# Basics of Computational Combustion Modelling

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# *Why study Combustion?*

Combustion of hydrocarbons – important fuel source

- Power generation
- Aircraft, rocket propulsion
- Cars etc
- Marine applications

Combustion – rapid chemical reaction between fuel and oxidant (air). Usually involves fluid flow.

Understand + model processes $\rightarrow$ improve power generation, decrease polutants.

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## *Physical basis*

Complex area of investigation :

- Combustion affects fluid flow. Heat release $\rightarrow \Delta T \rightarrow$ change physical properties. Also buoyancy drives flow
- Fluid flow affects combustion. Brings reactants together, removes products. Can determine rate of combustion, and even extinguish flame.

Overall, combustion $\equiv$ rapid chemical reaction between fuel and oxidiser.

However details vary – treat different regimes differently.

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# *Combustion regimes*

- Non-premixed combustion
  - Regions of fuel + oxidiser separate,
  - Combustion occurs at interface
- Premixed combustion
  - Fuel and oxidiser mixed at molecular level
  - Regions of burned and unburned gas, separated by (thin) flame
- Partially premixed combustion
  - somewhere between

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# *Some examples*

Premixed :

- Spark ignition (IC) petrol engines
- Lean burn gas turbines
- Household burners
- Bunsen burner (blue flame regime)

Partially premixed :

- Direct injection (DI) petrol engines
- Aircraft gas turbines

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# *Examples – non-premixed*

Non-premixed :

- Diesel engines
- Aircraft gas turbines
- Furnaces
- Candles, fires

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# *Flame structure*

Premixed combustion

– Flame propagating in laminar flow is characterised by :

| | |
|---|---|
| Laminar flame speed | $s_L$, |
| thickness | $l_F$ |

Combustion rate controlled by molecular diffusion processes ($D_L$ – diffusivity)

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## *Chemistry*

Dimensional analysis gives :

$$l_F = \frac{D_L}{s_L}$$

linking these processes.

Chemical reaction time

$$t_L = \frac{l_F}{s_L}$$

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# *Turbulent flame structure*

This is more complex. Turbulence characterised by

| | |
|---|---|
| turbulence intensity | $u'$ |
| Integral, Kolmogorov scales | $l_I,\ \eta$ |
| Turbulent Reynolds number | $\mathcal{R}e_T = \dfrac{u' l_I}{\nu}$ |

Characteristic turbulent eddy turnover time

$$t_T = \frac{l_I}{u'}$$

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# *Damköhler number*

Compare importance of turbulence and combustion – Damköhler number

$$\mathcal{D}a = \frac{t_T}{t_L} = \frac{l_I s_L}{u' l_F}$$

- ratio of eddy turnover time to burning
- effect of turbulence on chemical processes

Other measures :

$l_F/\eta$ Measure of local distortion of the flame

$u'/s_L$ Relative strength of turbulence.

