Lecture 11

Premixed Turbulent Combustion:
The Regime Diagram
Regimes in Premixed Turbulent Combustion

- Diagrams defining regimes of premixed turbulent combustion in terms of velocity and length scale ratios have been proposed by Borghi (1985), Peters (1986) and many others.

- For scaling purposes, it is useful to assume equal diffusivities for all reactive scalars, a Schmidt number of unity

\[ \text{Sc} = \frac{\nu}{D} = 1 \]

and to define the flame thickness and the flame time as

\[ \ell_F = \frac{D}{s_L}, \quad t_F = \frac{D}{s_L^2} \]
• Then, using $\nu = D$, the turbulent intensity and the turbulent length scale introduced in Lecture 10, we define the turbulent Reynolds number as

$$\text{Re} = \frac{\nu'\ell}{s_L\ell_F}$$

and the turbulent Damköhler number

$$\text{Da} = \frac{s_L\ell}{\nu'\ell_F}$$

• Furthermore, with the Kolmogorov time, length, and velocity scales defined in Lecture 10, we introduce two turbulent Karlovitz numbers

• The first one defined as

$$Ka = \frac{t_F}{t_\eta} = \frac{\ell_F^2}{\eta^2} = \frac{v_\eta^2}{s_L^2}$$

measures the ratios of the flame scales in terms of the Kolmogorov scales
• Using the definitions

\[ \eta = \left( \frac{\nu^3}{\varepsilon} \right)^{1/4}, \quad t_\eta = \left( \frac{\nu}{\varepsilon} \right)^{1/2}, \quad \nu_\eta = (\nu\varepsilon)^{1/4} \]

with \( \nu = D \) and

\[ \varepsilon \sim \frac{v_n^2}{t_n} \sim \frac{v_n^3}{\ell_n} \sim \frac{\ell_n^2}{t_n^3} \]

it is seen that

\[ \text{Re} = \frac{v'\ell}{s_L\ell_F}, \quad \text{Da} = \frac{s_L\ell}{v'\ell_F}, \quad \text{Ka} = \frac{t_F}{t_\eta} = \frac{\ell_F^2}{\eta^2} = \frac{v_\eta^2}{s_L^2} \]

can be combined to show that

\[ \text{Re} = \text{Da}^2\text{Ka}^2 \]
Referring to the discussion about the appropriate reaction zone thickness $\delta$ in premixed flames in Lecture 6, a second Karlovitz number $K_{a\delta}$ may be introduced as

$$K_{a\delta} = \frac{\ell_{\delta}^2}{\eta^2} = \delta^2 K_a$$

where for the reaction zone thickness

$$\ell_{\delta} = \delta \ell_F$$

has been used.
Regime diagram for premixed turbulent combustion

\[ \log(v'/s_L) \text{ versus } \log(\ell/\ell_F) \]

- Using

\[ \text{Ka} = \frac{\ell_F^2}{\eta^2} \quad \text{and} \quad \text{Re} = \frac{v'\ell}{s_L\ell_F} \]

where for scaling purposes we have set \( \varepsilon \equiv \frac{v'^3}{\ell} \), such that the Kolmogorov length scale squared becomes

\[ \eta^2 = \left( \frac{v^3}{\varepsilon} \right)^{1/2} = \left( s_L^3 \ell_F^3 \frac{\ell}{v'^3} \right)^{1/2} \]

the ratios \( v'/s_L, \ell/\ell_F \) may be expressed in terms of Re and Ka as

\[ \frac{v'}{s_L} = \text{Re} \left( \frac{\ell}{\ell_F} \right)^{-1} = \text{Ka}^{2/3} \left( \frac{\ell}{\ell_F} \right)^{1/3} \]
Regime diagram for premixed turbulent combustion

- Using these relations, the lines $Re = 1$, $Ka = 1$ represent boundaries between different regimes of premixed turbulent combustion.

- Other boundaries of interest are the line $\nu' / s_L = 1$ which separates the wrinkled flamelets from the corrugated flamelets, and the line denoted by $Ka_\delta = 1$, which separates thin reaction zones from broken reaction zones.
Regime diagram for premixed turbulent combustion

- The line $Re = 1$ separates all turbulent flame regimes characterized by $Re > 1$ from the regime of laminar flames ($Re < 1$), which is situated in the lower-left corner of the diagram.

