UNIT 5

Spray combustion:

Many practical applications liquid fuel is injected into the combustion chamber resulting in fuel spray.

Spray combustion involves many physical processes, including atomization, droplet collision and agglomeration, vaporization, heat and mass transfer, droplet-air and vapor-air mixing, ignition, turbulence, premixed and/or diffusion flames, pollutant production and flame extinction.

The liquid fuel is atomized by the combined action of aerodynamical shear, strain and surface tension producing a large number of small droplets which increase the overall surface area exposed to the oxidizer and enhance the rates of heat and mass transfer.

The atomization of a 1cm diameter droplet of liquid into droplets of 100 μm diameter, for example, produces a million droplets and increases the overall surface area by a factor of 10^4.

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The droplets distribution range from few microns to around 500μm, primarily because practical nozzles cannot produce sprays of uniform drop size at typical operating conditions. Furthermore, many of the larger droplets produced in the initial liquid disintegration undergo further breakup into smaller droplets.

Depending on the droplet distribution, the mode of operation and the state of the ambience, different regimes of burning occur, including

- a diffusion flame lies outside the cloud of droplets burning the ambient oxygen with the fuel that originates from the vaporizing droplets

- droplet burning occurring all throughout the cloud or in a layer on the edge of the cloud,

- internal group combustion with an internal flame that separates a group of vaporizing droplets from a group of individually burning droplets

- individual droplet combustion where individual droplets burn with oxygen diffusing across the resulting cloud of burning droplets

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Droplet Vaporization and Combustion:

Assumptions:

- droplet is a sphere

- single component fuel

- quiescent ambience

- no gravity

- spherical symmetry

- quasi-steady approximation

- one-step overall chemical reaction (F + O $\rightarrow$ Products)
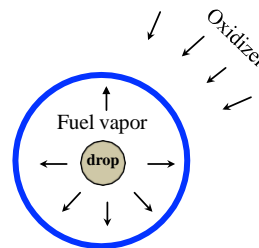
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overall mass conservation of the droplet

$$-\frac{d}{dt}\left(\frac{4}{3}\pi\rho_l r_s^3\right) = \dot{m}$$

mass flow rate
mass per unit time leaving the droplet

$$-4\pi\rho_l r_s^2 \frac{dr_s}{dt} = 4\pi r_s^2 \rho_g v$$

$$\boxed{\frac{dr_s}{dt} = -\frac{\rho_g}{\rho_l}v}$$

Since $\rho_g/\rho_l \ll 1$ (typically $\sim 10^{-2} - 10^{-3}$) the droplet recedes very slowly compared to the diffusion processes.

quasi-steady approximation

$\dot{m}$ or $\rho_g v$ can be determined from the steady equations in the gas phase, with the droplet history determined a-posteriori from the relation above

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In the following, the gas density will be denoted by ρ (with no subscript) and the droplet radius a.

The steady conservation equations are

$$\frac{d}{dr}(r^2\rho v) = 0$$

$$\rho v \frac{dY_F}{dr} - \frac{\rho D_F}{r^2}\frac{d}{dr}\left(r^2\frac{dY_F}{dr}\right) = -v_F W_F \omega$$

$$\rho v \frac{dY_O}{dr} - \frac{\rho D_O}{r^2}\frac{d}{dr}\left(r^2\frac{dY_O}{dr}\right) = -v_O W_O \omega$$
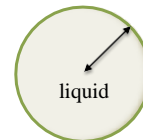
$$\rho v \frac{dT}{dr} - \frac{\lambda}{c_p}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dT}{dr}\right) = \frac{Q}{c_p}\omega$$

$$\rho T = \frac{P_0}{R/W}$$

$$\omega = B\left(\frac{\rho Y_F}{W_F}\right)\left(\frac{\rho Y_O}{W_O}\right)e^{-E/RT}$$

Conditions far away, as $r \rightarrow \infty$

$$T = T_\infty, \quad \rho = \rho_\infty \quad Y_F = 0 \quad Y_O = Y_O$$

liquid

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Conditions at the liquid-gas interface can be derived by integrating the energy (expressed in terms of enthalpy) and species equations across $r = a$.