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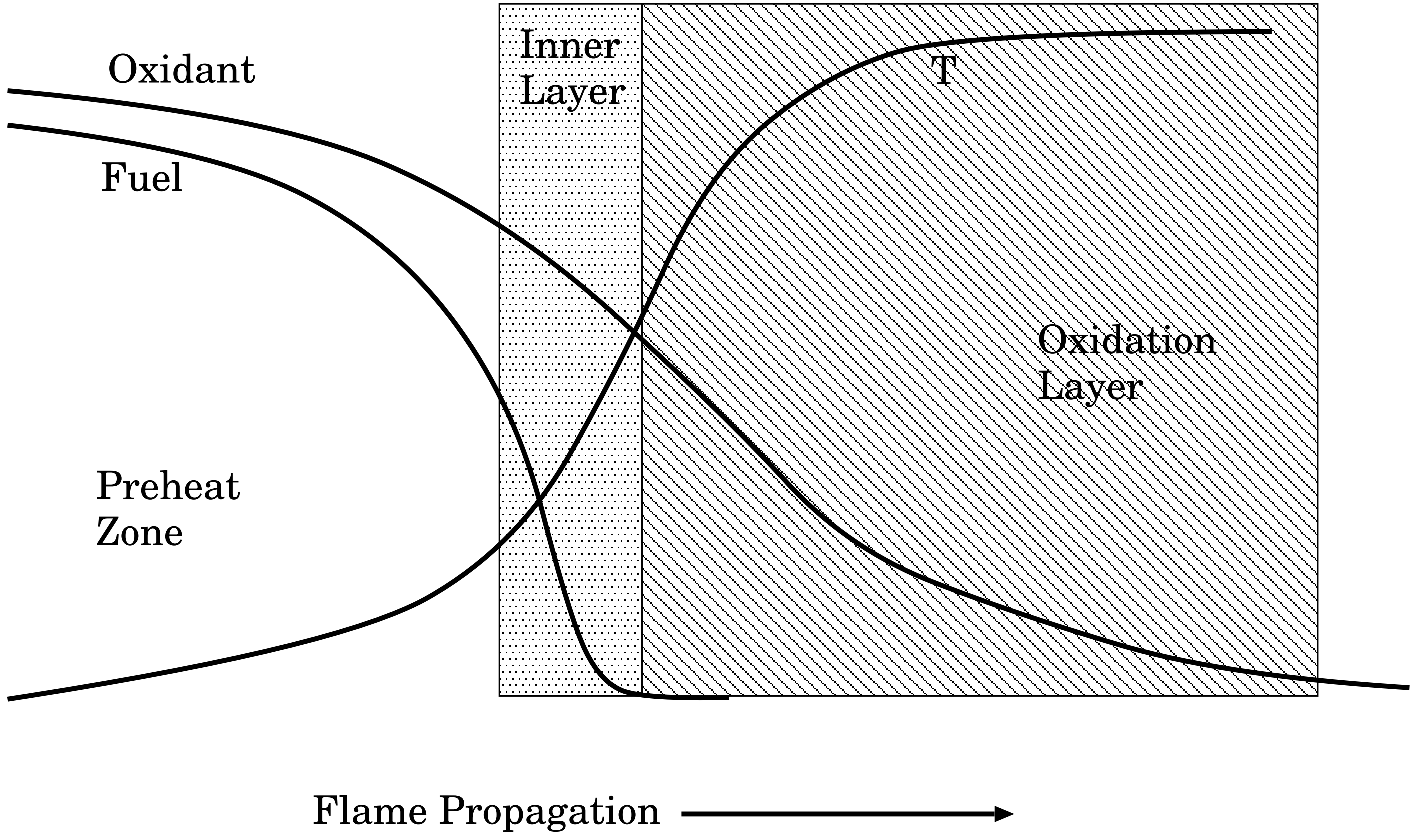
# *Flame structure*

In more detail, 3 regions :

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# *Flame structure*

1. a preheat zone,
2. an inner layer of fuel consumption,
3. the oxidation layer.

Thickness of the inner layer

$$l_\delta = l_F \delta$$

For stoichoimetric methane at $1$ atmosphere,

$$l_F = 0.175\,\mathrm{mm} \qquad \text{and} \qquad \delta = 0.1$$

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## *Non-premixed combustion*

- No obvious characteristic velocity scale
- Define a characteristic diffusion thickness $l_D$
- Flame still divided into fuel consumption and oxidation layers
- Oxidation layer

  $$l_\varepsilon = \varepsilon l_D$$

  of more importance.

# *Modelling – direct approach*

We can approach the problem in a simple way :

- Combustion $\equiv$ chemical reaction process combining reactants to form products
- Write balance equations for species
- Solve together with continuity and momentum equations

# *Mass fraction*

Define *Mass fraction* $Y_i$

– the mass of the species per unit mass of the mixture.

Transport equation

$$\frac{\partial \rho Y_i}{\partial t} + \nabla . \rho Y_i \underline{u} = \nabla . \rho D_i \nabla Y_i + \rho S_i$$

Source term represents addition/removal due to combustion

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# *Temperature equation*

Also need transport equation for some measure of the energy – say temperature $T$.

$$\frac{\partial \rho T}{\partial t} + \nabla . \rho T \underline{u} = \nabla . \rho D \nabla T + \rho S_T$$

Source term represents radiation, pressure work, energy release.

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# *Reactive scalars*

Often group everything together as "reactive scalars"

$$\psi_i = \{Y_1, Y_2, \ldots, Y_n, T\}$$

with transport equation

$$\frac{\partial \rho \psi_i}{\partial t} + \nabla . \rho \psi_i \underline{u} = \nabla . \rho D_i \nabla \psi_i + \rho S_{\psi_i}$$

## *Problems*

Problems with this approach :

1. $n$ often quite large!
   *Elementary reaction mechanisms* – detail 100's of reactions for combustion process. Invoke QSSA to reduce to manageable proportions (1-5).

2. Turbulence still unaccounted for!!
   Turbulence – introduces too many details to calculate. Use Reynolds averaging to eliminate details, replace by a model.

