

Analysis of Methane-Air Edge Flame Structure

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Acknowledgement

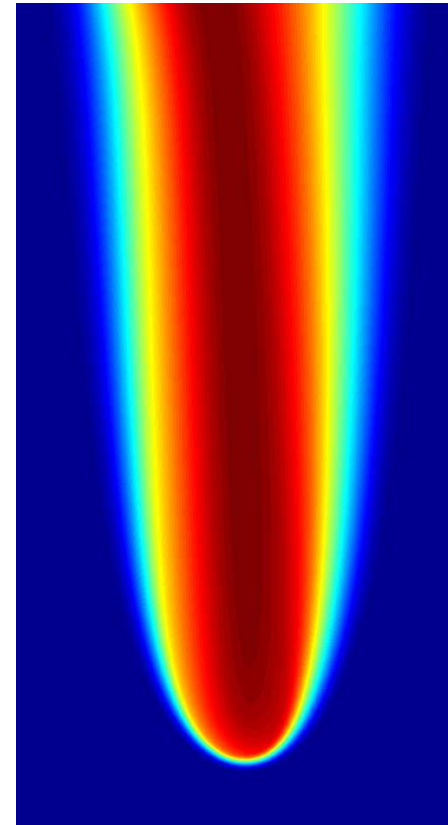
DOE Office of Science, Basic Energy Sciences, Chemical Sci. Div.

Introduction

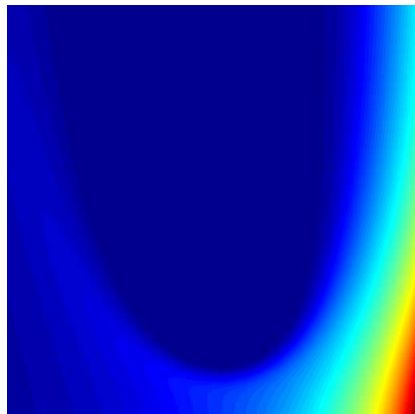
- Edge flames are an interesting class of flames that involve both premixed and non-premixed flame physics
- Relevance in microstructure of turbulent combustion
- Edge flame structure
 - Premixed flame front
 - Trailing non-premixed flame
- There have been many studies of edge flames, with a focus on flame stabilization and lift off height characteristics
- Fewer studies have probed the chemical structure of Hydrogen and Methane edge flames
- We explore the detailed structure of hydrocarbon and nitrogen chemistry in Methane-Air edge flames
 - Identify important processes in different flame regions

Problem Setup

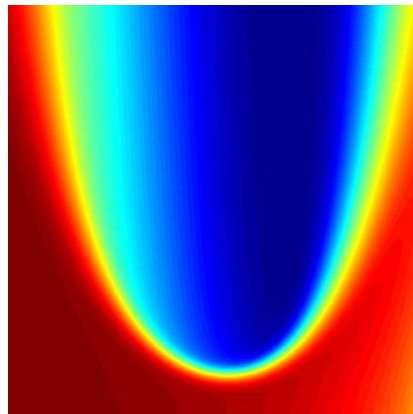
- Low Mach number detailed chemistry reacting flow model
- GRImech3.0 ($N = 53$ species, 325 reactions)
- $\sim 1.5 \times 3.0$ cm domain
- Uniform inflow velocity
- Inflow mixture: mixing layer pure CH₄ (right) and Air (left)
 - $\tanh()$ mixture fraction profile, $\xi_{st} = 0.055$
 - ξ is the elemental mixture fraction (Bilger)



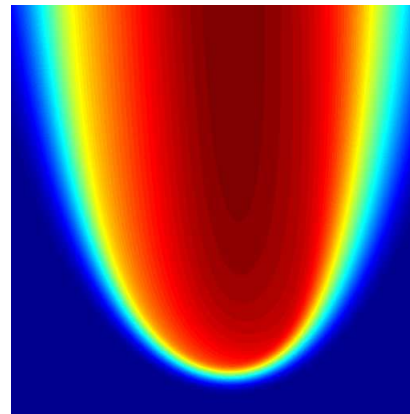
Edge flame detail: Y_i and w_i : CH_4 , O_2 , T , and NO



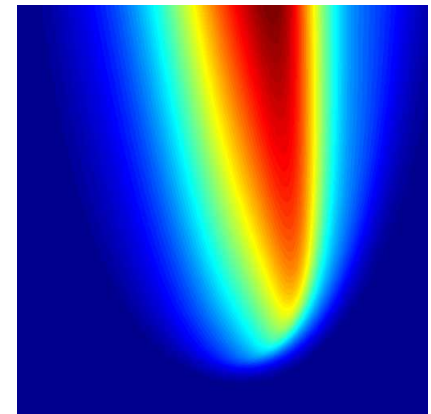
CH_4



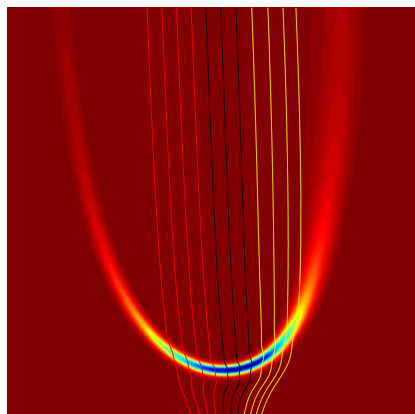
O_2



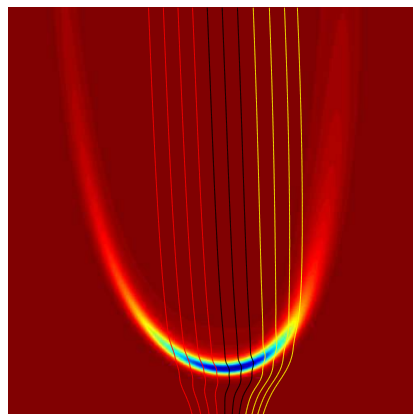
T



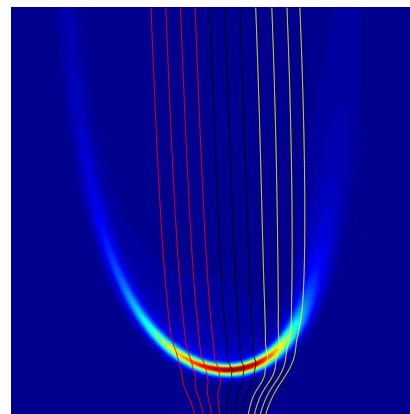
NO



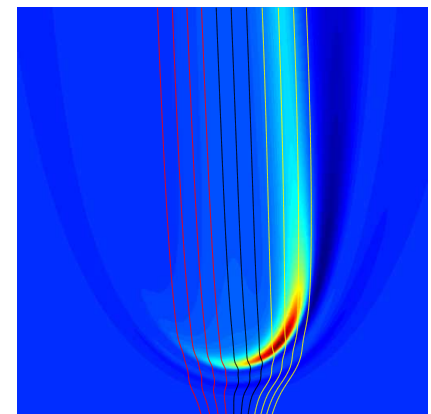
w_{CH_4}



w_{O_2}

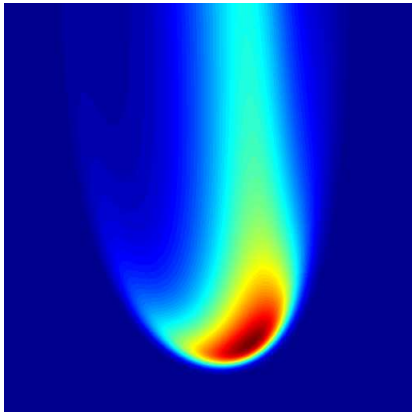


w_T

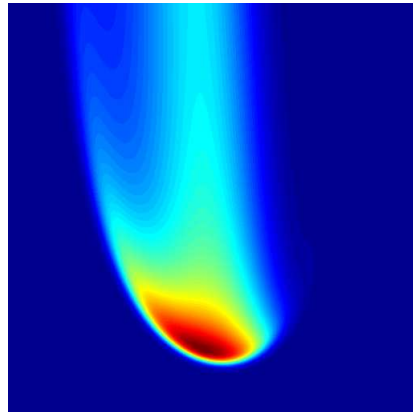


w_{NO}

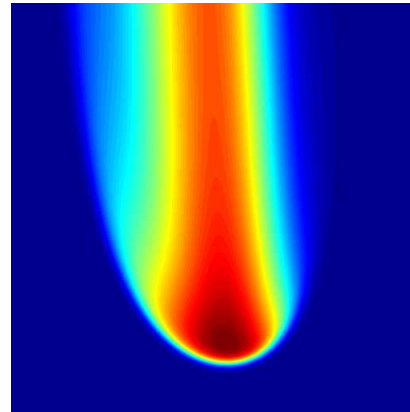
Edge flame detail: Y_i and w_i : H, O, OH, and N



