MECH 6120: Combustion
Notes on Droplet Combustion

1 Pure Evaporation

The problem here is to determine the rate of evaporation of a droplet. We start with the following assumptions.

1. The rate of change of the droplet radius R is sufficiently 'small' so that the problem can be considered steady (i.e., a quasi–steady assumption).

2. Properties k, c_p, ρ, and D are constant. The first two approximations are reasonable. The last two are not – especially since ρ will vary with $1/T$. It could be relaxed (i.e., $\rho \neq$ constant), but it makes the formulation somewhat more difficult. In the end, the results for $\rho =$ constant and $\rho \neq$ constant are equivalent.

3. The temperature of the droplet is uniform (this is the lumped–capacity assumption).

4. The Lewis number is unity, i.e., $D = \alpha$ (note that $\alpha = k/\rho\,c_p$, so assuming k and c_p constant would imply that $\rho\,D$ is constant, or $D \sim 1/\rho$. But here we assume that both D and ρ are constant).

We assume that we know the temperature and the species mass fractions both at the surface and at infinity (far from the droplet). The goal of the problem is to predict the velocity u of the vapor leaving the droplet surface. Once we have this, we can find the mass transfer from the surface and the evaporation rate.

First, review the relationships for the liquid–vapor interface (which exists at $r = R$). Mass conservation gives

$$\rho_l\,u_{l,R} = \rho\,u_R \tag{1}$$

where subscript l denotes the liquid phase, and R denotes that the property is evaluated at the surface. It is implied that the right–hand side corresponds to the gas phase (i.e., the g subscript is omitted). Also, $\rho_R = \rho =$ constant – per our assumptions.

The mass fraction of fuel in the liquid is $Y_{f,l}$, and in the gas phase at the surface it is $Y_{f,R}$. Note that $Y_{f,l} > Y_{f,R}$, i.e., there is a 'jump' in fuel mass fraction at the surface.

In the liquid, only convection brings the fuel to the surface (liquid–phase diffusion is negligible). In the gas, both convection and diffusion bring the fuel away from the surface. The species balance for fuel at the interface is then

$$\rho_l\,u_{l,R}\,Y_{f,l} = \rho\,u_R\,Y_{f,R} - \rho D\,\frac{dY_f}{dr}\bigg|_{r=R} \tag{2}$$

Use Eq. (1) and solve for u_R:

$$u_R = -\frac{D}{Y_{f,l} - Y_{f,R}}\,\frac{dY_f}{dr}\bigg|_{r=R} \tag{3}$$

We could also perform a similar balance on the transfer of O_2 across the interface, which would give the result

$$u_R = -\frac{D}{Y_{O_2,l} - Y_{O_2,R}}\,\frac{dY_{O_2}}{dr}\bigg|_{r=R} \tag{4}$$

in which $Y_{O_2,l}$ and $Y_{O_2,R}$ are the mass fractions of O_2 in the liquid (typically zero) and in the vapor at the surface.

The energy balance at the interface is similar to the species balance. We neglect conduction in the liquid phase (T is uniform). In the gas, both convection and conduction bring energy from the surface. The first law at the surface is:

$$\rho_l\,u_{l,R}\,h_l = \rho\,u_R\,h_{g,R} - k\,\frac{dT}{dr}\bigg|_{r=R} \tag{5}$$

Both the liquid enthalpy h_l and the vapor enthalpy h_g would be evaluated at the droplet temperature T_l (unlike mass fraction, the temperature is continuous from the liquid to the vapor phase). The difference in vapor and liquid enthalpies is h_{lg}, the latent heat of vaporization. Using Eq. (1) in the above, and making the substitution $\alpha = k/\rho\,c_p$, gives

$$u_R = \frac{\alpha\,c_p}{h_{lg}}\,\frac{dT}{dr}\bigg|_{r=R} \tag{6}$$

Equation (3) says that mass transfer (i.e., u_R) results from diffusion of the vapor away from the surface, whereas Eq. (6) says that mass

transfer results from heat transfer into the surface (and subsequent vaporization). Both are equivalent. Since there can only be one value of u_R, these two relations imply that the mass fraction and temperature fields are coupled – which they are.