- We will consider turbulent combustion for large Reynolds numbers, which corresponds to a region sufficiently removed from the line $Re = 1$ towards the upper r.h.s.
Regime diagram for premixed turbulent combustion

- We will not consider the wrinkled flamelets regime, because it is not of much practical interest.

- In that regime, where $v' < s_L$, the turn-over velocity $v'$ of even the large eddies is not large enough to compete with the advancement of the flame front with the laminar burning velocity $s_L$. Laminar flame propagation therefore is dominating over flame front corrugations by turbulence.
Regime diagram for premixed turbulent combustion

- We will also not consider the broken reaction zones Regime in any detail for reasons to be discussed at the end of this lecture.

- Among the remaining two regimes, the corrugated flamelets regime is characterized by the inequalities $\nu' > s_L$, $\text{Re} > 1$ and $\text{Ka}_\delta < 1$. 

\[ \frac{\nu'}{s_L} \]

\[ \text{Re} = 1 \]

\[ \text{Ka}_\delta = 1 \]

\[ \eta = \ell_\delta \]

\[ \eta = \ell_F \]

\[ \text{corrugated flamelets} \]

\[ \text{thin reaction zones} \]

\[ \text{broken reaction zones} \]

\[ \text{laminar flames} \]

\[ \text{wrinkled flamelets} \]

\[ \ell / \ell_F \]
The corrugated flamelet regime

- In view of

\[ \text{Ka} = \frac{t_F}{t_\eta} = \frac{\ell_F^2}{\eta^2} \]

for \( \text{Ka} < 1 \)

\[ \ell_F < \eta \]

which means that the entire reactive-diffusive flame structure of thickness \( \ell_F \) is embedded within eddies of the size of the Kolmogorov scale, where the flow is quasi-laminar.
The corrugated flamelet regime

- Therefore the flame structure is not perturbed by turbulent fluctuations and remains quasi-steady.
- The boundary of the corrugated flamelets regime to the thin reaction zones regime is given by $Ka = 1$, which, according to $\ell_F \equiv \eta$ is equivalent to the condition that the flame thickness is equal to the Kolmogorov length scale.

This is called the Klimov-Williams criterion.
• The thin reaction zones regime is characterized by $\text{Re} > 1$, $K_a \delta < 1$, and $K_a > 1$

• $K_a > 1$ indicates that the smallest eddies of size $\eta$ can enter into the reactive-diffusive flame structure since

$$\eta < \ell_F$$

• These small eddies are still larger than the inner layer thickness

$$\eta > \ell_\delta = \delta \ell_F$$

and can therefore not penetrate into that layer
• The non-dimensional thickness $\delta$ of the inner layer in a premixed flame is typically one tenth.

• Therefore the inner layer thickness is one tenth of the preheat zone thickness, which is of the same order of magnitude as the flame thickness.

• Using

$$K a_\delta = \frac{\ell_\delta^2}{\eta^2} = \delta^2 K a$$

we see that the line $K a_\delta = 1$ corresponds with $\delta = 0.1$ to $K a = 100$. 
• We will now enter into a more detailed discussion of the two flamelet regimes.

• In the regime of **corrugated flamelets** there is a **kinematic** interaction between turbulent eddies and the advancing quasi-laminar flame structure.

• With $Ka < 1$ we have: $v' \geq s_L \geq v_\eta$

• To determine the size of the eddy that interacts locally with the flame front, we set the turn-over velocity $v_n = s_L$ in

$$\varepsilon \sim \frac{v^n}{t_n} \sim \frac{v^n}{\ell_n} \sim \frac{l^n}{t^n}$$

• This determines the the **Gibson scale** (cf. Peters, 1986) as $\ell_G = \frac{s_L^3}{\varepsilon}$
• Eddies of the size of the Gibson scale

\[ \ell_G = \frac{s_L^3}{\varepsilon} \]

which have a turnover velocity \( v_n = s_L \) can interact with the flame front

• Since the turn-over velocity of the large eddies is larger than the laminar burning velocity, these eddies will push the flame front around, causing a substantial corrugation

• Smaller eddies of size \( \ell_n < \ell_G \) having a turnover velocity smaller than \( s_L \) will not even be able to wrinkle the flame front
• It has been shown by Peters (1992) that the Gibson scale is the lower cut-off scale of the scalar spectrum function in the corrugated flamelets regime.

• At that cut-off, there is only a weak change of slope in the scalar spectrum function.

