Turbulence – Combustion interaction

- What is fluid turbulence well known?
- Combustion modes premixed, diffusion and partially premixed
- Combustion times vs. fluid times or Damköhler number
- Extinction ignition steady reaction
- Learning from fundamental combustion configurations –
 mixing layer, stagnation point flow lifted flames for modeling
- Basic modeling features of combustion in turbulent flows single step reaction, full chemistry

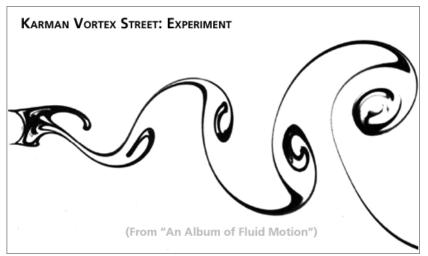
H. S. Mukunda, IISc Bangalore CFD workshop, GTRE, 24 May 2013

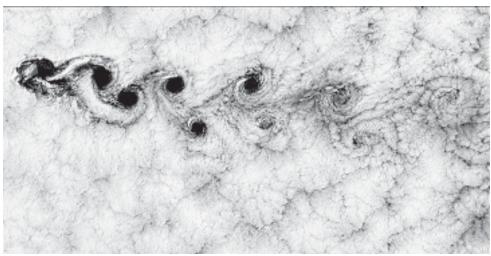
Answers needed from you to help focus on what we should discuss usefully

- How many of you have performed simulations involving chemistry?
- Are these only aerospace related problems gas turbine related or have you dealt with other engineering issues?
- What kind of physical sizes had you to deal with? 100 mm? 500 mm? 1000 mm?
- Only steady state solutions? Unsteady solutions as well?
 Acoustics involved as well?
- Have you encountered issues related to numerics only? If at all?
- How have had to figure out if the results are meaningful at all? Or was this not needed any time?

What is fluid turbulence – well known?

- 1. Just unsteady flow? Unsteady flow with random fluctuations developing from random inputs? Or something else?
- 2. Given a measurement platform how will you declare a flow is turbulent or unsteady random flow?
- 3. It is said to be difficult to understand it (and so model it). Why is it so? Is it controlled by local flow only? Or is it affected differently?
- 4. What will combustion add to it? More difficulties? More features with lessoned difficulties?





f = 0.185 U/D.

Strohaul number = fD/U = 0.195 (1 - 20.1v/UD)see Govardhan and Ramesh, Resonance, August 2005

Any organized simply understood system cannot be turbulent flow! Will oscillations of the cylinder or the free stream, even random lead to turbulent flow?

From Nonlinear dynamics of the wake of an oscillating cylinder – Olinger and Sreenivasan Let us see.......

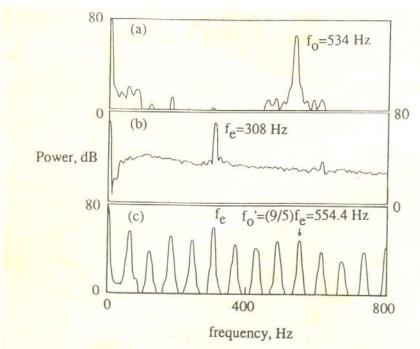


FIG. 1. (a) Power spectral density for the case of natural vortex shedding at $f_0 = 534$ Hz. (b) The corresponding data for the excitation source, measured with a photodiode; $f_e = 308$ Hz. (c) Frequency locking occurring as a result of excitation. The natural shedding frequency disappears in favor of the new peak at $\frac{9}{5} f_e$; peaks appear at other fractions of f_e .

Turbulent flow – random fluctuations with energy at all frequencies! These frequencies are not directly related to each other simply. The flow features control the relationships.