We can now proceed to the problem of determining the gas–phase mass fraction and temperature profiles. The continuity equation is

$$\nabla \cdot \rho \, \mathbf{u} = 0 \tag{7}$$

which, in spherical coordinates, is

$$\frac{1}{r^2} \frac{d}{dr} r^2 \, \rho \, u = 0 \tag{8}$$

or

$$r^2 \, \rho \, u = \text{constant} = R^2 \rho \, u_R \tag{9}$$

The species equation (in spherical coordinates) is

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \rho \, u \, Y_f \right) = \frac{\rho D}{r^2} \frac{d}{dr} r^2 \frac{dY_f}{dr} \tag{10}$$

Use Eq. (9) in the above and simplify:

$$R^2 u_R \frac{dY_f}{dr} = D \frac{d}{dr} r^2 \frac{dY_f}{dr} \tag{11}$$

Before we solve this DE, it is useful to define 'normalized' variables which make the boundary conditions somewhat easier to formulate. Define

$$b_f \equiv \frac{Y_f - Y_{f,\infty}}{Y_{f,l} - Y_{f,R}} \tag{12}$$

where $Y_{f,\infty}$ is the ambient (or free–stream) fuel mass fraction – which is typically zero. The interface velocity condition, Eq. (3), becomes

$$u_R = -D \left. \frac{db_f}{dr} \right|_{r=R} \tag{13}$$

The DE, Eq. (11), becomes

$$R^2 \, u_R \frac{db_f}{dr} = D \frac{d}{dr} r^2 \frac{db_f}{dr} \tag{14}$$

and the boundary conditions are

$$b_f = b_{f,R} = \frac{Y_{f,R} - Y_{f,\infty}}{Y_{f,l} - Y_{f,R}}, \quad r = R \tag{15}$$

$$b_f = 0, \quad r \to \infty \tag{16}$$

This DE/BC problem is easy to solve. Integrate Eq. (14) once:

$$R^2 u_R b_f = D \, r^2 \frac{db_f}{dr} + C_1 \tag{17}$$

Now set $r = R$, and use the interface condition in Eq. (13) to evaluate the integration constant:

$$C_1 = R^2 u_R b_{f,R} - D \, R^2 \left. \frac{db_f}{dr} \right|_{r=R} = R^2 u_R (b_{f,R} + 1) \tag{18}$$

Replace this back in Eq. (17):

$$-R^2 u_R (1 + b_{f,R} - b_f) = D \, r^2 \frac{db_f}{dr} \tag{19}$$

Separate the variables and integrate again:

$$\frac{R^2 u_R}{D \, r} = - \ln(1 + b_{f,R} - b_f) + C_2 \tag{20}$$

Let $r \to \infty$ and use Eq. (16):

$$C_2 = \ln(1 + b_{f,R}) \tag{21}$$

This gives us the complete solution to the problem. The implicit formula for b_f is

$$\ln \left(\frac{1 + b_{f,R}}{1 + b_{f,R} - b_f} \right) = \frac{R^2 \, u_R}{D} \cdot \frac{1}{r} \tag{22}$$

We could solve this explicitly for b_f, but the above form is useful enough. Now set $r = R$ (and $b_f = b_{f,R}$) and solve for the interface velocity:

$$u_R = \frac{D}{R} \ln(1 + b_{f,R}) = \frac{D}{R} \ln(1 + B_f) \tag{23}$$

where the transfer number B_f is defined

$$B_f = b_{f,R} = \frac{Y_{f,R} - Y_{f,\infty}}{Y_{f,l} - Y_{f,R}} \tag{24}$$

We can also work out the problem from a heat transfer approach. The energy equation will be

$$R^2 u_R \frac{dT}{dr} = \alpha \frac{d}{dr} r^2 \frac{dT}{dr} \tag{25}$$

Define the normalized variable

$$b_T \equiv \frac{c_P(T_\infty - T)}{h_{lg}} \tag{26}$$

Using the fact that $\alpha = D$, the interface velocity condition, Eq. (6), becomes

$$u_R = -\alpha \left. \frac{db_T}{dr} \right|_{r=R} = -D \left. \frac{db_T}{dr} \right|_{r=R} \tag{27}$$

and the DE becomes

$$R^2 u_R \frac{db_T}{dr} = D \frac{d}{dr} r^2 \frac{db_T}{dr} \tag{28}$$

with boundary conditions

$$b_T = b_{T,R} = \frac{c_P(T_\infty - T_l)}{h_{lg}}, \quad r = R \tag{29}$$

$$b_T = 0, \quad r \to \infty \tag{30}$$

This is the same DE and same BCs as for the species equation. The solution is therefore the same. We get

$$u_R = \frac{D}{R} \ln(1 + B_T) \tag{31}$$

$$B_T = b_{T,R} = \frac{c_P(T_\infty - T_l)}{h_{lg}} \tag{32}$$

Note that the mass transfer and heat transfer results imply that $B_T = B_f$. This is a feature of our assumptions – especially $D = \alpha$.