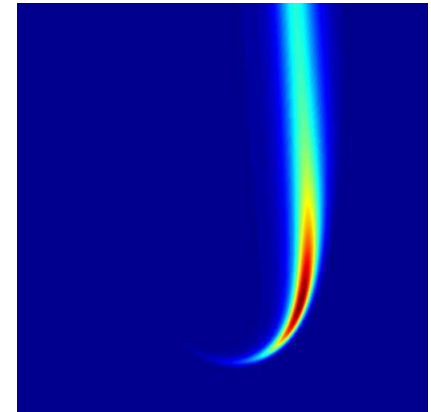
H



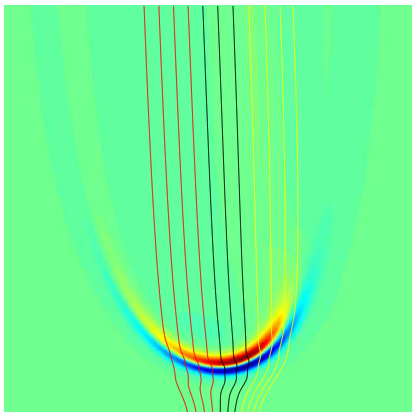
O



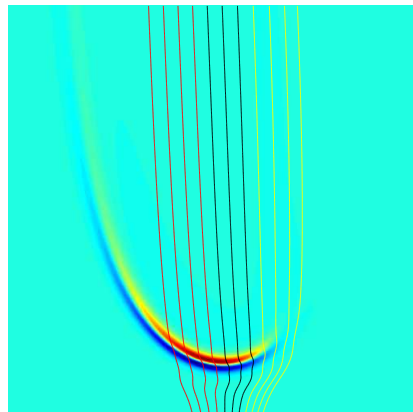
OH



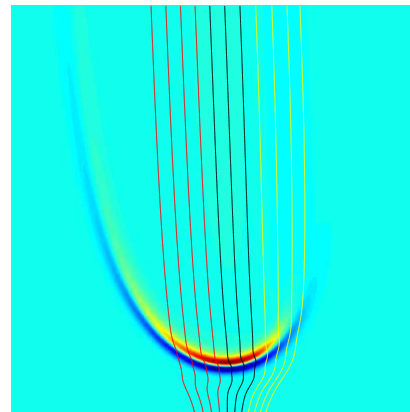
N



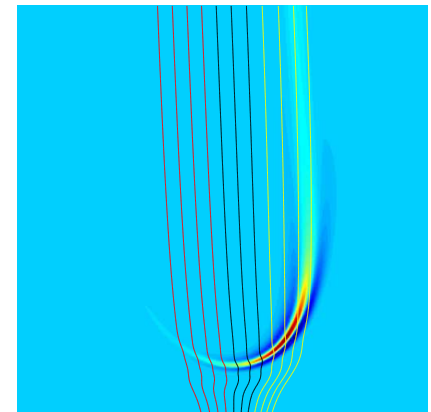
w_H



w_O



w_{OH}



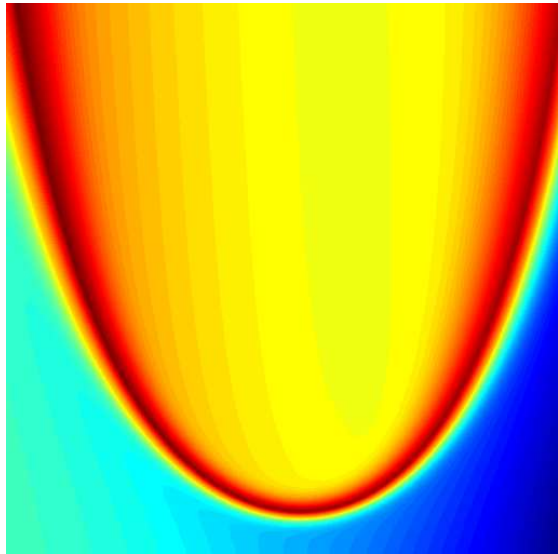
w_N

Fast-Slow Structure of Chemical Systems

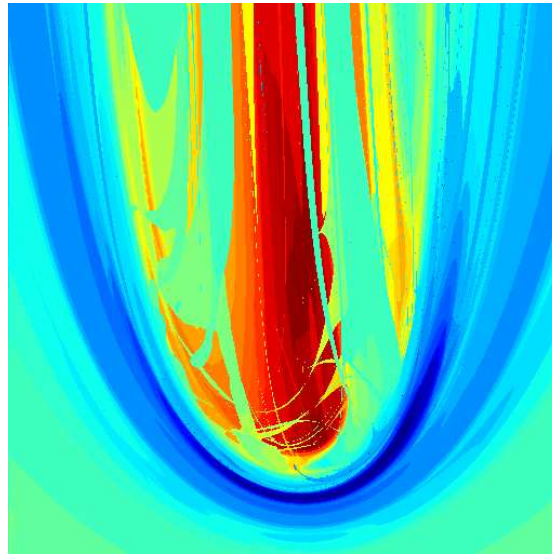
- Chemical systems are characterized by extreme stiffness
 - Typical range of time scales 1 ms — 1 ns
- Stiff/fast-slow ODE systems exhibit low order behavior
 - Fast processes are "slaved" to the slow processes
 - Slow processes govern evolution of the system along a low dimensional Slow Invariant Manifold (SIM)
- Computational Singular Perturbation (CSP) provides :
 - analysis of the dynamics of a chemical system
 - decoupling of fast and slow processes
 - cause-and-effect relationships
 - means for automated chemical model simplification strategies

Lam and Goussis, 22nd Comb. Symp., 1988.

