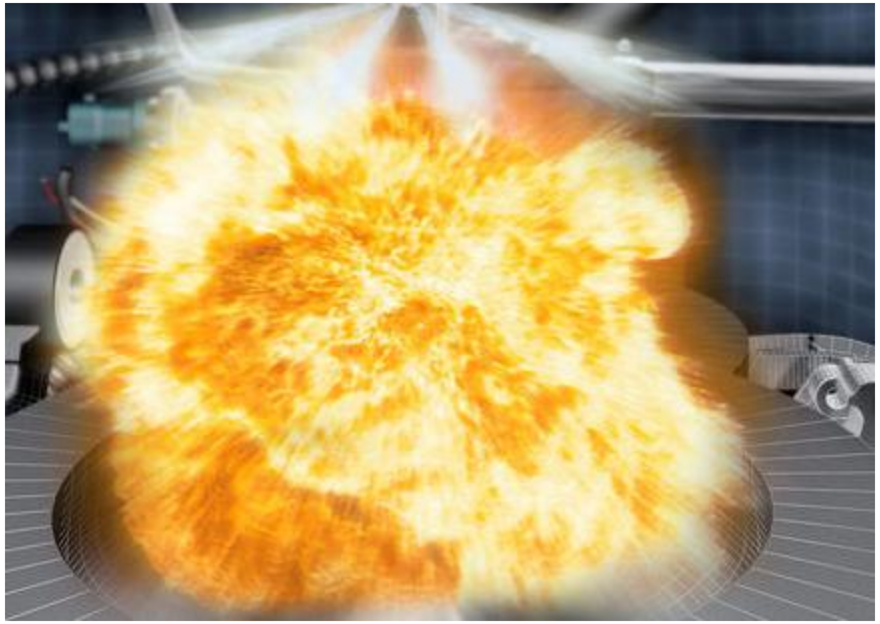
Aerospace Combustion

Lecture 13:

Spray Combustion Part 2



Kerosene Spray Combustion
(AMS kfztech.de)

Spray Combustion

Content

- Injectors and Injection Conditions
- Atomization and Droplet Formation and Break-up
- Droplet Transport
- Vaporization
- Description of 2-Phase Flows
- Spray Combustion

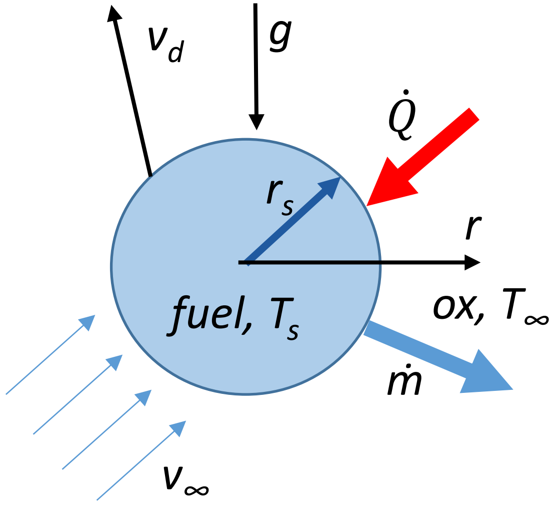
Boundary Conditions for Droplet Vaporization (1)

1) The simplest case is that droplet and surrounding gas at saturation temperature of droplet, droplet a single component fluid, no convection, no gravitational field, ambient pressure

   → the only driving potential is the concentration gradient in the environment

2) The next is that a cold droplet is put into a warm gas. The problem is simplified by the assumption that

   - heat transferred to the droplets raises its temperature from the initial value to the boiling temperature with only minor phase change phenomena and
   - then heat transferred to the droplets is entirely used to vaporize the droplet at a constant rate



The first assumption means that we have no temperature gradient in the droplet

→ infinitely fast heat conduction in the droplet;

The second assumption means the temperature in the environment is constant

→ infinitely fast transport in the gas, no gas-side temperature gradient

Boundary Conditions for Droplet Vaporization (2)

3) Droplet-side heat transfer isn't infinitely fast but heat transfer in the environment is still infinitely fast;
→ temperature gradient in the droplet
4) Both, droplet and environment heat transfer finite
→ temperature gradients in both fluids, concentration gradient in environment
5) Droplet is a mixture of different species, species
→ temperature and species concentration gradient in the droplet due to difference in the volatility (boiling curve)
→ temperature and species concentration gradients in the environment
6) Droplet in a moving environment (constant environment velocity and constant velocity difference between droplet and environment (be aware of difference between laminar and turbulent flow
→ additional convective boundary condition, temperature gradient in droplet and environment, velocity gradient in environment, droplet drag (momentum exchange between droplet and fluid)
7) Friction forces at droplet surface initiate convection inside droplet
→ enhanced mixing with consequences for temperature and concentration gradients inside droplet as well as concentration gradient in environment

Vaporization

Boundary Conditions for Droplet Vaporization (3)

8. Presence of a gravitational field
   → natural convection will come into play with impact, buoyance force interaction with temperature and density (species) gradients in the environment result in additional convection
9. Presence of other droplets (as long as the effect is negligible, problem may be treated as single droplet case, if there is a dense spray
   → severe impact on gas-side temperature, velocity and species profiles with consequences for heat transfer to droplet and droplet surface temperature
10. The next step in complication is to consider droplet contact with either secondary atomization or agglomeration. We could as well have transient effects such as condensation of gas-side species at the surface Let’s assume a dense spray so the droplets feel the presence of other droplets
11. Finally, account for droplet agglomeration and droplet breakup

12. Don’t forget the impact of combustion and resulting temperature increase due to the heat release, changes of species and species concentrations.

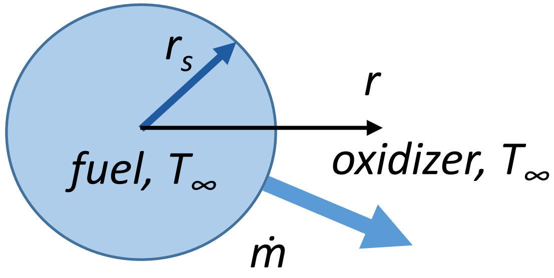
Vaporization

Different Vaporization Cases

Case Study 1 Assumptions:

- Quasi-steady process ($\dot{m}$ = const.; equivalent to an appropriate mass addition to droplet)
- All thermo-physical properties constant
- Temperature and pressure constant everywhere
- Vapor mass fraction at surface is at saturation conditions, i.e. vapor mass fraction away from surface is then smaller

Mass transfer

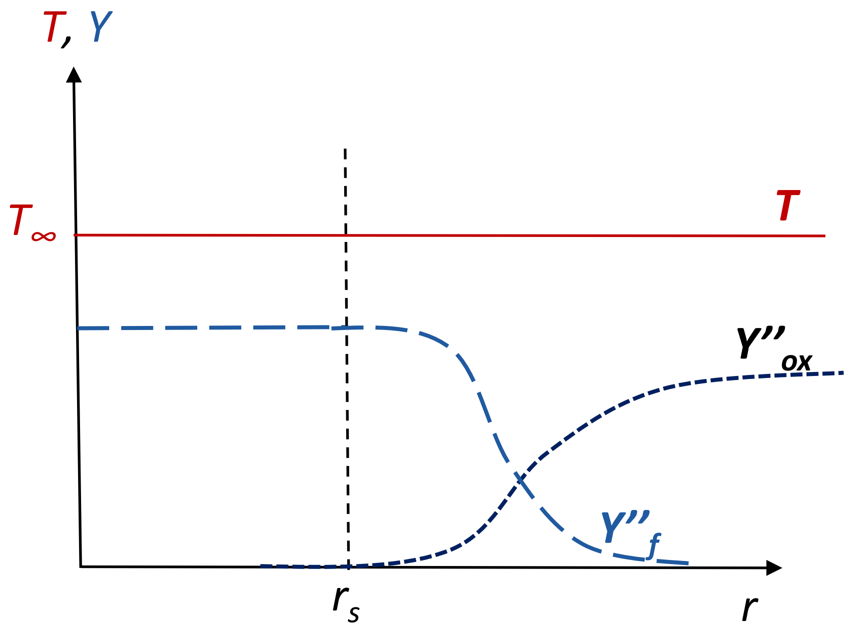


$$\dot{m}(r) = \dot{m}_f(r) = 4\pi r^2 \dot{m}''_f$$

m''_f : evaporated fuel mass
$D_{f,ox}$: binary diffusion coefficient of fuel in oxidizer
Y''_f, Y''_{ox}: fuel, oxidizer mass fraction in gas

$$\dot{m}''_f(r) = \frac{\rho_{ox} D_{f,ox}}{1-Y''_f}\frac{dY''_f}{dr} \Rightarrow \dot{m}(r) = -4\pi r^2 \frac{\rho_{ox} D_{f,ox}}{1-Y''_f}\frac{dY''_f}{dr}$$

with $C^* = 4\pi\rho_{ox} D_{f,ox} \Rightarrow \dfrac{dY''_f}{1-Y''_f} = -\dfrac{\dot{m}}{C^* r^2}\,dr$