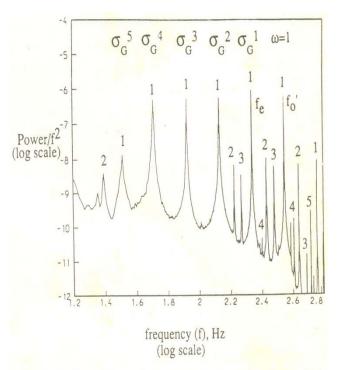
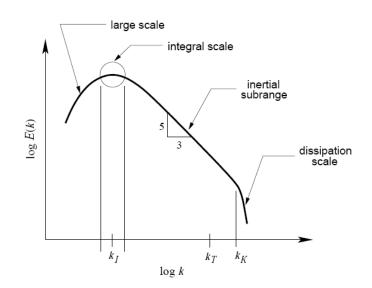


FIG. 5. Frequency-scaled power spectrum for the excited wake at the critical golden-mean point (to within 0.1%).



Turbulent length scales and time scales

RMS velocity fluctuation in terms of fluctuating kinetic energy

$$v' = \sqrt{\frac{2}{3}\tilde{k}}$$

L = Large eddy scale – normally size of the flow field

$$Re_L = \frac{v'L}{v}$$

$$\eta \ = \ \frac{1}{Re_L^{3/4}} L$$

Kolmogorov length scale

$$\eta = \left(\frac{\nu^3}{\tilde{\epsilon}}\right)^{\frac{1}{4}}$$

Energy dissipation

$$\epsilon = \frac{\mu}{\rho} \frac{\partial u_i'}{\partial x_i} \frac{\partial u_i'}{\partial x_i}$$

Kolmogorov time scale

$$\tau_{\eta} = \left(\frac{\nu}{\tilde{\epsilon}}\right)^{\frac{1}{2}}$$

$$\eta = \frac{1}{15^{1/4}} \frac{1}{Re_{\lambda}^{1/2}} \lambda$$

$$\lambda = \left(\frac{10\nu\tilde{k}}{\tilde{\epsilon}}\right)^{\frac{1}{2}}$$

$$Re_{\lambda} = \frac{v'\lambda}{\nu} = \left(\frac{20\tilde{k}^2}{3\nu\tilde{\epsilon}}\right)^{\frac{1}{2}}$$

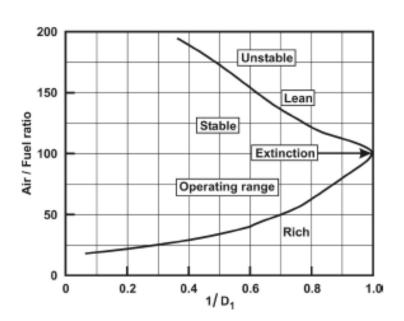
Fluid time/chemical time: First Damköhler number

$$Da = \frac{\tau_{fm}}{\tau_{ch}}$$

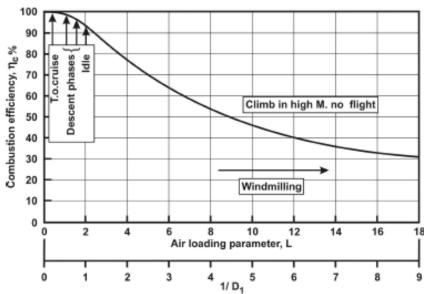
Various combustion devices and Damkohler numbers

Table 6.7: Comparison of various combustion devices; GT MC = Gas turbine main combustor, AB = Afterburner, RJ = ramjet, LR = Liquid Rocket

Type	$\operatorname{GT}\operatorname{MC}$	AB/ RJ	LR	Scramjet
Pressure, atm.	2 - 40	2 – 5	20 – 200	0.5 - 1.5
Temperature, K	500 - 750	600 - 2000	2500 - 3500	1200 - 1500
Mach number	0.2 - 0.4	0.3 - 0.5	0.5 - 0.7	1.5 - 3.5
Mean velocity, m/s	150 - 300	200 - 350	800 - 1000	700 - 1500
Reaction time, ms	0.3 - 1	3 - 4	1 - 2	1 - 1.5
Residence time, ms	3.5 - 5	4 - 5	2 - 3	0.7 - 1.0
Damkohler number	1 - 5	1 - 2	1 - 3	0.5 - 1.0
Pressure loss, %	6 - 8	4 - 5	5 - 20	15 - 25