2 Evaporation with combustion

We now have a situation in which a diffusion flame forms around the droplet. The position of the flame is $r = r_f$. In addition to the assumptions made in the pure evaporation case, we assume that the flame thickness is infinitesimally small – which is equivalent to an 'infinite–rate' kinetics model. The flame forms a boundary, separating a region with fuel and combustion products (on the inside) from a region with oxygen and combustion products (on the outside). Neither fuel nor O_2 can penetrate the flame, and their mass fractions directly at the flame go to zero.

As before, we want to predict the burning rates. The interface boundary conditions (i.e., Eqs. (3), (4), (6)) remain the same – since the reaction occurs completely in the gas phase. The DEs in the gas phase, however, will now include the source (or sink) terms corresponding to the reaction. In particular, the DEs for fuel, O_2, and energy will appear

$$R^2 u_R \frac{dY_f}{dr} = \alpha \frac{d}{dr} r^2 \frac{dY_f}{dr} + \frac{r^2 \dot{\omega}_f \, MW_f}{\rho} \tag{33}$$

$$R^2 u_R \frac{dY_{O_2}}{dr} = \alpha \frac{d}{dr} r^2 \frac{dY_{O_2}}{dr} + \frac{\nu \, r^2 \dot{\omega}_f \, MW_f}{\rho} \tag{34}$$

$$R^2 u_R \frac{dT}{dr} = \alpha \frac{d}{dr} r^2 \frac{dT}{dr} - \frac{r^2 \dot{\omega}_f \, MW_f \, LHV}{\rho \, c_p} \tag{35}$$

In the above, ν is the stoichiometric O_2/fuel ratio (kg O_2/kg fuel), and $\dot{\omega}_f \, MW_f$ is the fuel reaction rate (kg fuel/m$^3 \cdot s$). Note that the O_2 reaction rate, $\dot{\omega}_{O_2} \, MW_{O_2}$, would be ν times the fuel reaction rate. And both these numbers would be negative.

The presence of the reaction rate terms make solution of the DEs difficult. Note that, according to our 'infinite–rate' assumptions, the reaction rates would mathematically appear as delta functions – in that they would be zero for all positions except directly at the flame. We can avoid the reaction rate terms by defining 'coupling' functions. For example, divide Eq. (34) through by ν and subtract it from Eq. (33). If we define

$$f_{fo} = Y_f - \frac{Y_{O_2}}{\nu} \tag{36}$$

we find that f_{fo} satisfies

$$R^2 u_R \frac{df_{fo}}{dr} = \alpha \frac{d}{dr} r^2 \frac{df_{fo}}{dr} \tag{37}$$

Likewise, we can define

$$f_{Tf} = \frac{c_p T}{LHV} + Y_f \tag{38}$$

$$f_{To} = \frac{c_p T}{LHV} + \frac{Y_{O_2}}{\nu} \tag{39}$$

and each of these satisfies Eq. (37). So we have come up with variables which eliminate the reaction rate from the DE.

What we want to do now is 'renormalize' the f variables so that we get a problem identical to that solved for the pure evaporation case. If the DE and BCs are the same, the solution is the same. Referring to Eqs. (14) and (28), the DEs for the b variables – which were used for the pure evaporation model – are already identical to the DE for f, Eq. (37) (remember that $\alpha = D$). But the f variables will not, as currently defined, satisfy the same BCs as the b variables. However, Eq. (37) is homogeneous and linear. It follows that if f is a solution, then $b = c_1 f + c_2$ is also a solution – where c_1 and c_2 are constants. We therefore want to choose c_1 and c_2 so that the new, 'renormalized' b satisfies the pure evaporation boundary conditions.