Vaporization

Different Vaporization Cases

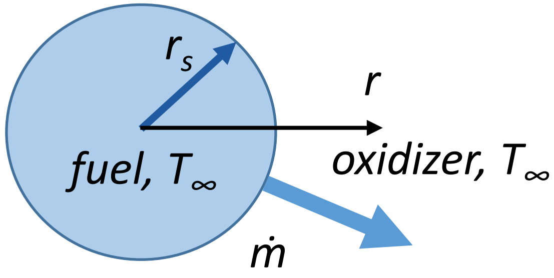
Case Study 1:

$$\frac{dY''_f}{1-Y''_f} = -\frac{\dot m}{C^* r^2}\,dr \quad \Rightarrow \quad \int_{Y_{r_s}}^{Y_r} \frac{dY''_f}{1-Y''_f} = \int_{r_s}^{r} \frac{\dot m}{C^* r^2}\,dr$$

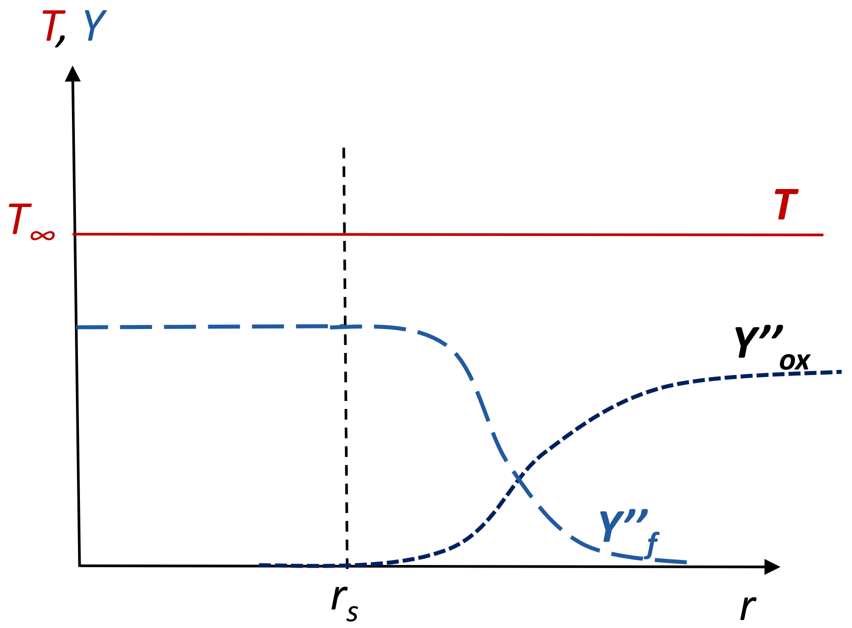
$$\Rightarrow Y''_f(r) = 1 - \frac{\left(1-Y''_{f,sat}\right)\exp\left(-\frac{\dot m}{C^* r}\right)}{\exp\left(-\frac{\dot m}{C^* r_s}\right)} =$$

$$= 1 - \left(1-Y''_{f,s}\right)\exp\left[-\frac{\dot m}{C^*}\left(\frac{1}{r_s}-\frac{1}{r}\right)\right]$$

Mass transfer



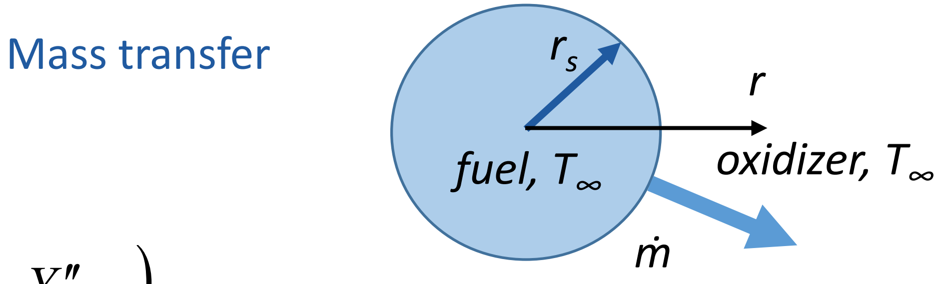
$$\dot m(r) = \dot m_f(r) = 4\pi r^2 \dot m''_f$$



Vaporization

Different Vaporization Cases

Case Study 1: Boundary Conditions



$$Y''_f(r=r_s)=Y''_{f,sat}\,; \qquad Y''_f(r\to\infty)=Y''_{f,\infty}$$

$$Y''_f(r\to\infty)=1-\frac{\left(1-Y''_{f,sat}\right)}{\exp\left(-\frac{\dot{m}}{C^*r}\frac{1}{r_s}\right)}=Y''_{f,\infty} \qquad \Rightarrow \exp\left(-\frac{\dot{m}}{C^*r_s}\right)=\frac{\left(1-Y''_{f,sat}\right)}{\left(1-Y''_{f,\infty}\right)}$$

$$\Rightarrow \dot{m}=4\pi\rho_{ox}r_sD_{f,ox}\ln\left(\frac{1-Y''_{f,\infty}}{1-Y''_{f,sat}}\right)$$

$Y''_{f,\infty}<Y''_{f,sat}\,;$ Evaporation

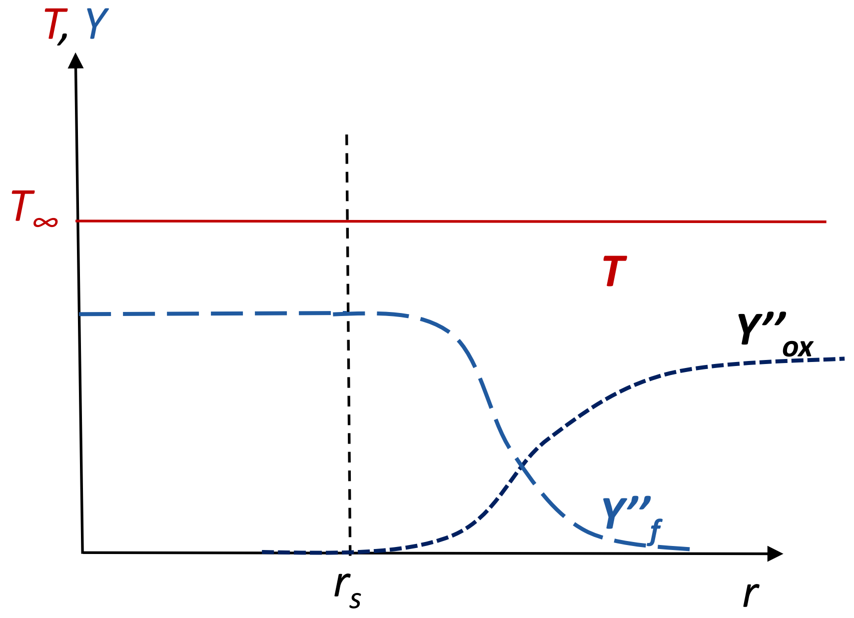
$Y''_{f,\infty}=Y''_{f,sat}\,;$ No net mass transfer

