density  
 $\sigma$ : surface tension  
 $\tau$ : non-dimensional time  
 $\tau_T$ : heat transfer time in the droplet  
 $\tau_v$ : 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  
 $\infty$ : 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,  $T_\infty \gg T_i$ , with  $T_\infty$  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  $\rho_m$  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  $\rho_0$  at the beginning of the strong density gradient area..

Let us name  $D_m$  the diameter of the domain bordered by the isochore  $\rho_m$  and  $D_0$  the diameter of the domain bordered by the isochore  $\rho_0$ . It was shown [6], [7] that the diameter  $D_m$  satisfies the “D<sup>2</sup>” law :  $D_m^2 = I - \tau$ , with,  $\tau$  the non-dimensional time, ratio between the time and the life time of the « droplet ». The diameter  $D_0$  satisfies (see figure 1):

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

The parameter  $\beta$  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,  $\beta$  is becoming greater. Given that the diameter  $D_o$  is made non-dimensional with the initial diameter of the “droplet”,  $D_o(\tau) \leq 1$  and, for great values of  $\beta$ , the previous equation becomes at first order :

$D_o^2 = I - \tau$ . The  $D^2$  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  $\dot{M} = 4\pi r^2 \dot{m}$ ,  $\dot{m} = \rho u$ ,

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

$$\dot{M} c_p \frac{dT}{dr} - 4\pi k r \frac{d^2(rT)}{dr^2} = 0, \text{ with the boundary}$$

conditions: at infinity ( $r = \infty$ ):  $Y_j = Y_{j\infty}$ ,  $T = T_\infty$ ,

and at the droplet surface ( $r_s = D/2$ ):

$$Y_{jS}, T_S, 4\pi \rho D r_s^2 \frac{dY_j}{dr} \Big|_S = -\dot{M} (Y_{jL} - Y_{jS}),$$

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

Then, solution of the diffusion equation writes

$$\dot{M} = 4\pi \rho D r_s \ln(1 + B_M), \text{ with}$$

$$B_M = (Y_{FS} - Y_{F\infty}) / (I - Y_{FS}).$$

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  $\dot{M} = 4\pi (k/c_p) r_s \ln(I + B_T)$ , 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  $\Delta t_{hu}$ , and droplet lifetime  $\Delta t_{ex}$  are of the same order of magnitude for kerosene droplets, but for LOX droplets  $\Delta t_{hu} \gg \Delta t_{ex}$ .

In the case of infinitely fast heat exchanges in the liquid phase, we need to solve the following system:

$$\frac{dT_S}{dt} = \frac{12k\ell}{\rho_L c_L c_p D^2} \left( \frac{B'_T}{B_T} - 1 \right) \ln(I + B_T),$$

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

where  $B_T$  was defined foregoing and where  $B'_T = c \frac{(T_\infty - T_s)}{p} \ell$ .

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  $\dot{M} = 2\pi \frac{k}{c} D \ln(1+B_T) = 2\pi \rho D D \ln(1+B_M)$ .

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  $\mu_L$  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

$$\ell = \frac{(M_A - M_F)Y_{FS} + M_F}{M_A M_F} \frac{b R T_s^2}{(T_s - c)^2}. \quad \text{As}$$

temperature and concentrations are not constant in the droplet surrounding, the averaged properties  $c_p$ ,  $k$  are evaluated at the reference temperature and composition  $\bar{T} = T_s + A_r (T_\infty - T_s)$ ,  $\bar{Y}_F = Y_{FS} + A_r (Y_{F\infty} - Y_{FS})$ .

$A_r = 1/3$  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  $\Delta t_{hu}$ , the other for the steady-state phase  $\Delta t_{QS}$ . 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  $\tau_T$  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:  $G(T_s) \rightarrow K_{QS}$  for  $T_s \rightarrow T_{QS}$ . 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:

$$F(T_s) \approx \frac{T_{QS} - T_s}{\tau_T} \left( D_i^2 - \frac{h}{\tau_T} (T_s - T_i) + \tau_T K_{QS} \ln \left( \frac{T_{QS} - T_s}{T_{QS} - T_i} \right) \right) \quad \text{and}$$

for the diameter :

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

$T_{QS}$  is such that  $F(T_{QS}) = 0$ ,  $K_{QS}$  is such that

$K_{QS} = -G(T_{QS})$ ,  $\tau_T$  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  $\beta$ .

- 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

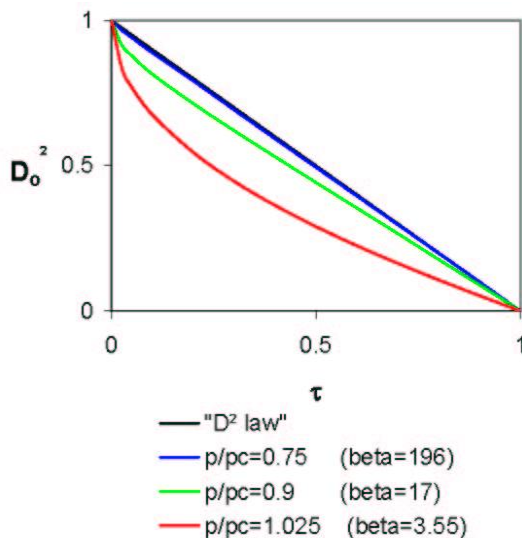


Figure 1. Square of the droplet diameter as a function of the reduced time  $\tau$  for different pressures.  $P_c$  is the critical pressure.

