

## **Simplified Drop-Wise Liquid Combustion Theory**

### **1. Introduction**

In this lecture we examine in more depth the fluid phenomena which dominate the operation, and hence the design, of a liquid rocket. We start by considering the two phase aspects of combustion, which usually determine the combustor size. Next we examine the stability of combustor operation and the design modification required to achieve it. Heat transfer to walls, wall compatibility and wall cooling form the next topic. We conclude with some notions in nozzle aerodynamic design and nozzle optimization.

### **2. Drop Vaporization and Spray Combustion**

Returning to Fig. 12.1 (lecture 12), we note again the existence of a zone AC where the propellants go from a series of liquid jets issuing through a multiplicity of small injector holes, through breakup of these jets into droplets, impingement (in some designs) of jets or droplet streams on each other, dispersion of the droplets into a recirculating mass of combustion products, evaporation of the droplets, interdiffusion of the vapors and kinetically controlled combustion. These are obviously complicated processes, and a comprehensive analysis good enough for first principles design requires large-scale computation [18, 19, 20]. In fact, the largest number of existing liquid rocket combustors, those dating from before 1970, were developed mainly through empirical methods, supplemented by very extensive testing. Improved modeling and computational capabilities have more recently permitted a more direct approach, with fewer hardware iterations, but theory is still far from completely developed in this area, and serves at this point mainly to ascertain trends and verify mechanisms. For an in-depth discussion of liquid propellant combustion, see Refs. 21 and 22. Here we will only review the fundamental concepts which underlie current spray combustion models.

#### **2.1 Single-Drop Combustion**

Even when liquids are originally injected into the chamber, actual combustion takes place in the gas phase, following vaporization of both, oxidizer and fuel. In fact, vaporization is usually the rate-controlling step in the whole process, although its rate is itself affected by the reactions occurring near each droplet. In a few instances, both propellants enter the chamber as gases or easily vaporized liquids, and then gas phase mixing is the limiting step. (An example is the Shuttle SSME, where the hydrogen is vaporized in the cooling circuit, and the oxygen is partially vaporized by the hydrogen in a co-flowing heat exchanger arrangement ahead of the injectors, the rest being atomized and evaporated shortly after injection).

In a fuel-rich environment, vapor from a fuel droplet diffuses without reacting into the surrounding gas, while heat diffuses inwards to supply the latent heat of evaporation. In the same environment, vapor from an oxidizer drop comes in contact, and reacts with the fuel-rich gas at some distance from the droplet, forming a spherical flame, from which heat diffuses both ways, while reaction products diffuse outwards and also stagnate in layer around the droplet. A similar description applies to a locally oxidizing environment. It will be sufficient to analyze, for example the case of a fuel drop in an oxidizing environment, from which we can easily derive other cases by suitable re-interpretations.

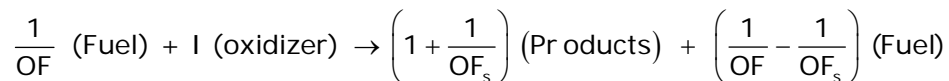
As a preliminary, some relationships will be derived between the overall stoichiometry (oxidizer/fuel ratio, or OF, by mass), and the mass fractions of products and excess oxidizer or fuel to be found in the burnt gas far from the droplets. Let the actual mass ratio be OF, and the stoichiometric mass fraction be  $OF_s$  (later called  $i$  for short), Assuming excess oxidizer, and complete combustion (a rough assumption), the reaction can be mass balanced as



and so the mass fraction of excess oxidization at infinity is

$$Y_{ox,\infty} = \frac{OF - OF_s}{(1 + OF_s) + (OF - OF_s)} = \frac{OF - OF_s}{1 + OF}$$

Similarly, for fuel-rich operation,



and the mass fraction of excess fuel at infinity is

$$Y_{F,\infty} = \frac{\frac{1}{OF} - \frac{1}{OF_s}}{\left(1 + \frac{1}{OF_s}\right) + \left(\frac{1}{OF} - \frac{1}{OF_s}\right)} = \frac{OF_s - OF}{(1 + OF) OF_s}$$

which could be also formally obtained from  $Y_{Ox,\infty}$  by reversing the roles of fuel and oxidizer (including  $OF \rightarrow \frac{1}{OF}$ )