$Y''_{f,\infty}>Y''_{f,sat}\,;$ Condensation

$$B_m=\left(\frac{Y''_{f,\infty}-Y''_{f,sat}}{Y''_{f,sat}-1}\right);$$

Introducing B_m : Spalding Mass Transfer Number

$$\Rightarrow \dot{m}=4\pi\rho_{ox}r_sD_{f,ox}\ln\left(1+B_m\right)$$



Vaporization

Different Vaporization Cases

Case Study 1: Change of Droplet Diameter

Mass of droplet $m_d = \rho_l \pi \frac{D_d^3}{6}$ Mass loss of droplet $\frac{dm_d}{dt} = -\dot{m}$ with $\dot{m} = 4\pi\rho_{ox} r_s D_{f,ox} \ln\left(1 + B_M\right)$

$$\Rightarrow \frac{d}{dt}\left[\rho_f \pi \frac{D_d^3}{6}\right] = -4\pi\rho_{ox} r_s D_{f,ox} \ln\left(1 + B_M\right) \Rightarrow \left[\rho_f \pi \frac{3D_d^2}{6}\right]\frac{dD_d}{dt} = -2\pi D_d \rho_{ox} D_{f,ox} \ln\left(1 + B_M\right)$$

$$\Rightarrow \left[\rho_f \pi \frac{3D_d}{6}\right]\frac{dD_d}{dt} = -2\pi\rho ox D_{f,ox} \ln\left(1 + B_M\right) \Rightarrow \frac{dD_d^2}{dt} = \boxed{-8\frac{\rho_{ox}}{\rho_l} D_{f,ox} \ln\left(1 + B_M\right)}$$

evaporation constant *k*

Evaporation D-square law which holds for almost all vaporization conditions

$$\Rightarrow D^2(t) = D_0^2 - kt$$

From this equation we can deduce the life time of a droplet

$$t_{life} = \frac{D_0^2}{kt}$$

Let's assume that the oxidizer is moving with a small velocity *U*

$$\Rightarrow \mathrm{Re} = \frac{\rho_{ox} U_{ox} D_d}{\mu_{ox}}$$

$$\Rightarrow k_U = k\left(1 + a\,\mathrm{Re}^n\right)$$

with a ~ 0.3 and
n ~ 0.26-0.3

Vaporization

Different Vaporization Cases

Case Study 2 Assumptions:

- Quasi-steady process ($\dot m$ = const.)
- All thermo-physical properties constant
- Droplet temperature at boiling condition, ambient temperature higher, constant pressure

m''_f : evaporated fuel mass
$D_{f,ox}$: binary diffusion coefficient of fuel in oxidizer
Y''_f, Y''_{ox}: fuel, oxidizer mass fraction in gas

$$\dot m = 4\pi r_s^2 \rho_{ox} D_{f,ox} \ln(1+B_M)$$

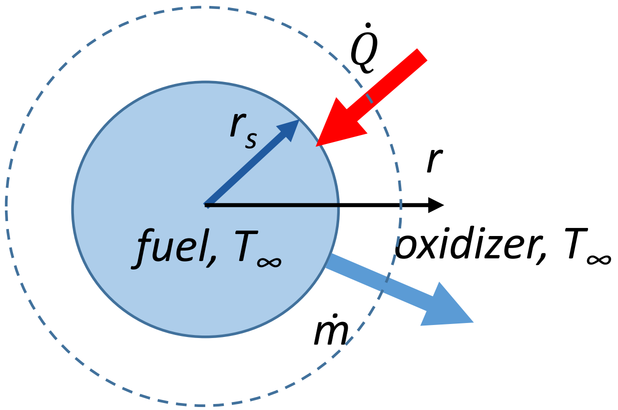
$$\dot m c_p \frac{dT}{dr} = \frac{d}{dr}\left(4\lambda\pi r^2 \frac{dT}{dr}\right) \Rightarrow \frac{\dot m c_p}{4\pi\lambda}\frac{dT}{dr} = \frac{d}{dr}\left(r^2 \frac{dT}{dr}\right)$$

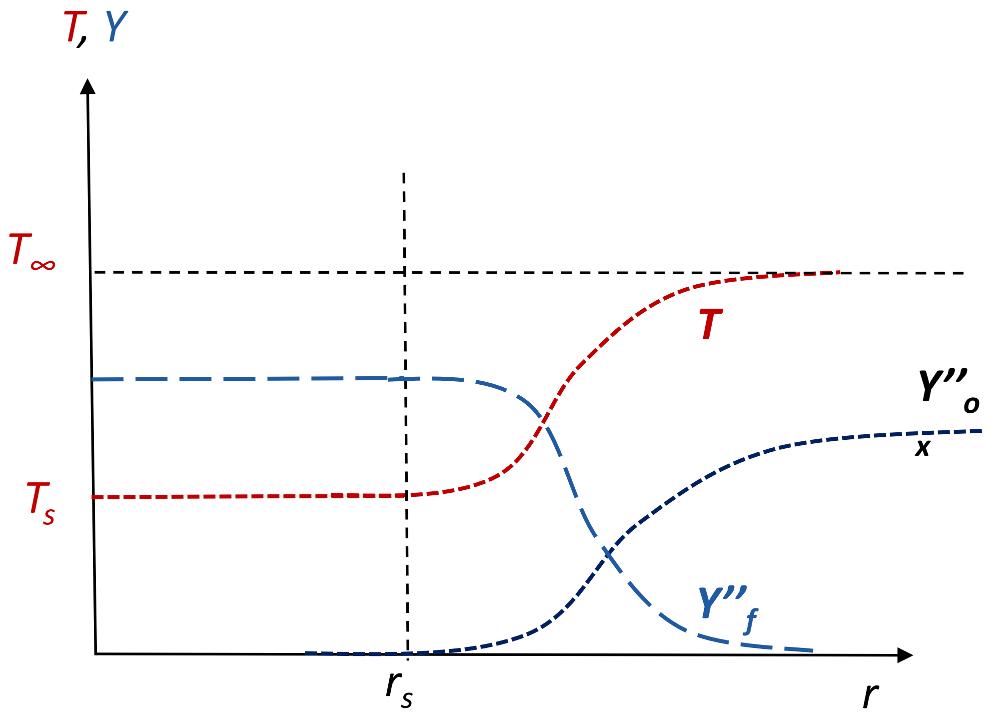
Integration yields:

$$const. + \frac{\dot m c_p}{4\lambda\pi}T = r^2 \frac{dT}{dr}$$

Heat transfer and mass transfer phenomena present

Heat transferred across droplet surface balanced by mass transferred into environment





Vaporization

Different Vaporization Cases

Case 2:

$$const. + \frac{\dot{m} c_p}{4\lambda\pi} T = r^2 \frac{dT}{dr}$$

At droplet surface ($r = r_s$ und $T = T_s$):

$$\lambda \left.\frac{dT}{dr}\right|_{r_s} = \dot{m}''\left(h_{vap} - h_l\right) = \dot{m}'' h_{fg}$$

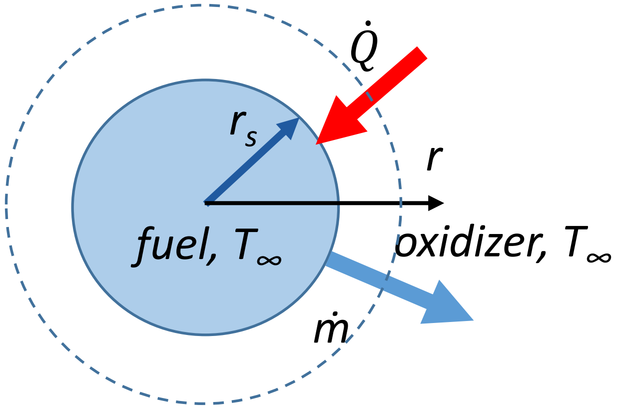
$$r_s^2 \left.\frac{dT}{dr}\right|_{r_s} = \frac{\dot{m}}{4\lambda\pi} h_{fg}$$

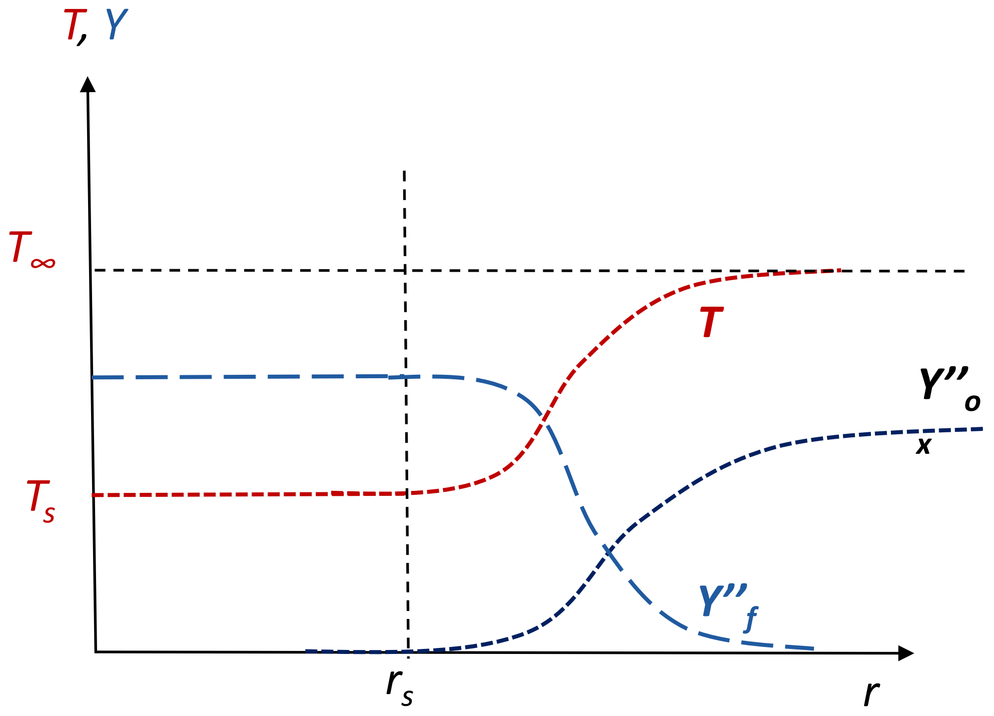
$$\Rightarrow const. = \frac{\dot{m} c_p}{4\lambda\pi}\left(\frac{h_{fg}}{c_p} - T_s\right) \qquad \Rightarrow r^2 \frac{dT}{dr} = \frac{\dot{m} c_p}{4\lambda\pi}\left(T - T_s + \frac{h_{fg}}{c_p}\right);$$

