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A Strain-Consistent Epsilon-Based Flamelet Model for Non-Premixed Turbulent Combustion

Sylvain L. Walsh, Wes Hellwig, Yalu Zhu, Feng Liu and William A. Sirignano.
University of California, Irvine

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Turbulent combustion: a multi-scale, multi-physics problem

Turbulent combustion is the coupled interaction of turbulent transport and chemical reaction, where turbulence controls mixing and flame structure while heat release feeds back on the flow.

Wide range of spatial scales

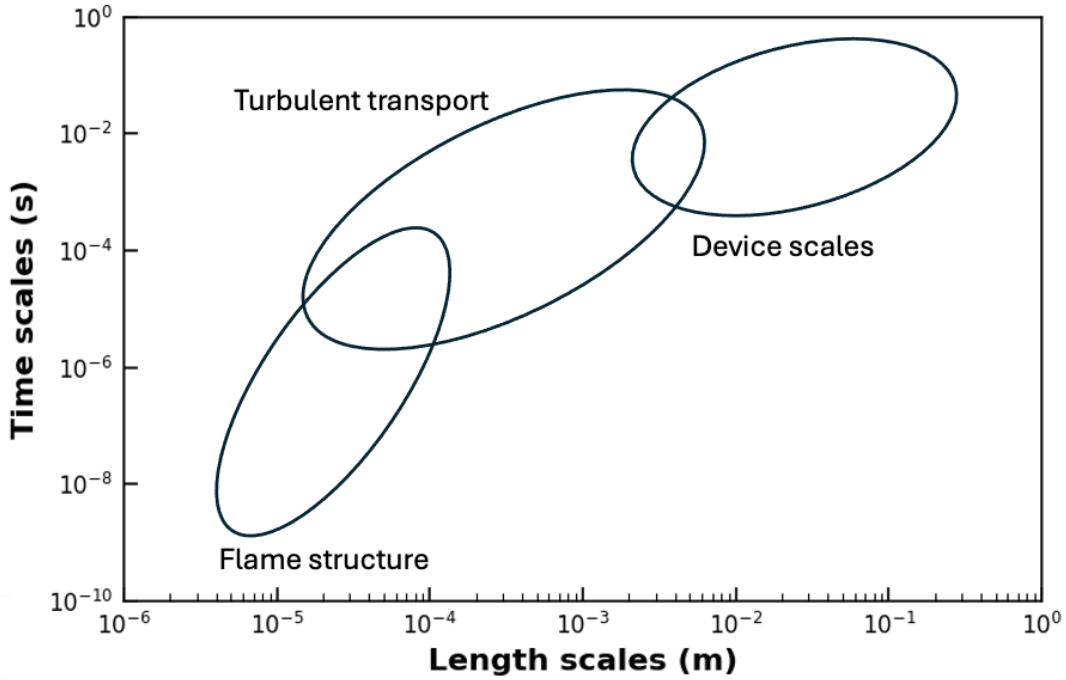
- Large turbulent structures → molecular mixing → reaction zones

Wide range of temporal scales

- Flow evolution → turbulent mixing → fast chemical kinetics

Strong two-way coupling

- Turbulence affects combustion; heat release and density changes modify the turbulence

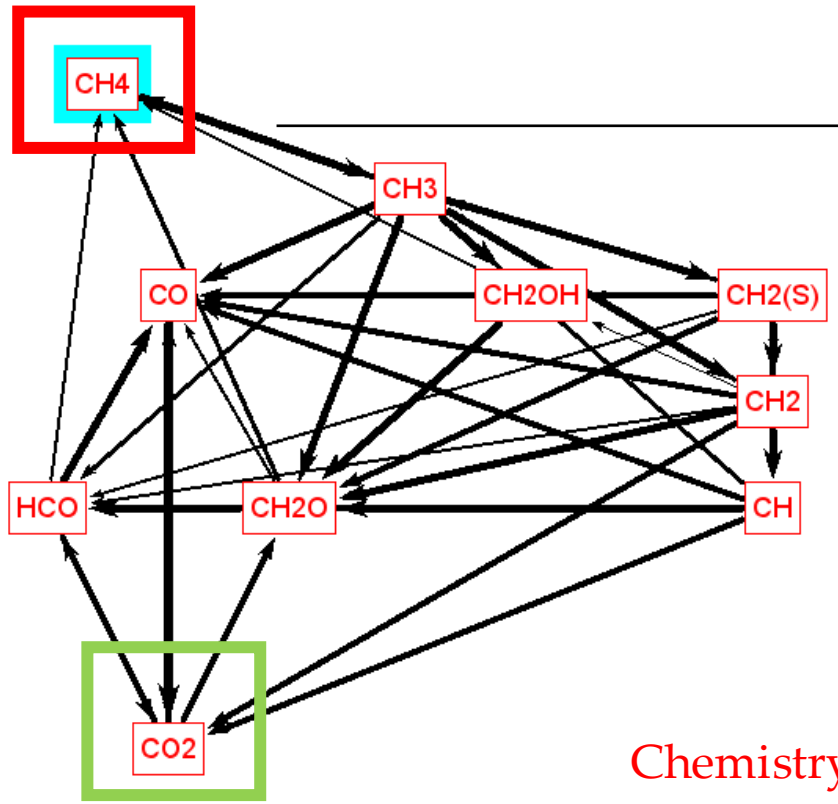




Ouroboros

Complexity of Detailed Chemical Kinetics

Start $\mathrm{CH_4 + 2O_2 + 7.52N_2} \rightarrow \mathrm{CO_2 + 2H_2O + 7.52N_2}$ End



Line thickness: absolute rate of production

Arrhenius chemistry

$$\mathrm{CH_4 + OH \leftrightarrow CH_3 + H_2O}$$
$$\mathrm{CH_4 + H \leftrightarrow CH_3 + H_2}$$
$$\mathrm{CH_4 + O \leftrightarrow CH_3 + OH}$$

Elementary reactions

Species production rates depend on reaction-rate coefficients and local species concentrations

Production rates $\dot{\omega}_i = \dot{\omega}_i(k_r, [X_1], [X_2], \ldots)$

Reaction-rate coeff. $k = \mathbf{A}T^n \exp\left(-E_A/RT\right)$

Chemistry is therefore strongly nonlinear in temperature and composition

Complexity of Detailed Chemical Kinetics

Reaction mechanisms give us rate coefficients $k = \mathbf{A}T^n \exp\left(-E_A/RT\right)$

```
ELEMENTS
O H C N AR HE
END
SPECIES
    AR          HE          N2          H2
    H           O           O2          OH
    H2O         HO2         H2O2        CO
    CO2         C           CH          CH2
    CH2(S)      CH3         CH4         HCO
    CH2O        CH2OH       CH3O        CH3OH
    C2H         C2H2        C2H3        C2H4
    C2H5        C2H6        HCCO        CH2CO
    CH2CHO      CH3CHO      CH3CO       H2CC
    OH*         CH*
END
REACTIONS
H+O2<=>O+OH                 9.841E+13   0.000   15310.00
O+H2<=>H+OH                 3.848E+12   0.000    7950.00
 DUPLICATE
O+H2<=>H+OH                 6.687E+14   0.000   19180.00
 DUPLICATE
OH+H2<=>H+H2O               2.256E+08   1.510    3437.00
2OH<=>O+H2O                 3.161E+04   2.420   -1928.00
H2+M<=>2H+M                 4.580E+19  -1.400  104390.00
AR/ 0.00/ HE/ 0.00/ N2/ 1.01/ H2/ 2.55/ H2O/12.02/ CO/ 1.95/ CO2/
3.83/
CH4/ 2.00/ CH2O/ 2.50/ CH3OH/ 3.00/ C2H6/ 3.00/
H2+AR<=>2H+AR               5.176E+18  -1.100  104390.00
H2+HE<=>2H+HE               5.840E+18  -1.100  104390.00
2O+M<=>O2+M                 6.160E+15  -0.500       0.00
AR/ 0.00/ HE/ 0.00/ H2/ 2.50/ H2O/12.00/ CO/ 1.90/ CO2/ 3.80/ CH4/
2.00/
CH2O/ 2.50/ CH3OH/ 3.00/ C2H6/ 3.00/
2O+AR<=>O2+AR               1.890E+13   0.000   -1788.00
2O+HE<=>O2+HE               1.890E+13   0.000   -1788.00
O+H+M<=>OH+M                4.710E+18  -1.000       0.00
AR/ 0.75/ HE/ 0.75/ N2/ 1.32/ H2/ 2.50/ H2O/15.80/ CO/ 2.52/ CO2/
5.01/
CH4/ 2.00/ CH2O/ 2.50/ CH3OH/ 3.00/ C2H6/ 3.00/
H2O+M<=>H+OH+M              6.060E+27  -3.322
120800.00
AR/1.23/ HE/1.33/ N2/2.46/ H2/3.77/ O2/1.50/ H2O/0.00/ CO/2.40/
CO2/4.67/ CH4/2.00/ CH2O/2.50/ CH3OH/3.00/ C2H6/3.00/
2H2O<=>H+OH+H2O             7.528E+25  -2.440  120200.00
H+O2(+M)<=>HO2(+M)          4.565E+12   0.440       0.00
   LOW  /  6.370E+20  -1.720   525.00/
   TROE/  0.5000   30.00  90000.00  90000.00 /
AR/ 0.60/ HE/ 0.71/ N2/ 0.96/ H2/ 1.87/ O2/ 0.75/ H2O/15.81/ CO/
1.90/
CO2/ 3.45/ CH4/ 2.00/ CH2O/ 2.50/ CH3OH/ 3.00/ C2H6/ 3.00/
HO2+H<=>H2+O2               2.945E+06   2.087   -1455.00
HO2+H<=>2OH                 5.888E+13   0.000     300.00
HO2+H<=>O+H2O               1.632E+12   0.000       0.00
HO2+O<=>OH+O2               1.609E+13   0.000    -445.00
HO2+OH<=>H2O+O2             7.347E+12   0.000   -1093.00
 DUPLICATE
HO2+OH<=>H2O+O2             4.534E+14   0.000   10930.00
 DUPLICATE
2HO2<=>H2O2+O2              1.958E+11   0.000   -1409.00
 DUPLICATE
2HO2<=>H2O2+O2              1.111E+14   0.000   11040.00
 DUPLICATE
H2O2(+M)<=>2OH(+M)          2.187E+12   0.900   48750.00
   LOW  /  2.490E+24  -2.300  48750.00/
   TROE/  0.5800   30.00  90000.00  90000.00 /
AR/0.85/ HE/0.65/ N2/1.33/ H2/3.27/ O2/1.20/ H2O/6.63/ H2O2/6.61/
CO/2.80/ CO2/1.60/ CH4/2.00/ CH2O/2.33/ CH3OH/3.00/ C2H6/3.00/
H2O2+H<=>OH+H2O             2.045E+13   0.000    3970.00
H2O2+H<=>HO2+H2             5.856E+13   0.000    7950.00
H2O2+O<=>OH+HO2             8.513E+06   2.000    3970.00
H2O2+OH<=>H2O+HO2           1.565E+12   0.000     318.00
 DUPLICATE
H2O2+OH<=>H2O+HO2           7.340E+13   0.000
7270.00
 DUPLICATE
CO+O(+M)<=>CO2(+M)          1.880E+11   0.000    2430.00
   LOW  /  1.400E+21  -2.100  5500.00/
AR/ 0.87/ H2/ 2.50/ H2O/12.00/ CO/ 1.90/ CO2/ 3.80/ CH4/ 2.00/
CH2O/ 2.50/
CH3OH/ 3.00/ C2H6/ 3.00/
CO+O2<=>O+CO2               1.533E+12   0.000   47700.00
CO+OH<=>H+CO2               6.187E+04   2.053    -356.00
 DUPLICATE
CO+OH<=>H+CO2               5.017E+12  -0.664     332.00
 DUPLICATE
CO+HO2<=>OH+CO2             1.570E+05   2.180   17944.00
HCO+M<=>H+CO+M              4.800E+17  -1.200   17734.00
AR/ 1.40/ HE/ 1.31/ N2/ 1.31/ H2/ 1.31/ O2/ 1.32/ H2O/15.31/ CO/
2.04/
CO2/ 2.00/ CH4/ 2.60/ CH2O/ 3.29/ CH3OH/ 3.00/ C2H6/ 3.00/
HCO+H<=>H2+CO               8.482E+13   0.000       0.00
HCO+O<=>OH+CO               3.010E+13   0.000       0.00
HCO+O<=>H+CO2               3.001E+13   0.000       0.00
HCO+OH<=>H2O+CO             1.199E+14   0.000       0.00
HCO+O2<=>HO2+CO             7.562E+10   0.521    -521.00
C+OH<=>H+CO                 5.000E+13   0.000       0.00
C+O2<=>O+CO                 6.620E+13   0.000     636.00
CH+H<=>C+H2                 1.089E+14   0.000       0.00
CH+O<=>H+CO                 5.700E+13   0.000       0.00
CH+OH<=>H+HCO               3.000E+13   0.000       0.00
CH+H2<=>H+CH2               1.612E+14   0.000    3320.00
CH+H2(+M)<=>CH3(+M)         5.130E+13   0.150       0.00
   LOW  /  2.430E+22  -1.600     0.00/
   TROE/  0.5140   152.00  22850.00  10350.00 /
AR/0.71/ HE/0.70/ H2O/6.00/ CO/1.50/ CO2/2.00/ CH4/2.00/
CH2O/2.50/
```

FFCM-1 Reaction mechanism:

- 38 species
- 291 elementary reactions

Detailed mechanisms: O(10-100) species, O(10^2-10^3) elementary reactions

Smith, G., Tao, Y., and Wang, H., "Foundational Fuel Chemistry Model Version 1.0 (FFCM-1)," , 2016

What are the computational challenges?