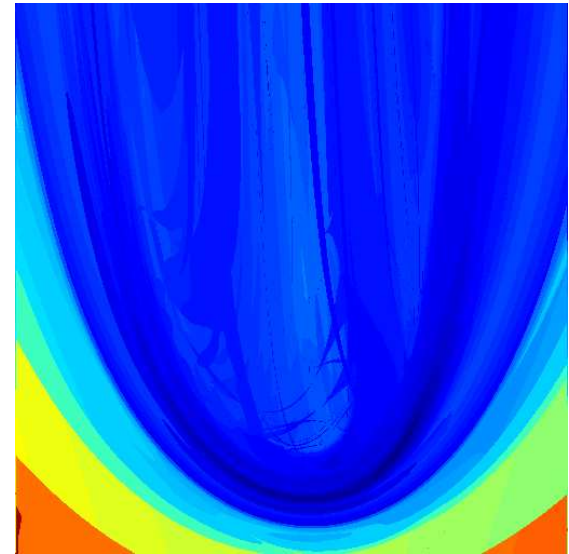
Time Scales and the SIM Dimension M



τ_1



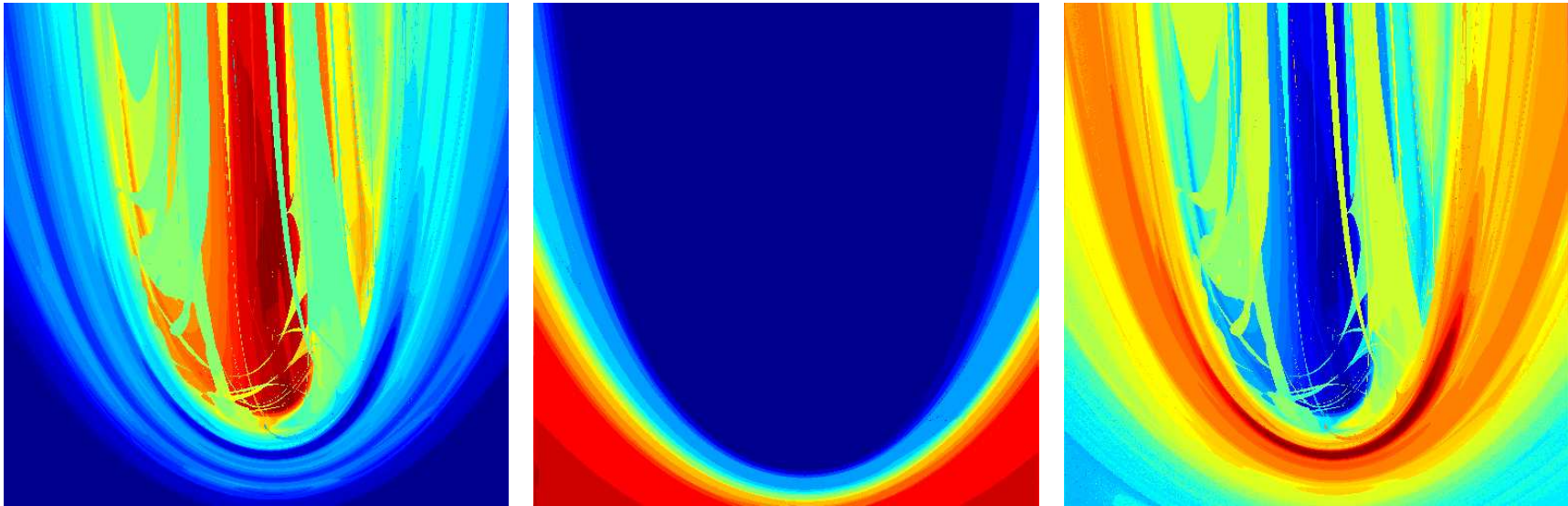
M



τ_{M+1}

- Fastest time scale $\tau_1 \sim \mathcal{O}(1 \text{ ns})$
- SIM dimension M :
 - ~ 4 in the premixed reaction zone
 - ~ 40 in the diffusion flame behind the edge flame
- Driving time scale (fastest of the slow) τ_{M+1}
 - $\sim \mathcal{O}(10 \text{ ns})$ in the premixed reaction zone

Composition of M — the SIM Dimension



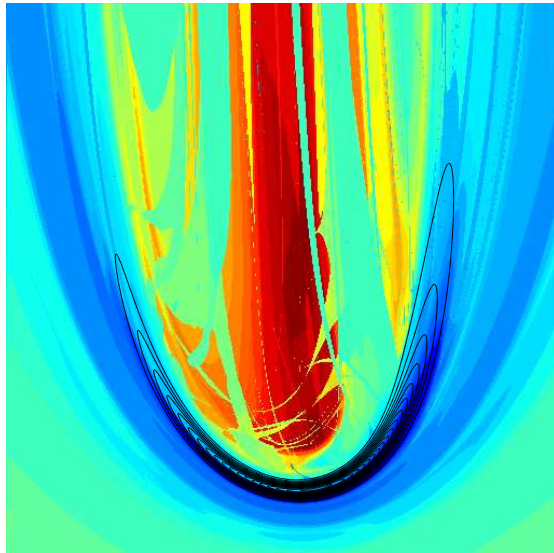
Exhausted Modes

Frozen Modes

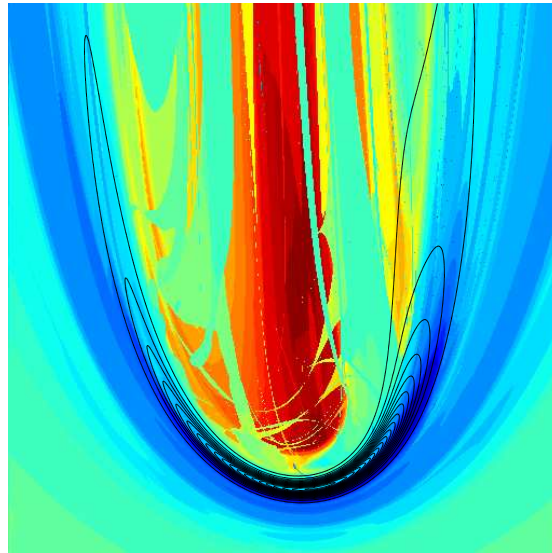
Active Modes

- $M = \# \text{ Exhausted Modes} + \# \text{ Frozen Modes}$
- $\# \text{ Active Modes} = N - M$
 - Highest activity in premixed reaction zone

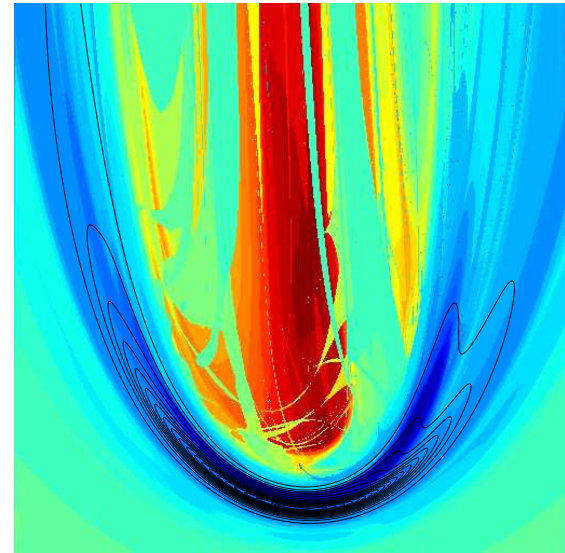
Internal Structure within the Premixed Front



w_{CH_4}



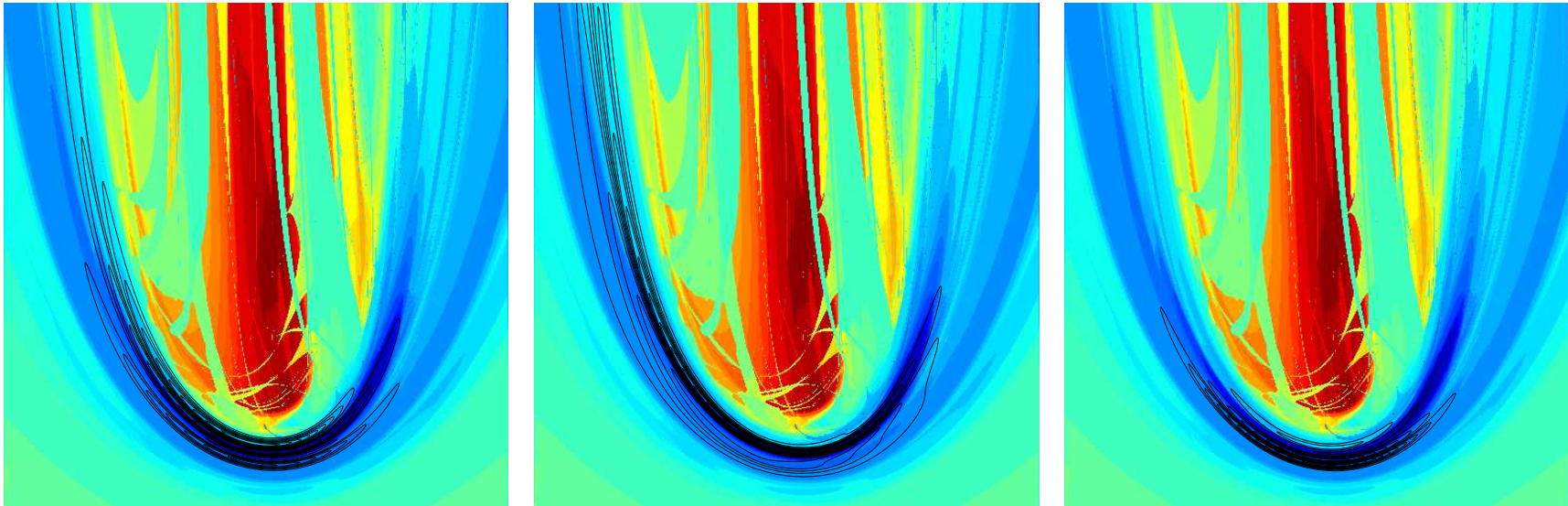
Y_{HCO}



$Y_{\text{CH}_3\text{O}}$

- M field indicates a two-layer structure in the premixed front
- The two layers are separated significantly on the rich side
- Internal layer coincides with the main hydrocarbon fuel consumption zone
- High mass fraction of CH_3O in the outer layer