 $Table \ 6.6: Combustor \ performance \ for \ Olympus \ and \ JT \ 9D \ engines \ (The \ normalized \ quantities \ have \ been \ calculated \ with \ the \ units \ for \ primary \ quantities \ shown \ below)$

Parameter	Olympus 593	JT 9 D
Combustor volume, m ³	0.08	0.19
Comp. Pr. ratio	15.5	25.5
Sea level Take-off		
Thrust, kN	167.0	240.0
mair, kg/s	186.0	118.0 (core)
\dot{m}_{fuel} , kg/s	1.5	2.4
$p_{ambient}$, atm	1.01	1.01
$T_{ambient}$, K	288.0	288.0
T_{stag} , K	288.0	288.0
p_{comb} , atm	15.5	25.5
T_{comb} , K	627.0	722.0
Heat release rate, MW/m^3	787.5	530.5
$m\sqrt{T_{stag}}/p_{stag}$	3125.2	2502.0
$L = \dot{m}/p_{comb}^{1.8}T_{comb} \times 10^4$	21.5	4.9
t_r , ms	2.5	9.5
t_t , ms	1.4 to 1.6	1.3 - 1.5
D_1	1.6 - 1.8	6.3 - 7.3
Cruise		
Flight altitude, km	16.0	11.0
Flight M	2.0	0.85
$T_{ambient}$, K	216.0	216.0
$p_{ambient}$, atm	0.101	0.226
T_{stag} @ ISA + 5, K	398.0	253.0
p_{stag} , atm	0.79	0.362
$\dot{m}_{air},$ kg/s	105.0	52.0 (core)
\dot{m}_{fuel} , kg/s	1.5	0.864
p_{comb} , atm	12.25	9.23
T_{comb} , K	867.0	635.0
$\dot{m}\sqrt{T_{stag}}/p_{stag}$	2651.6	2284.8
$L = \dot{m}/p_{comb}^{1.8}T_{comb} \times 10^4$	13.4	14.9
t_r, \mathbf{ms}	2.33	5.1
t_t , ms	1.4 - 1.6	1.4 - 1.6
D_1	1.5 - 1.7	3.2 - 3.7

$$D_1$$
 = Da $Da = \frac{\tau_{fm}}{\tau_{ch}}$

What does combustion do to the flow?

- Combustion introduces zones that are at high temperature in a fluid which is otherwise at low (or lower) temperature.
- These occur at low speeds (compared to acoustic speeds) deflagration.
- If heat release occurs over a distance of maximum of hundreds of mean free path,
 one has detonation. We are not discussing them here.
- If heat release occurs over distances 1000 times the mean free path or more, then
 one has deflagration.
- The distance over which deflagration occurs is about 50 to 1000 μ m, the distance going down with pressure ($\delta_f \sim 1/p$). This distance $\delta_f <<$ meaningful combustion device size 10 to 500 mm
- Thus one can look upon the flames as "thin" except under certain conditions –
 extinction, ignition.
- Since fluid viscosity $\sim T^{0.7}$, it will be much higher in the high temperature zone (products) compared to low temperature zone (reactants)
- Re in the hot zone much smaller (by a factor 3 to 5) compared to cold zone
- Acoustic speeds are much higher in the hot zone (1000 m/s) compared to cold zone (340 m/s)

Combustion modes – premixed and diffusion

Fuel/oxidizer mixing	Fluid motion	Examples
Premixed	Turbulent	Spark-Ignited gasoline engines Low-NO _x stationary gas turbine
	Laminar	Flat flame Bunsen flame (followed by a nonpremixed candle for φ>1)
Nonpremixed (Diffusion)	Turbulent	Diesel engine Aircraft turbine H ₂ /O ₂ rocket engine
	Laminar	Wood fire Candle Radiant burners for heating