Governing equations for compressible reacting flow consisting of N species

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0 \qquad \text{(Continuity)}$$

$$\frac{\partial (\rho \mathbf{V})}{\partial t} + \nabla \cdot (\rho \mathbf{V}\mathbf{V}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} \qquad \text{(Momentum)}$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho E \mathbf{V}) = -\nabla \cdot (p\mathbf{V}) + \nabla \cdot (\mathbf{V} \cdot \boldsymbol{\tau}) - \nabla \cdot \mathbf{q} + \dot{Q} \qquad \text{(Energy)}$$

$$\frac{\partial \rho Y_n}{\partial t} + \nabla \cdot (\rho Y_n \mathbf{V}) = -\nabla \cdot \mathbf{j}_n + \dot{\omega}_n, \; n = 1, \; 2, \; \ldots, \; N \qquad \text{(Species)}$$

Heat-release rate $\dot{Q} = -\sum_{n=1}^{N} h_{f,n}^{0} \dot{\omega}_n$

Total sensible energy $E = h - \frac{p}{\rho} + \frac{1}{2}\mathbf{V} \cdot \mathbf{V}$

With h as sensible only $h = \sum_{n=1}^{N} Y_n h_n \quad \text{and} \quad h_n = \int_{T_{\text{ref}}}^{T} C_{p,n}(T)\mathrm{d}T$

1. Direct simulation is computationally prohibitive

- Detailed chemistry involves many species and reactions.
- The chemical source terms are stiff, requiring small timesteps.
- At engineering Reynolds numbers, DNS that resolve the full range of turbulent and reactive spatial and temporal scales becomes unfeasible.

2. RANS/LES resolve only part of the problem

- RANS: solves for the mean flow; all turbulent fluctuations are modeled.
- LES: resolved large turbulent scales; subgrid scales are modeled.
- In both cases, the smallest turbulent and reactive scales are not explicitly resolved on the computational mesh.

3. Nonlinear chemistry leads to unclosed source terms

Because the chemical source terms are nonlinear functions of temperature and composition, the mean/filtered reaction rates cannot be obtained by evaluating the chemistry at the resolved/mean state:

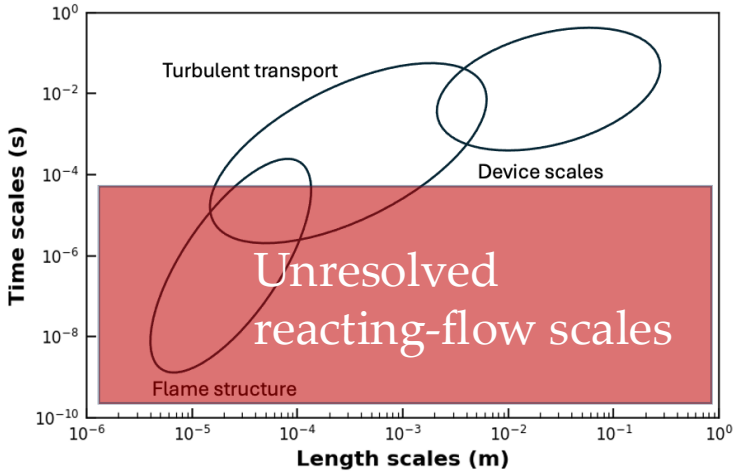
$$\langle \dot{\omega}_n(T, \rho, \mathbf{Y}) \rangle \neq \dot{\omega}_n \left(\langle T \rangle, \langle \rho \rangle, \langle \mathbf{Y} \rangle \right)$$

Unresolved fluctuations in temperature, composition and mixing directly affect the mean/filtered reaction rates.

4. Combustion closure problem

A combustion model must represent the unresolved chemical state and its interaction with turbulent mixing.

What does this have to do with the price of eggs?



Historical assessment of predictive computational modeling capability – Bilger (2011)

Every day use, very-high confidence on quantitative prediction.

Frequent use with engineering value for qualitive information on trends.

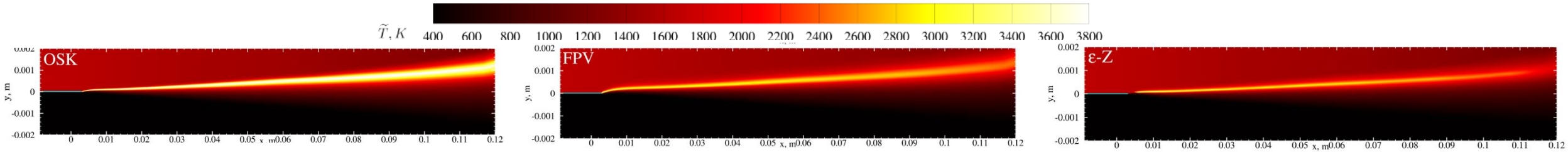
Occasional use with only marginal input into the design and optimization process.

Status	Physics
⋆ ⋆ ⋆ ⋆ ⋆	Stress and deformation prediction.
⋆ ⋆ ⋆ ⋆	Heat transfer and solid temperature prediction.
⋆ ⋆ ⋆	Fluid flow and convective heat transfer prediction in the absence of combustion.
⋆ ⋆	General flow and mixing prediction of combustion systems.
⋆	Prediction of finite-rate chemistry effects, such as ignition, extinction, and pollutant formation of CO, NOx, soot, etc.

R. W. Bilger, "The role of combustion technology in the 21st century", in "Turbulent Combustion Modelling", Echekki & Mastorakos (Eds.), Springer, 2011.

Predictive capability is sensitive to the combustion closure!

Same flow and and turbulence model, different combustion closures



Combustion closure is not a minor detail: it can strongly affect predictive capabilities. Accurate and computationally affordable combustion closures are therefore needed.

The Non-Premixed Flamelet Model

Fundamental assumptions

Flamelet assumption

At sufficiently large Damköhler number $\mathrm{Da} = \dfrac{\tau_{\mathrm{flow}}}{\tau_{\mathrm{chem}}} \gg 1$

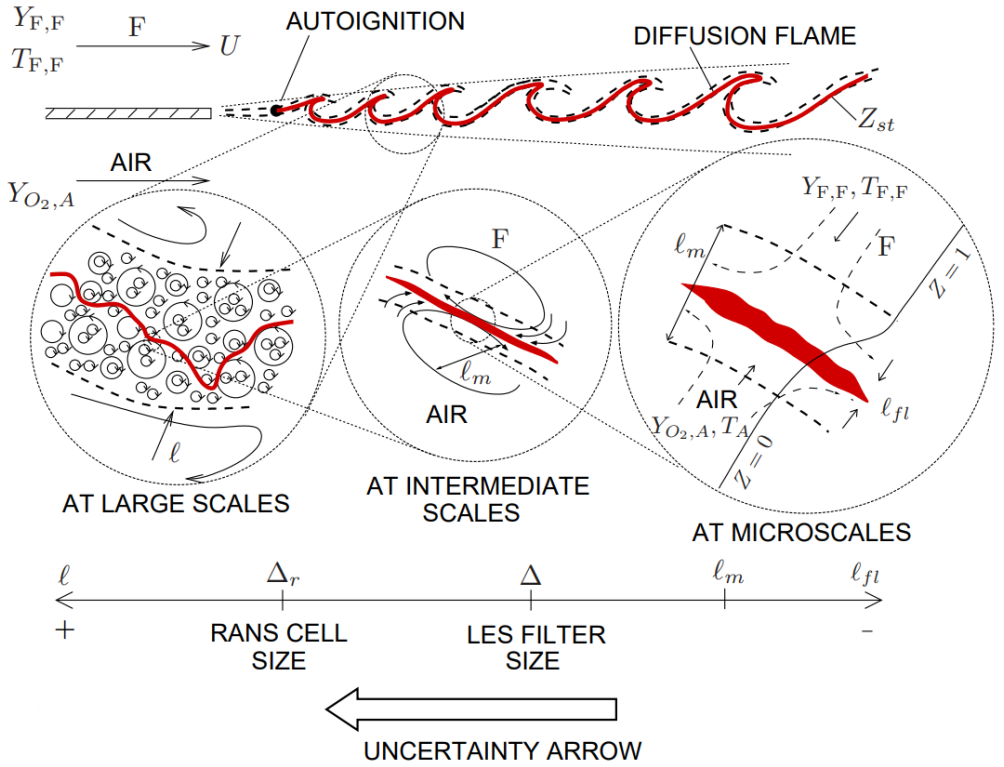
- Reaction zone remains thin relative to the smallest turbulent structures.
- Turbulence affects the flame primarily through mixing and strain.
- Internal flame structure remains diffusion-reaction dominated.

Non-premixed interpretation

- A complex turbulent diffusion flame is represented as an ensemble **of locally laminar diffusion flame structures (flamelets)** existing below the resolved-scale.
- Canonical flamelets are modeled as counterflow diffusion flames.
- Each flamelet is subject to different magnitude of strain imposed by the surrounding turbulent flow.

Why is this useful

- Detailed chemistry can be pre-computed and tabulated to be accessed later by the CFD.
- Increase in kinetics detail does not translate to a proportional increase in CFD cost.



Urzay et al., CTR Annual Research Briefs, 2012.

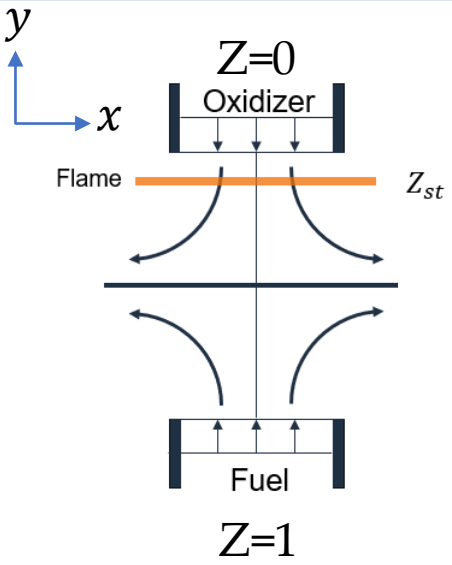
Pre-computed flamelet library representation

$$\psi_j = F(\mathrm{mixture}, \mathrm{strain}, \ldots)$$

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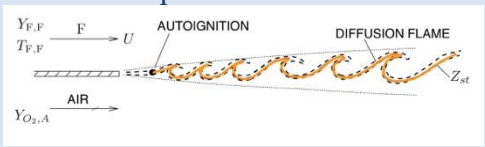
Classical Non-Premixed Flamelet Equations

1. Counterflow Diffusion Flame



Scalar boundary conditions

- Fuel stream: $Y_{j,F}$, T_F, p $(Z = 1)$
- Oxidizer stream: $Y_{j,O}$, T_O, p $(Z = 0)$
- These are taken from global-flow inlet conditions and used to solve the flamelet equations.