Consider a spherical fuel droplet of radius  $R$  and density  $\rho_l$ . Its rate of vaporization is

$$\Gamma = -4 \pi R^2 \rho_p \frac{dR}{dt}$$

and the main purpose of the analysis is the calculation of  $\Gamma$  from given  $R$  and gas properties. Let  $Y_f(r)$ ,  $Y_{pr}(r)$  be the mass fractions of fuel and of combustion products in the region  $R < r < r_{fl}$  between the drop and the flame location (no oxidizer is to be found there, so  $Y_f + Y_{pr} = 1$ ). These two constituents are both convected by the mean outwards flow, and diffuse according to their concentration gradients. Since the products do not penetrate the drop surface, the net outflow of fuel at radius  $r$  is equal to the total mass flow, and is given by

$$\Gamma Y_f - 4 \pi r^2 \rho D_f \frac{dY_f}{dr} = \Gamma$$

where  $D_f$  is the diffusivity in the products. The net flux of products remain zero in this region (but not their concentration  $Y_{pr} = 1 - Y_f$ ). Imposing that  $Y_f$  approaches zero at the flame radius, the above equation integrates to

$$Y_f = 1 - e^{-\lambda_f \left( \frac{1}{r} - \frac{1}{r_{fl}} \right)} \quad (R < r < r_{fl})$$

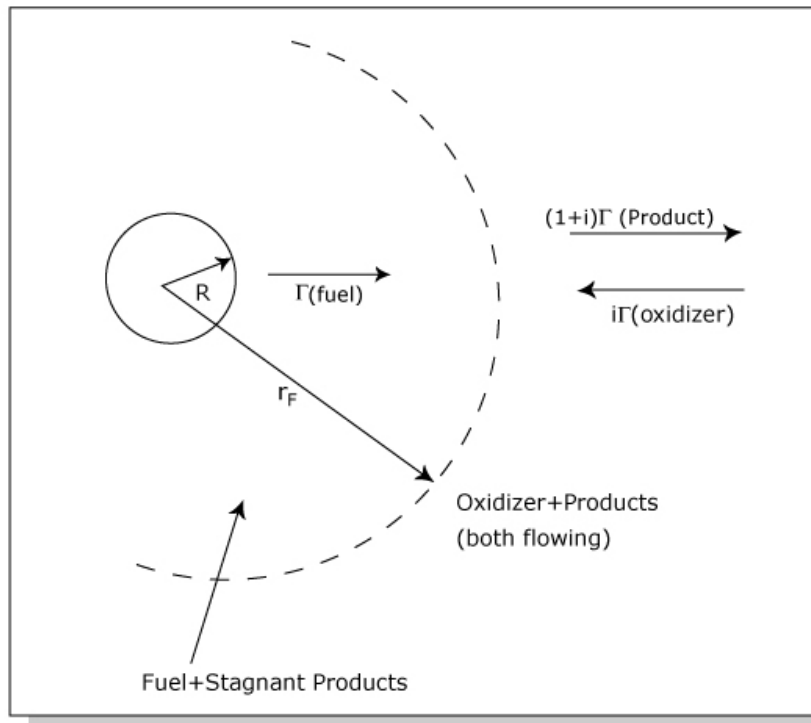
where

$$\lambda_f = \frac{\Gamma}{4 \pi (\rho D_f)}$$

and the product  $\rho D_f$  is taken to be constant.

While this gives information about the composition of the gas near the droplet, the more important results come from a similar mass balance outside the flame radius ( $r > r_f$ ).