- Combustion can occur only when the collisions between molecules are energetic molecules with velocity much higher than the mean only contribute to reactions.
- These collisions between molecules of different species creates new species.
- Only the most stable molecules under the prevailing conditions of temp and pressure remain.
- Combustion at the core is always "molecular" with sizes very small $\sim 1 10 \mu m$.
- Turbulence affects the availability of "fuel" and "oxidizer" packets in appropriate zones

Premixed flames - Diffusion flames

Premixed flames Fuel and air is mixed before combustion Product zone Reaction zone Pre-heat zone Unburned gas zone Porous-plug burner Fuel + air

Nonpremixed flames (Diffusion flames) Fuel and air burn when they meet

Laminar flames

- Premixed
 - e.g. Bunsen flame
 - Rather low flame velocity







Nonpremixed (Diffusion)

- e.g. candle flame
- Fuel: wax, Oxidizer: air
- Reaction zone between wax vapors and air

Premixed flames



Example: Spark-Ignition Engine

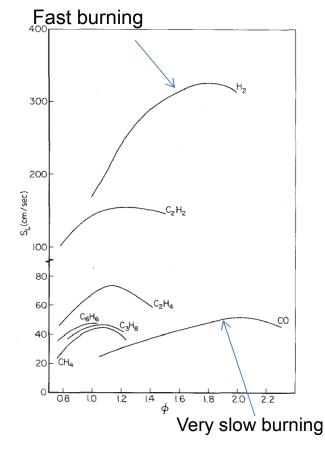
- Gaseous fuel and oxidizer are mixed on a molecular level prior to combustion
- Hydrocarbon/air flames have burning velocities around 0.5 m/s

Nonpremixed flames (Diffusion flames)



Example: Diesel Engine

- Fuel and oxidizer are introduced separately and mix during combustion
- Energy release rate limited by mixing process
- Reaction zone between oxidant and fuel zone



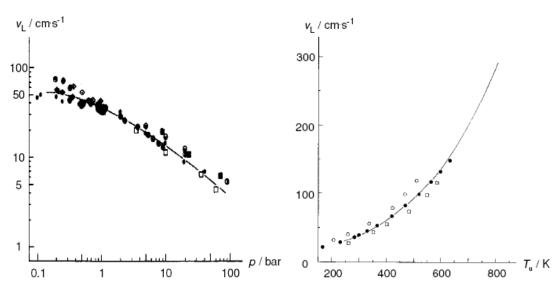
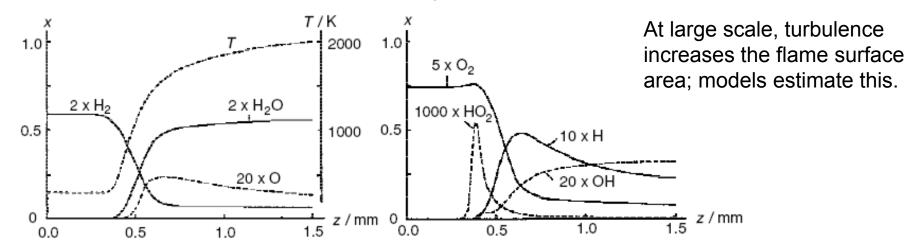


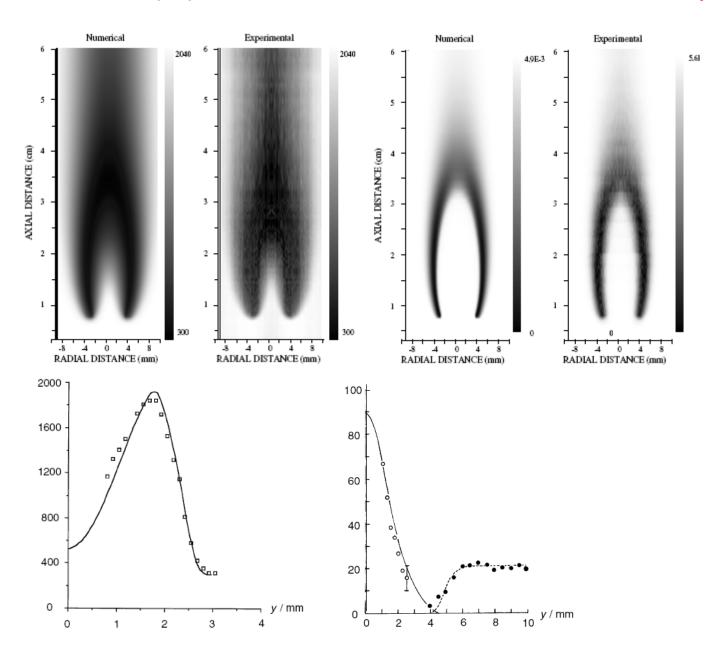
Fig. 8.8. Pressure dependence of v_L for $T_u = 298$ K (left) and temperature dependence of v_L for p = 1 bar (right) in stoichiometric CH₄-air mixtures (Warnatz 1988)