The first criterion is that $b \to 0$ for $r \to \infty$. So we can define b as $b = c_1(f - f_\infty)$, where f_∞ is the value of f evaluated at $r \to \infty$. Secondly, we want b to satisfy the interface velocity condition:

$$u = -\alpha \left. \frac{db}{dr} \right|_{r=R} \tag{40}$$

or, using $b = c_1(f - f_\infty)$,

$$c_1 = -u \cdot \left(\alpha \left. \frac{df}{dr} \right|_{r=R} \right)^{-1} \tag{41}$$

To figure out the right–hand–side, we need to substitute in the specific definitions of the f variables (Eqs. (36), (38) and (39)) and the interface relations given in Eqs. (3), (4), and (6). (Ignore, for the time being, that the O_2 concentration – and dY_{O_2}/dr – will be zero at the surface, per our diffusion flame assumption, which means that Eq. (4) would be

indeterminant). For the fo coupling, we get

$$\alpha \left. \frac{df_{fo}}{dr} \right|_{r=R} = \alpha \left(\left. \frac{dY_f}{dr} \right|_{r=R} - \frac{1}{\nu} \left. \frac{dY_{O_2}}{dr} \right|_{r=R} \right)$$
$$= -u \left(Y_{f,l} - Y_{f,R} - \frac{1}{\nu}(Y_{O_2,l} - Y_{O_2,R}) \right)$$

Combine this with Eq. (41) and we get our definition of b_{fo}:

$$b_{fo} = \frac{Y_f - Y_{f,\infty} - \frac{1}{\nu}(Y_{O_2} - Y_{O_2,\infty})}{Y_{f,l} - Y_{f,R} - \frac{1}{\nu}(Y_{O_2,l} - Y_{O_2,R})} \tag{42}$$

Likewise, for the Tf and To couplings, we get

$$b_{Tf} = \frac{\frac{c_p}{LHV}(T_\infty - T) + Y_{f,\infty} - Y_f}{\frac{h_{lg}}{LHV} + Y_{f,l} - Y_{f,R}} \tag{43}$$

$$b_{To} = \frac{\frac{c_p}{LHV}(T_\infty - T) + \frac{1}{\nu}(Y_{O_2,\infty} - Y_{O_2})}{\frac{h_{lg}}{LHV} + \frac{1}{\nu}(Y_{O_2,l} - Y_{O_2,R})} \tag{44}$$

Our problem is now completely equivalent to the pure evaporation case. The velocity at the surface is given by

$$u_R = \frac{\alpha}{R} \ln(1 + B) \tag{45}$$

where the transfer number B is b evaluated at the surface, and can be

obtained from the fo, Tf, or To couplings:

$$B = B_{fo} = B_{Tf} = B_{To}$$

$$B_{fo} = \frac{Y_{f,R} - Y_{f,\infty} - \frac{1}{\nu}(Y_{O_2,R} - Y_{O_2,\infty})}{Y_{f,l} - Y_{f,R} - \frac{1}{\nu}(Y_{O_2,l} - Y_{O_2,R})} \qquad (46)$$

$$B_{Tf} = \frac{\frac{c_p}{LHV}(T_\infty - T_l) + Y_{f,\infty} - Y_{f,R}}{\frac{h_{lg}}{LHV} + Y_{f,l} - Y_{f,R}} \qquad (47)$$

$$B_{To} = \frac{\frac{c_p}{LHV}(T_\infty - T_l) + \frac{1}{\nu}(Y_{O_2,\infty} - Y_{O_2,R})}{\frac{h_{lg}}{LHV} + \frac{1}{\nu}(Y_{O_2,l} - Y_{O_2,R})} \qquad (48)$$

Commonly, the droplet will consist of pure fuel, so $Y_{f,l} = 1$ and $Y_{O_2,l} = Y_{O_2,R} = 0$. At infinity, we can also assume that the fuel concentration is zero, so $Y_{f,\infty} = 0$. When combustion is present, the temperature of the droplet will be close to the boiling (or saturation) temperature of the fuel at the given total pressure, so $T_l = T_B$. We could obtain the fuel mass fraction at the surface, $Y_{f,R}$, by assuming that the partial pressure of the fuel at the surface is equal to the saturation pressure (thermodynamic equilibrium) – and then relate the partial pressure to the mass fraction. An easier route is to use the To formula for B – since this does not involve mass fractions at the surface. Using the above assumptions:

$$B_{To} = \frac{c_p}{h_{lg}}(T_\infty - T_B) + \frac{LHV\,Y_{O_2,\infty}}{\nu\,h_{lg}} \qquad (49)$$