$$\Rightarrow T(r) = \left(T_s - \frac{h_{fg}}{c_p}\right) + \left(T_\infty - T_s + \frac{h_{fg}}{c_p}\right)\exp^{\frac{\dot{m} c_p}{4\pi\lambda}\frac{1}{r}};$$

Heat transfer and mass transfer phenomena present

Heat transferred across droplet surface balanced by mass transferred into environment





Vaporization

Different Vaporization Cases

Case 2:

$$const. + \frac{\dot{m} c_p}{4\lambda\pi} T = r^2 \frac{dT}{dr}$$

Integration similar to previous species equation:

$$\frac{\frac{\dot{m} c_p}{4\lambda\pi}}{r} = \ln\left[\frac{c_p\left(T_\infty - T_s\right) + h_{fg}}{c_p\left(T - T_s\right) + h_{fg}}\right] \Rightarrow \frac{\frac{\dot{m} c_p}{4\lambda\pi}}{r_s} = \ln\left[1 + \frac{c_p\left(T_\infty - T_s\right)}{h_{fg}}\right]$$

$$\dot{m} = -4\pi \frac{\lambda}{c_p} \ln\left[1 + \frac{c_p\left(T_\infty - T_s\right)}{h_{fg}}\right] = -4\pi\rho_f \alpha \ln\left[1 + \frac{c_p\left(T_\infty - T_s\right)}{h_{fg}}\right]$$

$$B_h = \left(\frac{c_p\left(T_\infty - T_s\right)}{h_{fg}}\right);$$

Introducing B_h : Spalding Energy Transfer Number

$$\Rightarrow \dot{m} = -4\pi\rho_f \alpha \ln\left[1 + B_h\right]$$

but we have as well

$$\dot{m} = 4\pi\rho_{ox} r_s D_{f,ox} \ln\left(1 + B_m\right)$$

Vaporization

Different Vaporization Cases

Case 2:

$$\dot{m} = -4\pi\rho_{ox} r_s D_{f,ox} \ln\left(1+B_m\right) = -4\pi\rho_f \alpha \ln\left[1+B_h\right]$$

Let's assume *Le=1*:

$$B_h = B_m \Rightarrow \frac{Y''_{f,\infty} - Y''_{f,sat}}{Y''_{f,sat} - 1} = \frac{c_p\left(T_\infty - T_s\right)}{h_{fg}}$$

Surface temperature is linked to the saturation concentration.

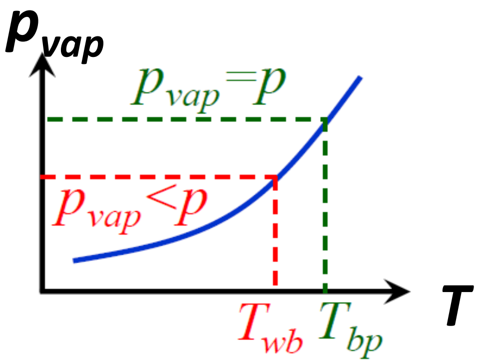
Now let's assume that we have phase equilibrium between liquid and gas at the surface. (Clausius-Clapeyron Equation)

$$\left.\frac{dp}{dT}\right|_{sat} = \frac{h_{fg}}{T v_{fg}} > 0 \qquad v_{fg} = \frac{1}{\rho_g} - \frac{1}{\rho_l} = \frac{RT}{p_{vap}} - \frac{1}{\rho_l} \cong \frac{RT}{p_{vap}}$$

$$\frac{dp_{vap}}{p} \cong \frac{dT}{T^2}\frac{h_{fg}}{R} \Rightarrow \ln\left(p_{vap}\right) \cong -\frac{h_{fg}}{RT} + C; \qquad C = pe^{-h_{fg}(T_{bp})/RT_{bp}}$$

$$p_{vap} \cong pe^{-h_{fg}(T_{bp})/RT_{bp}} e^{-h_{fg}(T_{wb})/RT_{wb}}$$

$$p_{f,sat} = px_{f,sat}; Y_{f,sat} = x_{f,sat} W_f \Big/ \sum_i x_i W_i$$



T_{wb} is the wet bulb temperature: Lowest temperature air can be cooled by vaporization of water into the air; more general, the temperature which is reached when the surrounding gas is saturated with the vaporized species.

Vaporization

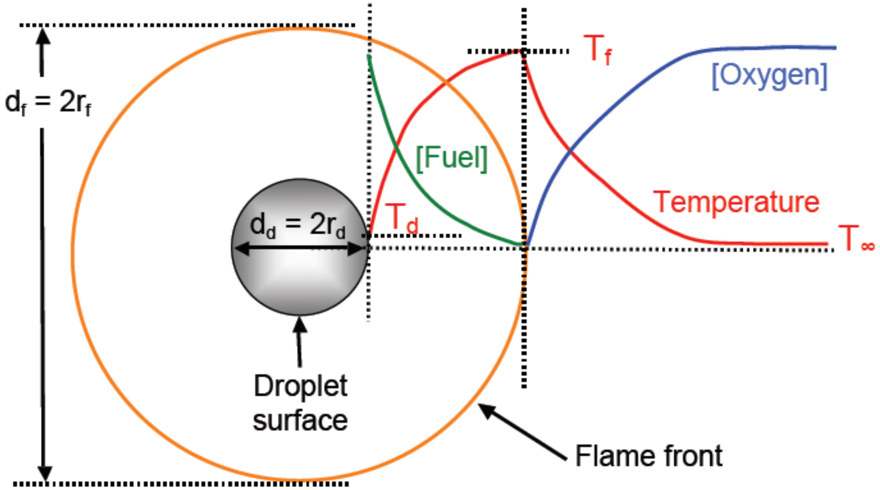
Collection of useful non-dimensional numbers

$$B_h = \left(\frac{c_p \left(T_\infty - T_s \right)}{h_{fg}} \right); \qquad B_m = \left(\frac{Y''_{f,\infty} - Y''_{f,sat}}{Y''_{f,sat} - 1} \right); \qquad \mathrm{Nu} = 2 \frac{\ln\left(1 + B_h\right)}{B_h}; \qquad \mathrm{Sh} = 2 \frac{\ln\left(1 + B_m\right)}{B_m}$$

Simplified models	provide necessary computational simplicity to predict droplet vaporization in spray combustor (scale >> scale of droplet)
Exact models	Predict drag coefficient, Nusselt & Sherwood numbers for simplified models, provide detailed insight, study droplet interaction
Infinite conductivity	Old approach, useful for code development, not useful for spray predictions
Finite conductivity	Zero Reynolds number limit of simplified models
Constant liquid temperature	Old approach, not recommended for spray predictions

Droplet Combustion

Balance Equations



Similar analysis to a 1D planar flame instead 1D steady spherical version of convection-diffusion equations for mass fraction of fuel Y_f, mass fraction of oxidizer Y_o and temperature T.