These equations are:

$$\rho v \frac{dh}{dr} - \frac{\lambda}{r^2} \frac{d}{dr}\left(r^2 \frac{dT}{dr} \right) = 0$$

$$\rho v \frac{dY_i}{dr} - \frac{\rho D_i}{r^2} \frac{d}{dr}\left(r^2 \frac{dY_i}{dr} \right) = -v_i W_i \omega \qquad \text{for } i = F, O$$

and, in view of mass conservation $r^2 \rho v = $ const. can be written as

$$\frac{d}{dr}(r^2 \rho v Y_i) - \frac{d}{dr}\left(\rho D_i r^2 \frac{dY_i}{dr} \right) = -v_i W_i \omega \qquad \text{for } i = F, O$$

$$\frac{d}{dr}(r^2 \rho v h) - \frac{d}{dr}\left(\lambda r^2 \frac{dT}{dr} \right) = 0$$

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Integrating the species equations from $r = a^-$ to $r = a^+$, assuming that no reaction occurs at the interface, yields

$$\left. r^2 \rho v Y_i - \rho D_i r^2 \frac{dY_i}{dr} \right|_{a^-}^{a^+} = 0$$

Concentration gradients inside the droplet will be assumed negligible, and the droplet's content will be assumed to be a pure fuel so that $Y_F = 1$, $Y_O = 0$. Consequently, the conditions at $r = a$ becomes

$$\rho v Y_F - \rho D_F \frac{dY_F}{dr} = \rho v$$

$$\rho v Y_O - \rho D_O \frac{dY_O}{dr} = 0$$

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When the energy equation is similarly integrated, we obtain

$$\left. r^2 \rho v h - \lambda r^2 \frac{dT}{dr} \right|_{a^-}^{a^+} = 0$$

$$\rho v a^2 \, (\underline{h_v} - \underline{h_L}) - \lambda a^2 \left[\left.\frac{dT}{dr}\right|_{a^+} - \left.\frac{dT}{dr}\right|_{a^-} \right] = 0$$

Q_v
latent heat of
vaporization

where $_v$ and $_L$ stand
for vapor and liquid.

$$4\pi a^2 \lambda \left.\frac{dT}{dr}\right|_{a^-} \approx \tfrac{4}{3}\pi a^3 \rho_l c_{pl} \frac{dT}{dt}$$

assuming all the heat conducted inwards
goes to heating the liquid fuel,

Otherwise one needs to solve the
heat equation inside the droplet.

$$\lambda \frac{dT}{dr} = \rho v Q_v + \underbrace{\tfrac{4}{3}\pi a^3 \rho_l c_{p\,l} \left.\frac{dT}{dt}\right|_l}_{\text{often neglected.}}$$

Alternatively it may be accounted for
by replacing Q_v with an "effective"
value that accounts for internal heating.

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If one assumes that the phase change at the interface occurs very fast, equilib-
rium conditions prevail and a definite relation exists between the vapor partial
pressure and the droplet surface temperature. This relation is of the form

$$p Y_F = k \exp\left[\frac{Q_v}{R} \left(\frac{1}{T_B} - \frac{1}{T} \right) \right]$$

known as the **Claussius Clapeyron relation**. Instead we shall use for sim-
plicity that the surface temperature is constant, and at $r = a$

$$T = T_B$$

Boundary conditions at $r = a$

$$\rho v Y_F - \rho D_F \frac{dY_F}{dr} = \rho v$$

$$\rho v Y_O - \rho D_O \frac{dY_O}{dr} = 0$$

$$\lambda \frac{dT}{dr} = \rho v Q_v$$

$$T = T_B$$

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We write dimensionless equations using a as a unit of distance, D_{th}/a as a unit of velocity and normalize the density and temperature with respect to their ambient values ρ_∞ and T_∞.