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# *Moment methods*

Turbulence modelling – replace ‘small scale’ detail of turbulence with (cheaper) turbulence model.

Similar process used in combustion modelling – average to remove details, then substitute a model.

Density of fluid variable $\Rightarrow$ use *Favre* averaging.

$$u_x(\underline{x}, t) = \widetilde{u_x} + u_x''$$

Here

$$\overline{\rho u_x} = 0 \quad \text{and thus} \quad \widetilde{u_x} = \frac{\overline{\rho u_x}}{\overline{\rho}}$$

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# *Favre averaging*

Useful for modelling when density varies : NSE contain terms such as

$$\overline{\rho u_x u_y}$$

Using Favre averaging this becomes

$$\overline{\rho u_x u_y} = \overline{\rho}\widetilde{u_x}\widetilde{u_y} + \overline{\rho}\widetilde{u_x'' u_y''}$$

Use this to derive mean flow equations (Favre-averaged NSE) and equations for $k$ and $\epsilon$ – a turbulence model for compressible flow.

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# Moment methods cont.

Favre averaged equation for reactive scalars :

$$\frac{\partial \overline{\rho} \widetilde{\psi_i}}{\partial t} + \nabla . \overline{\rho} \widetilde{\psi_i} \widetilde{\underline{u}} = \nabla . \overline{\rho D_i \nabla \psi_i} - \nabla . \overline{\rho} \widetilde{\underline{u}'' \psi_i''} + \overline{\rho} \widetilde{S_{\psi_i}}$$

High $\mathcal{R}e$, so molecular diffusivity $D$ can be ignored.
Two terms cause problems :

$-\nabla . \overline{\rho} \widetilde{\underline{u}'' \psi_i''}$ representing turbulent transport

and

$\overline{\rho} \widetilde{S_{\psi_i}}$ the mean chemical source term

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## *Specific models*

Different combustion models arrise from different approaches to these terms – range from cheap and inaccurate to precise and expensive.

E.g. Eddy Breakup Model – Spalding (1971)

- assumes turbulent mixing determines chemical reaction rate
- gives simple model for chemical source term
- combine with $k - \epsilon$ model for turbulence
- cheap to compute. Requires extensive tuning.

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# *PDF Transport*

**P**robability **D**istribution **F**unction methods

- turbulence can be described/modelled in terms of correlation functions
- turbulent processes – combustion – can also be described/modelled in terms of correlations
- joint PDF of velocity and reactive scalars

$$P(\underline{u}, \underline{\psi}; \underline{x}, t)$$

- Potentially more accurate. Also very expensive.

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# *Flamelet methods*

Main alternative methodology.

High $\mathcal{R}e, \mathcal{D}a \Rightarrow$ flame fronts very thin – consider as 2d sheet which :

- separates burnt and unburnt gas (premixed combustion)
- separates fuel and air (non-premixed)
- is distorted by mean flow and by turbulence
- propagates by burning.

Location of flame sheet specified by *indicator function*.

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# *Indicator function*

Premixed combustion : *progress variable*

$$c = \frac{T - T_u}{T_b - T_u} \quad \text{or} \quad c = \frac{Y_P}{Y_{P,b}}$$

$0 < c < 1$ : $1$ represents burned gas, $0$ unburned.

Some intermediate value represents flame centre.