Assume  $c_{p_f} = c_{p_{ox}} = c_{p_{prods.}}$ ,  $k^+ = k^- = k$ ,  $\rho_g D = \frac{k}{C_p}$



For  $r > r_F$ , the oxidizer mass balance is

$$\Gamma Y_{ox} = 4 \pi r^2 \rho D \frac{dY_{ox}}{dr} = -i \Gamma \quad (1)$$

or

$$\frac{dY_{ox}}{d(1/r)} + \frac{\Gamma}{4 \pi \rho D} Y_{ox} = -\frac{i \Gamma}{4 \pi \rho D} \quad (2)$$

Define  $\lambda = \frac{\Gamma}{4 \pi \rho D} \approx \frac{\Gamma C_p}{4 \pi k}$  (3)

and impose  $Y_{ox}(r = \infty) = Y_{ox,\infty}$  (4)

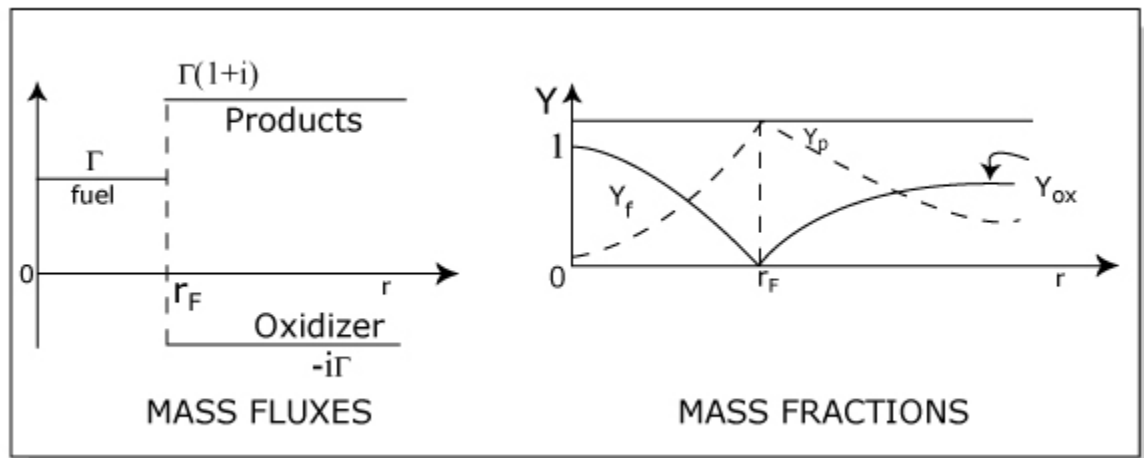
$$Y_{ox} = (i + Y_{ox,\infty}) e^{-\frac{\lambda}{r}} - i \quad (5)$$

Impose also  $Y_{ox}(r = r_F) = 0$ , solve for  $\frac{\lambda}{r_F}$ :

$$\frac{\lambda}{r_F} = \ln\left(1 + \frac{Y_{ox,\infty}}{i}\right) \quad (6)$$

which is a relationship between  $\Gamma$  and  $r_F$  ( $r_F$  turns out to be proportional to  $\Gamma$ , i.e., a “blowing” effect)

The distribution of both, mass fluxes and mass fractions are displayed below:



We now need the heat flux balance, both inside and outside the flame:

$R < r < r_F$  - Taking  $T = T_v$  as the (temporary) enthalpy zero, the convected heat flow inside the flame, where only fuel vapor moves, is  $\Gamma c_p (T - T_v)$ . The conductive flow is  $-4 \pi r^2 k \frac{dT}{dr}$ , The total, flowing inward (negative) is used at  $r = R$  to vaporize liquid, at  $L$  (latent heat) per unit mass:

$$\Gamma c_p (T - T_r) - 4 \pi r^2 k \frac{dT}{dr} = -\Gamma L \quad (7)$$

$$\frac{dT}{d(1/r)} + \frac{\Gamma c_p}{4 \pi k} (T - T_v) = -\frac{\Gamma L}{4 \pi k} \quad (8)$$

λ again

Imposing  $T(R) = T_v$ , this integrates to

$$T - T_v = \frac{L}{c_p} \left[ e^{\lambda \left( \frac{1}{R} - \frac{1}{r} \right)} - 1 \right] \quad (9)$$

and, in particular, at  $r = r_f$

$$\boxed{T_f - T_v = \frac{L}{c_p} \left[ e^{\lambda \left( \frac{1}{R} - \frac{1}{r_f} \right)} - 1 \right]} \quad (10)$$

which also relates  $\Gamma$  (in  $\lambda$ ) to  $r_f$ , but also introduces  $T_f$ , the flame temperature, as a third unknown. We will need the heat flux balance for  $r > r_f$  to complete the formulation. For this purpose, we now move the enthalpy zero to  $T = T_f$ , the flame temperature. The total heat flow (convection plus diffusive) is now