We also use $\quad M = \dfrac{\dot{m}/4\pi}{a(\lambda/c_p)}\quad$ to denote the dimensionless mass flux .

$$M = r^2 \rho v \qquad\qquad \rho T = 1$$

$$\frac{M}{r^2}\frac{dY_F}{dr} - \frac{Le_F^{-1}}{r^2}\frac{d}{dr}\left(r^2\frac{dY_F}{dr}\right) = -\omega$$

$$\frac{M}{r^2}\frac{dY_O}{dr} - \frac{Le_O^{-1}}{r^2}\frac{d}{dr}\left(r^2\frac{dY_O}{dr}\right) = -v\,\omega$$

$$\frac{M}{r^2}\frac{dT}{dr} - \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dT}{dr}\right) = q\,\omega$$

$$\omega = D\,\rho^2 Y_F Y_O e^{-B_0/T}$$

at $r = 1$:

$$MY_F - Le_F^{-1}\frac{dY_F}{dr} = M$$

$$MY_O - Le_O^{-1}\frac{dY_O}{dr} = 0$$

$$\frac{dT}{dr} = ML_v, \qquad T = T_s$$

as r

$$T = \rho = 1, \quad Y_O = Y_O \qquad Y_F = 0$$

We have a 6th-order system, with 7 BCs; the extra one for the determination of M.

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The parameters are

$$v = v_O W_O / v_F W_F \qquad\qquad \beta_0 = E/\mathrm{R}T_\infty$$

$$q = Q/v_F W_F c_p T_\infty \qquad\qquad D = \frac{\rho_\infty^2\, a^2 v_F B}{(\lambda/c_p)W_O}$$

$$L_v = Q_v/c_p T_\infty \qquad\qquad T_s = T_B/T_\infty$$

We note in, particular, the dependence on the Damköhler number on the droplet radius $D \sim a^2$ and on the ambient pressure $D \sim P_0$.

We also assume unity Lewis numbers.

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The general solution of the differential equation

$$\frac{M}{r^2}\frac{dZ}{dr} - \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dZ}{dr}\right) = 0$$

$$Z = C_1 e^{-M/r} + C_2$$

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Pure vaporization: $D = 0$

$$Y_F = 1 - e^{-M/r}$$

$$Y_O = Y_{O\infty} e^{-M/r} \qquad M = \ln\left(1 + \frac{1 - T_s}{L_v}\right)$$
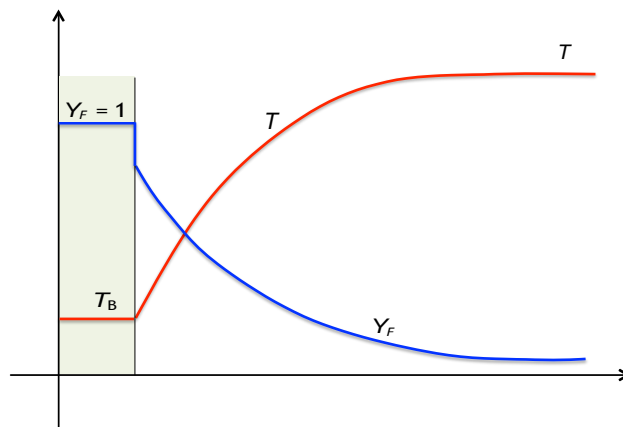
$$T = T_s - L_v + L_v e^{M(1-1/r)}$$

In dimensional form, the vaporization rate is

$$\dot{m} = \frac{4\pi a \lambda}{c_p} \ln\left(1 + \frac{c_p(T_\infty - T_B)}{Q_v}\right)$$

transfer number $\qquad B_v = \dfrac{c_p(T_\infty - T_B)}{Q_v} = \dfrac{\text{impetus for transfer}}{\text{resistance to transfer}}$

Clearly $B_v > 0$, which implies that, for vaporization, $T_\infty > T_B$.