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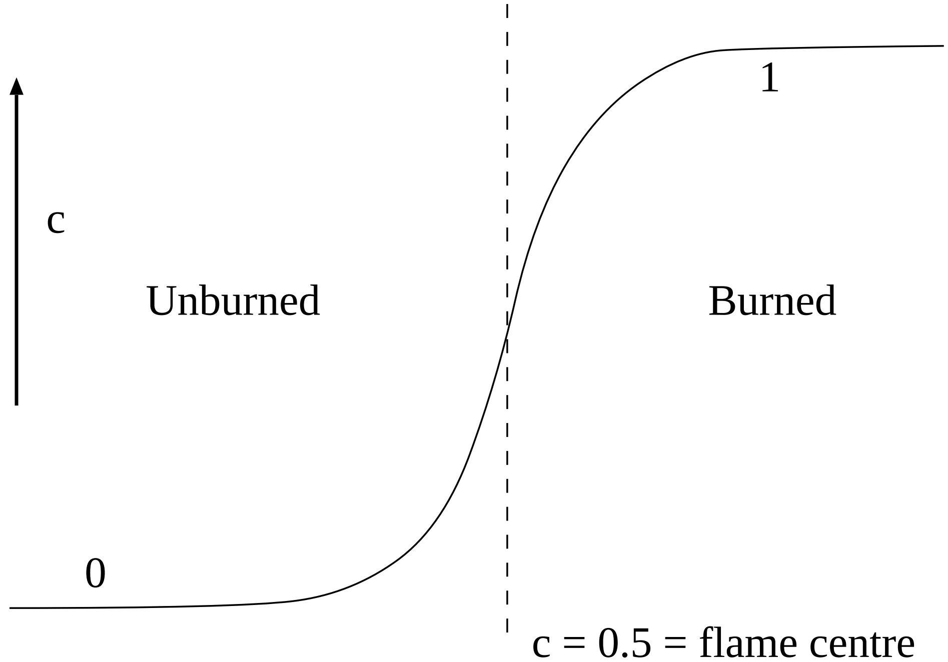
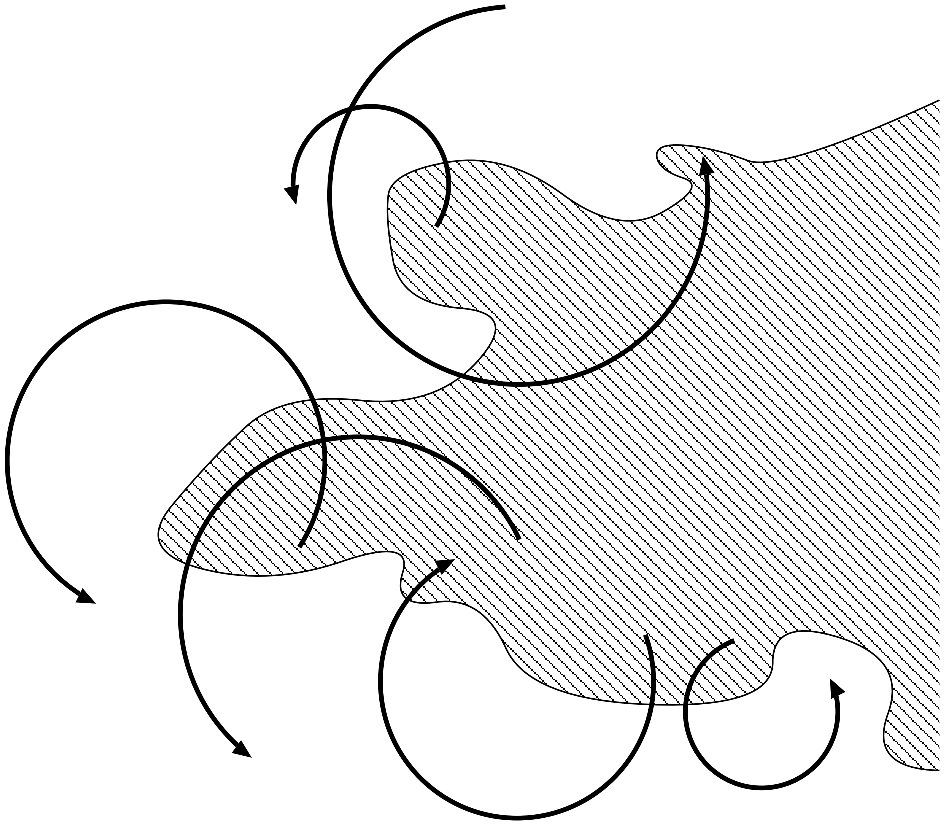
# *1-d representation*

Plotting $c$ across the flame :



## *Flame wrinking*

Flame will be wrinkled by turbulence on scales too small to simulate



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## *Averaging*

Average equation

$$\frac{\partial \overline{\rho}\widetilde{c}}{\partial t} + \nabla . \overline{\rho}\widetilde{c}\underline{u} = -\nabla . \overline{\rho}\widetilde{\underline{u}''c''} + \overline{\rho}\widetilde{S}_c$$

Need to model :

$\widetilde{\underline{u}''c''}$ turbulent transport term

$\widetilde{S}_c$ reaction term

– but now have a manageable set of equations.

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## *Other models*

Other versions

- *flame surface density* $\Sigma$
- $\mathcal{G}$-equation
- Non-premixed combustion
  – use mixture fraction $Z$.

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# ***Counter-gradient transport***

Final note : modelling of $\widetilde{\underline{u}''c''}$ often uses *gradient transport* assumption

$$\widetilde{\underline{u}''c''} = -D_t \nabla \widetilde{c}$$

However this is frequently wrong – *counter-gradient transport*.

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