$$S_u \simeq \sqrt{(k/c_p)A_f} \frac{RT_{in}}{p} p^{n/2} e^{-E/2RT_f} \simeq p^{(n/2)-1} e^{-E/RT_f}$$

$$\rho_u S_u = \sqrt{(k/c_p)\dot{w}_f'''} \qquad \qquad d_f = (k/c_p) \times (1/\rho_u S_u)$$



Diffusion flames – fuel and oxidizer fluxes in stoichiometric proportions arrive at the flame – flame is formed there only



Extinction/Ignition in flames

Assumptions: equal diffusivities of chemical species and temperature

$$Le_i = \lambda/(c_p \rho D_i) = 1, \quad i = 1, 2, \dots, k$$
 \Rightarrow $D = \lambda/(\rho c_p)$

The balance equation for mixture fraction, temperature and species read:

$$\rho \frac{\partial Z}{\partial t} + \rho v_{\alpha} \frac{\partial Z}{\partial x_{\alpha}} - \frac{\partial}{\partial x_{\alpha}} \left(\rho D \frac{\partial Z}{\partial x_{\alpha}} \right) = 0$$

$$\rho \frac{\partial T}{\partial t} + \rho v_{\alpha} \frac{\partial T}{\partial x_{\alpha}} - \frac{\partial}{\partial x_{\alpha}} \left(\rho D \frac{\partial T}{\partial x_{\alpha}} \right) = \sum_{i=1}^{k} \dot{m}_{i} \frac{h_{i}}{c_{p}} + \frac{\dot{q}_{R}}{c_{p}} + \frac{1}{c_{p}} \frac{\partial p}{\partial t}$$

$$\rho \frac{\partial Y_{i}}{\partial t} + \rho v_{\alpha} \frac{\partial Y_{i}}{\partial x_{\alpha}} - \frac{\partial}{\partial x_{\alpha}} \left(\rho D \frac{\partial Y_{i}}{\partial x_{\alpha}} \right) = \dot{m}_{i} \quad i = 1, 2, \dots, k$$

$$\rho \frac{\partial T}{\partial \tau} - \rho D \left(\frac{\partial Z}{\partial x_{\alpha}} \right)^{2} \frac{\partial^{2} T}{\partial Z^{2}} \approx \sum_{i=1}^{k} \dot{m}_{i} \frac{h_{i}}{c_{p}} + \frac{\dot{q}_{R}}{c_{p}} + \frac{1}{c_{p}} \frac{\partial p}{\partial t}$$

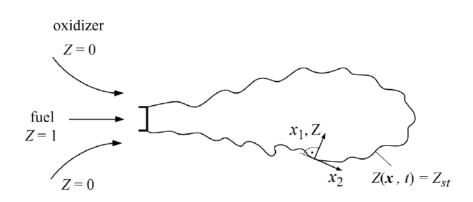
Z replaces x

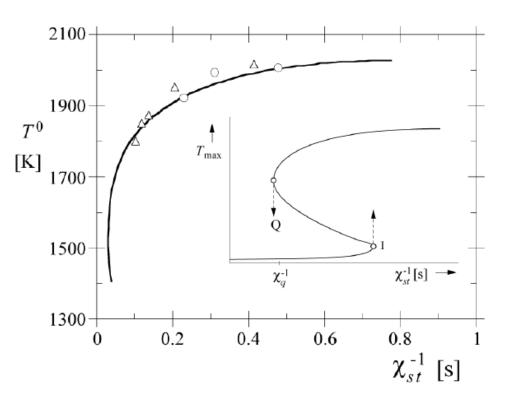
$$\rho \frac{\partial T}{\partial t} - \rho \frac{\chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = \sum_{l=1}^r \frac{Q_l}{c_p} \omega_l + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