2. From Physical Space to Mixture-Fraction Space

Mixture fraction

- $\boldsymbol{Z}$ is a conserved scalar that parametrizes local composition.
- $Z = 1$ in the fuel stream, $Z = 0$ in the oxidizer stream.
- Using Z as the independent variable transforms the counterflow flame into a 1D boundary value-problem.

Scalar dissipation rate

$$\chi = 2D|\nabla Z|^2$$

- Measures the local rate of molecular mixing.
- Its stoichiometric value $\boldsymbol{\chi_{st}}$ is used to parametrize the flamelet.
- In a counterflow configuration, $\boldsymbol{\chi_{st}}$ is proportional to the imposed strain rate $\boldsymbol{a}$ (axial velocity of in the oxidizer stream).

$$a = -\frac{\partial v_\infty}{\partial y} \quad \text{(at the inlet)} \qquad \chi_{st} \propto a$$

Classical steady flamelet equations (N. Peters)

$$-\rho\frac{\chi(Z)}{2}\frac{\partial^2\psi_j}{\partial Z^2} = \dot{\omega}_j,\ j = 1, 2, \ldots, M+1$$

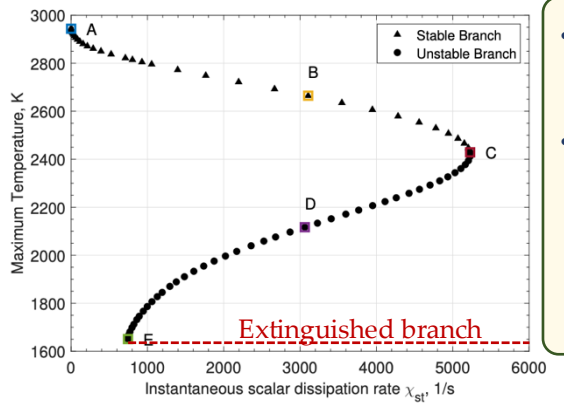
- ψ_j represents species mass fractions and temperature.
- Momentum equations do not appear; the flow enters through a prescribed $\boldsymbol{\chi(Z)}$ through a similarity solution.
- Solution provides $\boldsymbol{\psi_j = \psi_j(Z, \chi_{st} \propto a)}$

Key assumptions of the classical formulation

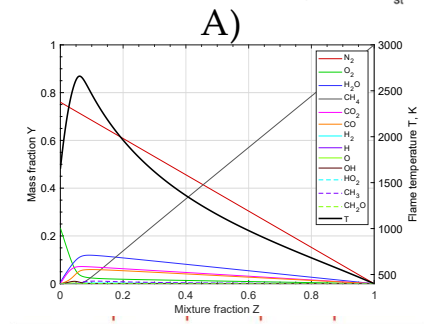
- Fickian diffusion + equal Lewis number.
- Low-Mach number / constant pressure flamelet.
- Steady state flamelet $(\partial/\partial t = 0)$.

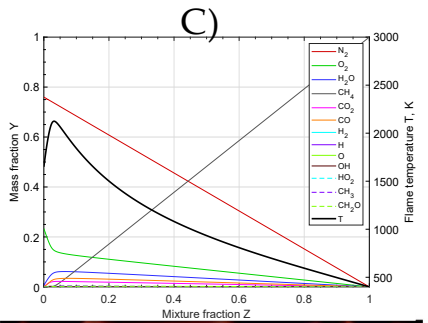
3. Flamelet Solutions and Response to Strain

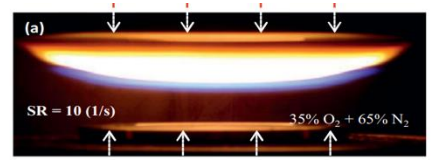
S-shaped response (flame temperature)

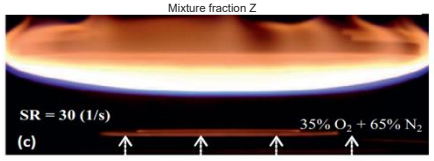


- Multiple steady solutions exist for a given strain value.
- Higher χ means shorter mixing/residence time. Beyond a critical χ (point C), chemistry cannot keep pace and the flame quenches.









Increasing strain rate (a) or scalar dissipation rate (χ_{st})

Takeaway: The classical flamelet equations provide 1D solutions $\psi_j(Z, \chi_{st} \propto a)$ for given inlet compositions and temperatures. Increasing strain modifies the flame structure and can lead to extinction

Images: Agrawal A, Baukal, Jr. CE. Fundamental Flames. In: Agarwal AK, Olson S, Golber MJ, Jacobs TJ, Vaccari M, eds. A Gallery of Combustion and Fire. Cambridge University Press; 2020:4-38.

Coupling the Flamelet Library to the Computational Flow Field

Presumed PDF approach for turbulence-chemistry interaction

1. Transport on the CFD mesh

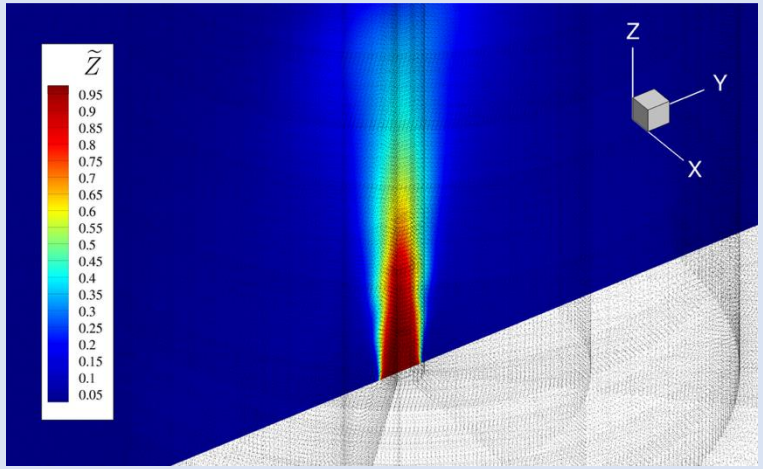
Solve transport equations for the mixture fraction (conserved scalar) and its variance

Mixture fraction

$$\frac{\partial \bar{\rho}\widetilde{Z}}{\partial t} + \nabla \cdot (\bar{\rho}\widetilde{Z}\widetilde{\mathbf{V}}) = -\nabla \cdot \mathbf{j}_Z$$

Mixture fraction variance

$$\frac{\partial \bar{\rho}\widetilde{Z''^2}}{\partial t} + \nabla \cdot (\bar{\rho}\widetilde{Z''^2}\widetilde{\mathbf{V}}) = -\nabla \cdot \mathbf{j}_{Z''^2} + 2\frac{\mu_T}{Sc_T}\nabla\widetilde{Z} \cdot \nabla\widetilde{Z} - \bar{\rho}\widetilde{\chi}$$



CFD mesh – jet flame example – Mixture fraction field

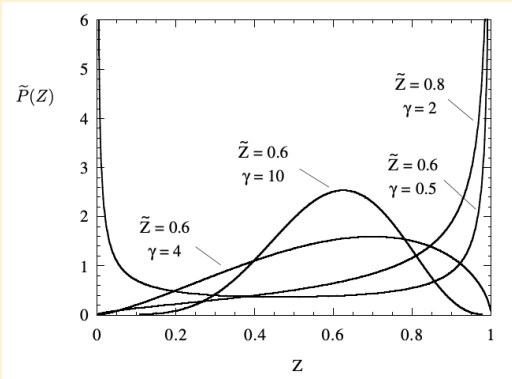
2. Presumed PDF and averaging (OFFLINE)

The resolved state does not uniquely determine the flamelet state due to unresolved mixture-fraction fluctuations

$$\widetilde{\psi}_j \neq \psi_j(\widetilde{Z})$$

Use a presumed PDF:

- β-PDF for Z (from $\widetilde{Z}$ and $\widetilde{Z''^2}$)
- δ-PDF for χ (fluctuations neglected)

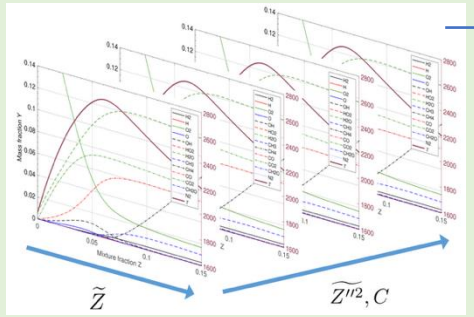


β-PDF for mixture fraction Z

$$\widetilde{\psi}_j(\widetilde{Z}, \widetilde{Z''^2}, \widetilde{\chi}) = \int_0^1 \psi_j(Z, \chi)\, \widetilde{P}(Z, \widetilde{Z}, \widetilde{Z''^2})\, \mathrm{d}Z$$

3. Precomputed mean flamelet libraries return to the CFD solver

At every LES/RANS computational cell, given $\widetilde{Z}$, $\widetilde{Z''^2}$ and $\widetilde{\chi}$



Representation of Flamelet library

Retrieve PDF-averaged

$$\widetilde{Y_n}, \widetilde{\dot{Q}}$$

and feed back to the flow solver.

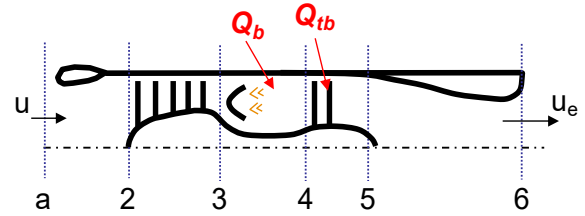
Why is this useful

$$\frac{\partial \bar{\rho}\widetilde{Y}_n}{\partial t} + \nabla \cdot (\bar{\rho}\widetilde{Y}_n\widetilde{\mathbf{V}}) = -\nabla \cdot \mathbf{j}_n + \widetilde{\dot{\omega}}_n,\ n = 1,\ 2,\ \ldots,\ N$$

- 5+N governing equations become 5 + 2 equations, independent of the detail of the reaction mechanism.
- Provided there is a model for $\widetilde{\chi}$

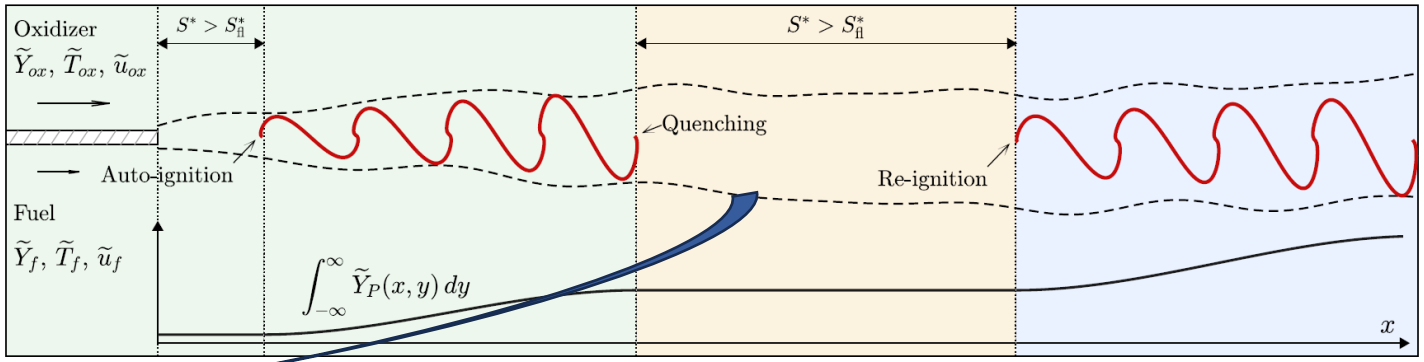
The presumed PDF approach models the effect of unresolved mixture-fraction fluctuations.