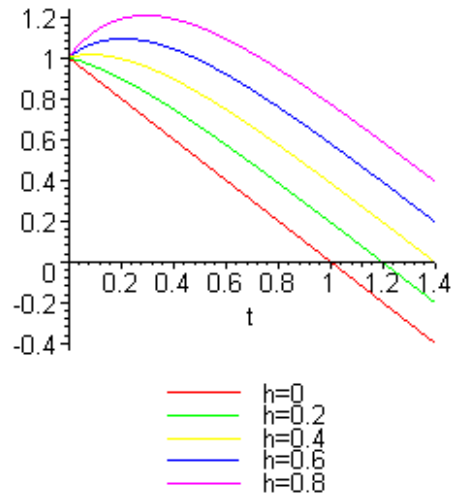


Figure 2.  $(D/D_i)^3$  as a function of reduced time  $\tau = K_{QS} t / D_i$ , for  $\tau_T = 0.3$ , for a subcritical droplet.

**REFERENCES**

1. Borghi, R. & Lacas, F. (1995) : « Modeling of liquid-propellant spray combustion in rocket engine combustor », *Proceedings of the Second International Symposium on Liquid Rocket Propulsion, ONERA, Chatillon, June 19-21, 7.1 – 7.26.*
2. Dietrich, D. L., Struk, P. M., Kitano & Ikegami (1999): « Combustion of interacting droplet arrays in a micro-gravity environment », *Fifth International Micro-gravity Combustion Workshop, Proceedings, NASA Glenn Research Center and NCMR, Cleveland, OH, May 18-20, 281-284.*
3. Rangel, R.H. and Sirignano, W. A. (1989) : « Combustion of parallel fuel droplet streams », *Combustion and flame*, **75**, 241-254.
4. Virepinte, J.F., Adam, O., Lavergne, G. and Bicos, Y. (1999): Droplet spacing on drag measurement and burning rate for isothermal and reacting conditions”, *Journal of Propulsion and Power*, 15, N°1, 97-102.
5. Sanchez-Tarifa C., Crespo A., Fraga E.A., 1972, “Theoretical Model for the Combustion of Droplets in Super-critical Conditions and Gas Pockets”, *Astron. Acta*, 17, pp. 685-692.
6. Préau S., Prud’homme R., Ouazzani J., Zappoli B., 2004, “Supercritical density

- relaxation as a new approach of droplet vaporization”, *Phys. Fluids*, 16, pp 4075-4087.
7. Préau S., 2003, “Etude théorique et numérique de l’«évaporation » d’une « goutte » de densité critique le long d’une isobare légèrement supercritique”, Ph.D. thesis, University Paris VI, France.
  8. Gagniol, R. & Prud’homme, R., 2001, Mechanical and thermodynamical modeling of fluid interfaces- Series on Advances in Mathematics for Applied Sciences, 58, World Scientific, Singapore.
  9. Defay, R. & Sanfeld, A., 1975, “Surface tension of interfaces outside equilibrium”, *Anales de Chimie*, 71, pp. 856-860.
  10. Petitjeans, P., 1996, “Une tension de surface pour les fluides miscibles”, *C.R. Acad. Sci. Paris II B*, 322, pp. 673-679.
  11. Kojima M., Hinch E. J., Acrivos A., 1984, “The formation and expansion of a toroidal drop moving in a viscous fluid”, *Phys. Fluids*, 27 (1), pp. 19-32.
  12. Godsave, G.A.E. (1953): “Studies of the combustion of drops in a fuel spray. The burning of single drops of fuel”, *Fourth Symposium (International) on Combustion*, The Combustion Institute, 818-830.
  13. Spalding, D. B. (1953): “Studies of the combustion of drops in a fuel spray. The burning of single drops of fuel”, *Fourth Symposium (International) on Combustion*, The Combustion Institute, 847-864.
  14. Chin, J. S. & Lefebvre A. H. (1985) : « The role of the heat-up period in fuel drop evaporation », *Int. J. Turbo Jet Engines*, 2, 315-325.
  15. Lefebvre, A.H. (1989) : « *Atomization and sprays* », Hemisphere Publishing Corporation.
  16. Law, C. K. & Sirignano, W. A. (1977) : « Unsteady droplet combustion with droplet heating-II: conduction limit », *Combustion and flame*, 28, 175-186.
  17. Prud’homme, R., Habiballah M., Nicole, A. & Mauriot, Y. (2005) : « Instabilités liées au phénomène d’évaporation : Réponse dynamique d’une goutte à un champ acoustique », soumis au 17<sup>ème</sup> Congrès Français de Mécanique, Troyes.
  18. Abramson, B. & Sirignano, W. A. (1989) : « Droplet vaporization model for spray combustion calculations », *Int. J. Heat Mass Transfer*, 32, N° 9, 1605-1618.