$$\rho \frac{\partial Y_i}{\partial t} - \rho \frac{\chi_{st}}{Z} \frac{\partial Y_i}{\partial Z^2} = \dot{m}_i \quad i = 1, 2, \dots, k.$$

Scalar dissipation rate

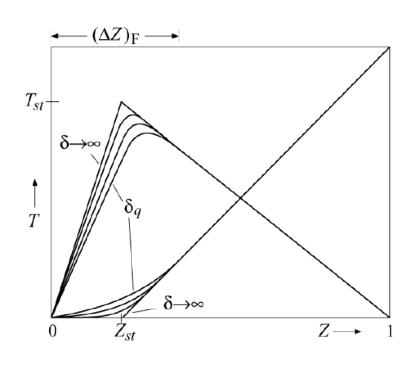
$$\chi_{st} = 2D \left(\frac{\partial Z}{\partial x_{\alpha}}\right)_{st}^{2}$$





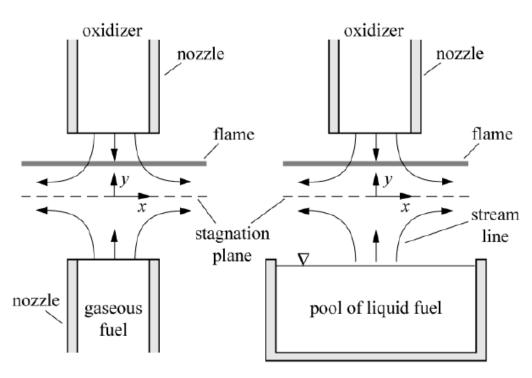
$$-\rho \frac{\chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = \frac{Q}{c_p} \omega$$

$$\chi = 4aZ^2 \left[\text{erfc}^{-1}(2Z^2) \right]$$



Thus the maximum temperature will decrease until the flamelet is quenched at a value of $\chi_{st} = \chi_q$.

Why does extinction occur?



$$\chi = 4aZ^2 \left[\text{erfc}^{-1}(2Z^2) \right]$$

$$\mathrm{Da} = \frac{B\rho_{\mathrm{st}}\nu_{\mathrm{O_2}}'Y_{F,1}}{\chi_{\mathrm{st}}W_F(1-Z_{\mathrm{st}})}\exp\left(-\frac{E}{\mathcal{R}T}\right)$$

Experimental observation: When the stream speeds are increased, beyond a speed, the flame extinguishes.