What we do not know

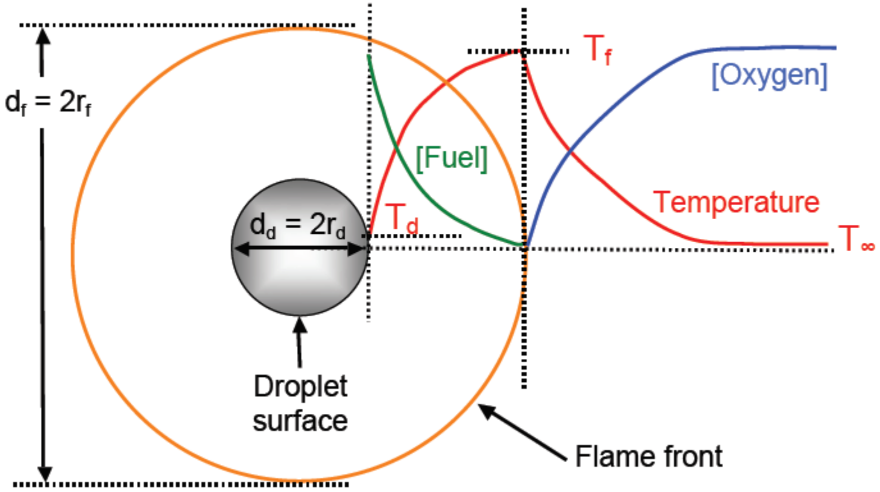
- Flame temperature and location
- Fuel mass flux from droplet surface (mass flux is constant but fue mass flow isn't due to change of surface)
- Fuel concentration at droplet surface

Hence, we need four equations

- Reactant diffusive fluxes into flame sheet in stoichiometric portions
- Fuel enthalpy flux into flame sheet (thermal enthalpy flux out by conduction)
- Energy balance at droplet surface
- Mass balance at droplet surface

Droplet Combustion

Balance Equations



Fuel (from droplet surface to flame position, $r_d \le r \le r_f$)

$$\rho u \frac{dY_F}{dr} r - \rho \frac{D_F}{r^2}\frac{d}{dr}\left(r^2 \frac{dY_F}{dr}\right) = 0; \quad \dot{m} = 4\pi r^2 \rho u = const$$

$$PeLe_F Y_F \frac{dY_F}{d\tilde{r}} = \frac{d}{d\tilde{r}}\left(\tilde{r}^2 \frac{dY_F}{d\tilde{r}}\right); \text{ with } Pe = \frac{\dot{m} c_p}{4\pi\lambda r_d}; \quad \tilde{r} = \frac{r}{r_d}; \quad Le_F = \frac{\lambda}{D_F c_p \rho}$$

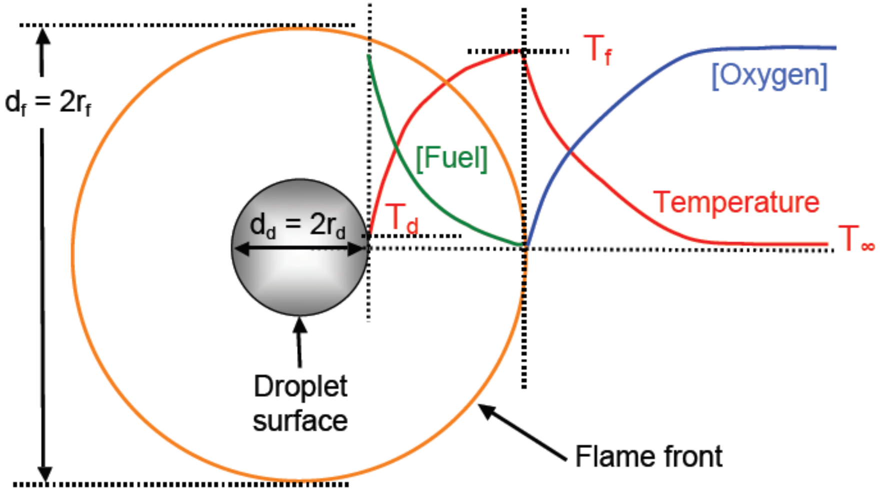
$$\Downarrow$$

$$Y_F(\tilde{r}) = \frac{dY_{F,d}\left(e^{-PeLe_F/\tilde{r}_f} - e^{-PeLe_F/\tilde{r}}\right)}{e^{-PeLe_F/\tilde{r}_f} - e^{-PeLe_F}}; \quad \frac{dY_F}{d\tilde{r}} = \frac{-PeLe_F}{\tilde{r}^2}\frac{Y_{F,d}e^{-PeLe_F/\tilde{r}}}{e^{-PeLe_F/\tilde{r}} - e^{-PeLe_F}};$$

$$\left.\frac{dY_F}{d\tilde{r}}\right|_{\tilde{r}=1} = -PeLe_F \frac{Y_{F,d}e^{-PeLe_F}}{e^{-PeLe_F/\tilde{r}_f} - e^{-PeLe_F}}; \quad \left.\frac{dY_F}{d\tilde{r}}\right|_{\tilde{r}=\tilde{r}_f} = \frac{PeLe_F}{\tilde{r}_f^2}\frac{Y_{F,d}}{e^{-PeLe_F\left(1-1/\tilde{r}_f\right)} - 1};$$

Droplet Combustion

Balance Equations



Oxidizer (from flame further out, $r \geq r_f$)

$$Y_{Ox}(\tilde{r}) = Y_{Ox,\infty} \frac{\left(e^{-PeLe_{Ox}/\tilde{r}} - e^{-PeLe_{Ox}/\tilde{r}_f}\right)}{1 - e^{-PeLe_{Ox}/\tilde{r}_f}}; \quad \frac{dY_{Ox}}{d\tilde{r}} = Y_{Ox,\infty} \frac{-PeLe_{Ox}}{\tilde{r}^2} \frac{e^{-PeLe_{Ox}/\tilde{r}}}{1 - e^{-PeLe_{Ox}/\tilde{r}_f}};$$

$$\left.\frac{dY_{Ox}}{d\tilde{r}}\right|_{\tilde{r}=\tilde{r}_f} = \frac{PeLe_{Ox}}{\tilde{r}_f^2} \frac{Y_{Ox,\infty}}{e^{-PeLe_{Ox}/\tilde{r}_f} - 1}; \quad \left.\frac{dY_{Ox}}{d\tilde{r}}\right|_{\tilde{r}=\infty} = 0$$

$$Pe = O(1); Le_{Ox} = O(1); \tilde{r}_f >> 1; \Rightarrow 1 - e^{-PeLe_{Ox}/\tilde{r}_f} \approx \frac{1}{\tilde{r}_f} \Rightarrow \frac{Y_{Ox}(\tilde{r})}{Y_{Ox,\infty}} \approx \frac{\tilde{r}_f}{\tilde{r}}$$

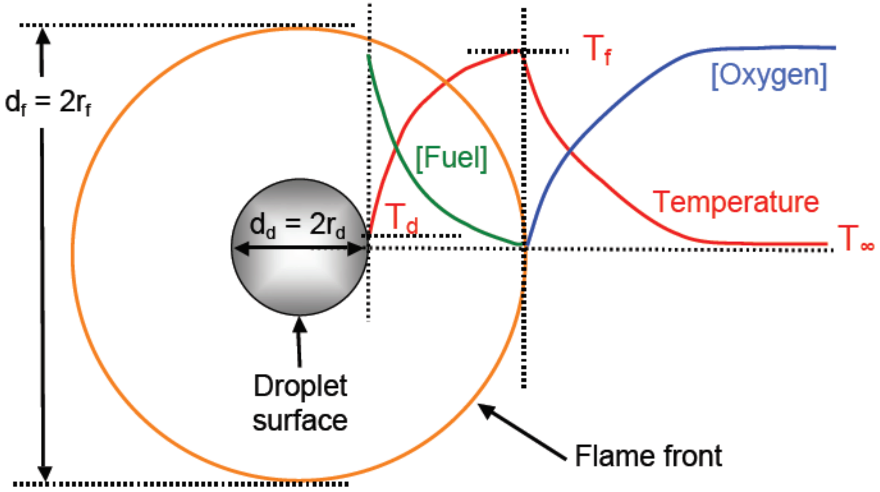
Temperature ($r_\mathrm{d} \leq r \leq r_f$)

$$T(\tilde{r}) = \frac{(T_f - T_\infty)e^{-Pe/\tilde{r}} - \left(T_f e^{-Pe} - T_d e^{-Pe/\tilde{r}_f}\right)}{e^{-Pe/\tilde{r}_f} - e^{-Pe}}; \quad \frac{dT}{d\tilde{r}} = -\frac{Pe}{\tilde{r}^2} \frac{(T_f - T_\infty)e^{-Pe/\tilde{r}}}{1 - e^{-Pe(1-1/\tilde{r}_f)}};$$

$$\left.\frac{dT}{d\tilde{r}}\right|_{\tilde{r}=\tilde{r}_f} = -\frac{Pe}{\tilde{r}_f^2} \frac{(T_f - T_\infty)e^{-Pe/\tilde{r}_f}}{1 - e^{-Pe/\tilde{r}_f}}; \quad \left.\frac{dT}{d\tilde{r}}\right|_{\tilde{r}=\infty} = 0$$