Internal Structure within the Premixed Front



w_{HO_2}

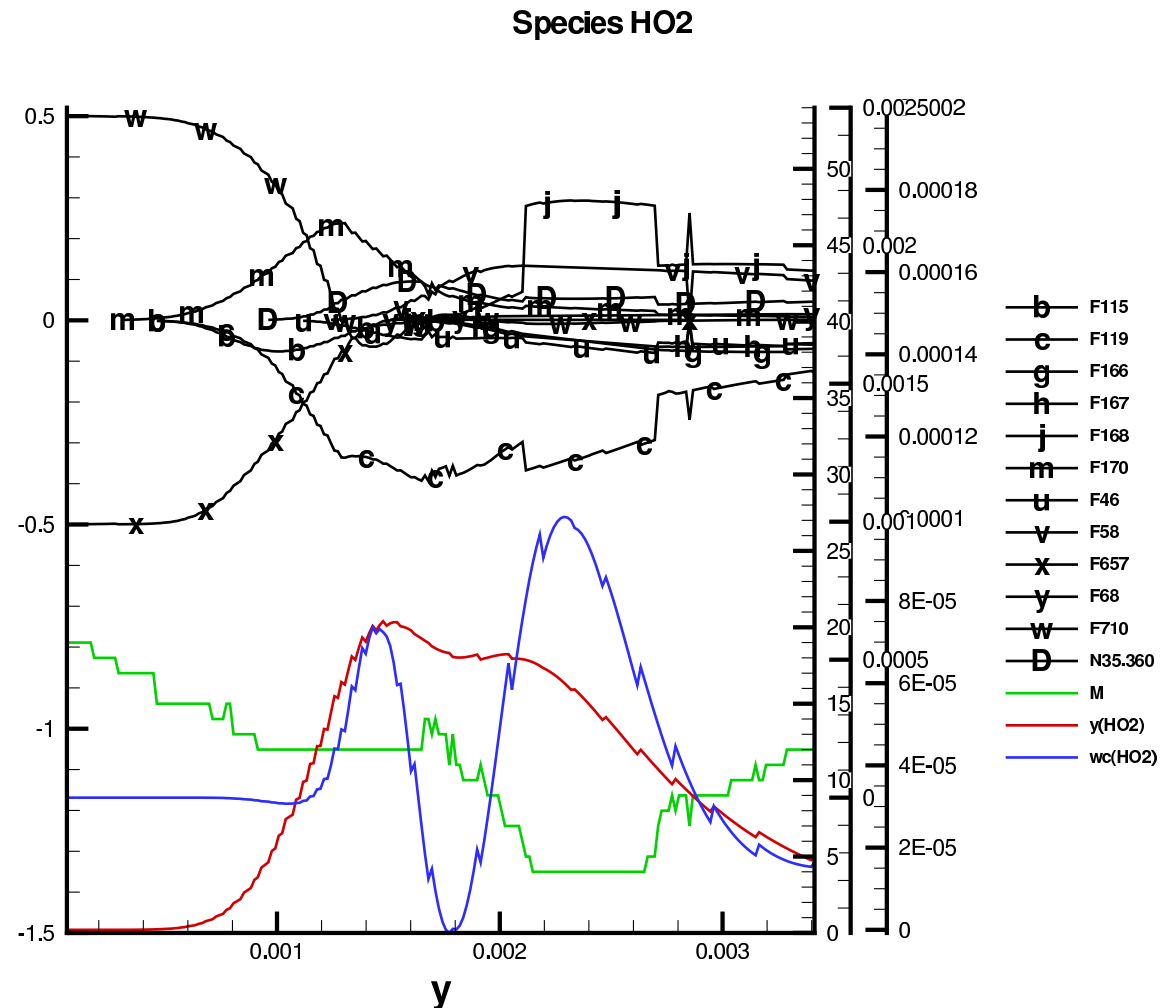
$w_{\text{H}_2\text{O}_2}$

$w_{\text{CH}_3\text{O}}$

- Outer layer associated with low temperature chemistry
- Participation by HO_2 , H_2O_2 , and CH_3O reactions
- Why the larger separation on the rich side?
 - Examine flow structure along a $\xi = 0.075$ line in the rich region

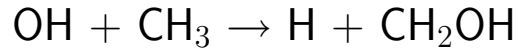
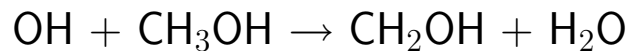
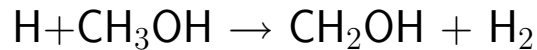
HO2 Importance Indices along $\xi = 0.075$

- Two minimum plateaus of M coincide with maxima in w_{HO_2}
- Cold inflow:
Convection < 0 ; Diffusion > 0
- Preheat region/First layer:
Convection $\lesssim 0$; Diffusion $\gtrsim 0$
R170: $\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{HO}_2 + \text{CH}_2\text{O} > 0$
R119: $\text{HO}_2 + \text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{O} < 0$
- Main Premixed front/Second layer:
R168: $\text{HCO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{CO} > 0$
R119: $\text{HO}_2 + \text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{O} < 0$

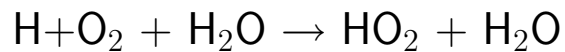
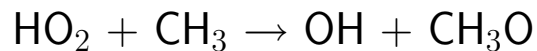
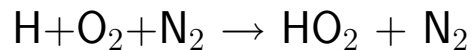


Active Timescale and Driving Process Analysis

- $\xi = 0.035$: One low M plateau: $M = 7$: $\tau_{M+1} = 0.07 \mu\text{sec}$
Reactions with highest participation indices in P_{M+1} :



- $\xi = 0.075$: Low- T low- M plateau: $M = 8$: $\tau_{M+1} = 1 \mu\text{sec}$
Reactions with highest participation indices in P_{M+1} :

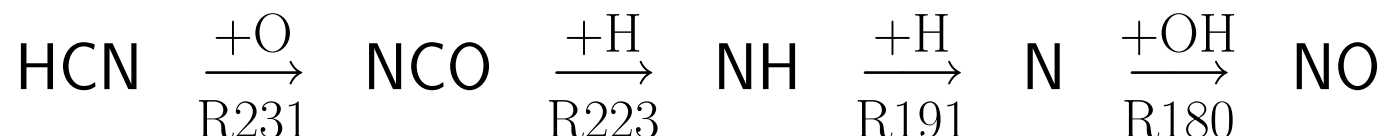


- On the rich side, low T chemistry is slower than on the lean side, such that a longer residence time is needed for activation of the fast fuel breakdown reactions
— hence the larger separation between the two M -layers

- Thermal (Zeldovich) mechanism



- Prompt pathway initiated by Rxns of Hydrocarbon radicals with N_2 to produce HCN and N, which are converted to NO:

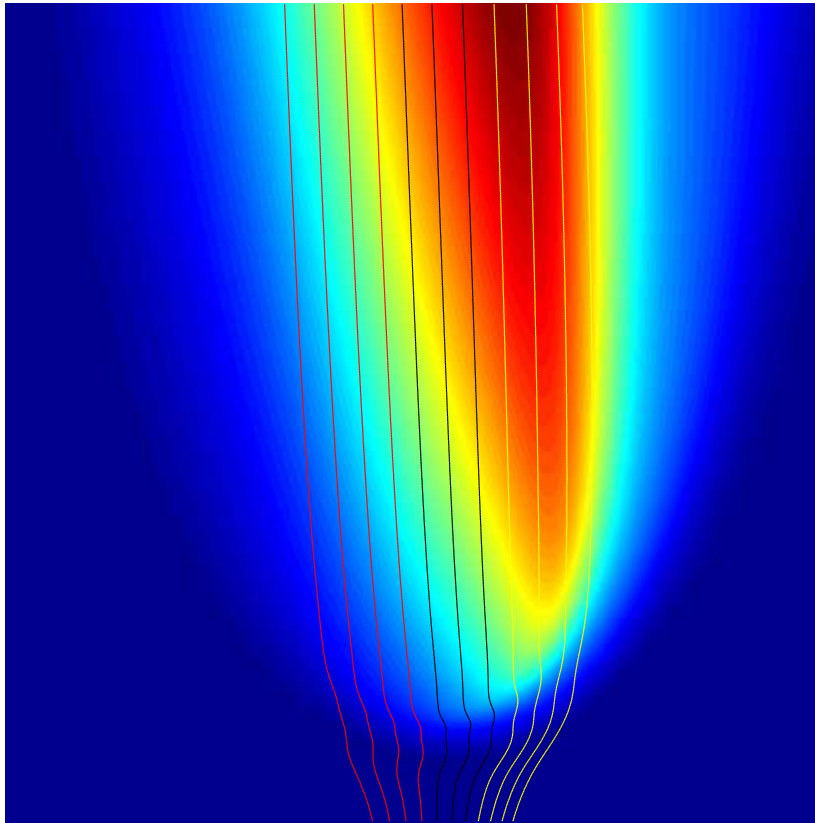


- Other NO production/consumption pathways, involving HNO and HNCO, have also been included in the prompt path

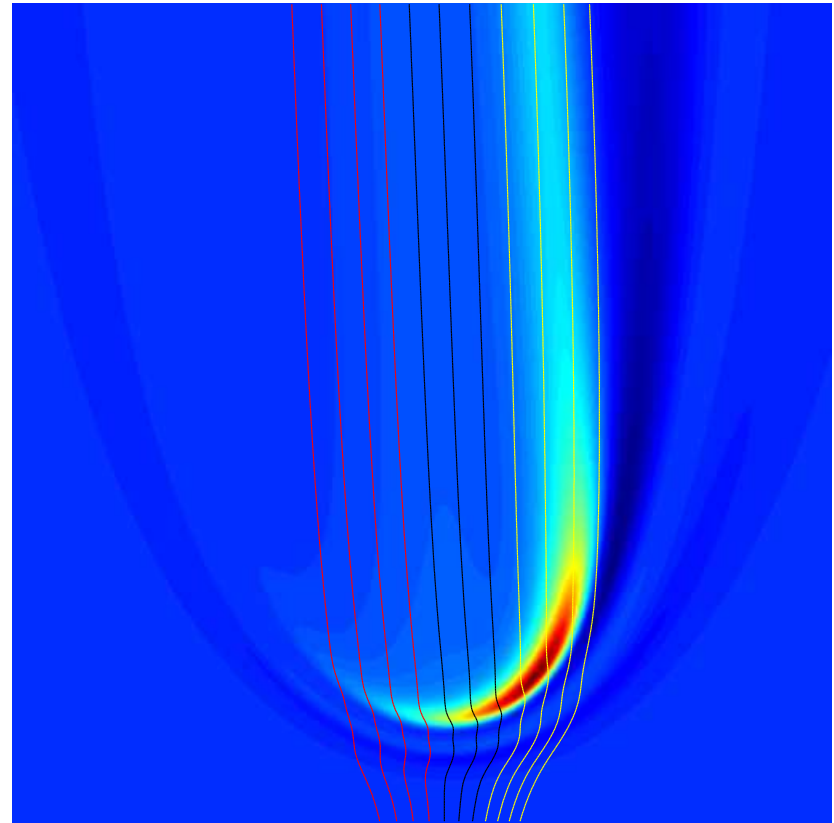
- N_2O intermediate pathway



Edge Flame Structure – NO



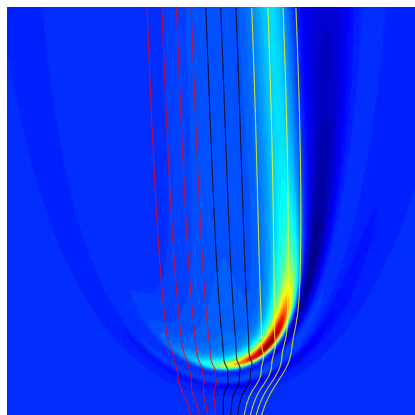
NO



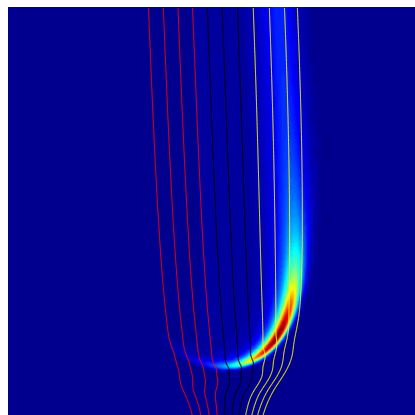
w_{NO}

- Bulk NO production is on the rich side of the edge flame
- Transported to the lean side

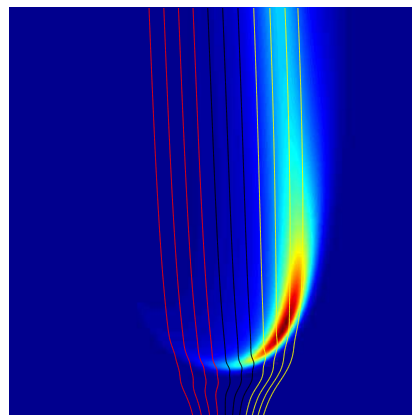
Basic Edge Flame Structure — NO Reactions



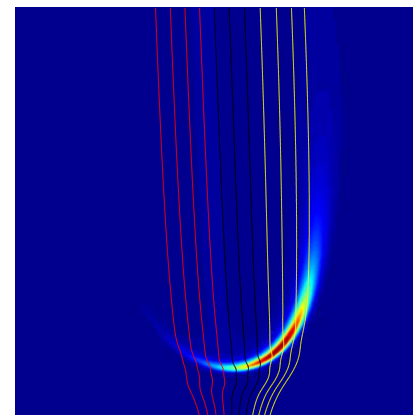
w_{NO}



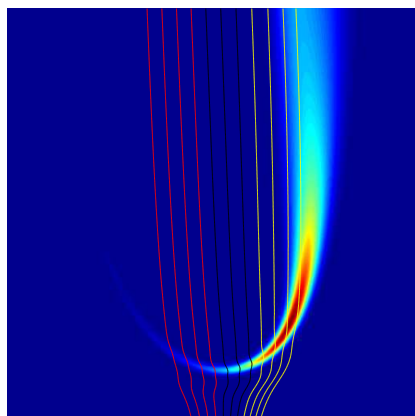
$\text{N} + \text{OH} = \text{NO} + \text{H}$
R180: 1.4×10^{-6}



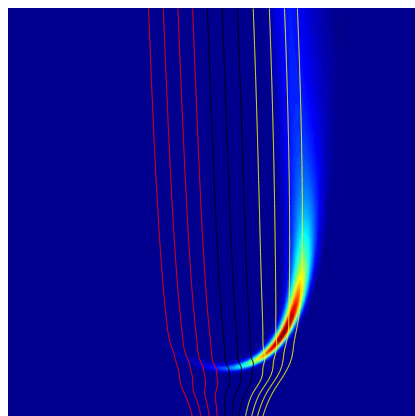
$\text{HNO} + \text{H} = \text{H}_2 + \text{NO}$
R214: 0.87×10^{-6}



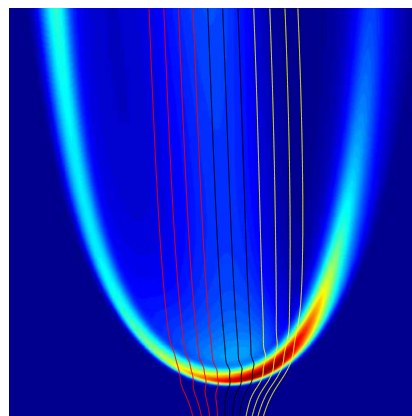
$\text{N} + \text{O}_2 = \text{NO} + \text{O}$
R179: 0.73×10^{-6}