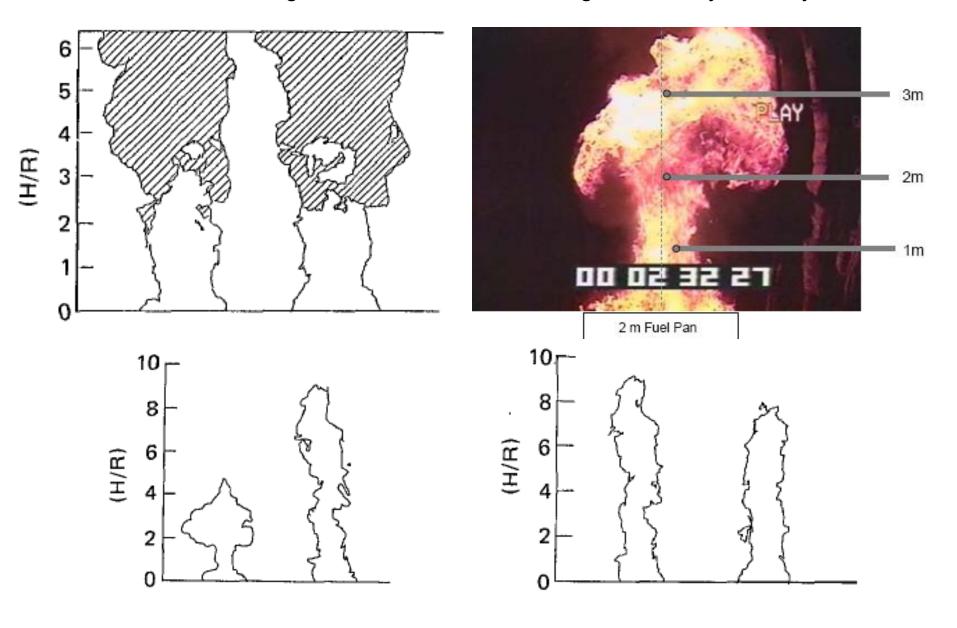
a = stag vel. gradient ~ U/d

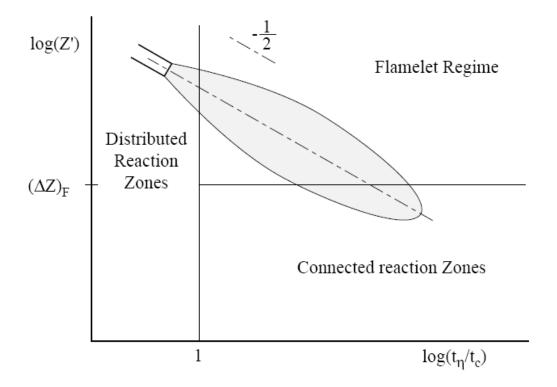
Increase in a leads to increase in stretch. Too much positive stretch causes extinction Because there is inadequate residence time.

In dimensionless terms, Da = Damkohler number = fluid time/chemical kinetic time;

In a turbulent flow, the eddies cause stretching of the flame and this leads to enhancement of the flame or extinguishment.

Nature of large diffusion flames at ambient pressure Notice broken segments due to extinction-reignition – why are they there?.





The second criterion, based on time scales, should as in premixed combustion, consider the ratio of the Kolmogorov to the chemical time. The Kolmogorov time $t_{\eta} = (\nu/\tilde{\varepsilon})^{1/2}$ is the turnover time of the smallest eddies and therefore the shortest characteristic time of turbulence. If combustion is fast with respect to this time scale, it may be considered as quasi-steady and the diffusion flamelet concept is valid. If however, the Kolmogorov time is of the same order or shorter than the chemical time, the flamelet regime breaks down and regions of intense mixing and reaction will appear. As in premixed combustion, we will call this regime the distributed reaction zones regime (conf. [11.4]).

Turbulent diffusion model - EDC

EDC assumes that the fluid state is determined by the fine structure state, the surrounding state and the fraction of fine structures. The turbulent fine structures are assumed to be concentrated in fine-structure regions. On the basis of similarity considerations of the transfer of energy from the macroscale to the fine structure, Magnussen proposes the following expression for the fraction of the flow occupied by such regions.

$$C_{D1} = 0.134 \text{ and } C_{D2} = 0.5 \qquad \gamma = \left(\frac{3C_{D2}}{4C_{D1}^2}\right)^{\frac{1}{4}} \left(\frac{\nu^* \tilde{\epsilon}}{\tilde{k}^2}\right)^{\frac{1}{4}}$$
 (1.31)

Scalar dissipation rate

$$\frac{\tilde{w}_f}{\rho} = -\frac{\gamma^2 \chi_{\text{remin}} \left[\hat{Y}_{\text{min}}, \ \hat{Y}_P, \ (\hat{Y}_{\text{min}} + \hat{Y}_P) \gamma \right]}{\tau^* \min \left[\hat{Y}_{\text{min}}, \ \hat{Y}_P, \ (\hat{Y}_{\text{min}} + \hat{Y}_P) \gamma \right]}$$