Droplet Combustion

Balance Equations



Stoichiometric balance at flame sheet

$$\rho D_F \frac{dY_F}{d\tilde r}\bigg|_{\tilde r=\tilde r_{f-}} = -\frac{\nu_F}{\upsilon_{Ox}}\frac{M_F}{M_{Ox}}\rho D_{Ox}\frac{dY_F}{d\tilde r}\bigg|_{\tilde r=\tilde r_{f+}}$$

$$\rho D_F \frac{PeLe_F}{\tilde r_f^{\,2}}\frac{Y_{F,d}}{e^{-PeLe_F\left(1-1/\tilde r_f\right)}-1} = -\frac{\nu_F}{\upsilon_{Ox}}\frac{M_F}{M_{Ox}}\rho D_{Ox}\frac{PeLe_{Ox}}{\tilde r_f^{\,2}}\frac{Y_{Ox,\infty}}{e^{-PeLe_{Ox}/\tilde r_f}-1}$$

$$\frac{1}{e^{-PeLe_F\left(1-1/\tilde r_f\right)}-1} = -\frac{\nu_F}{\upsilon_{Ox}}\frac{M_F}{M_{Ox}}\frac{Y_{Ox,\infty}}{Y_{F,d}}\frac{Le_{Ox}}{Le_F}\frac{D_{Ox}}{D_F}\frac{1}{e^{-PeLe_{Ox}/\tilde r_f}-1}$$

$$\Rightarrow e^{-PeLe_F\left(1/\tilde r_f-1\right)} + Se^{-PeLe_{Ox}/\tilde r_f} = 1+S$$

$$Le_F = Le_{Ox} = 1 \Rightarrow e^{-Pe/\tilde r_f} = \frac{e^{-Pe}+S}{1+S}$$

Energy balance at flame sheet

$$-Q_R\rho D_F\frac{dY_F}{d\tilde r} = \lambda\frac{dT}{d\tilde r}\bigg|_{\tilde r=\tilde r_{f-}} - \lambda\frac{dT}{d\tilde r}\bigg|_{\tilde r=\tilde r_{f+}}$$

$$\Rightarrow \frac{Y_{F,d}Q_R/c_p}{1-e^{-PeLe_F\left(1-1/\tilde r_f\right)}} = \frac{\left(T_f-T_d\right)e^{-Pe/\tilde r}}{1-e^{-Pe\left(1-1/\tilde r_f\right)}} + \frac{\left(T_f-T_\infty\right)}{1-e^{-Pe/\tilde r_f}}$$

$$Le_F = 1$$

$$\Rightarrow \frac{Y_{F,d}Q_R}{c_p} = \left(T_f-T_d\right)+\left(T_f-T_\infty\right)\left[\frac{e^{-Pe/\tilde r_f}-e^{-Pe}}{1-e^{-Pe/\tilde r_f}}\right]$$

Droplet Combustion

Balance Equations

Conducted heat flux to droplet equals enthalpy need to vaporize fuel mass flux

$$\lambda\left(4\pi r_d^2\right)\frac{dT}{d\tilde{r}}\bigg|_{\tilde{r}=1} = \dot{m}h_V;\ \Rightarrow \frac{dT}{d\tilde{r}}\bigg|_{\tilde{r}=1} = \frac{\dot{m}c_p}{4\pi\lambda r_d}\frac{h_V}{c_p} = Pe\frac{h_V}{c_p}$$

$$\Rightarrow Pe\frac{\left(T_f - T_d\right)}{e^{-Pe(1-1/\tilde{r}_f)}-1} = Pe\frac{h_V}{c_p};\Rightarrow e^{-Pe(1-1/\tilde{r}_f)} = 1+\frac{c_p\left(T_f - T_d\right)}{h_V}$$

Mass flow from surface = rate of fuel convected + rate of fuel diffused into gas

$$\dot{m} = \rho D_F 4\pi r_d^2 \frac{dY_F}{dr}\bigg|_{r=r_d};+\dot{m}Y_{F,d};\Rightarrow \frac{\dot{m}c_p}{4\pi\lambda r_d}\frac{\lambda}{\rho c_p D_F}\left(1-Y_{F,d}\right) = -\frac{dY_F}{d\tilde{r}}\bigg|_{\tilde{r}=1}$$

$$dY_{F,d} = 1-e^{-PeLe_F(1-1/\tilde{r}_f)}$$

Droplet Combustion

Solutions

Flame temperature

$$Pe = \ln\left(1 + \left[Q_R\left(Y_{Ox,\infty}\frac{\nu_F}{\upsilon_{Ox}}\frac{M_F}{M_{Ox}}\right) + c_p\left(T_\infty - T_d\right)\right] / h_V\right);$$

$$B = \frac{Q_R\left(Y_{Ox,\infty}\frac{\nu_F}{\upsilon_{Ox}}\frac{M_F}{M_{Ox}}\right) + c_p\left(T_\infty - T_d\right)}{h_V}$$

$$T_f = \frac{\frac{\left(Q_R - h_V\right)}{c_p} + T_d + \left(\frac{S}{Y_{F,d}}\right)T_\infty}{1 + \frac{S}{Y_{F,d}}};$$

B transfer number,

for hydrocarbons *B ≈ 10*; however,

for CH_3OH; *B ≈ 3*

Burning rate

$$\Rightarrow d_d^2(t) = d_0^2 + \boxed{\frac{8\lambda}{\rho_d c_p}}\ln(1+B);$$

burning rate
constant

Droplet Combustion

Solutions

Flame radius

$$\tilde{r}_{\mathrm{f}} = \frac{r_f}{r_d} = \frac{d_f}{d_d} = \frac{\ln\left(1+B\right)}{\ln(1+Y_F/S)} = \frac{n\left(1+B\right)}{\ln\left(1+Y_{Ox,\infty}\dfrac{\nu_F}{\upsilon_{Ox}}\dfrac{M_F}{M_{Ox}}\right)}$$

Fuel mass fraction at droplet surface

$$Y_{F,d} = \frac{B-(Y_{F,d}/S)}{1-S(Y_{F,d}/S)} = \frac{B-Y_{Ox,\infty}\dfrac{\nu_F}{\upsilon_{Ox}}\dfrac{M_F}{M_{Ox}}}{1+B}$$

Droplet Combustion

Results

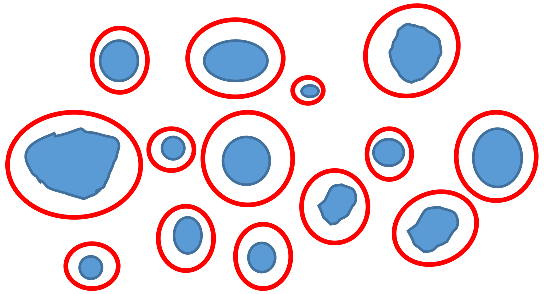
- B is independent of transport properties
- Burning time mainly dependent on droplet diameter
- Fuel temperature hardly affects burning rate (Stefan problem; holds only for quiescent conditions, has to be checked for cryogenic propellants)
- Decreasing oxygen mass fractions yield larger flame radia
- No pressure dependency (however, reaction rates are pressure dependent)
- As long as heat is required to vaporize and pre-heat fuel, the concept of adiabatic flame temperature is questionable
- Concepts of spray combustion

Spray Combustion

Case 1: Combustion of Individual Droplets

Cluster of individual droplets each covered by a flame. Near the droplet, mixture is too rich to burn, very far away, the mixture is to lean to burn. Distance between flame and droplet depends on flammability limit

- Advantages, since case can be handled as combustion of individual droplets
- When droplets becomes very small, the amount of evaporated mass may be not sufficient to sustain combustion around the droplet (flammability limit) → extinction



Cluster of burning droplets

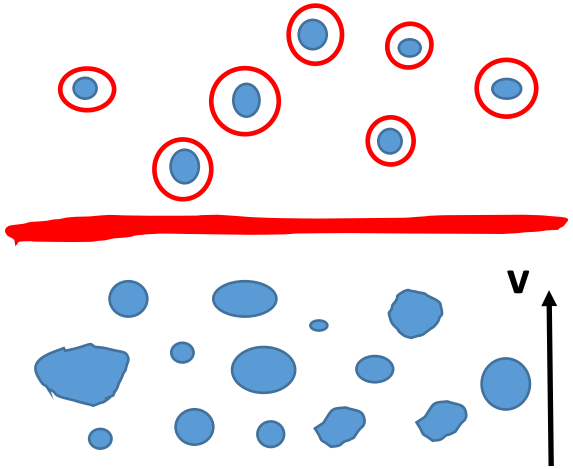
Occurs inside the combustion chamber when propellant supply is very fast (shear coax injection in a rocket engine)

Spray Combustion

Case 2: Internal Group Combustion

Clusters of individual droplets moves towards flame, if convection time scale is smaller than that of vaporization, some droplets eventually may penetrate the flame and continue burning in the product zone (favorable mixture necessary).