2.1 Location of the flame and flame temperature

Go back to Eq. (22). The general solution for the b variable is

$$\ln\left(\frac{1+B}{1+B-b}\right) = \frac{R^2\,u_R}{\alpha} \cdot \frac{1}{r}$$

where we've used the fact that $b_R \equiv B$. Combine this with

$$u_R = \frac{\alpha}{R}\ln(1+B) \qquad (50)$$

to get

$$\frac{r}{R} = \frac{\ln(1+B)}{\ln\left(\dfrac{1+B}{1+B-b}\right)} \qquad (51)$$

Realize that the above is the solution for any of the 3 b variables given in Eqs. (42–44). And – at any point in the flame, all of the three b variables must be equal to each other.

Per our infinite–kinetics assumption, both Y_f and Y_{O_2} will be zero at the flame. It follows from Eq. (42) that the value of b_{fo} at the flame (denoted $b_{fo,F}$) will be

$$b_{fo,F} = \frac{Y_{O_2,\infty}}{\nu(1 - Y_{f,R})} \qquad (52)$$

Likewise, if we assume zero O_2 on the fuel side of the flame, and zero fuel on the O_2 side of the flame, the equation for B_{fo}, Eq. (46), gives

$$B_{fo} = \frac{Y_{f,R} + \dfrac{Y_{O_2,\infty}}{\nu}}{1 - Y_{f,R}} \qquad (53)$$

Combine the previous two equations with Eq. (51), and the flame position is

$$\frac{r_F}{R} = \frac{\ln(1+B)}{\ln\left(1 + \dfrac{Y_{O_2,\infty}}{\nu}\right)} \qquad (54)$$

We see that the distance from the surface to the flame will depend on the mass transfer rate through the $\ln(1 + B)$ term. As the burning rate increases, the flame moves farther away from the droplet.

The expression for r_F/R usually predicts results different than experimental measurements for two reasons:

1. Buoyancy of hot combustion gases affects the flame shape so that it is not spherical – experimental values of r_F/R may be difficult to assign.

2. The region of maximum luminosity is usually used to define r_F, and this will generally be different than the position of maximum temperature which, as we will see below, theoretically defines the flame location. Maximum luminosity occurs where the concentration of carbonaceous soot particles is greatest, and this occurs on the fuel–side of the flame.

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In the expression for r_F, we have (implicitly) assumed that $r_F > R$ – i.e., the flame is in the gas phase. We see from Eq. (54) that in the limit of $B \to Y_{O_2,\infty}/\nu$ the flame 'collapses' onto the fuel surface. From Eq. (53), this limit would be attained for $Y_{f,R} \to 0$ – which would correspond to a fuel that does not vaporize prior to combustion (such as solid carbon). For such a combustion process, the reaction occurs in the solid rather than the gas phase. Consequently, the gas phase equations for solid combustion no longer contain reaction rate terms – but the boundary conditions will.

2.2 Flame temperature

To predict the flame temperature, we use the fact that the solution for b_{fo} will be identical to the solution for b_{To}, since both satisfy the same DE and BC's. We know the value of b_{fo} at the flame – therefore we know the value of b_{To} at the flame, from which we can get the flame temperature. Using the thin flame assumption and Eqs. (44) and (52), we have

$$b_{To,F} = \frac{c_p}{h_{lg}} \left(T_\infty - T_F \right) + \frac{Y_{O_2,\infty} LHV}{\nu h_{lg}}$$
$$= b_{fo,F} = \frac{Y_{O_2,\infty}}{\nu(1 - Y_{f,R})} \qquad (55)$$

We can determine $Y_{f,R}$ in the above by equating B_{fo} and B_{To}, i.e.,

$$B_{fo} = \frac{Y_{f,R} + \dfrac{Y_{O_2,\infty}}{\nu}}{1 - Y_{f,R}} = B_{To} = \frac{c_p}{h_{lg}}(T_\infty - T_B) + \frac{LHV Y_{O_2,\infty}}{\nu\, h_{lg}} \qquad (56)$$

where T_B is again the boiling temperature of the liquid. Eliminating $Y_{f,R}$ between the above two equations and solving for T_F yields

$$T_F = T_B + \frac{T_\infty - T_B + \dfrac{Y_{O_2,\infty}}{\nu c_p}(LHV - h_{lg})}{\dfrac{Y_{O_2,\infty}}{\nu} + 1} \qquad (57)$$