• This is the reason why the Gibson scale is difficult to measure.

• The stronger diffusive cut-off occurs at the Obukhov-Corrsin scale defined by

\[ \ell_C = \left( \frac{D^3}{\varepsilon} \right)^{1/4} \]

• Since we have assumed \( D = \nu \), this scale is equal to the Kolmogorov scale.

\[ D = \nu \quad \Rightarrow \quad \ell_C = \eta \]
• The next flamelet regime in the regime diagram is the regime of thin reaction zones

• As noted earlier, in the thin reaction zone regime

\[ \eta < \ell_f \]

small eddies can enter into the preheat zone and increase scalar mixing

• However, these eddies cannot penetrate into the inner layer since

\[ \eta > \ell_\delta \]

• The burning velocity is smaller than the Kolmogorov velocity, which would lead to a Gibson scale that is smaller than the Kolmogorov scale

• The Gibson scale is therefore irrelevant in that regime
• A time scale, however, can be used in the thin reaction zones regime to define a characteristic length scale using Kolmogorov scaling in the inertial range.

• That time scale should represent the response of the thin reaction zone and the surrounding diffusive layer to unsteady perturbations.

• The appropriate time is the same as the flame time $t_F$.

• Using Kolmogorov scaling $\varepsilon \sim \frac{\ell_n^2}{t_n^3}$, the turbulent length scale interacting with the flame is

$$\ell_m = (\varepsilon t_F^3)^{1/2}$$

• This mixing length scale is the size of an eddy within the inertial range which has a turnover time equal to the time needed to diffuse scalars over a distance equal to the diffusion thickness $t_m = t_D$. 

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11.-23
• During its turnover time, an eddy of size $\ell_m$ will interact with advancing reaction front and transport preheated fluid from a region of thickness $\ell_D$ in front of the reaction zone over a distance corresponding to its own size.

• Much smaller eddies will also do this, but since their size is smaller, their action will be masked by eddies of size $\ell_m$.

• Larger eddies have a longer turnover time and would therefore be able to transport thicker structures than those of thickness $\ell_D$.

• They will therefore corrugate the broadened flame structure at scales larger than $\ell_m$. 
• The physical interpretation of $\ell_m$ is therefore that of the maximum distance that preheated fluid can be transported ahead of the flame.

• Differently from the Gibson length scale the mixing length scale can be observed experimentally.

• Changes of the instantaneous flame structure with increasing Karlovitz numbers have been measured by Buschmann et al. (1996) who used 2D-Rayleigh thermometry combined with 2D laser-induced fluorescence on a turbulent premixed Bunsen flame.

• They varied the Karlovitz number between 0.03 and 13.6 and observed at $Ka > 5$ thermal thicknesses that largely exceed the size of the smallest eddies in the flow.
Beyond the line $K\alpha_\delta = 1$, there is a regime called the **broken reaction zones regime** where Kolmogorov eddies are smaller than the inner layer thickness.

- They may therefore enter into the inner layer and perturb it with the consequence that chemistry breaks down locally due to enhanced heat loss to the preheat zone followed by temperature decrease and the loss of radicals.

- When this happens, the flame will extinguish and fuel and oxidizer will mix with burnt regions where combustion reactions have ceased.

- In a series of papers, Mansour et al. (1992), Chen et al. (1996), Chen and Mansour (1997) and Mansour et al. (1998) have investigated highly stretched premixed flames on a Bunsen burner which were surrounded by a large pilot.
- Simultaneous temperature and CH measurements
• They found a thin reaction zone, as deduced from the CH profile, and steep temperature gradients in the vicinity of that zone.

• There also was evidence of occasional extinction of the reaction zone.

• This corresponds to instantaneous shots where the CH profile was absent as in the picture on the upper r.h.s.

• Such extinction events do not occur in the flame F3 which has a Karlovitz number of 23 and is located in the middle of the thin reaction zones regime.

• It can be expected that local extinction events would appear more frequently, if the exit velocity is increased and the flame enters into the broken reaction zones regime.
• Local extinction events will occur at an exit velocity close to 75m/s so frequently that the entire flame extinguishes

• Therefore one may conclude that in the broken reaction zones regime, a premixed flame is unable to survive

• The measurements also show strong perturbations of the temperature profile on the unburnt side of the reaction zone

• This is most evident in the picture on the lower l.h.s., where the temperature reaches more than 1100 K but falls back to 800 K again

• This seems to be due to small eddies that enter into the preheat zone and confirms the concept of the thin reaction zones regime
Regimes in Premixed Combustion LES

- A similar regime diagram can be constructed for LES using the filter size $\Delta$ as the length scale and the subfilter velocity fluctuation $v'_{\Delta}$ as the velocity scale.