$$\Gamma c_p (T - T_f) - 4 \pi r^2 k \frac{dT}{dr}$$

and this must be the heat released at the flame front, minus the heat sent inwards from the flame to the liquid. The former is  $\Gamma Q$  ( $Q =$  heat of combustion per unit fuel mass). The latter would be  $\Gamma L$ , except for the extra  $\Gamma c_p (T_f - T_v)$  due to the change of enthalpy references. Altogether,

$$\Gamma c_p (T - T_f) - 4 \pi r^2 k \frac{dT}{dr} = \Gamma [Q - L - c_p (T_f - T_v)] \quad (11)$$

or

$$\frac{dT}{d(1/r)} + \frac{\Gamma c_p}{4 \pi k} (T - T_f) = \frac{\Gamma}{4 \pi k} [Q - L - c_p (T_f - T_v)] \quad (12)$$

Integrating with  $T(\infty) = T_\infty$  as a boundary condition,

$$T - T_f = \frac{Q - L - c_p (T_f - T_v)}{c_p} \left( 1 - e^{-\frac{\lambda}{r}} \right) + (T_\infty - T_f) e^{-\frac{\lambda}{r}} \quad (13)$$

and particularizing at  $r = r_f$  ( $T = T_f$ ),

$$\boxed{T_F - T_\infty = \frac{Q - L - c_p (T_F - T_v)}{c_p} \left( e^{\frac{\lambda}{r_F}} - 1 \right)} \quad (14)$$

which is the needed extra relationship to complement (6) and (10)

Eqs. (10) and (14) can be simplified if  $\frac{\lambda}{r_F}$  is substituted from (6):

$$T_F - T_v = \frac{L}{c_p} \left( \frac{e^{\lambda/R} - 1}{1 + \frac{Y_{ox,\infty}}{i}} \right) \quad (10')$$

$$T_F - T_\infty = \frac{Q - L - c_p (T_F - T_v) Y_{ox,\infty}}{c_p i} \quad (14')$$

Eliminate  $T_F$  between these two equations:

$$T_v + \frac{L}{c_p} \left( \frac{e^{\lambda/R} - 1}{1 + \frac{Y_{ox,\infty}}{i}} \right) - T_\infty = \left[ \frac{Q - L}{c_p} - \frac{L}{c_p} \left( \frac{e^{\lambda/R} - 1}{1 + \frac{Y_{ox,\infty}}{i}} \right) \right] \frac{Y_{ox,\infty}}{i}$$

$$\frac{L}{c_p} \frac{e^{\lambda/R}}{1 + \frac{Y_{ox,\infty}}{i}} \left( 1 + \frac{Y_{ox,\infty}}{i} \right) = \frac{Q}{c_p} \frac{Y_{ox,\infty}}{i} + \frac{L}{c_p} + T_\infty - T_v \quad (15)$$

Solve for  $\frac{\lambda}{R}$ , and use  $\lambda = \frac{\Gamma c_p}{4 \pi k}$ :

$$\boxed{\Gamma = \frac{4 \pi k}{c_p} R \ln \left[ 1 + \frac{Q Y_{ox,\infty} / i + c_p (T_\infty - T_v)}{L} \right]} \quad (16)$$

In the literature, this is written as

$$\Gamma = \frac{4 \pi k}{c_p} R \ln[1 + B] \quad (17)$$

with  $B \equiv \frac{Q Y_{\text{ox},\infty} / i + c_p (T_\infty - T_v)}{L}$  (18)

(the Spaulding parameter).

We have solved for  $\Gamma$ , and can go back to (6) to get the flame radius

$$r_f = R \frac{\ln(1 + B)}{\ln\left(1 + \frac{Y_{\text{ox},\infty}}{i}\right)} \quad (19)$$

and to (10') to get  $T_F$ . From (15), (18),  $i^{1/R} = 1 + B$ , and then, from (10'),

$$T_F = T_v + \frac{L}{c_p} \frac{B - Y_{\text{ox},\infty} / i}{1 + Y_{\text{ox},\infty} / i} \quad (20)$$



### Order of Magnitude:

Assume an oxidizer-rich LOX-kerosene burner, with  $(O/F)_s = i = 2.4$ , and  $O/F = 3$ .