- Case can be handled as vaporization of droplets, gas / gas combustion and combustion of individual droplets
- Problematic in aero engines since high temperatures may lead to NOx production
- Occurs in the reactive shear of a coax injector



Cluster of droplets moving towards a flame front

Spray Combustion

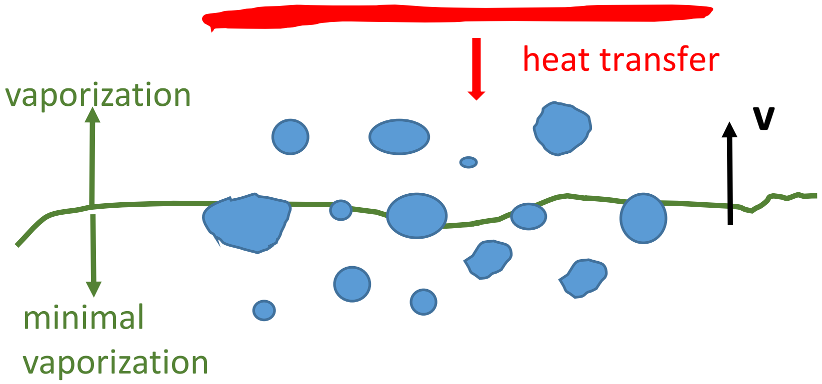
Case 3: External Group Combustion

Existence of two Zones where (convective transport small)

a) droplet number density so high that vaporization is almost negligible; ambient gas is saturated with vapor

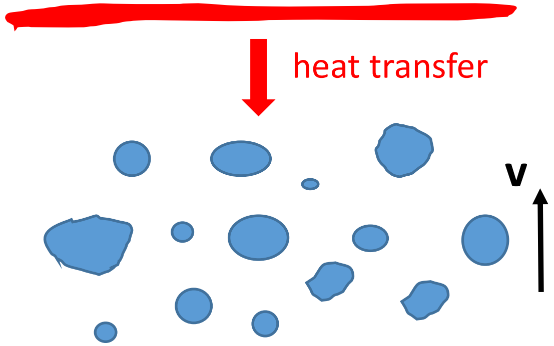
b) Vaporization due to heat transfer from the flame to the droplets and gas/gas combustion

- Favorable, can be handled as phase change due to concentration gradient, and gas / gas combustion



Occurs in the absolute vicinity of the injectors

Case 4: External Group Combustion without negligible vaporization



Occurs in the absolute vicinity injector post (flame holding)

Group Combustion Model of Chu

Group Combustion Number of second kind

$$G \equiv \frac{\text{rate of heat exchange between two phases}}{\text{rate of vaporization}}$$

$$G \equiv \frac{D}{R_\infty U_\infty} G_1$$

with

$$G_1 = \frac{2\pi \lambda_l r_{l0} n_0 R_\infty^2 T_0}{\rho_\infty D_\infty L}\left(2 + 0.6\,\mathrm{Re}_{dl0}^{1/2}\,\mathrm{Pr}^{1/3}\right)$$

G_1, the Group combustion number of first kind.

D_∞, mass diffusivity of gas

n_0, droplet number density at reference conditions

L, latent heat of vaporization per unit mass

r_∞, density of gas

R_∞, radius of two-phase zone

N, total number of droplets

r_{l0}, reference radius of droplet

$$n_0 \equiv \frac{3N}{4R_\infty^3}$$

Spray Combustion

Group Combustion Model of Chu

A more recent paper by Chu redefines *G* to:

$$G \equiv \frac{\text{rate of heat exchange between two phases}}{\text{rate of energy transport by convection}}$$

with

$$G_1 = \frac{4\pi\lambda_l \rho_{l0} n_0 R_\infty^2}{\rho_\infty D_\infty c_p}\left(1 + 0.276\,\mathrm{Re}_{dl0}^{1/2}\, Sc^{1/3}\right)$$

which enables to rewrite *G₁*:

$$G_1 = 3\left(1 + 0.276\,\mathrm{Re}_{dl0}^{1/2}\, Sc^{1/3}\right) Le N \left(\frac{r_{l0}}{R_\infty}\right)$$

of further importance is the air/fuel mass density ratio.

$$\beta = \frac{4}{3}\frac{\pi r_{l0}^3 n_0 \rho_l}{\rho_\infty}$$

Sprays with large b are characterized by high speed jets and large droplets which yields short residence times and poor vaporization with lower group burning rates.

For a fixed b, high G-sprays have a higher burning rate, are characterized by dense small droplets with high vaporization rates and thus higher group burning rate.

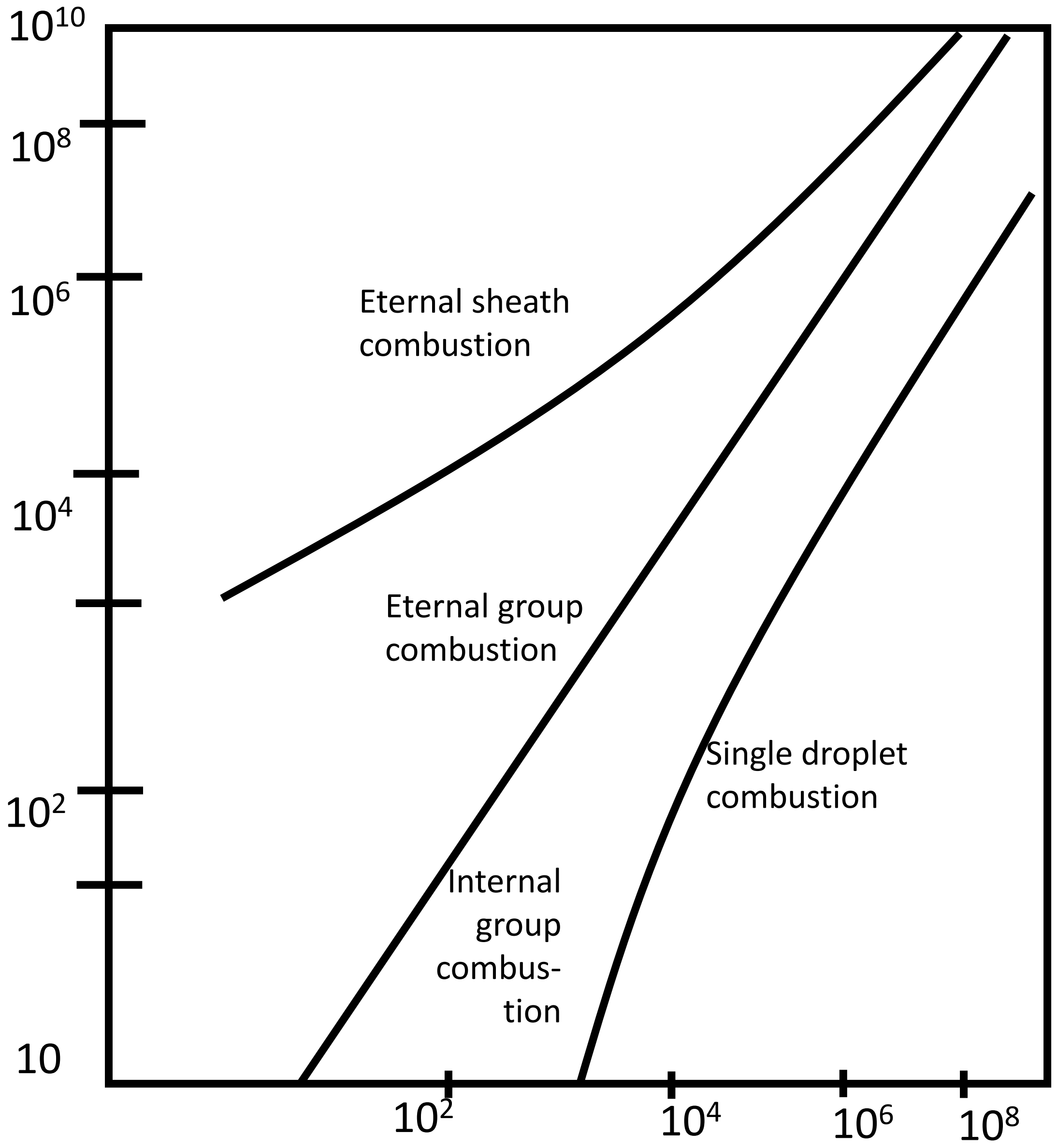
Spray Combustion

Group Combustion Model of Chu

Plotting *N*, the total number of droplets as a function of the non-dimensional separation distance *s* yields:

$$s = 0.05 \frac{d_i / r_i}{1 + 0.276 \,\mathrm{Re}_{dl0}^{1/2}\, Sc^{1/3}}$$

However, this model still misses effects such as radiation, particle dispersion by turbulence, and more.