For fast chemistry limit,
$$\tau = \left(\frac{C_{D2}}{3}\right)^{1/2} \left(\frac{\nu^*}{\epsilon}\right)^{1/2} = \left(\frac{C_{D2}}{3}\right)^{\frac{1}{2}} \tau_\eta^* \qquad \tau_\eta = \left(\frac{\nu}{\tilde{\epsilon}}\right)^{\frac{1}{2}}$$

For full chemistry,

$$\frac{\overline{\dot{w}_i}}{\rho} = 11.17 \frac{\epsilon}{k} \left(\frac{\overline{Y_i} - Y_i^*}{1 - \gamma^3} \right)$$

Eddy dissipation

For moderate Re_{λ} , the factor $1/(1-\gamma^3)$ is close to unity as $\gamma = 3.43/\sqrt{Re_{\lambda}}$. Recognising $\hat{Y}_{\min} = \min(Y_f, Y_o x/s) = \hat{Y}_L$ and $\gamma^2/\tau^* = 11.17 \epsilon/k$, the mean reaction rate equation [Eq. 1.54] can be written as:

$$\frac{\tilde{w_f}}{\rho} = -\operatorname{const.} \frac{\epsilon}{k} \, \tilde{Y_L} \tag{1.55}$$

which is essentially same as Eq. 1.21 - the model proposed by Spalding for predicting mean reaction rate.

How to identify in the flow premixedness or diffusion state

$$D = \nabla Y_{\rm H_2} \cdot \nabla Y_{O_2}$$

The term D determines the nature of combustion

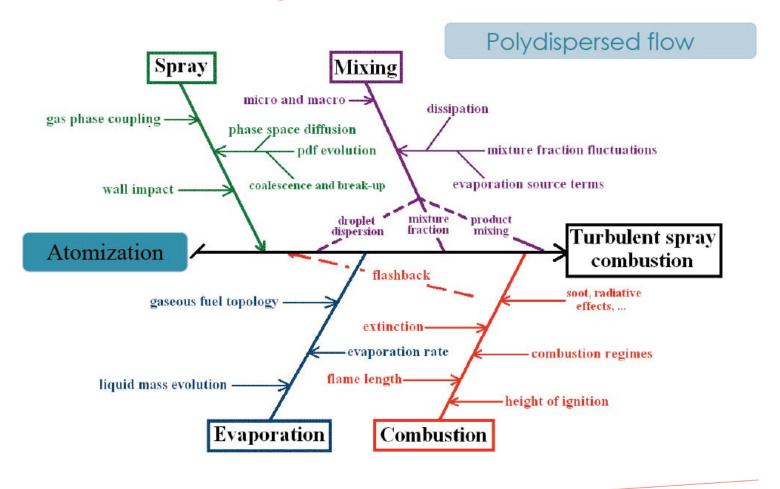
$$E = Y_{\rm H_2} Y_{\rm O_2} / z_{\rm H} z_{\rm O}$$

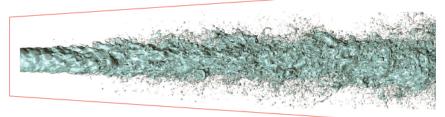
The parameter E is the measure of unreactedness

For No reaction,
$$Y_{H2} = Z_H$$
 and $Y_{O2} = Z_O$ so $E = 1$

For Fast Chemistry
$$Y_{H2} = 0$$
 or $Y_{O2} = 0$ so $E = 0$

Multi-phase flows





Brief summary

- Combustion process occurs at fine scales. Flow variations are at varying scales – mostly large.
- Treating combustion as fast is a good approximation for mean thermal properties.
- Most combustion process is diffusion dominated. Modeling such systems at various levels of sophistication exist (not discussed here).
- For pollution estimation (CO, NO_x), this information is used in several ways - not discussed here.
- Knowledge of basic combustion principles is valuable (may even be essential) to interpret results meaningfully since the interactions are complex.