Actually, we could derive the above temperature from a pure energy–balance point of view. Per unit mass of fuel, the quantity of heat released from the reaction is LHV. This heat does three things: 1) it vaporizes a unit mass of fuel, 2) it raises the temperature of the vaporized fuel from T_B to T_F, and 3) it raises the temperature of the oxygen and inert species from T_∞ to T_F. In the free stream, all we have is oxygen and inerts (i.e., N_2). So for every 1 g of oxygen, we have $(1 - Y_{O_2,\infty})/Y_{O_2,\infty}$ g of inerts. Since it takes ν g of oxygen to react with 1 g of fuel, we have

$$\begin{matrix} \text{mass oxygen \&} \\ \text{inerts per unit} \\ \text{mass of fuel} \end{matrix} = \nu(1 + \frac{1 - Y_{O_2,\infty}}{Y_{O_2,\infty}}) = \frac{\nu}{Y_{O_2,\infty}} \qquad (58)$$

The energy balance can then be written

$$LHV = h_{lg} + c_p(T_F - T_B) + \frac{\nu}{Y_{O_2,\infty}} c_p(T_F - T_\infty) \qquad (59)$$

which, upon solving for T_F, yields the exact same formula as that given by Eq. (57). The energy balance approach defines the adiabatic flame temperature for the liquid fuel. This temperature will be lower that the adiabatic flame temperature for the same fuel in a vapor phase because of the heat required to vaporize the fuel.

2.3 Spray Combustion

In most combustion devices using liquid fuels (i.e., diesel engines, jet engines) the fuel is atomized, or broken up into droplets, prior to the combustion process. The degree of atomization profoundly affects the performance of liquid fuel combustion devices. Commonly, it is desirable to produce the minimum droplet size – because this will produce the maximum total surface area for a given mass of fuel. Another design criteria of atomizers is the nature of the spray pattern. Some atomizers are designed to produce a region relatively free of drops along the spray axis (hollow cone), where others produce a uniform density of drops (full cone).

Atomizers used in combustion devices (commonly referred to as injectors) can be classified into two major categories:

1. *Pressure–atomizing injectors:* Here the fuel injector is simply a small orifice through which the fuel is forced with a high velocity into relatively quiescent air. A common example is the nozzle on a garden hose. The fuel, as it issues from the nozzle, forms into a conical surface. Instabilities arising from surface tension and fluid turbulence break up the surface into droplets.

2. *Twin–fluid injectors:* Atomization is accomplished here by inject-
ing the fuel jet at a relatively low velocity into a high–velocity air
stream. The drag between the fuel and the air breaks the fuel into
droplets. Although twin–fluid injectors are more complicated, they
can produce smaller droplets than pressure atomization.

A table of typical injector devices used in combustion systems is given
in Fig. 1 (from Kuo, p. 519).

The simultaneous burning of a multitude of drops in a combustion
chamber can alter the picture somewhat from the single drop analysis
performed in the previous section. Two major complications arise when
dealing with groups of drops. Firstly, the environment surrounding each
drop is altered due to the combustion of neighboring drops. Each drop is
competing for the same supply of oxidizer, so the oxidizer mass fraction
in the free stream for group combustion will be somewhat lower than
the case for a single drop in an infinite oxidizer. Also, the ambient
temperature 'seen' by each drop will be higher because of the burning
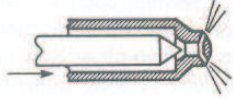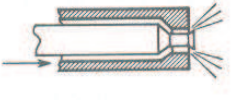of neighboring drops.

The second complicating factor deals with the diffusion of oxidizer into
the 'cloud' of droplets. If the droplet vaporization rate is much higher
than the oxidizer diffusion rate, then it is possible for the droplets to
completely vaporize before combustion occurs. The combustion process
in this situation would then be governed by the laws of gaseous diffu-
sion flames. Also, the length of the spray will be controlled by either
the droplet evaporation time or the oxidizer diffusion time – whichever
is longer. To adequately address this problem, one would have to inves-
tigate the transport of oxidizer into the spray jet – much in the same
way that we investigated jet diffusion flames.