Spray Combustion

Spray Combustion Models

Locally Homogeneous Flow Models

Basic Assumptions:

- Transport coefficients of all species and heat are the same (*D, α ,v*) (holds for molecular and turbulent quantities)
- Combustion is adiabatic
- Radiation, viscous dissipation and kinetic energy are negligible
- Molecular rates of reaction are infinitely fast, thus local thermodynamic equilibrium is maintained
- Mean flow is steady and axisymmetric
- Quite often the *k*-*ε* model is applied with the isotropic turbulent viscosity modelled as

$$\Rightarrow \mu_t = C_\mu \bar{\rho} \frac{k^2}{\varepsilon};$$

→ Local state of mixture is entirely specified by pressure and mixture fraction solely.

Spray Combustion

Spray Combustion Models

Locally Homogeneous Flow Models

Various modeling approaches for two situations: non-swirling and swirling injection, w/wo boundary layer combustion for axisymmetric, steady state flows.

Sample approach for non-swirling flow, axisymmetric, steady state

$$\frac{\partial}{\partial x}\left(\bar{\rho}\bar{u}\phi\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\bar{\rho}\bar{v}^{\phi}\phi\right)=\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\mu_l}{\sigma_\phi}\frac{\partial\phi}{\partial r}\right)+S_\phi;$$

$$H_t=\sum Y_i h_i+\frac{1}{2}\left(u^2+v^2+w^2\right);$$

$$h_i=\Delta h^0_{f,i}+\int_{T_{red}}^{T}c_{p,i}\,dT$$

Table

for variable source terms

ϕ	S_ϕ
1	0
$\bar{u}^b$	$\pm a(\rho_\infty-\bar{\rho})$
k	$\mu_l=\left(\frac{\partial\bar{u}}{\partial r}\right)^2-\rho\varepsilon$
ε	$\frac{\varepsilon}{k}\left(c_{\varepsilon 1}\mu_l\left(\frac{\partial\bar{f}}{\partial r}\right)^2-c_{\varepsilon 2}\bar{\rho}\varepsilon\right)$
$\bar{f}$	0
$\bar{H}^+$	S_{rad}
g	$c_{g2}\mu_l\left(\frac{\partial\bar{f}}{\partial r}\right)^2-c_{g2}\bar{\rho}\frac{\varepsilon g}{k}$
Y_i	$C_i R_f$

Spray Combustion

Spray Combustion Models

Separated (Two-Phase) Flow Models treat finite rates of exchange of mass, momentum and energy between liquid and gas phase. However, they usually don’t model individual droplets but employ empirical correlations for drag, mass and heat transfer.

Particle-Source-in-Cell Model (Discrete Droplet Model)

a) Deterministic Separated Flow Model

b) Stochastic Separated Flow Model

- A finite number of droplet groups are applied to represent the entire spray
- The movement of such samples are tracked through the flow applying a Lagrangian formulation while a Eulerian formulation is used to solve the governing equations of the gaseous phase
- Effects of droplets on gas phase are accounted for by appropriate source terms of the gas phase equations

Spray Combustion

Spray Combustion Models

a) Deterministic Separated Flow Model

Here slip and interface transport rates are considered but effects of droplet dispersion by turbulence and effects of turbulence on interphase transport are ignored. Droplets are assumed to interact with the mean gas motion. Usually, standard drag coefficients for spheres are employed and virtual mass and Basset forces as well as particle interactions are ignored.

Models works well for high void fractions and high liquid-to-gas density ratios.

b) Stochastic Separated Flow Model

Here, slip and interaction of droplets on turbulence are considered while effects of turbulent fluctuations on droplets are ignored. Several authors have propose variations of the model for different boundary conditons (low Mach number, small particle loading, high Reynolds number, …)

Spray Combustion

Spray Combustion Models

Continuous Droplet Model

Based on a statistical distribution function of the spray which describes the probable number of particles of chemical composition *j* in the radius range *dr* around *r* located in the spatial range *dx* about ***x*** and velocities in the range *dv* about ***v*** at time *t*,

$$f_j = \left(r, \mathbf{x}, \mathbf{v}, t\right) dr d\mathbf{x} d\mathbf{v}$$

applying this distribution function, the statistical distributions of droplet temperature, concentration, …… will be available.

Spray Combustion

Mixture Ratio Inhomogeneity

Varying droplet diameters in a spray and different vaporization/combustion case yield a resulting inhomogeneous mixture ratio field which result in

- formation of local fuel-rich or oxidizer-rich combustion zones (consequences for soot or NOx formation in aero engines)
- time- and space dependent ignition limits and ignition times (problem of extinction / flame blow-out)

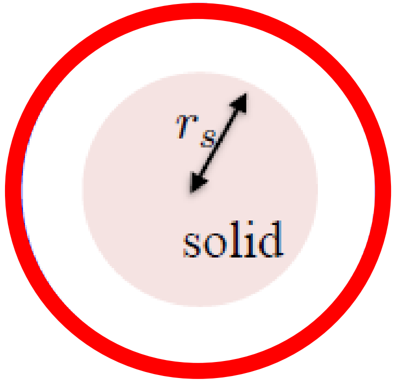
General Characteristics of Spray Flames

- Progress is controlled the slowest process which is either mixing (mixing may be dominated by diffusive transport in case on no or small velocities in case of no or laminar flow or by turbulent transport in case of turbulent flow) or vaporization (vaporization may be dominated by either large temperature or pressure gradients (flashing) and additionally radiation)
- Spray flames are usually thicker than gas/gas flames because quite often all four different combustion regimes are present inside the combustion chamber.

Combustion of a Solid Particle

Problem may be handled similarly to a single liquid droplet

→ Solid particle is surrounded by a diffusion flame



Two possible cases

a) Flame close to the surface : diffusion controlled

$$r_d^{\,2}(t) = r_0^2 - \frac{2\rho D}{\rho_s}\left(1 - \frac{\nu_f W_f}{\upsilon_O W_O} Y_O\right) t$$

b) Surface combustion: kinetic controlled (B_s energy transfer to solid)

$$r_d(t) = r_0 - \frac{2\rho}{\rho_s} Y_O B_s \exp\left(-\frac{E}{RT_s}\right) t$$

Combustion of a Solid Particle

Particle Life-Time

$$t = \begin{cases} \dfrac{r_0^2 \rho_s}{2\rho D} \dfrac{1}{\ln\left(1 + \dfrac{\nu_f W_f}{\upsilon_O W_O} Y_O\right)} \\[2ex] \dfrac{r_0 \rho_s}{\rho Y_O B_s} \exp\left(-\dfrac{E}{R T_s}\right) \end{cases}$$

diffusion controlled, life time is independent of temperature, usual d² law holds

kinetic controlled, life time is inversely proportional to temperature and is thus linearly dependent on diameter

Controlling mechanism is determined by a surface Damköhler number *Da*$_s$:

$$Da_s = \frac{t_{diff}}{t_{kin}} = \frac{r_0 B_s Y_O \exp\left(-\dfrac{E}{R T_s}\right)}{2 D_O \ln\left(1 + \dfrac{\nu_f W_f}{\upsilon_O W_O} Y_O\right)}$$

Large particles or high temperature
→ diffusion controlled

Small particles, low temperature
→ kinetic controlled

Droplet and Spray Combustion

What you should not forget

- Typical injectors
- Atomization diagram
- Droplet formation and forces on droplet
- Droplet tracking methods
- What is D^2 law ?
- What do Spalding transfer numbers describe ?
- Droplet combustion
- Spray combustion cases and their importance for emissions
- Solid particle combustion and limiting cases