This gives  $Y_{ox,\infty} = \frac{3 - 2.4}{1 + 3} = 0.15$ . The heat of reaction is roughly  $Q = 4.3 \times 10^7$

J/Kg/fuel and the fuel latent heat is  $L = 2.5 \times 10^5$  J/Kg. Assume the surrounding gas is at  $T_\infty - T_v = 2000$ K, and take  $C_p \approx 2000$  J/Kg/K. We calculate

$$\frac{Y_{ox,\infty}}{i} = \frac{0.15}{2.4} = 0.0625$$

$$B = \frac{4.3 \times 10^7 \times 0.0625 + 2 \times 10^3 \times 2 \times 10^3}{2.5 \times 10^5} = 26.8$$

In view of these numbers,  $\ln\left(1 + \frac{Y_{ox,\infty}}{i}\right) \approx \frac{Y_{ox,\infty}}{i} \ll 1$ , but  $B \gg 1$ , so (19) and (20) can simplify further to

$$r_f \approx R \frac{i}{Y_{ox,\infty}} \ln(1 + B) \quad (19')$$

$$T_f \approx T_v + \frac{L}{c_p} B = T_\infty + \frac{Q Y_{ox,\infty}}{c_p} / i \quad (20')$$

**Vaporization time** - The droplet is actually being consumed, so its radius varies (on a slower time than the gas transit time), according to

$$\rho_l 4 \pi R^2 \frac{dR}{dt} = -\Gamma \quad (21)$$

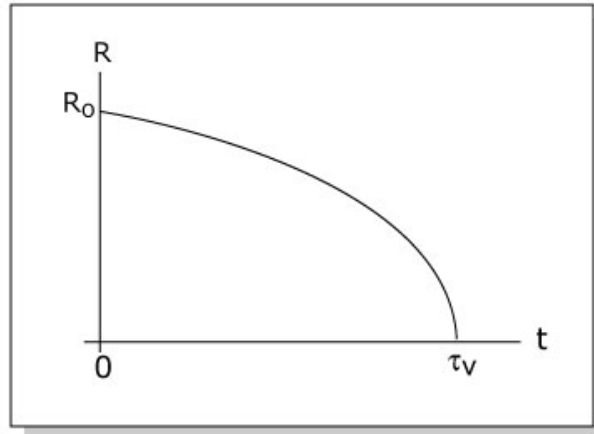
and since  $\Gamma$  is given by (17)

$$\rho_e \cancel{4\pi R^2} \frac{dR}{dt} = -\cancel{4\pi} \frac{k}{c_p} R \ln(1 + B)$$

$$\rho_l \frac{R_0^2 - R^2}{2} = \frac{k}{c_p} \ln(1 + B) t \quad R = R_0 \sqrt{1 - \frac{2k \ln(1 + B)}{\rho_l c_p R_0^2} t}$$

or  $\boxed{\frac{R}{R_0} = \sqrt{1 - \frac{t}{\tau_v}}}$  ;  $\boxed{\tau_v = \frac{\rho_l c_p R_0^2}{2k \ln(1+B)}}$  (22)

$\tau_v$  is the deep vaporization time



For an order of magnitude, assume  $R_0 = 50 \mu\text{m} = 5 \times 10^{-5} \text{m}$ ,  $\rho_l = 800 \text{ Kg/m}^3$ ,  $K \approx 0.1 \text{ W/m/k}$ , plus the numbers used in the previous examples. We calculate

$$\tau_v = \frac{800 \times 2000 \times (5 \times 10^{-5})^2}{2 \times 0.1 \times \ln(1+26.8)} = 6.0 \times 10^{-3} \text{ s} = 6 \text{ ms.}$$

On the other hand, since  $\tau_v \sim R_0^2$ , if  $R_0$  were instead  $10 \mu\text{m}$ ,  $\tau_v$  would be 25 times shorter, or  $2.4 \times 10^{-4}$ . To see the significance of this, assume the gas moves in the combustion chamber at  $M \approx 0.2$ , or  $u_g \sim 240 \text{ m/s}$ . A droplet of radius  $50 \mu\text{m}$  would then require a combustor length no less than  $240 \times 0.006 = 1.44 \text{ m}$ , which is excessive from the mass point of view. A drop of  $R_0 = 10 \mu\text{m}$ , on the other hand, require only 6 cm to evaporate. This brings out clearly the importance of good atomization.