3 Combustion of Solid Fuels

3.1 Introduction

The combustion of solid fuels has been used since the dawn of time to
provide heat and cook food. This form of fuel is also often associated
with the more unpleasant aspects of combustion – i.e., destructive fires.
Solid fuels are attractive because they have been relatively cheap and
abundant (e.g., wood and coal), are easy to handle and store, and can
provide high flame temperature and heat of combustion. In the past,

Figure 1: Typical atomization methods

solid fuels have been used primarily in stationary power plants or large
locomotive or marine propulsion systems. Recently, solid fuels have been
developed for rocket and aircraft propulsion.

When heated, some solids sublime directly to a vapor (such as naphthalene) and some melt into a liquid which then vaporizes (such as candle wax). Combustion of such solid fuels will occur in the gas phase, and our relations for liquid fuels can be used to predict the burning rates, flame positions, and flame temperatures providing the solid–vapor or solid–liquid enthalpy change is accounted for.

Some solids undergo a chemical reaction (known as pyrolyzation) when exposed to heat. Products of this reaction are combustible volatile gases and carbonaceous char. For example, when wood is heated CO, CO_2 and volatile hydrocarbons are formed from pyrolysis reactions and diffuse from the fuel. Determination of the burning rate during the pyrolysis (or devolatilization) stage involves two steps: 1) finding the rate of evolution of the volatiles from the solid as a function of the applied heat flux, and 2) applying the liquid–fuel relations to find the flame position and heat flux to the surface. A key difference between pyrolyzing solid combustion and liquid fuel combustion is that the liquid vaporization is a surface process, whereas the solid devolatilization is volumetric process. To precisely predict the rate of devolatilization from a pyrolyzing solid, one must analyze the heat and mass transfer processes and chemical reactions in the interior of the solid. This can be a formidable process, especially for non–homogeneous solid fuels such as coal. Often devolatilization rates are obtained empirically as a function of heat flux, ambient oxygen concentration and temperature, and other governing parameters.

Note that during devolatilization of a solid fuel, the combustion process occurs in the gas phase. Once all volatiles have been driven off of the fuel, the carbonaceous solid residue (char) is directly attacked by oxygen to yield 'glowing combustion'. In this process combustion is taking place directly in the solid phase.

Metals will burn in either a vapor or a solid phase mode depending upon the boiling temperatures of the metal and the corresponding metal oxide. For nearly all metals, the oxide boiling temperature is greater than the pure metal boiling temperature. The metal will thus vaporize before it oxidizes and combustion occurs in the vapor phase (as in liquid fuels). A few metals, notably boron, silicon, titanium, and zirconium, have boiling temperatures higher than their oxides. Combustion of these metals occurs in the solid phase, similar to solid carbon.

3.2 Combustion of a solid sphere

Here we consider small spherical particles of solid fuels that do not vaporize prior to combustion, i.e., they burn on the surface as oxygen diffuses to the surface.

Since the fuel does not vaporize, $Y_{f,R} = 0$. If we assume infinite–rate kinetics for the surface reaction, the mass fraction of O_2 at the surface will also be zero, and we can directly borrow from the relationships developed for liquid droplet combustion. The mass flux at the surface would be given by

$$\dot{m}_R'' = \frac{\rho\alpha}{R}\ln(1 + B) \qquad (60)$$

and the transfer number would be given by (from Eq. (53))

$$B = B_{fo} = \frac{1}{\nu}(Y_{O_2,\infty} - Y_{O_2,R}) \approx \frac{Y_{O_2,\infty}}{\nu} \qquad (61)$$

The burning rate – which is the rate at which the solid fuel is oxidized – is the mass flux times the particle area:

$$\dot{m} = 4\pi R^2 \dot{m}_R'' = 4\pi R\rho\alpha\ln(1 + B) \qquad (62)$$

The burning rate for this situation depends on (among other things) the value of ν – which in turn will depend on the fuel and the species produced at the surface. For most carbonacueous solid fuels (i.e., wood, coal), the fuel can be approximated as elemental solid carbon, C. Two types of oxidation reactions can occur with this fuel – forming either CO_2 or CO. If carbon dioxide is formed at the surface, then the reaction is

$$C + O_2 \longrightarrow CO_2 \qquad (63)$$

and $\nu = 32/12$. For air, $Y_{O_2,\infty} = 0.233$, so B would have the value 0.087 – which is quite small. We can then make the 'small B' assumption: namely that

$$\ln(1 + B) \approx B = \frac{Y_{O_2,\infty}}{\nu} \qquad (64)$$

and the burning rate is thus proportional to the ambient oxygen content.