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Combustion:

We will consider the Burke-Schumann limit $D \rightarrow \infty$ and make use of the coupling functions.

$$T + qY_F = 1 + (T_s - 1 + q - L_v)(1 - e^{-M/r})$$

$$T + qv^{-1}Y_O = (T_s - L_v)(1 - e^{-M/r}) + (1 + qv^{-1}Y_{O\infty})e^{-M/r}$$

from which we can also write

$$Y_F - v^{-1}Y_O = 1 - (1 + v^{-1}Y_O)e^{-M/r}$$

The profiles are readily available

$$Y_F = \begin{cases} 1 - (1 + v^{-1}Y_{O\infty})e^{-M/r} & (r < r_f) \\ 0 & (r > r_f) \end{cases}$$

$$Y_O = \begin{cases} 0 & (r < r_f) \\ (v + Y_{O\infty})e^{-M/r} - v & (r > r_f) \end{cases}$$

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$$T = \begin{cases} (T_s - L_v)(1 - e^{-M/r}) + (1 + qv^{-1}Y_{O\infty})e^{-M/r} & (r < r_f) \\ 1 + (T_s - 1 + q - L_v)(1 - e^{-M/r}) & (r > r_f) \end{cases}$$

There are few conditions that remain to be satisfied; these are $T = T_s$ at $r = 1$, and continuity of all variables at $r = r_f$. The first provides and expression for M and the others determine the flame standoff distance and the flame temperature.

$$M = \ln\left[1 + \frac{1 + qv^{-1}Y_{O\infty} - T_s}{L_v}\right]$$

In dimensional form, the burning rate is

$$\boxed{\dot{m} = \frac{4\pi a \lambda}{c_p} \ln\left[1 + \frac{c_p(T_\infty - T_B) + QY_{O\infty}/v_O W_O}{Q_v}\right]}$$

$$B_c = \frac{c_p(T_\infty - T_B) + QY_{O\infty}/v_O W_O}{Q_v} = \frac{\text{impetus for transfer}}{\text{resistance to transfer}}$$

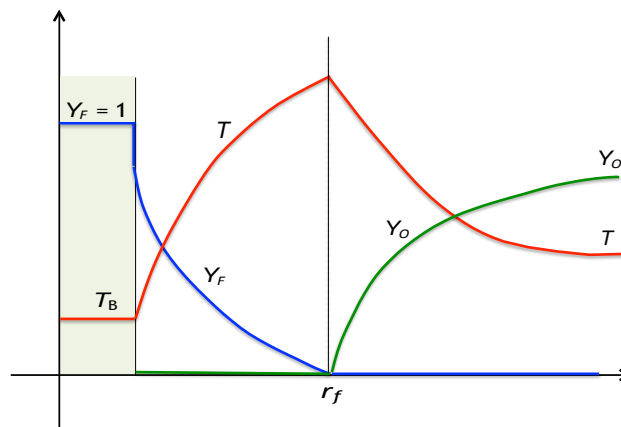**transfer number**

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The flame standoff distance

$$\tilde{r}_f = \frac{a \ \ln(1 + B_c)}{\ln(1 + v_F W_F Y_O \ /v_O W_O)}$$

Note that $r_f > 1$ implies that $c_p(T_\infty - T_B) > (Q_v - Q/v_F W_F)v^{-1}Y_{O\ \infty}$ which is not restrictive because typically $Q > Q_v$.

The flame temperature

$$\tilde{T}_f = T_\infty + \frac{(Q/v_F W_F - Q_v)/c_p - (T_\infty - T_B)}{1 + v_O W_O/v_F W_F Y_O}$$

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Droplet history:

(use back the notation $a = r_s$ and $\rho = \rho_g$)

The vaporization and burning rates were found to have the form
$\dot{m} = 4\pi r_s(\lambda/c_p)\ln(1 + B)$ with the appropriate transfer number.