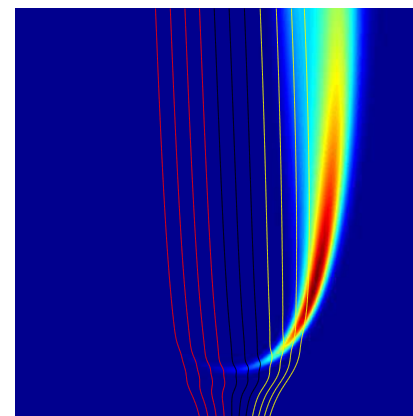
$\text{CH}_2 + \text{NO} = \text{H} + \text{HNCO}$
R249: 0.43×10^{-6}



$\text{CH} + \text{NO} = \text{HCN} + \text{O}$
R246: 0.32×10^{-6}



$\text{NO}_2 + \text{H} = \text{NO} + \text{OH}$
R189: 0.32×10^{-6}



$\text{HCCO} + \text{NO} = \text{HCNO} + \text{CO}$
R274: 0.27×10^{-6}

NO Importance Indices — Stoich. Mixture Fraction line ($\xi = 0.055$)

- Cold inflow:

Convection < 0 ; Diffusion > 0

- Preheat region:

Convection < 0 ; Diffusion > 0

R189: $\text{NO}_2 + \text{H} = \text{NO} + \text{OH} > 0$

R186: $\text{HO}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{O} < 0$

- Premixed front:

Convection < 0 ; Diffusion $> / < 0$

R179: $\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O} > 0$

R214: $\text{HNO} + \text{H} \rightarrow \text{H}_2 + \text{NO} > 0$

R249: $\text{CH}_2 + \text{NO} \rightarrow \text{H} + \text{HNCO} < 0$

R223: $\text{NCO} + \text{H} \rightarrow \text{NH} + \text{CO} < 0$

R186: $\text{HO}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{O} < 0$

- Trailing Diff flame:

Convection < 0 ; Diffusion $\gtrsim 0$

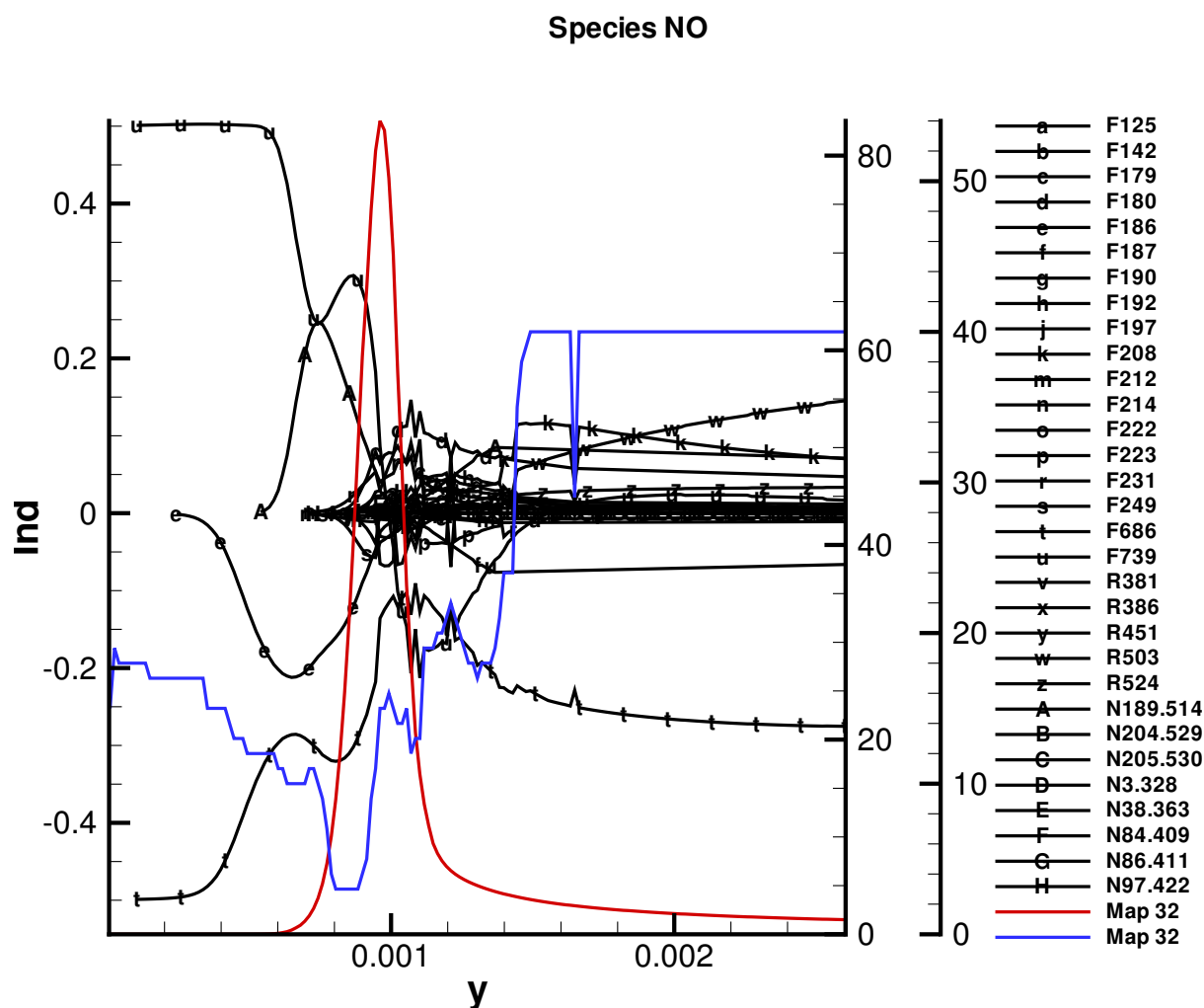
R178: $\text{N} + \text{NO} \leftarrow \text{N}_2 + \text{O} > 0$

R208: $\text{NNH} + \text{O} \rightarrow \text{NH} + \text{NO} > 0$

R189: $\text{NO}_2 + \text{H} = \text{NO} + \text{OH} > 0$

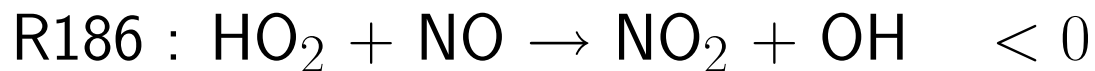
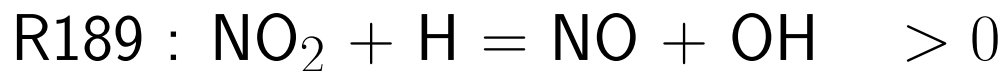
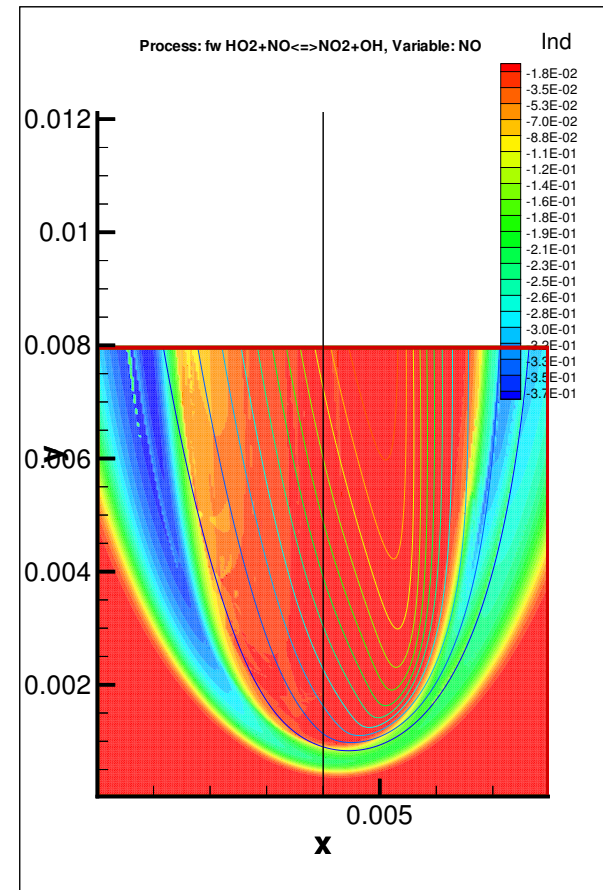
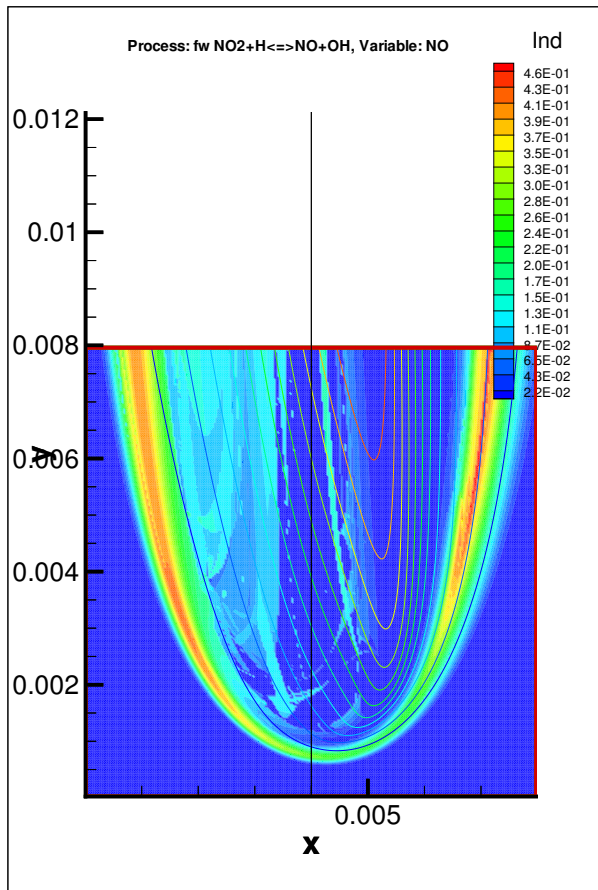
R180: $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H} > 0$