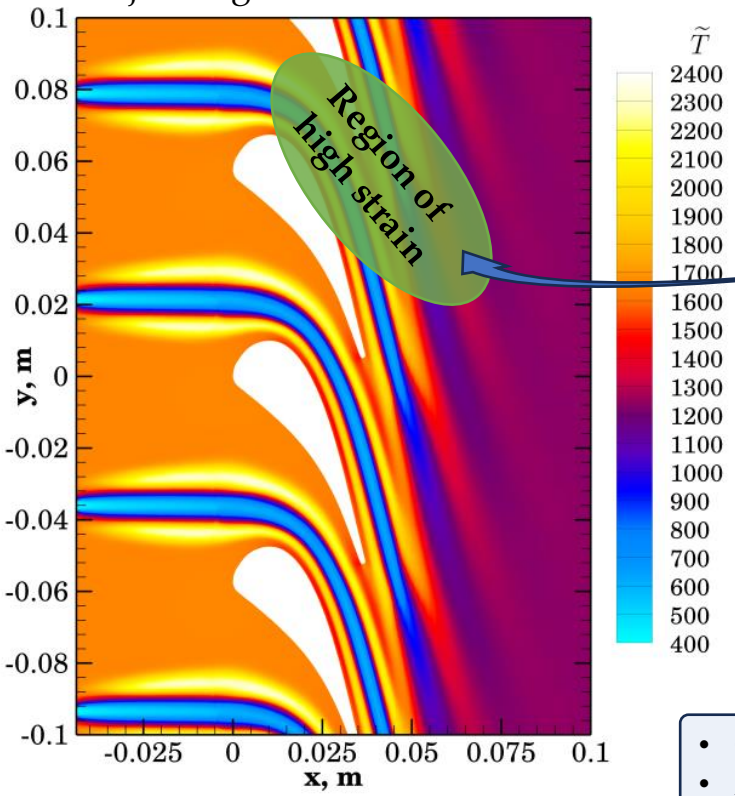
A Limitation of Strain-Based Flamelet Coupling



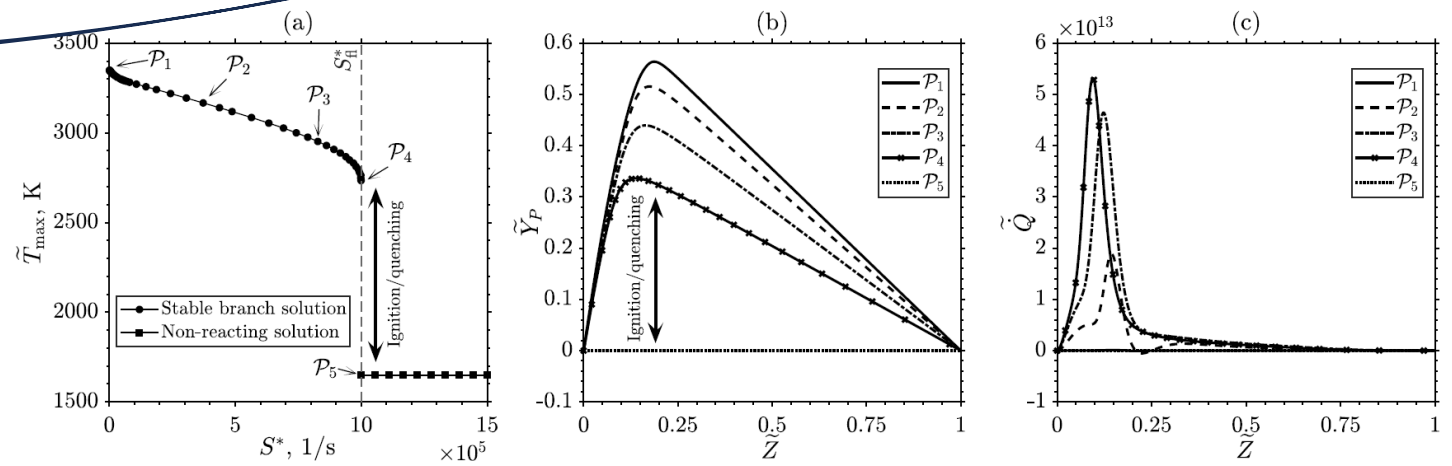
Turbojet diagram with turbine-burner.

Turbine-burner: Jet fuel (JP-5) has complex chemical kinetics involving hundreds of species and thousands of elementary reactions. Good case for a flamelet model.





(a) OSK.



- Crossing the flamelet extinction limit can map a smooth strain field to a discontinuous thermochemical state.
- A robust coupling strategy should preserve a physically continuous thermochemical response through extinction and reignition.

The Flamelet Progress Variable (FPV) Approach

1. Define a progress variable C

Progress variable

$$C = \alpha_1 Y_1(Z) + \alpha_2 Y_2(Z) + \ldots + \alpha_M Y_M(Z)$$

Chosen to measure a degree of reaction progress towards products. The specific choice is ad-hoc and becomes a model parameter. Example:

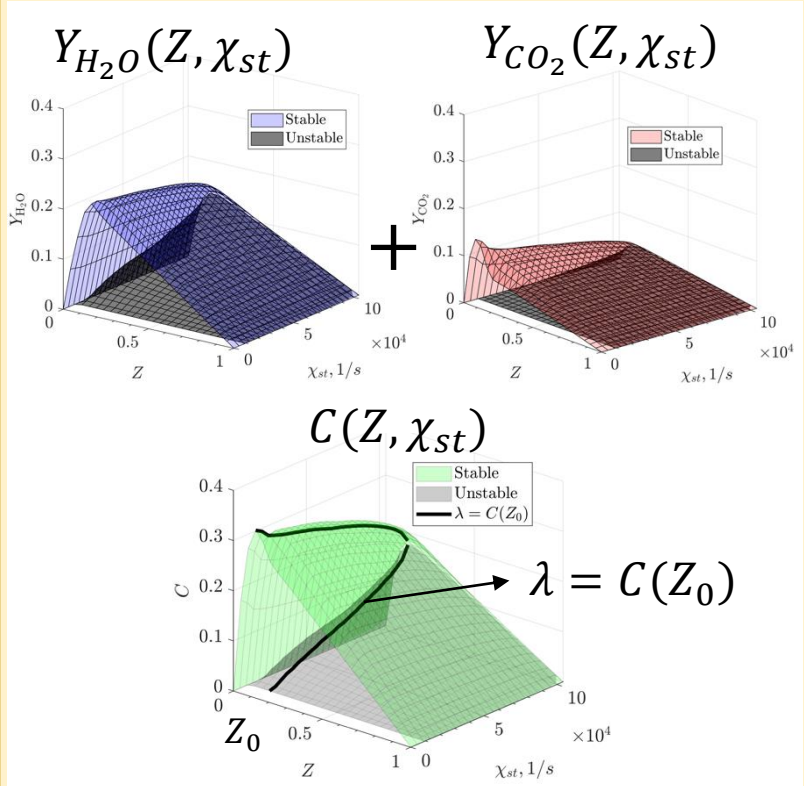
$$C = Y_{H_2O} + Y_{CO_2}$$

Flamelet parameter

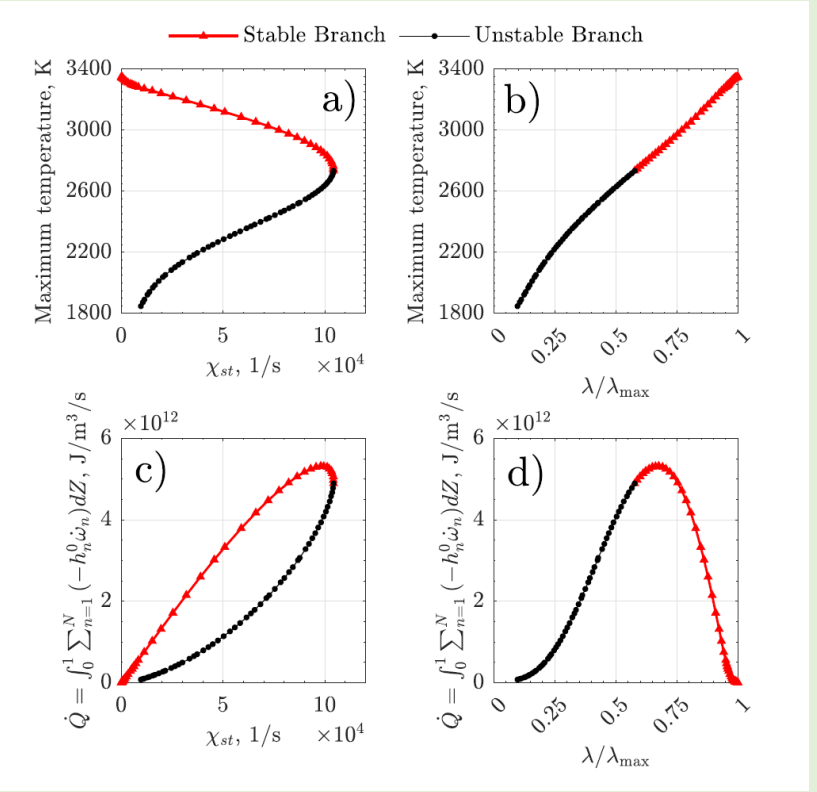
$$\lambda = C(Z_0)$$

Choose Z_0 so that λ varies monotonically along the flamelet manifold.

2. Construct C on the flamelet library



3. Map the flamelet solutions to λ



Takeaway: $\lambda = C(Z_0)$ provides a monotonic coordinate for parametrizing the flamelet libraries and removes the limitation of strain-based mapping near extinction. FPV is introduced to better represent ignition and extinction.

Coupling the Progress-Variable Library to CFD

1. Transport on the CFD mesh

Solve transport equations for the mixture fraction (conserved scalar), its variance and the progress variable

Mixture fraction

$$\frac{\partial \bar{\rho}\widetilde{Z}}{\partial t} + \nabla \cdot (\bar{\rho}\widetilde{Z}\widetilde{\mathbf{V}}) = -\nabla \cdot \mathbf{j}_Z$$

Mixture fraction variance

$$\frac{\partial \bar{\rho}\widetilde{Z''^2}}{\partial t} + \nabla \cdot (\bar{\rho}\widetilde{Z''^2}\widetilde{\mathbf{V}}) = -\nabla \cdot \mathbf{j}_{Z''^2} + 2\frac{\mu_T}{Sc_T}\nabla\widetilde{Z} \cdot \nabla\widetilde{Z} - \bar{\rho}\widetilde{\chi}$$

Resolved progress variable

$$\frac{\partial \bar{\rho}\widetilde{C}}{\partial t} + \nabla \cdot (\bar{\rho}\widetilde{C}\widetilde{\mathbf{V}}) = -\nabla \cdot \mathbf{j}_C + \widetilde{\dot{\omega}}_C$$

Progress variable source term

$$\dot{\omega}_C = \dot{\omega}_{H_2O} + \dot{\omega}_{CO_2}$$

Thus, the progress variable equation transports the bulk species defined as $H_2O + CO_2$

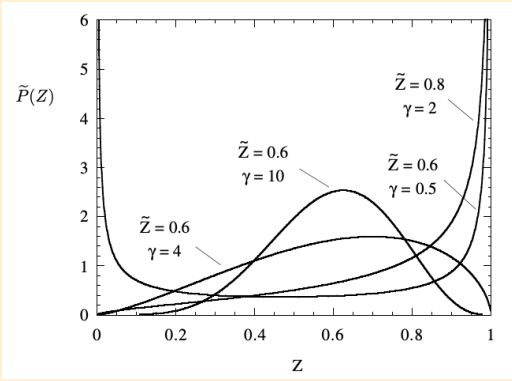
2. Presumed PDF and averaging (OFFLINE)

The resolved state does not uniquely determine the flamelet state due to unresolved mixture-fraction fluctuations

$$\widetilde{\psi}_j \neq \psi_j(\widetilde{Z})$$

Use a presumed PDF:

- β-PDF for Z (from $\tilde{Z}$ and $\widetilde{Z''^2}$)
- δ-PDF for λ (fluctuations neglected)