$$\dot{m} = 4\pi r_s^2 \rho_g v \qquad \Rightarrow \qquad \rho_g v = \frac{\lambda}{c_p}\ln(1 + B)\frac{1}{r_s}$$
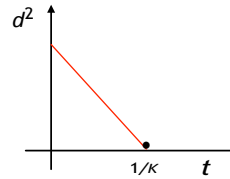
$$\frac{dr_s}{dt} = -\frac{\rho_g}{\rho_l}v = \frac{k}{2r_s} \qquad \text{with} \qquad k = \frac{2\lambda}{c_p}\frac{\ln(1 + B)}{\rho_l}$$

$$2r_s\frac{dr_s}{dt} = -k \qquad \Rightarrow \qquad r_s^2 = r_s^2(0) - kt$$

d^2-law

$$\boxed{\begin{aligned} d^2 &= d^2(0) - Kt \\ K &= \frac{8(\lambda/c_p)}{\rho_l}\ln(1 + B) \end{aligned}}$$
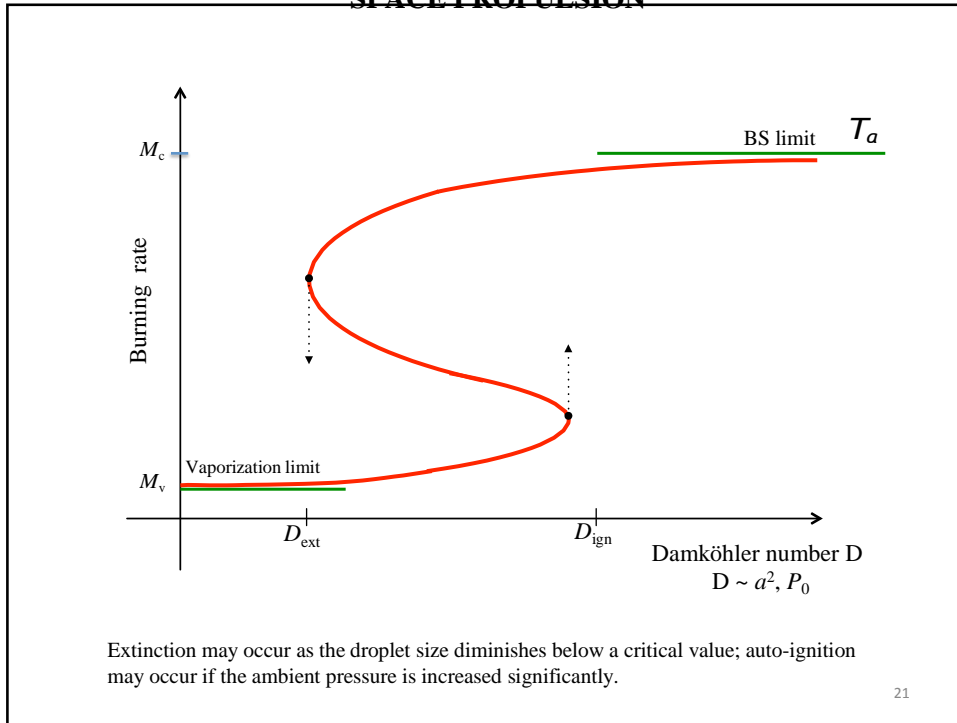

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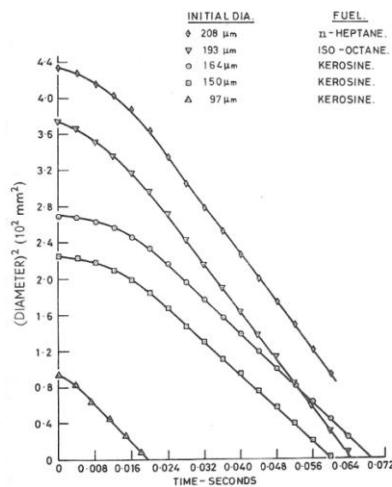
Nuruzzaman et al. PCI, 1971

The d^2-law prediction is verified experimentally for most of the droplet lifetime with the exception, perhaps, of a short initial period following ignition

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Extinction may occur as the droplet size diminishes below a critical value; auto-ignition may occur if the ambient pressure is increased significantly.
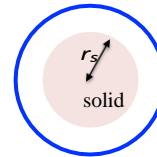
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Combustion of a solid particle:

Similar to a fuel droplet a solid particle may be surrounded by a diffusion flame, so that

$$\dot{m} = \frac{4\pi r_s \lambda}{c_p} \ln(1 + B)$$

if the flame is close enough to the surface, $r_f \approx 1$

$$\ln(1 + B) = \ln\left(1 + v^{-1}Y_O\right)$$

$$\boxed{\dot{m} = 4\pi r_s \rho D_O \ln\left(1 + v^{-1}Y_O\right)}$$

This is the diffusion-controlled limit, where the diffusion of oxidizer towards the particle controls the burning.
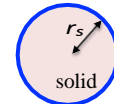
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For $Le = 1$, we have $\lambda/c_p = \rho D_O$.