### Other cases

For a fuel drop in a fuel-rich background, everything is the same if we make  $Q=0$  (no flame), and, of course, ignore  $r_f$  and  $T_f$ . In fact, the only equation needed is the  $r < r_f$  heat flow balance (Eq. 9), which, using  $T(\infty) = T_\infty$ , gives

$$T_\infty - T_v = \frac{L}{c_p} [e^{\lambda/R} - 1]$$

and so, finally

$$\frac{\lambda}{R} = \ln \left( 1 + \frac{c_p (T_\infty - T_v)}{L} \right)$$

or  
with

$$\Gamma = \frac{4 \pi k}{c_p} R \ln(1 + B)$$

(as in (17)),

$$B = \frac{c_p (T_\infty - T_v)}{L} \quad (\text{F / F Case}) \quad (23)$$

Again, this is as in (18) if  $Q=0$ .

So, the fuel drop evaporates faster if it is in an oxidizing environment (larger  $B$ ). The reason, clearly, is the extra heating from the nearby flame in that case.

For an oxidizer drop in an oxidizing background (O/O), we have a very similar situation (no flame), so, once again,  $\Gamma_{ox}$  is given by (17), with  $B$  given by (23), but now  $T_v$  and  $L$  must be reinterpreted to be those for the oxidizer liquid.

Finally, for an oxidizer drop in a fuel-rich background, we return to the first case (fuel drop in oxidizing gas), and switch the roles of fuel and oxidizer throughout. For, example,  $Q$  must be the heat of reaction per unit oxidizer mass,  $Y_{ox,\infty}$  must be replaced by  $Y_{f,\infty}$ ,  $i = (O/F)_{st}$  becomes  $1/i$ , and  $(T_v, L)$  refer to the oxidizing liquid.

CALCULATION OF CHAMBER LENGTH  
(Generalizing Spaulding's)

(2000 version)

The drop vaporization time  $T_v = \frac{\rho_l c_p R_0^2}{2k \ln(1+B)}$  depend on B. For a fuel-rich background, as normally seen in rocket, we have two types of droplets:

Fuel drop in fuel-rich medium: 
$$B_{F,F} = \frac{c_p (T_\infty - T_{v,f})}{L_f} \quad (23)$$

Oxidizer drop in fuel-rich medium: 
$$B_{O,F} = \frac{Q Y_{f,\infty} + c_p (T_\infty - T_{v,ox})}{L_{ox}} \quad (24)$$

(notice Q is still the heat of reaction per unit fuel mass). In many cases  $L_{ox} < L_f$  (especially for Lox), and also Q is a large quantity appearing in  $B_{O,F}$ , but not in  $B_{F,F}$ . So,  $B_{O,F} \gg B_{F,F}$ , meaning the oxidizer drops are likely to evaporate much earlier than the fuel drops. For chamber length calculations, then, we focus on the fuel drops mostly.

Assume fuel drops are injected into the chamber at a velocity  $u_{D0}$ . Oxidizer drops are assumed to vaporize very fast (or to be fully evaporated at injection, as when Lox is used). At any section prior to fuel vaporization, the fuel liquid fraction (by flux) is

$$\gamma = \frac{4}{3} \pi R^3 \rho_l n_D u_D \frac{A}{\dot{m}_F} \quad (25)$$

The number-flux of drops  $n_D u_D A$  is conserved, so  $\gamma \sim R^3$  and from (22), since the initial  $\gamma$  is unity,

$$\gamma = \left(1 - \frac{t}{\tau_v}\right)^{3/2} \quad (\tau_v = \text{fuel drop vap. time}) \quad (26)$$