β-PDF for mixture fraction Z

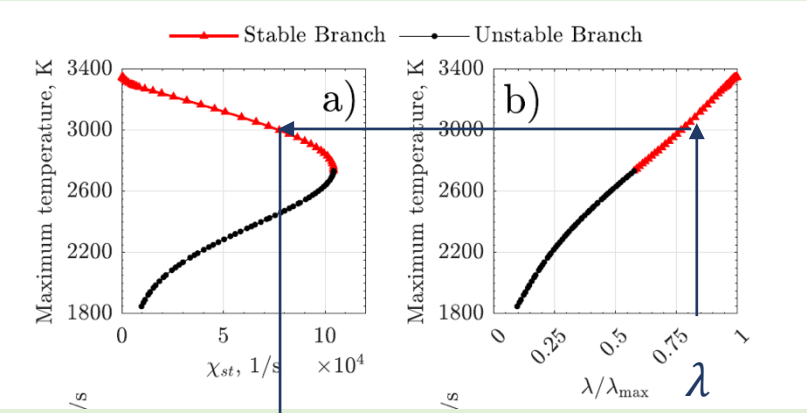
$$\widetilde{\psi}_j(\widetilde{Z}, \widetilde{Z''^2}, \lambda, \bar{p}) = \int_0^1 \psi_j(Z, \lambda, \bar{p})\widetilde{P}(Z, \widetilde{Z}, \widetilde{Z''^2})dZ$$

3. Precomputed mean flamelet libraries return to the CFD solver

At every LES/RANS computational cell, given $\widetilde{Z}$, $\widetilde{Z''^2}$ and $\widetilde{C}$

Invert $\widetilde{C}_{tab}(\lambda) = \widetilde{C}(\widetilde{Z}, \widetilde{Z''^2}, \lambda, \bar{p})$

To get the flamelet parameter, λ from which we can traceback to strain rate



$\widetilde{Y_n}$, $\widetilde{\dot{Q}}$ and $\widetilde{\dot{\omega}}_C$

Each tabulated λ corresponds to a flamelet originally generated at some χ_{st} (or strain rate). But is that generating strain representative of the local turbulent flow?

Accelerating Reacting Mixing-Layer Configuration

Numerical method

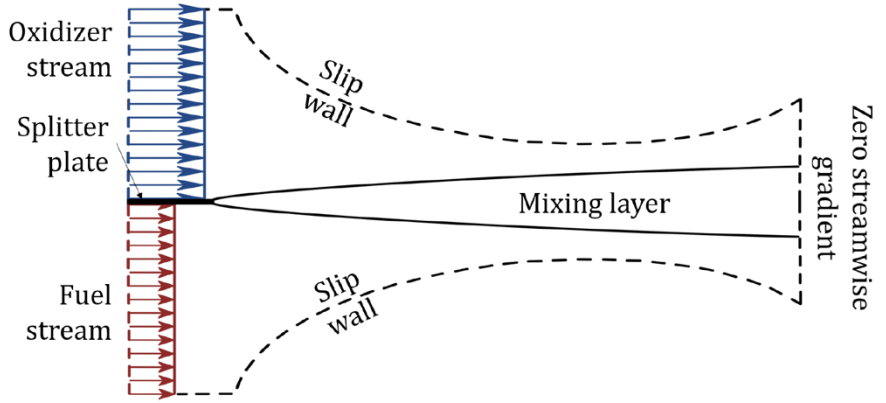
- 2D steady RANS of transonic accelerating mixing layer in a converging-diverging nozzle.
- In-house, reacting, compressible flow solver. Second-order cell-centered finite-volume solver on curvilinear multiblock structured grids, parallelized on CPUs with MPI.
- Steady-state-preserving operator splitting with explicit-Euler chemistry subintegration; Δt_{chem} set from the chemical Jacobian spectral radius
- SST $k-\omega$ turbulence model.
- Methane combustion using the Flamelet Progress Variable (FPV) model.

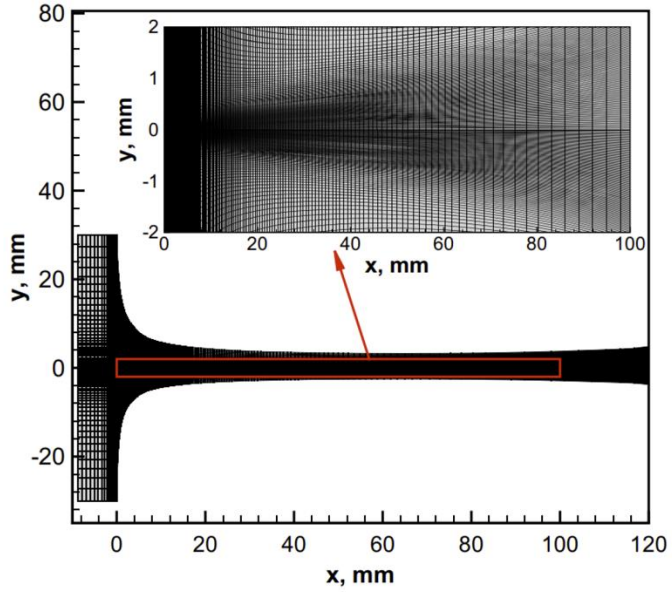
Inlet conditions

- **Oxidizer stream:** $Y_{O_2} = 0.5$, $Y_{N_2} = 0.5$, T = 1650 K, u = 100 m/s.
- **Fuel stream:** Pure CH_4, T = 400 K, u = 50 m/s.
- Inlet pressure = 30 bar.

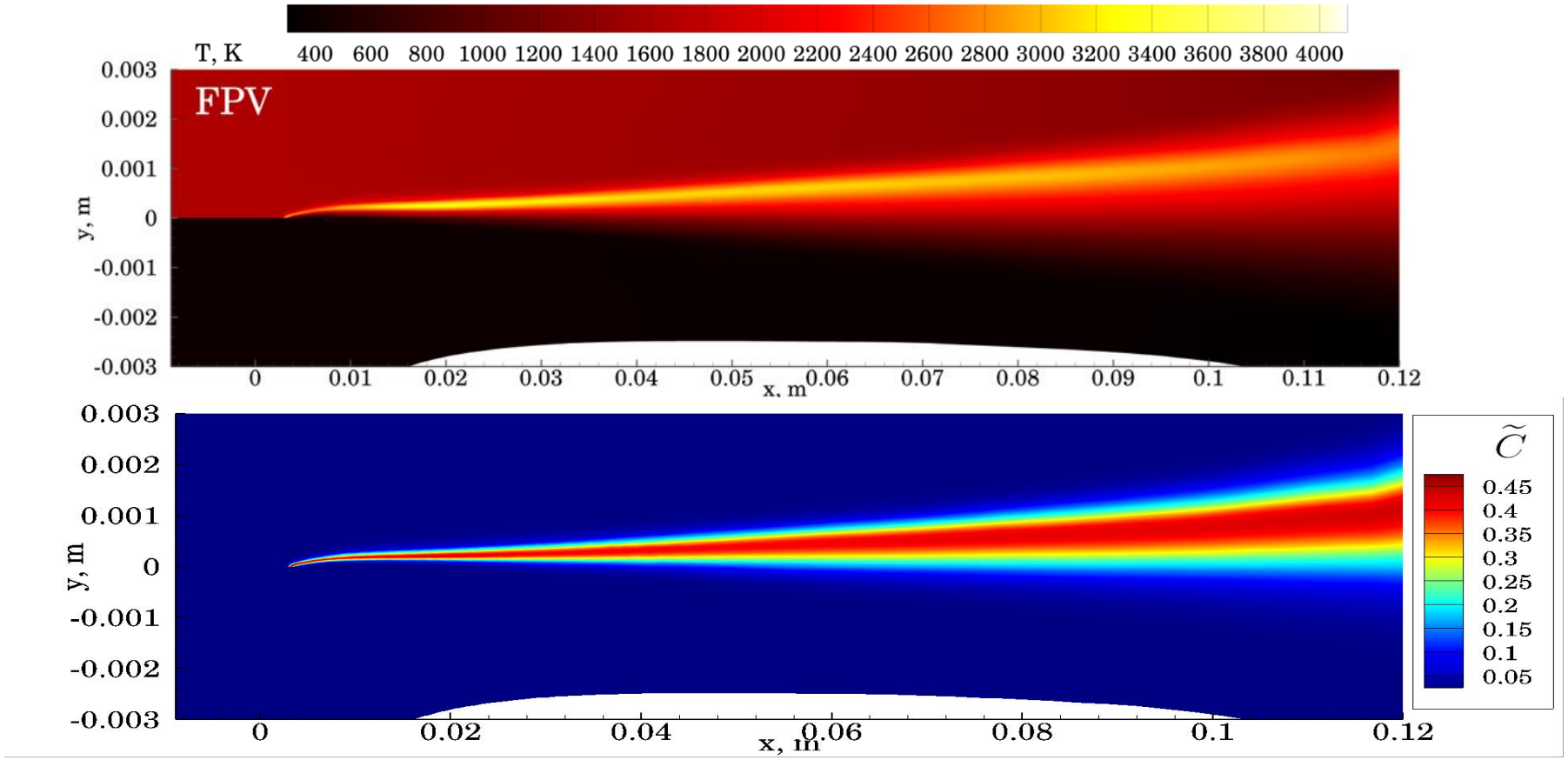
Boundary conditions

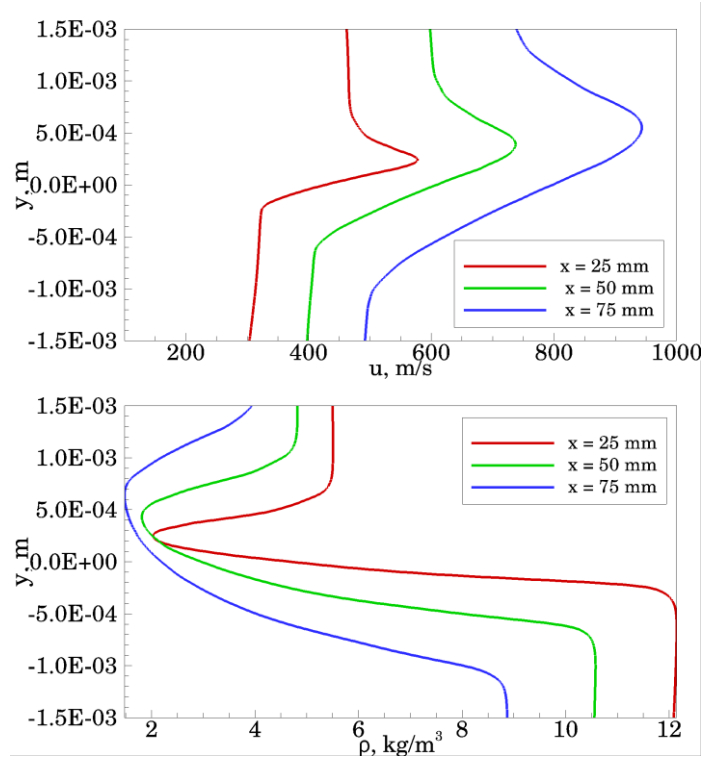
- No-slip wall along the splitter plate.
- Streamwise pressure gradient of 200 atm/m (representative of turbine conditions) imposed by the slip walls along the nozzle.