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If burning occurs on the surface (and possibly inside the pores) of the particle, the burning rate is controlled by the chemical kinetics. For an Arrhenius-type heterogenous surface chemical reaction rate, we have

$$\dot{m} = 4\pi r_s^2 k_s \rho Y_O$$

r_s

solid

kinetic-controlled burning

$$k_s = B_s e^{-E/RT_s}$$

This is the kinetic-controlled limit, where the chemical reaction rate controls the burning.

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Using

$$\dot{m} = -\frac{d}{dt}\left[\frac{4}{3}\pi\rho_s r_s^3\right] = -4\pi\rho_s\, r_s^2 \frac{dr_s}{dt}$$

we find that in the diffusion-controlled limit

$$r_s^2 = r_s^2(0) - \frac{2\rho D_O}{\rho_s} \ln\left(1 + v^{-1}Y_O\right)\, t$$

and in the kinetic-controlled limit

$$r_s = r_s(0) - \frac{k_s}{\rho_s}\rho Y_O\, t$$

The lifetime of a particle

$$t = \begin{cases} \cdot \ \dfrac{r_s^2(0)\,\rho_s}{2\rho D_O\, \ln(1+v^{-1}Y_O)} & \text{diffusion-controlled} \\[2em] \cdot \ \dfrac{r_s(0)\,\rho_s}{\rho B_s Y_O} e^{E/RT_s} & \text{kinetic-controlled} \end{cases}$$

t independent of T
$t \sim r_s^2$

$t \quad r_s$
t inversely proportional to T

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The controlling mechanism is determined by a surface Damköhler number

$$D_s = \frac{t_{\text{diff}}}{t_{\text{kin}}} = \frac{r_s(0)\ B_s Y_O e^{-E/RT_s}}{2D_O\ \ln(1+V^{-1}Y_O)}$$

large particles, or higher ambient temperature $\Rightarrow$ D_s large

diffusion-controlled

small particles, or low ambient temperature $\Rightarrow$ D_s small

kinetic-controlled

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Spray Modeling:

The accurate description of spray combustion, say by DNS, requires identifi-cation of whether liquid or gas is present at every point in space, to employ appropriate equations of state in each of the separate phases and to determine the evolution of a large number of liquid-gas interfaces with boundary condi-tions that involve phase transformation. The large number of droplets required to simulate real dispersed flows in turbulent environments that are encountered in practical applications, make such calculations prohibiitve.

There are a practically three approaches to spray combustion modeling.

· Continuum formulation

· Lagrangian formulation

· Probabilistic formulation

We will not be discussing any of these in detail, but we will try to get a general idea of what each of these formulations involve.

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Continuum Formulation. Properties of both the particles and the gas are as-sumed to exist at every spatial point (the average value of a small parcel that includes both phases) regardless of whether that point is actually in the liquid, solid or gas at that instant.

The gas bulk density ρ (mass of gas in a volume that occupies both liquid and gas) differs from the gas density ρ_g which is the mass per unit volume that includes only gas. If ϕ is the ratio of the volume occupied by the gas to the total volume of the mixture, then $\rho_g = \rho/\phi$.

Similarly the bulk liquid density $\hat{\rho}$ differs from the liquid density $\rho_l = \hat{\rho}/(1-\phi)$.

For a dilute spray the condensed phase volume fraction is small $(1-\phi \; 1)$ so that $\rho \sim \rho_g$, but

$$\hat{\rho} = (1-\phi)\rho_l \sim \frac{1-\phi}{\rho_g/\rho_l}\rho = O(1)$$

since $\rho_g/\rho_l \; 1$.