R187: $\text{NO} + \text{O} + \text{M} \rightarrow \text{NO}_2 + \text{M} < 0$





Highest NO Importance Indices — Preheat Zone — $\xi \in [0.035, 0.075]$



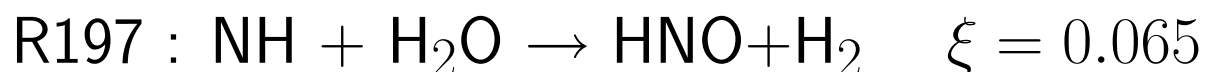
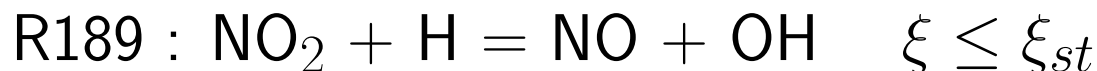
with decaying relative influence inside the premixed front

Highest NO Importance Indices — Premixed front

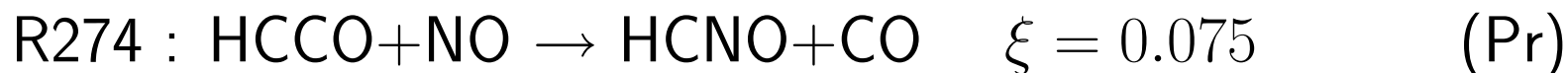
- Rxns with Large *+ve* Importance, $\xi \in [0.035, 0.075]$:
 - R189 : $\text{NO}_2 + \text{H} = \text{NO} + \text{OH}$
 - R179 : $\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$ (Zeldovich)
 - R180 : $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ (Z)
 - R214 : $\text{HNO} + \text{H} \rightarrow \text{H}_2 + \text{NO}$ (Prompt)
- R189 most Imp. *+ve* for $\xi = \{0.035, 0.075\}$
- Rxns with Large *-ve* Importance :
 - R249 : $\text{CH}_2 + \text{NO} \rightarrow \text{H} + \text{HNCO}$ $\xi \in [0.045, 0.075]$ (Pr)
 - R223 : $\text{NCO} + \text{H} \rightarrow \text{NH} + \text{CO}$ ξ_{st} post-flame (Pr)
 - R274 : $\text{HCCO} + \text{NO} \rightarrow \text{HCNO} + \text{CO}$ $\xi > 0.055$ (Pr)
 - R097 : $\text{OH} + \text{CH}_3 = \text{CH}_2(\text{S}) + \text{H}_2\text{O}$ $\xi \leq 0.055$

Highest NO Importance Indices — Trailing Diffusion Flame

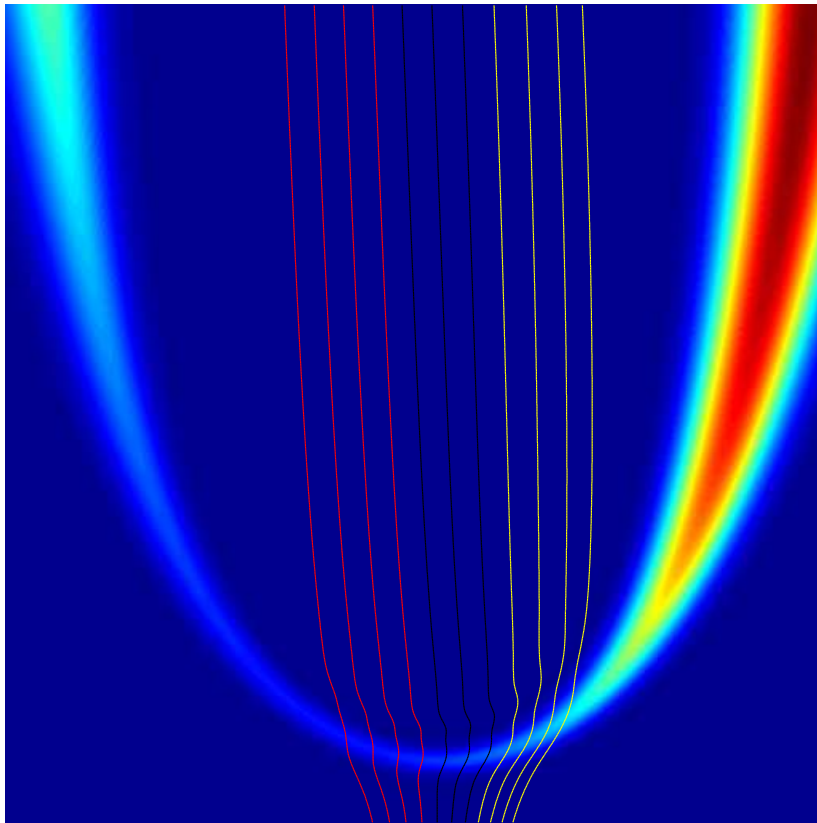
- Rxns with Large *+ve* Importance Indices



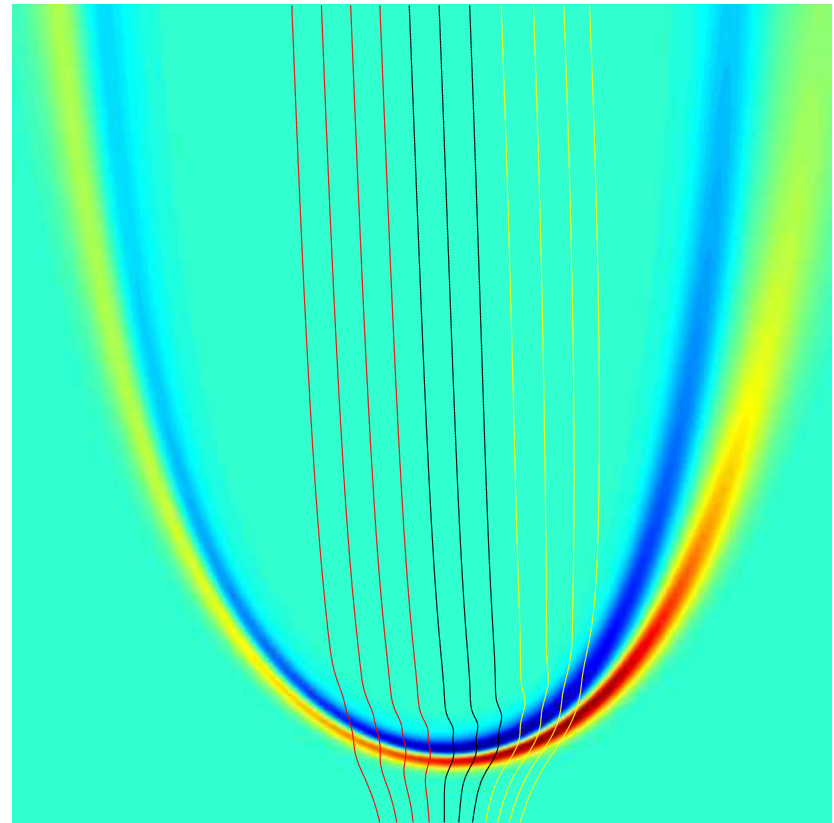
- Rxns with Large *-ve* Importance Indices