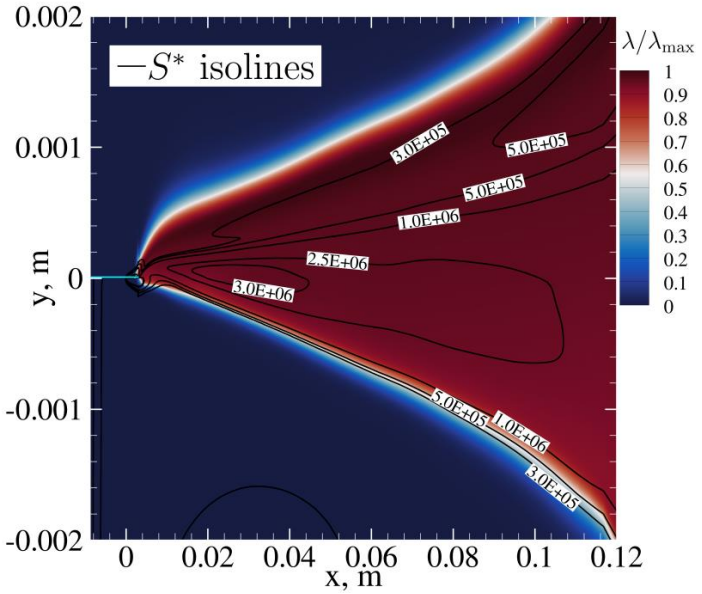
Accelerating Reacting Mixing-Layer Configuration



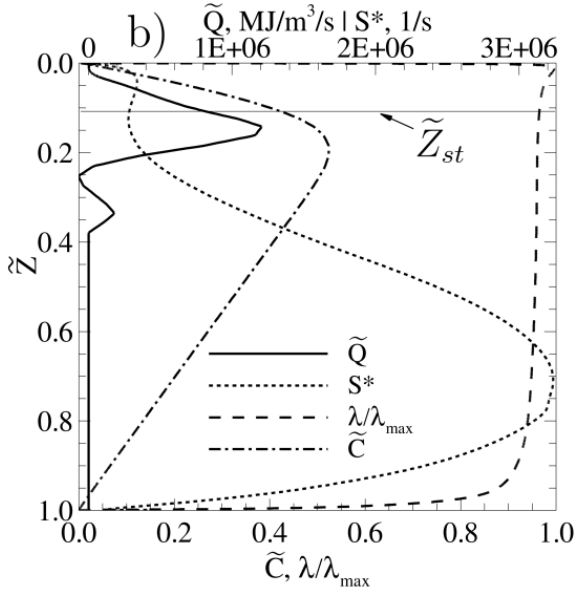


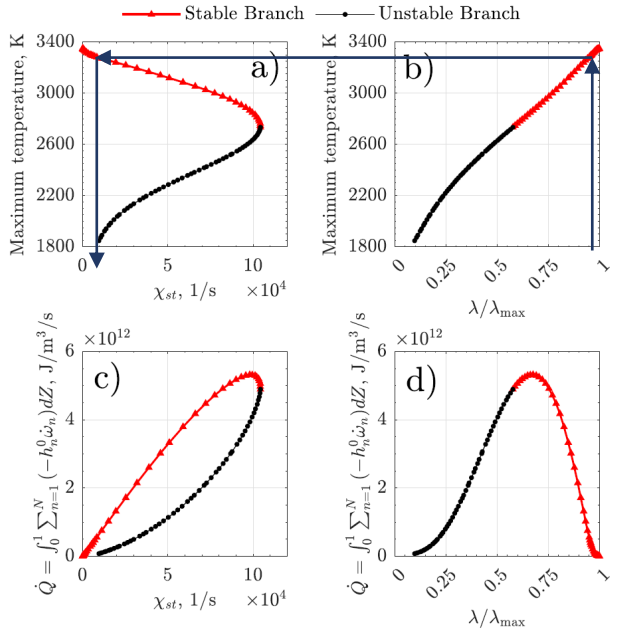
Accelerating Reacting Mixing-Layer Configuration

Flamelet parameter, λ contours



Profiles at x = 0.025 m





- Flamelets are controlled by an advective-diffusive-reactive balance; progress-variable mapping can **decouple strain from flamelet libraries**.
- Regions of finite strain rate are assigned **near-equilibrium flamelets** ($\chi_{st} \rightarrow 0$).
- The resulting strain from λ **does not necessarily match** the strain imposed by the local turbulent flow.
- Flamelet modeling assumes turbulence influences flame structure **primarily through strain.**

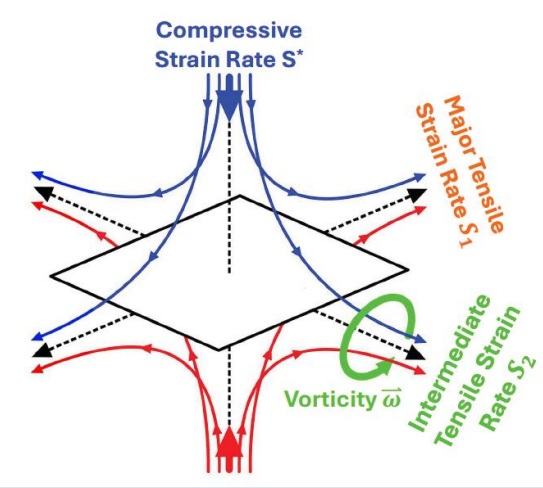
Objective

Develop a coupling strategy that connects flamelets to the surrounding turbulent flow field directly through strain rate.

Proposed ϵ-Based Flamelet Coupling

Use turbulent kinetic-energy dissipation rate to connect the turbulent flow directly to the strain imposed on the flamelet.

3D counterflow configuration



Three-dimensional flamelet with compressive, major and intermediate strain rates and vorticity to capture the centrifugal effects on the flammability limits.

Small-scale (flamelet) turbulent strain from ϵ

Viscous dissipation of the 3D counterflow related to the inflow/outflow strain rates:

$$\epsilon = 2\nu\left[(S^*S_1)^2 + S^{*2} + (S^*S_2)^2\right]$$

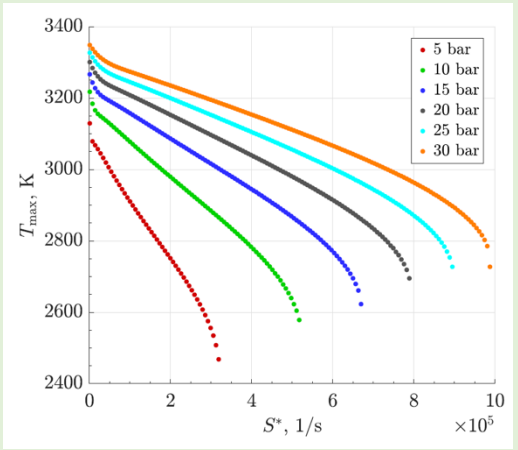
yields a direct relationship between ϵ and flamelet inflow strain rate, S*

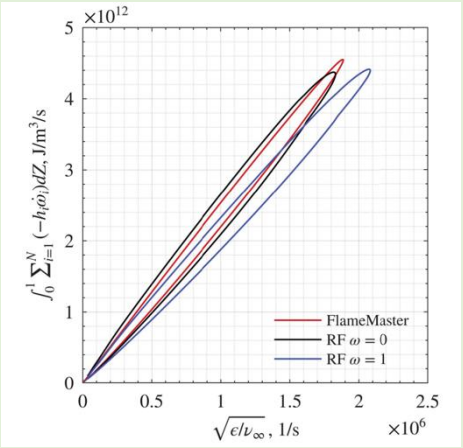
$$S^* = \frac{1}{2}\sqrt{\frac{C_{vd}\,\epsilon}{\nu[S_1^2 + 1 - S_1]}}$$

- C_{vd} model coefficient to take in account that viscous dissipation occurs over a range of the smallest scales. TBD with DNS.
- Setting $S_1 = S_2 = 0.5$ yields the axisymmetric configuration used in the classical flamelet model.

ϵ/ν, which is available or modeled in standard RANS/LES turbulence closures, provides a measure of the smallest turbulent time and length scales, which are the scales most directly interacting with a thin flamelet.

Mapping of flamelet quantities to $S^* \propto \sqrt{\epsilon/\nu}$





Direct turbulence-flamelet coupling

$$\{\widetilde{\dot{Q}}, \widetilde{\dot{\omega}}_n\} = f(\widetilde{Z}, \widetilde{Z''^2}, \bar{p}, S^*(\epsilon/\nu))$$

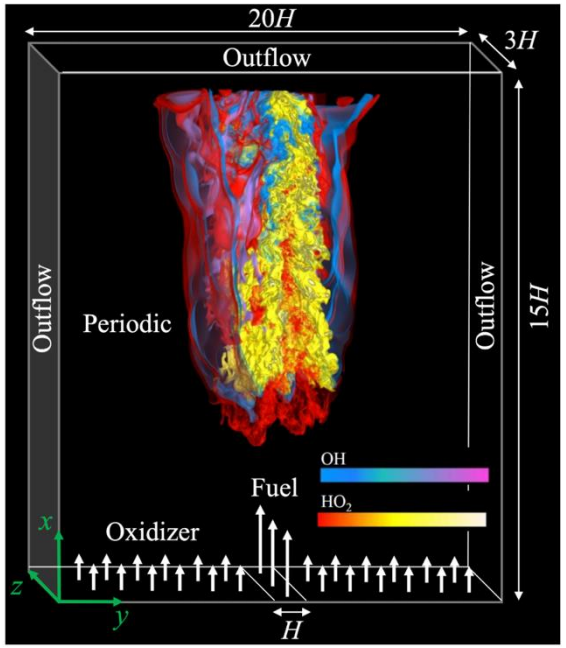
- Standard mixture fraction-based formulation.
- Presumed shape PDF approach (β for Z; δ for ϵ).

Takeaway: Instead of inferring strain rate indirectly through the progress variable, use the local turbulence dissipation rate to prescribe the strain rate experienced by the flamelet.

William A. Sirignano, Wes Hellwig & Sylvain L. Walsh (2026) Flamelet connection to turbulence kinetic energy dissipation rate, Combustion Theory and Modelling, 30:3, 267-294, DOI: 10.1080/13647830.2026.2635467

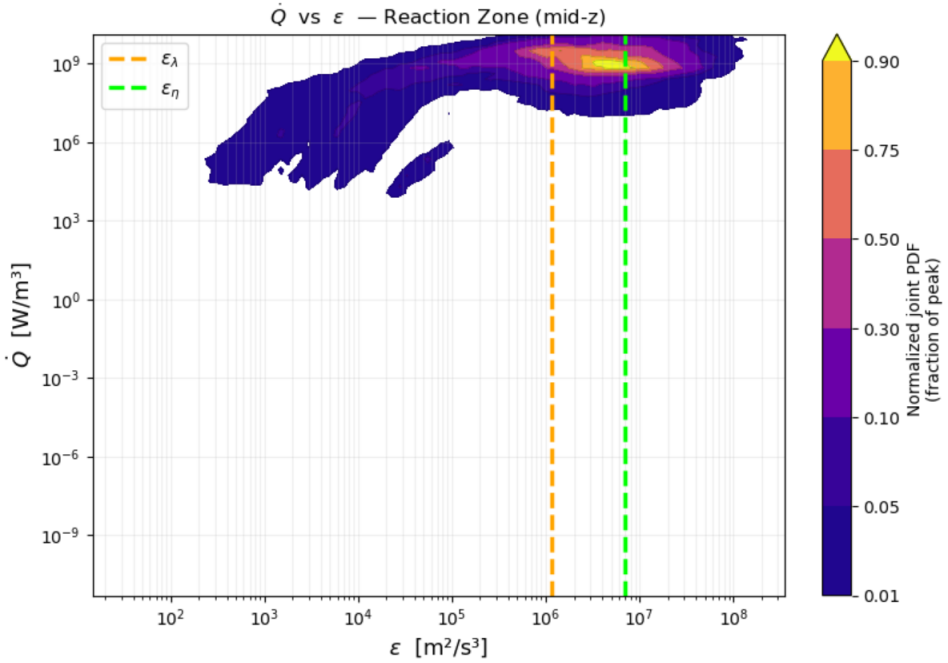
DNS Evidence for Dissipation-Reaction Coupling

3D lifted H_2/air flame (Chung et al. 2022)

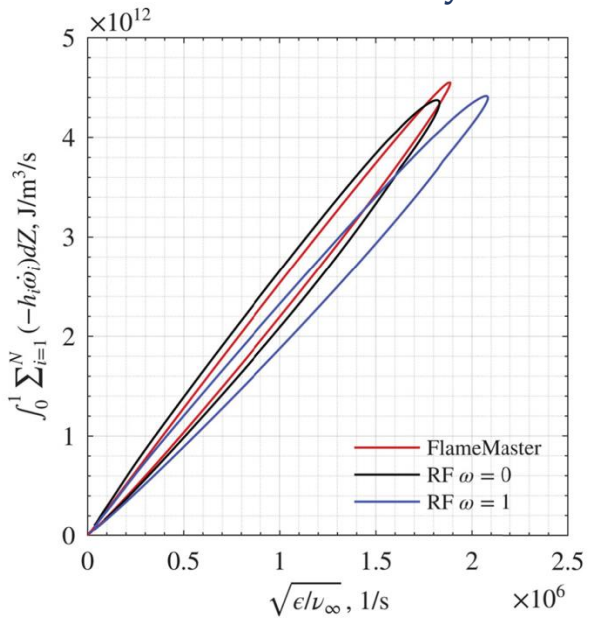


Chung, Ananda Mishra & Ihme (2022)
Combustion and Flame, 239:111758

Joint PDF of heat release and dissipation (DNS)