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Statements of mass conservation of the gas and condensed phases lead to

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = \dot{M}$$

$$\frac{\partial \hat{\rho}}{\partial t} + \nabla \cdot \hat{\rho}\hat{\mathbf{v}} = -\dot{M}$$

Here $\dot{M}$ is the total mass flux (per unit volume) added to the gas phase due to vaporization and $\mathbf{v}, \hat{\mathbf{v}}$ are the gas and particle velocities.

We have assumed here one class of particles; in general the spray must be divided into a number of classes identified by fuel content, size and velocity. Then $\dot{M}$ will be the sum of the individual fluxes from all the particles in a given class multiplied by the number density of particles in that class, and the velocity $\hat{\mathbf{v}}$ will be the mass-weighted velocity of all the particles.

Similarly, separate statements of momentum and energy conservation are writ-ten for the gas and liquid phases with appropriate source/sink terms repre-senting the total momentum and energy carried to the gas from the vaporizing droplets, the total force exerted on the particles from their surroundings and the internal heating of the droplets which, in general, could have a different temperature than the bulk gas.

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<u>Probabilistic Formulation</u>. In this approach the condensed phase is described by a distribution function, or probability density function (*pdf*)

$$f(r, \mathbf{x}, \mathbf{v}, e, t)$$

f dr d$\mathbf{x}$ d$\mathbf{v}$ de... is the probable number of particles in the radius range *dr* about *r*, in the spatial range *d$\mathbf{x}$* about the position *$\mathbf{x}$*, with velocities in the range *d$\mathbf{v}$* about *$\mathbf{v}$* and internal energy in the range *e* about *de*, etc..., at time *t*.

The time evolution of the distribution function *f* is given by

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}}\cdot(\mathbf{v}f) + \nabla_{\mathbf{v}}\cdot(\mathbf{a}f) + \frac{\partial}{\partial r}(\dot{r}f) + \frac{\partial}{\partial e}(\dot{e}f) + \cdots = Q,$$

and is known as the **spray equation**.

the terms on the l.h.s. of the spray equation represent drop-carrier gas interactions, the source term Q on the r.h.s. represents particle-particle interactions (fragmentation, coalescence, etc..).

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The quantities in the spray equation are determined by the laws governing the dynamics of individual droplets

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}, \quad \frac{d\mathbf{v}}{dt} = \mathbf{a}, \quad \frac{dr}{dt} = \dot{r}, \quad \frac{de}{dt} = \dot{e}, \quad \text{etc....}$$

For example, the dependence of $\dot{r}$ on the radius for liquid drops can be specified by adopting the d^2-law

$$\dot{r} = \frac{\lambda/c_p}{\rho_l}\frac{\ln(1+B)}{r},$$

The conservation laws for the gas-droplet mixture will include additional source terms involving the integral of *f*. For example, the mass and momentum equations are

$$\frac{\partial \rho_f}{\partial t} + \nabla\cdot(\rho_f\mathbf{u}) = -\ 4\pi r^2\rho_l\dot{r}f\,drd\mathbf{v}de,$$

$$\rho_f\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla P + \rho_f\mathbf{g} - \frac{4}{3}\pi r^3\rho_l\mathbf{a} + 4\pi r^2\rho_l\dot{r}(\mathbf{v}-\mathbf{u})\ f\,drd\mathbf{v}de,$$

where ρ_f is the fluid density, namely the mass of the gas mixture per unit volume of space, which due to the presence of the particles differs from the gas density ρ_g that corresponds to the mass per unit volume occupied by the gas.

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The main difficulty in this approach is the high dimensionality of the distribution function f (r, **x**, **v**, e, t) which, under the simplest assumptions, contains nine variables.

Lagrangian Discrete Particle Formulation. The droplets are considered as individual point-particles and their trajectories are solved for, separately from the flow field which exists only where there are no droplets. The main difficulty is probably the inability to track a sufficiently large number of particles in order to

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