The vaporized fuel fraction is  $1 - \gamma$ , so the gas mean velocity is

$$u_g = \frac{(1 - \gamma) \dot{m}_F + \dot{m}_{ox}}{\rho_g A} \quad (27)$$

and, at the end of the vaporization, this becomes

$$u_2 = \frac{\dot{m}}{\rho_{g_2} A} \quad (28)$$

If the molecular mass difference between fuel and oxidizer fuel and oxidizer vapors is ignored (consistent with earlier approximations), and  $\rho_g$ ,  $T_g$  are nearly uniform, then we treat  $\rho_g$  as a constant, and so

$$\frac{u_g}{u_2} \approx \frac{\dot{m}_F}{\dot{m}} (1 - \gamma) + \frac{\dot{m}_{ox}}{\dot{m}} = \frac{1 - \gamma + O/F}{1 + O/F} \quad (29)$$

or

$$u_g \approx \frac{u_2}{1 + O/F} \left[ 1 + O/F - \left( 1 - \frac{t}{\tau_v} \right)^{3/2} \right] \quad (30)$$

Notice that (29) implies an initial gas mean velocity  $u_g(0) \approx \frac{O/F}{1 + O/F} u_2$ , which is due to the vaporized oxidizer flow.

The particle velocity,  $u_b$  is different from  $u_g$  in general, so there is slip, and therefore drag force. Assuming small Reynolds number around each drop, Stokes flow occurs, so

$$\frac{4}{3} \pi R^3 \rho_l \frac{du_b}{dt} = 6 \pi R \mu_g (u_g - u_b) \quad (31)$$

or, defining a velocity relaxation time

$$\tau_{Rel} = \frac{2 R_0^2 \rho_l}{9 \mu_g} \quad (32)$$

$$\tau_{Rel} \left( \frac{R}{R_0} \right)^2 \frac{du_b}{dt} = u_g - u_b \quad (33)$$

We now introduce non dimensional variable

$$\frac{\tau_v}{\tau_{Ru}} = b \quad ; \quad 1 - \frac{t}{\tau_v} = \theta \quad ; \quad \frac{u_b}{u_2} = v \quad (34)$$

and write (33) as

$$\frac{\theta}{b} \frac{dv}{d\theta} = -\frac{1 + O/F - \theta^{3/2}}{1 + O/F} + v \quad (35)$$

This is a linear, first-order equation for  $v(\theta)$ , although with non-constant coefficients. It can be integrated by standard methods, like parameter variation.

Imposing  $u_D(t=0) = u_{D_0}$ , or  $v(\theta=1) = \frac{u_{D_0}}{u_2}$ , the solution is found to be

$$v = 1 + \left[ \frac{u_{D_0}}{2} - 1 - \frac{2b}{(3-2b)(1+O/F)} \right] \theta^b + \frac{2b}{(3-2b)(1+O/F)} \theta^{3/2} \quad (36)$$

One more integration will yield the vaporization length:

$$L = \int_0^{\tau_v} u_D dt = u_2 \tau_v \int_0^1 v(\theta) d\theta \quad (37)$$

After simplification, this gives the result

$$\frac{L}{u_2 \tau_v} = \frac{1}{1+b} \left[ \frac{u_{D_0}}{u_2} + \left( 1 - \frac{2/5}{1+O/F} \right) b \right] \quad (38)$$

Notice that, from (22) and (32), the parameter  $b$  can be written as

$$b = \frac{\tau_v}{\tau_{Rel}} = \frac{\rho_l c_p R_0^2}{2k \ln(1+B)} \frac{1}{\frac{2}{9} \frac{\rho_l R_0^2}{\mu_g}} = \frac{9 (\mu_g c_p / k)}{4 \ln(1+B)}$$