Heat release scaling with $S^* \propto \sqrt{\epsilon/\nu}$ (flamelet library)



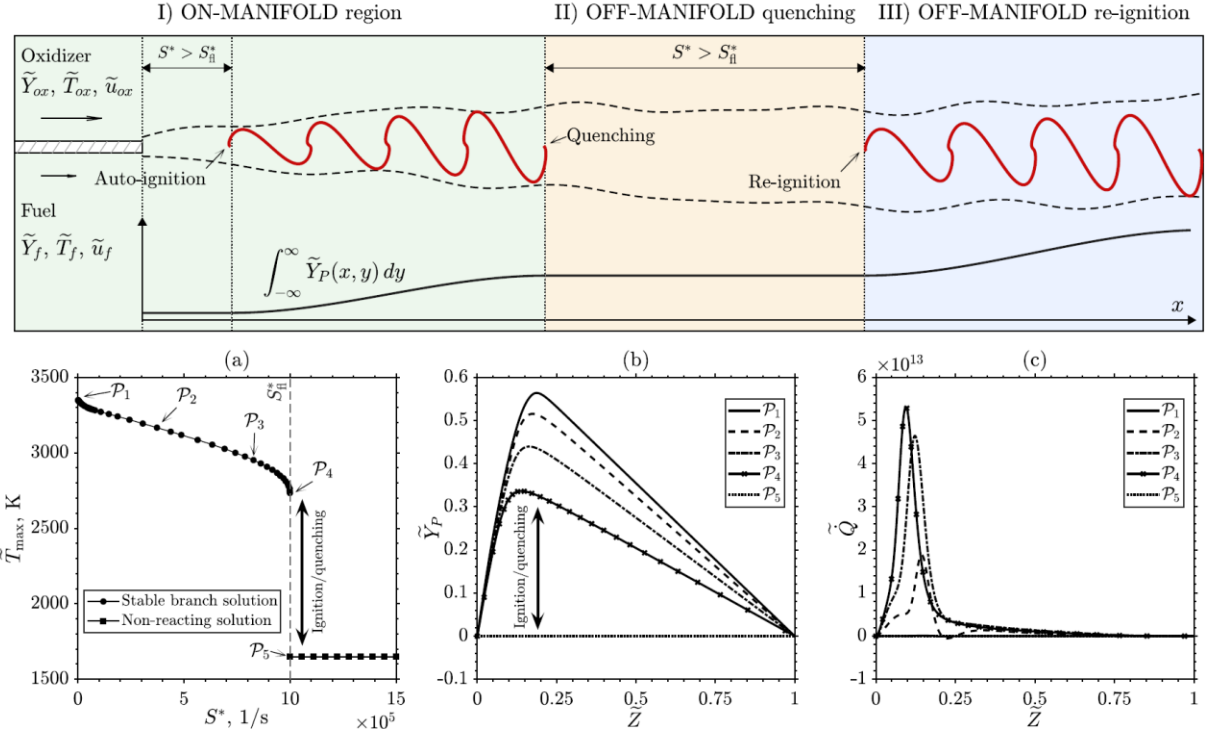
Peak heat release preferentially occurs in regions of elevated turbulent dissipation.
Since the characteristic small-scale strain rate scales as

$$S^* \propto \sqrt{\epsilon/\nu},$$

this supports the use of ϵ as a physically motivated measure of the strain experienced by the flame.

Handling Extinction and Off-Manifold States

Recap: steady flamelet manifold terminates at the extinction limit



Takeaway: allow the chemistry source terms to switch off at extinction while the transported species retain memory of the local state.

Transport through extinction

- Use flamelet libraries for the reaction source terms, while transporting a reduced set of major species.
- When the local strain rate exceeds the extinction limit,

$$S^* > S^*_{fl} \Longrightarrow \widetilde{\dot{\omega}}_n \to 0.$$

- Advection and diffusion then evolve the composition continuously through quenching and reignition.

The source term may be discontinuous; the transported thermochemical state need not be. A multi-progress variable approach where strain is still controlling.

Reactant availability correction

Off-manifold reacting states can differ from the inlet-based states used to generate the flamelet table.

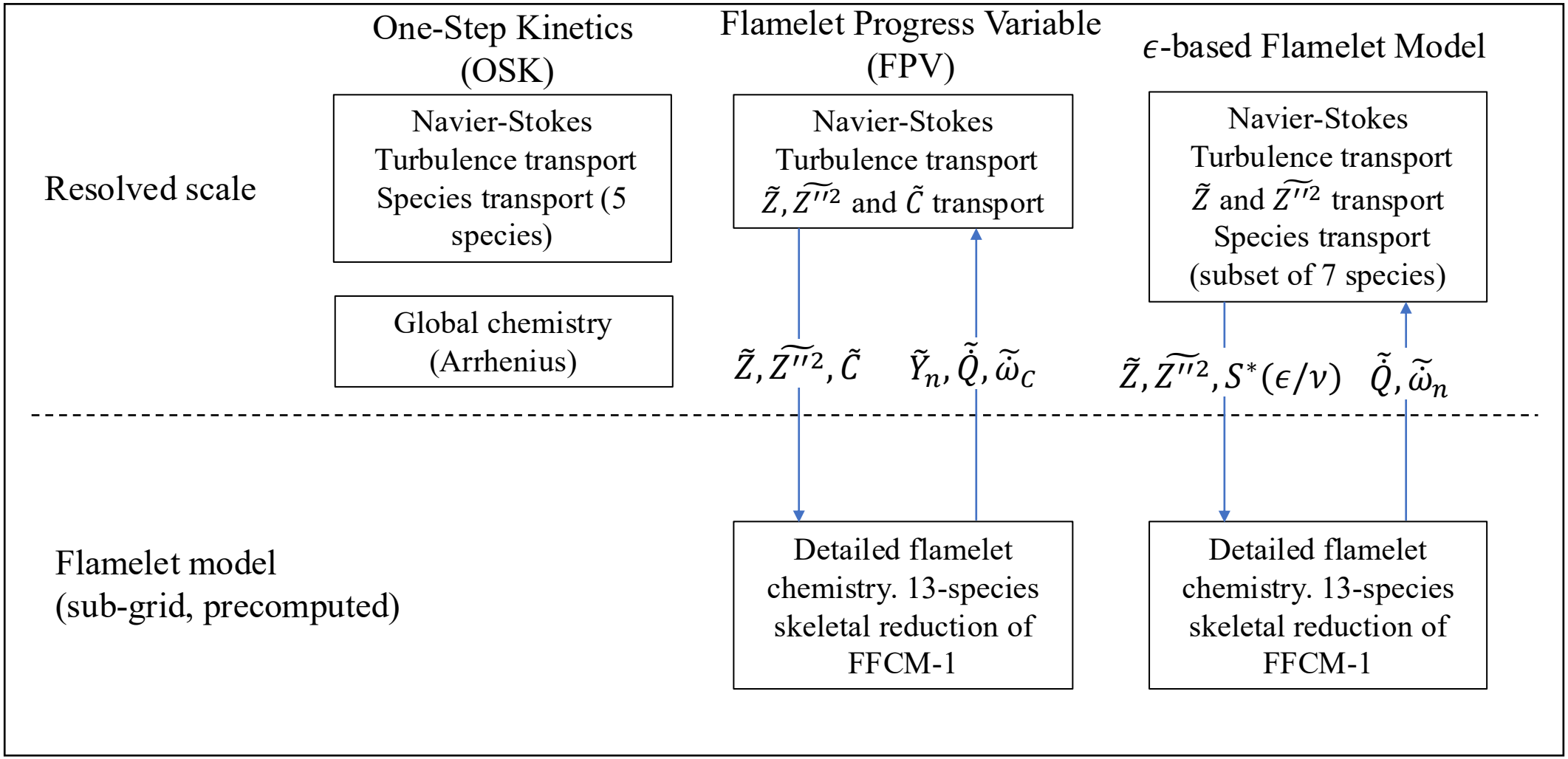
$$\alpha = \left(\frac{\tilde{Y}_F}{\tilde{Y}_F^{tab}}\right)\left(\frac{\tilde{Y}_{Ox}}{\tilde{Y}_{Ox}^{tab}}\right) \Longrightarrow \widetilde{\dot{\omega}}_n = \alpha \widetilde{\dot{\omega}}_n^{tab}$$

Scales tabulated reaction rates according to locally available reactants, preventing excessive consumption in off-manifold states.

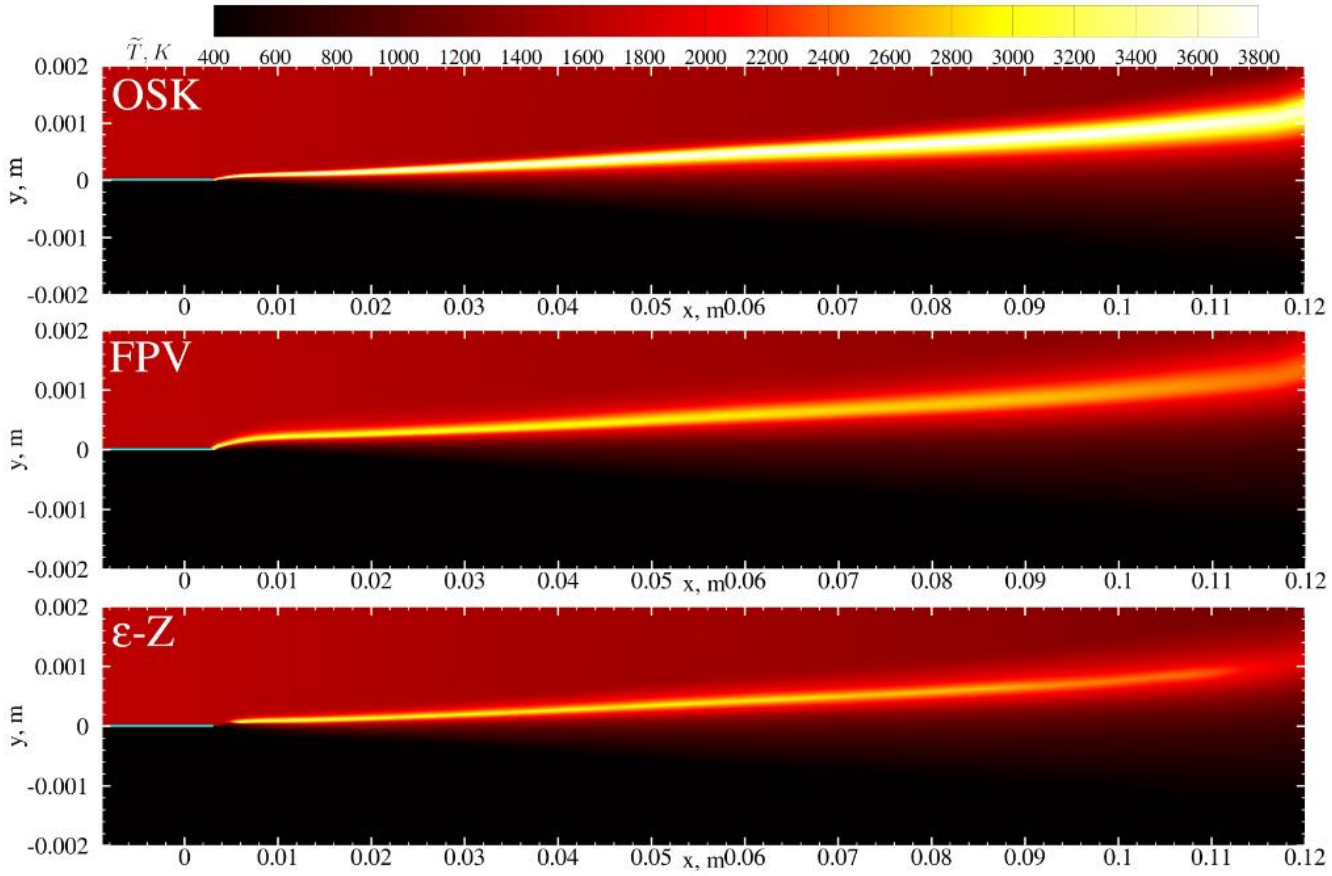
Limitations and future direction

- Complete flamelet tables that can represent all thermochemical states require modifying temperatures and compositions. Library dimensions → 2N+2.
- Future direction could be to solve local flamelet equation online using cell-local thermochemical states; naturally parallel across CFD cells and potentially suited to GPUs.