For solid carbon combustion the assumption that reaction rates are significantly faster than diffusion rates is often not accurate. If the reaction rates are comparable to or slower than the oxygen diffusion rate, then the thin–flame assumption will not hold and oxygen will build

up at the particle surface. For this situation the transfer number is approximated by

$$B \approx \frac{1}{\nu}(Y_{O_2,\infty} - Y_{O_2,R}) \qquad (65)$$

Since $Y_{O_2,R}$ will be smaller than $Y_{O_2,\infty}$, and $Y_{O_2,\infty}$ is a small number in itself, we can use the small B assumption to write the mass flux from the particle:

$$\dot{m}_R'' = \frac{\rho\alpha}{R}\ln(1+B) \approx \frac{\rho\alpha}{\nu R}(Y_{O_2,\infty} - Y_{O_2,R}) \qquad (66)$$

The above equation is not very useful at this point because the mass fraction of O_2 at the surface, $Y_{O_2,R}$, is an unknown. To complete the problem, we need to introduce chemical kinetics into the analysis. Say the reaction is represented by Eq. (63). The rate at which this reaction occurs would be given by the law of mass action – except some of the quantities are different than what we encountered for pure gas–phase reactions. First, the relevant rate will be the rate of mass consumption (or mole consumption) of carbon per unit <u>surface area</u> of particle – not per unit volume. This is because the reaction occurs on a surface. Secondly, the carbon is in the solid phase, and its concentration does not appear in the rate law. Only the concentration of the O_2 will appear. We can assume that the rate is first–order with respect to O_2 concentration. Since the O_2 concentration at the surface would be proportional to the O_2 mass fraction at the surface, the rate law for carbon consumption could be put into the form

$$\dot{m}_f'' = kY_{O_2,R} \qquad (67)$$

where k is a 'surface reaction rate constant' and would have units of kg/m²·s (i.e., a mass flux). The rate constant k would be dependent mostly on temperature, and to a lesser extent on total pressure. See the text for more discussion on this.

The mass fluxes predicted in the previous two equation would have to be equal. By combining the equations and solving for $Y_{O_2,R}$, we get

$$Y_{O_2,R} = \frac{\frac{\rho\alpha}{R}Y_{O_2,\infty}}{k + \frac{\rho\alpha}{R}} \qquad (68)$$

Using this in Eq. (9) results in

$$\dot{m}_R'' = \frac{Y_{O_2,\infty}}{\nu} \cdot \left(\frac{\frac{k\rho\alpha}{R}}{k + \frac{\rho\alpha}{R}}\right) \qquad (69)$$

We gain two limiting cases from the above equation.

1. <u>Diffusion control:</u> Here $k \gg \rho\alpha/R$ and the mass flux is obtained from our thin–flame approximation, i.e.

$$\dot{m}_R'' = \frac{Y_{O_2,\infty}\rho\alpha}{\nu R} \qquad (70)$$

This condition will occur for large particles (say $> 100\ \mu$m in diameter) and when the surface temperature is high so that k is high.

2. <u>Chemistry control:</u> Here $k \ll \rho\alpha/R$ and the mass flux becomes

$$\dot{m}'' = \frac{kY_{O_2,\infty}}{\nu} \qquad (71)$$

This will occur for small particles and low temperatures.

As noted above, the value of ν will depend on the product formed at the surface. Formation of CO_2 is actually unlikely due to the chemical structure of CO_2 – the C is in between the O atoms. A more probable product is CO. The CO formed at the surface can then diffuse outward to react with the inward diffusing oxygen and the ultimate product CO_2 is formed in the gas phase. In this situation, both a gas phase and a surface reaction are present.

Acutally, little oxygen gets to the surface since it is consumed in oxidizing the CO. Some of the CO_2 formed in this reaction diffuses back to the surface where it is reduced by the solid carbon to form CO. The realistic reaction steps in carbon combustion are thus

$$C + CO_2 \longrightarrow 2CO \quad \text{(surface)}$$

$$CO + \frac{1}{2}O_2 \longrightarrow CO_2 \quad \text{(gas)}$$