- Such a representation introduces both physical and modeling parameters into the diagram.

- A change in the filter size, however, also leads to a change in the subfilter velocity fluctuation.

- An LES regime diagram for characterizing subfilter turbulence/flame interactions in premixed turbulent combustion was proposed by Pitsch & Duchamp de Lageneste (2002) and was recently extended by Pitsch (2005).
• In contrast to the RANS regime diagrams, $\Delta/\ell_F$ and the Karlovitz number $Ka$ are used as the axes of the diagram.

• The Karlovitz number, defined as the ratio of the Kolmogorov timescale to the chemical timescale, describes the physical interaction of flow and combustion on the smallest turbulent scales.

• It is defined solely on the basis of physical quantities, and is hence independent of the filter size.

• The subfilter Reynolds and Damköhler numbers and the Karlovitz number relevant in the diagram are defined as

$$\text{Re}_\Delta = \frac{v'\Delta}{s_L\ell_F}, \quad \text{Da}_\Delta = \frac{s_L\Delta}{v'\ell_F}, \quad \text{and} \quad Ka = \frac{\ell_F^2}{\eta^2} = \left(\frac{v'^3\ell_F}{s_L^3\Delta}\right)^{1/2}$$
• In LES, the Karlovitz number is a fluctuating quantity, but for a given flow field and chemistry it is fixed.

• The effect of changes in filter size can therefore easily be assessed at constant Ka number.

• An additional benefit of this regime diagram is that it can be used equally well for DNS if Δ is associated with the mesh size.

• In the following, the physical regimes are briefly reviewed and relevant issues for LES are discussed.
• The effect of changing the LES filter width can be assessed by starting from any one of these regimes at large ratios

\[ \frac{\Delta}{\ell_F} \gg 1 \]

• As the filter width is decreased, the subfilter Reynolds number, \( \text{Re}_\Delta \), eventually becomes smaller than one

• Then the filter size is smaller than the Kolmogorov scale, and no subfilter modeling for the turbulence is required

• However, the entire flame including the reaction zone is only resolved if \( \Delta < \delta \)
• In the corrugated flamelets regime, if the filter is decreased below the Gibson scale,
  \[ \Delta < \ell_G \]
  which is the smallest scale of the subfilter flame-front wrinkling, the flame-front wrinkling is completely resolved

• It is apparent that in the corrugated flamelet regime, where the flame structure is laminar, the entire flame remains on the subfilter scale, if
  \[ \Delta / \ell_F > 1 \]

• This is always the case for LES
• In the thin reaction zones regime, the preheat region is broadened by turbulence

• Peters (1999) estimated the broadened flame thickness from the assumption that the timescale of the turbulent transport in the preheat zone has to be equal to the chemical time scale, which for laminar flames leads to the burning velocity scaling given in the beginning of this section

• From this, the ratio of the broadened flame thickness $\ell_m$ and the filter size can be estimated as (Pitsch, 2006)

$$\frac{\ell_m}{\Delta} = \left(\frac{\nu'_\Delta \ell_F}{s_L \Delta}\right)^{3/2} = K a \frac{\ell_F}{\Delta} = Da_\Delta^{-3/2}.$$

• Hence, the flame is entirely on the subfilter scale as long as $Da_\Delta > 1$, and is partly resolved otherwise
• It is important to realize that the turbulence quantities, especially $v'_\Delta$, and hence most of the non-dimensional numbers used to characterize the flame/turbulence interactions, are fluctuating quantities and can significantly change in space and time.

• To give an example, the variation of these quantities from a specific turbulent stoichiometric premixed methane/air flame simulation is shown in the regime diagram.

• This simulation was done for an experimental configuration with a nominal Karlovitz number of $Ka = 11$, based on experimentally observed integral scales.

• The simulated conditions correspond to flame F3 of Chen et al. (1996), and details of the simulation can be found in Pitsch & Duchamp de Lageneste (2002).
Summary:
Distinguishing different premixed turbulent combustion regimes

OH radical distribution in turbulent premixed flame

Buschmann 1996

Density distribution from premixed combustion DNS