Model Architecture Comparison



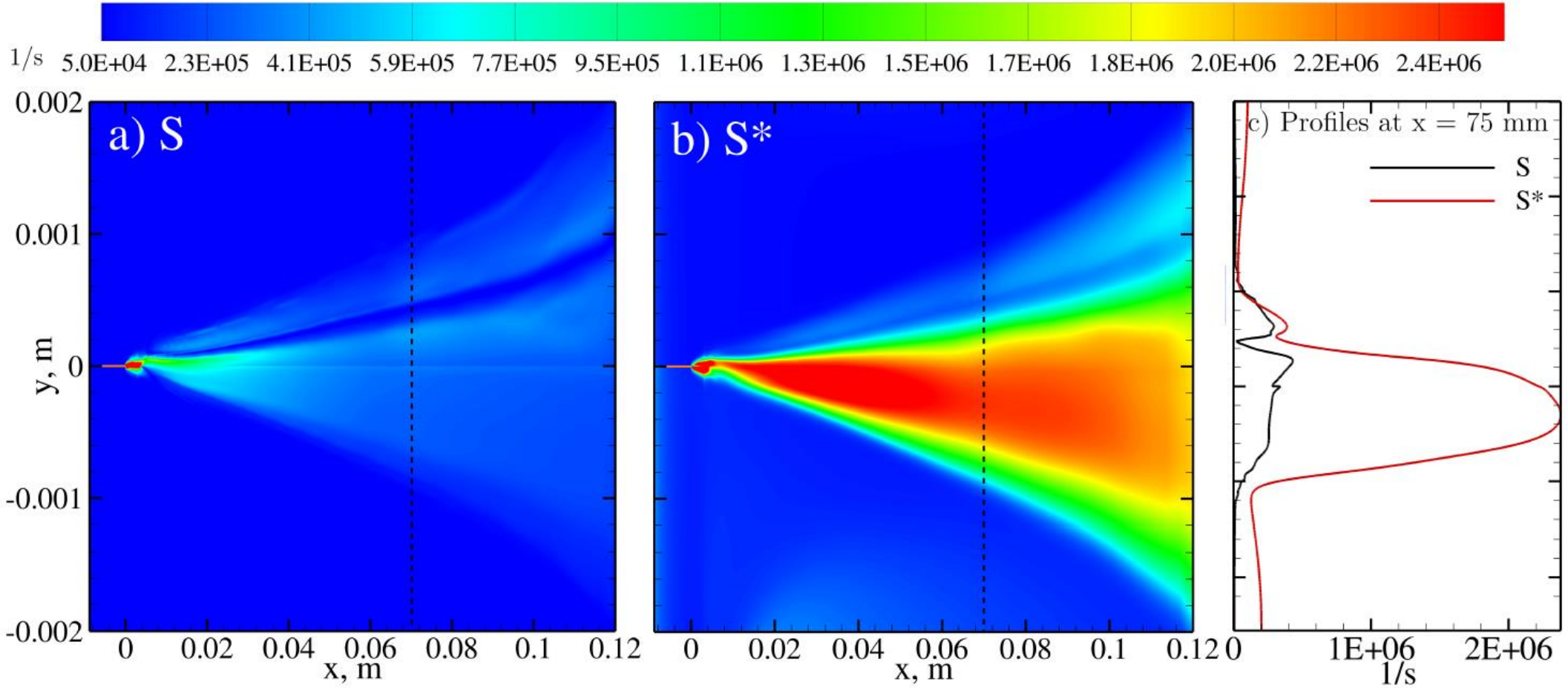
Combustion Model Comparison



- **OSK (one-step kinetics)**
  - Highest peak temperatures.
  - The global mechanism does not capture detailed finite-rate chemistry and dissociation, leading to overprediction of temperature.
- **FPV (flamelet progress variable)**
  - Detailed chemistry reduces peak temperature.
  - The progress-variable mapping does not directly couple the local turbulent strain to the selected flamelet state.
- **$\epsilon - Z$ (ϵ-based coupling)**
  - Local turbulent dissipation determines the flamelet strain.
  - Produces flame stand-off and downstream quenching where the inferred strain exceeds the flamelet flammability limit.

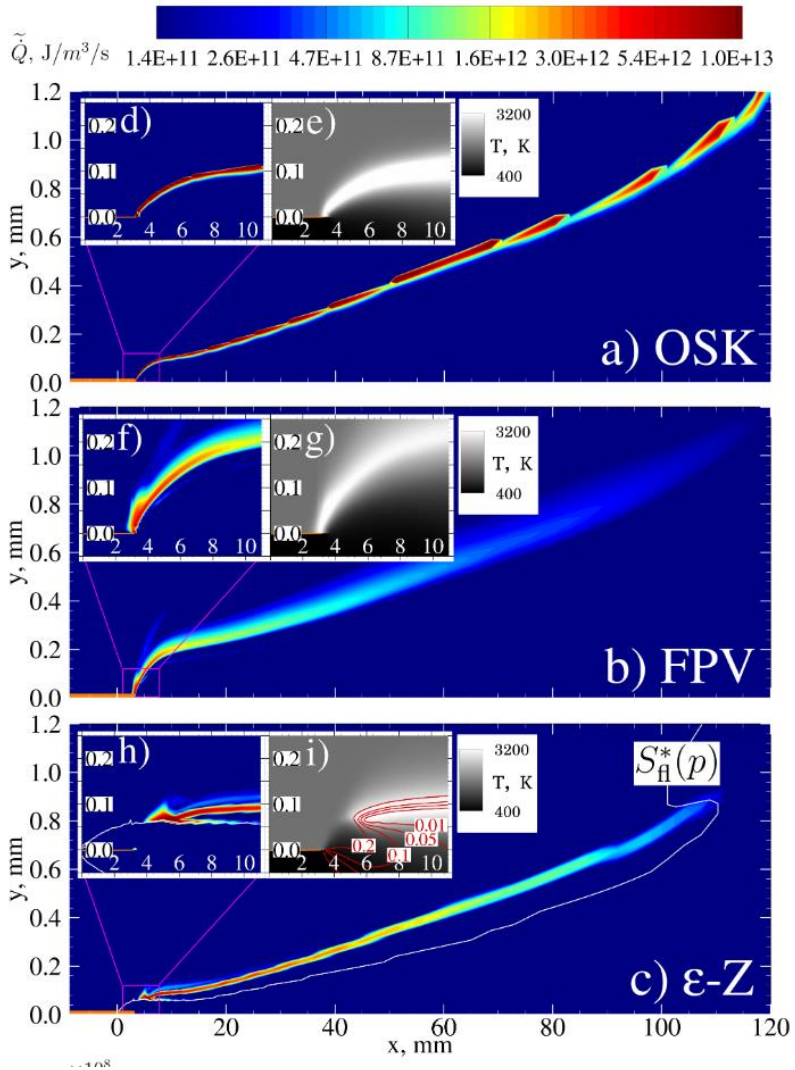
Takeaway: direct turbulence-flamelet coupling changes both the flame location and the downstream survival of the flame.

Direct Coupling Between Flow-Field and Flamelet Strain

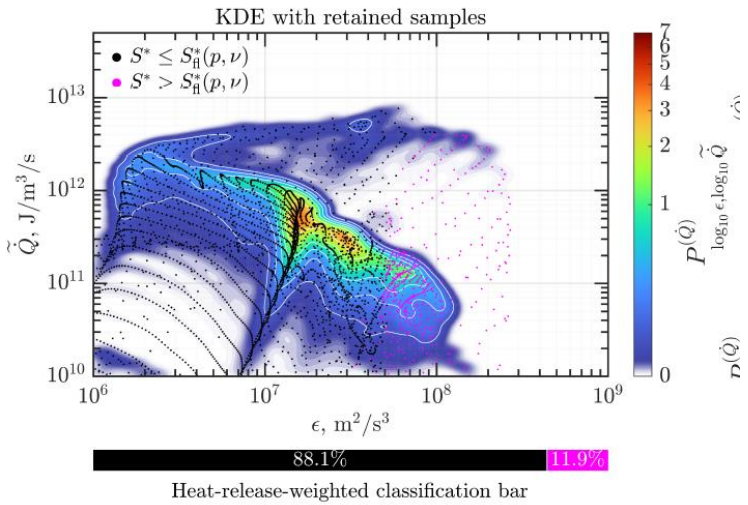


- ϵ-based model transfers the spatial structure of the turbulent strain field directly to the flamelet strain. It is not a chemically driven progress variable, but rather a tracking variable linking the local turbulence characteristics to the flamelet response.

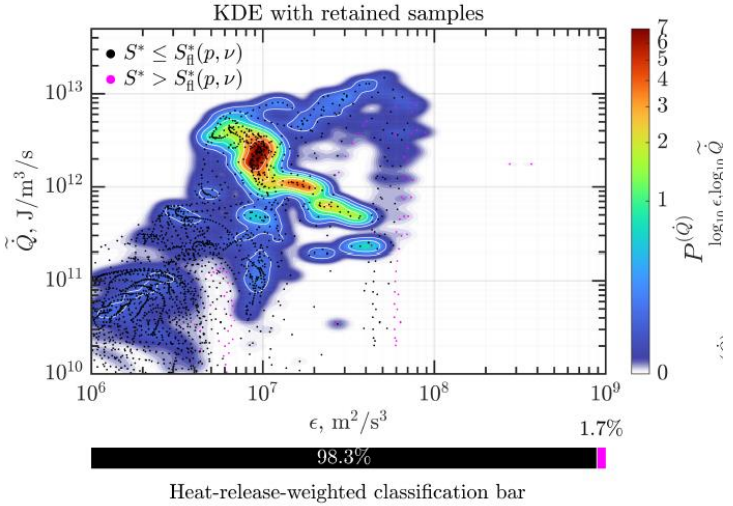
Heat-release-rate fields



Heat-release-weighted joint distribution: $\tilde{Q}$ vs ϵ



Fraction of total heat release in each regime



Fraction of total heat release in each regime

- $\epsilon - Z$ places a larger fraction of heat release rate in regions where the local strain remains below the flamelet extinction limit, yielding improved consistency between the turbulent flow state and retrieved flamelet state.
- $\epsilon - Z$ model exhibits a stronger association between heat release and elevated ϵ, qualitatively consistent with the DNS trend.

Conclusions

- Non-premixed progress-variable flamelet formulations do not guarantee consistent coupling between the local turbulent strain and the selected flame state, because the transported progress variable evolves independently of strain.
- The turbulent kinetic energy dissipation rate, ϵ, provides a physically motivated flamelet coupling variable enabling estimation of the smallest turbulent time and length scales, and associated flamelet strain rates consistent with the local turbulence cascade.
- Using ϵ-based coupling restores a direct turbulence-flamelet connection, enabling strain-rate-driven behavior such as flame standoff and downstream extinction to emerge from the local turbulent state.
- Transporting a reduced set of major species preserves thermochemical history through extinction and reignition. Products generated upstream can be advected and diffused through quenched regions without imposing a discontinuous tabulated composition.
- ϵ should not be thought as a progress variable. It need not evolve monotonically in space or time; instead, it communicates the local turbulent state to the flamelet model. We should think in terms of a "coupling variable" rather than a progress variable.
- **Ongoing work:** The model remains under development. DNS is needed to calibrate model coefficients, while ongoing LES of the Sydney Bluff-Body flame will provide an independent validation test. The present results should therefore be viewed as **preliminary verification**: the model responds qualitatively as intended to the introduced coupling physics.

Thank you