or  $b = \frac{9}{4} \frac{Pr}{\ln(1+B)} \quad (39)$

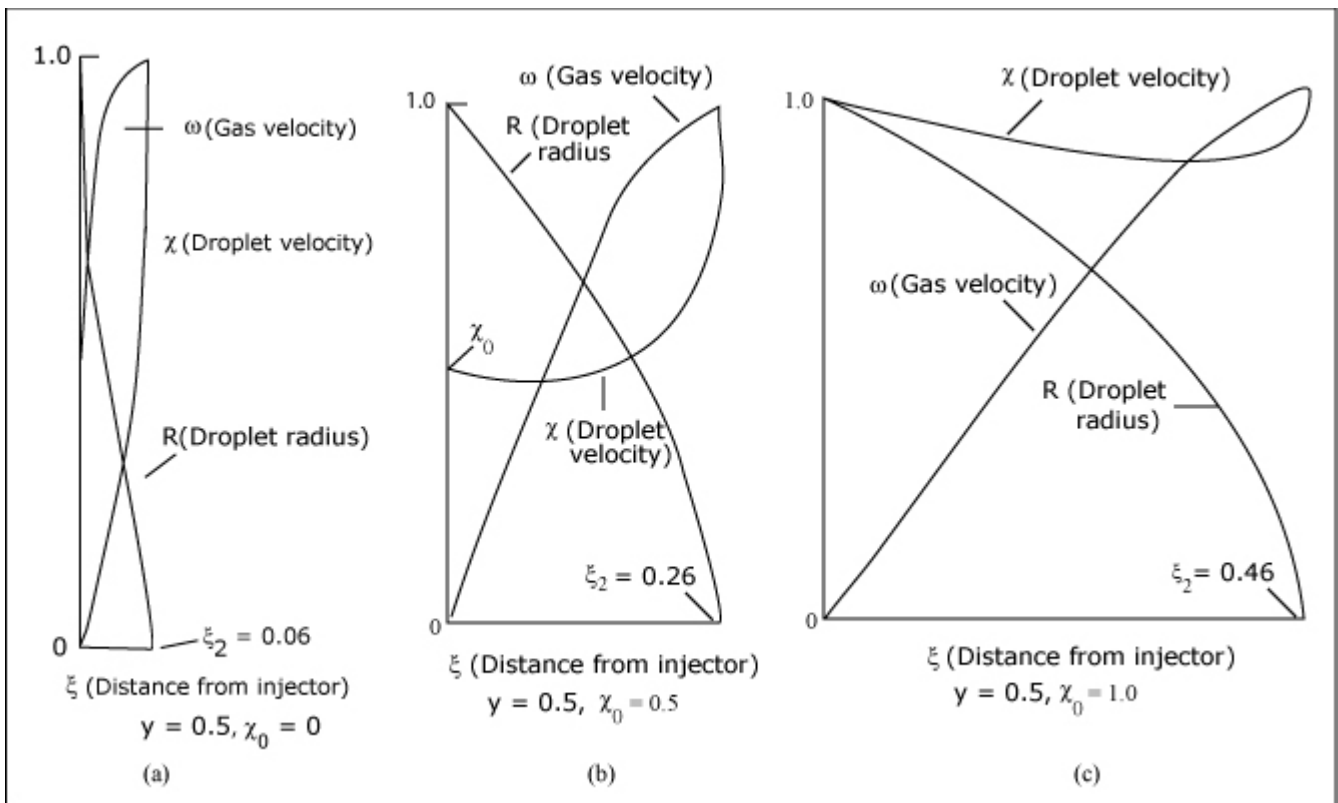
For  $B=30$  and  $Pr=0.8$ , this gives  $b=0.52$ .

Spaulding defined a related parameter  $\xi = 2b$  and presented results for the monopropellant case. We can reduce to that case by setting  $O/F=0$ . Result are shown in the next figure for  $\xi = 0.5$  ( $b = 0.25$ ). The parameter  $\chi_0$  is  $\frac{u_{D_0}}{u_2}$ , and

$$\xi = \frac{x}{2u_2 \tau_v}$$

As an example, for the middle graph  $\chi_0 = 0.5$ , so using  $O/F = 0$  in Eq. (38) we calculate  $\xi_2 = \frac{L}{2u_2 \tau_v} = \frac{1}{2 \times 1.5} (0.5 \times 0.6 \times 0.5)$  or  $\xi_2 = 0.267$ . This coincides with the result in the figure.

Notice how the droplets are initially slowed down by gas drag, but later, as the gas evolves and accelerates, they are pulled along. Near the end of vaporization, the rates accelerate, because the droplets are so light.



Evolution of evaporating droplet size and velocity. Here the reference  $v_{ref}$  for velocity is that of the gas after complete evaporation, and for length,  $l_{ref} = 2v_{ref} \tau_v$

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