Edge Flame Structure – NO_2



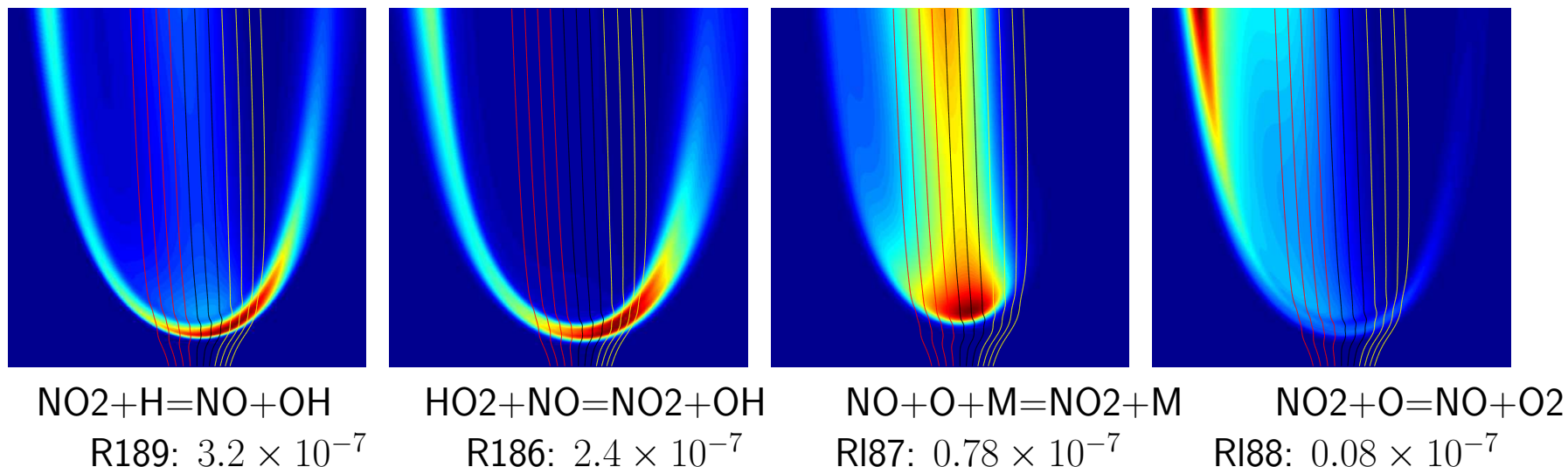
NO_2



w_{NO_2}

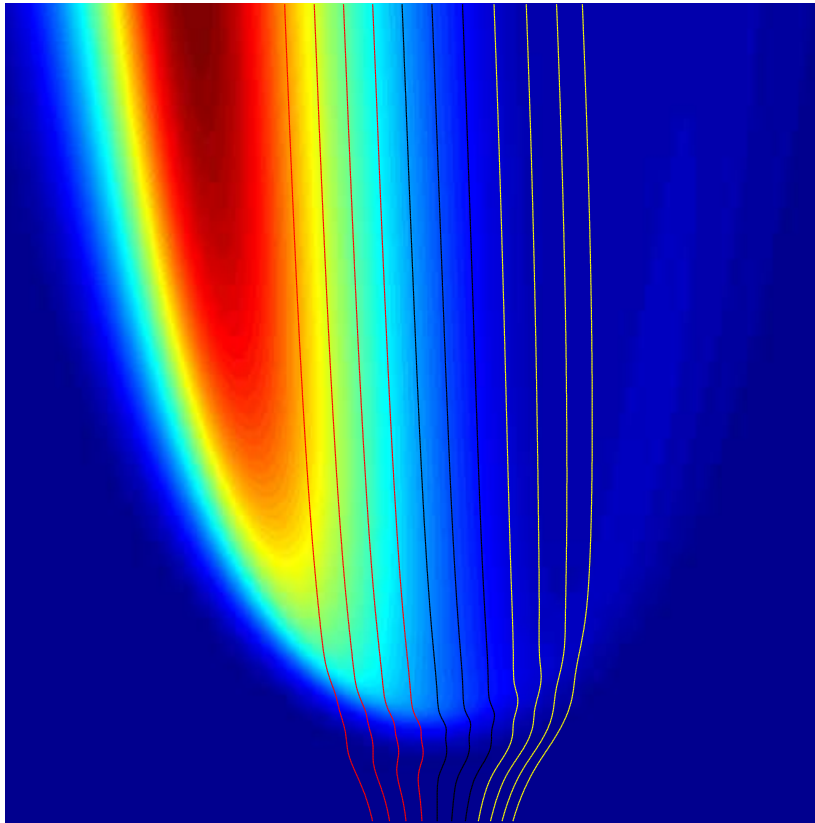
- NO_2 is a component of NO_x

Basic Edge Flame Structure — NO₂ Reactions

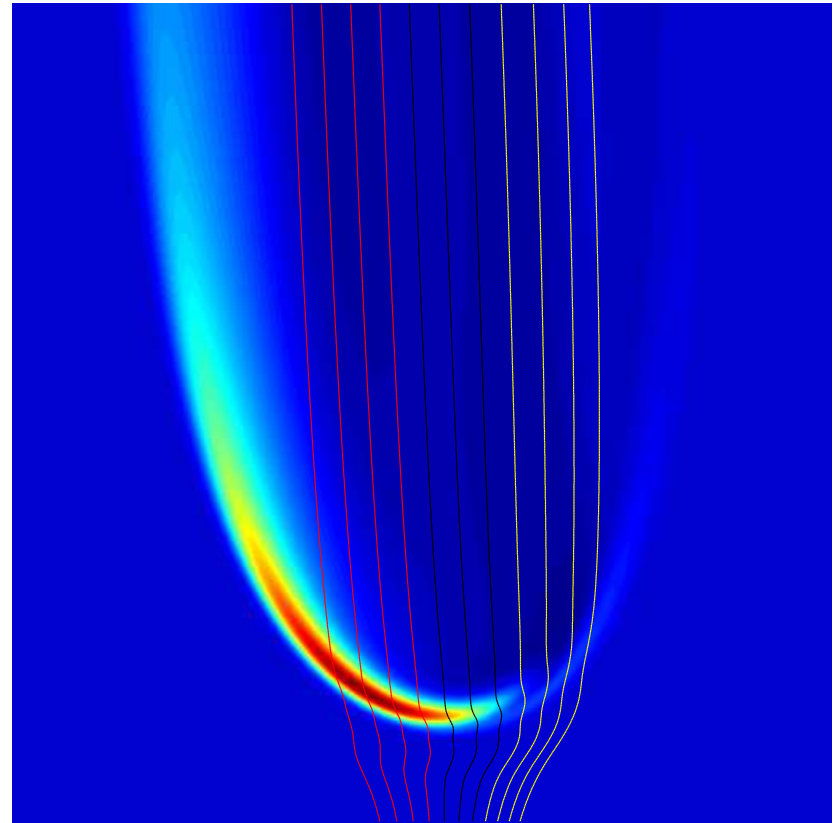


- Reactions with Large positive Importance to NO₂
 - R186 : HO₂+NO=NO₂+OH all ξ ($\rightarrow$ for $\xi = 0.075$)
 - R187 : NO+O+M=NO₂+M $\xi \in [0.035, \xi_{st}]$
- Reactions with Large negative Importance to NO₂
 - R189 : NO₂+H=NO+OH all ξ

Edge Flame Structure – N_2O



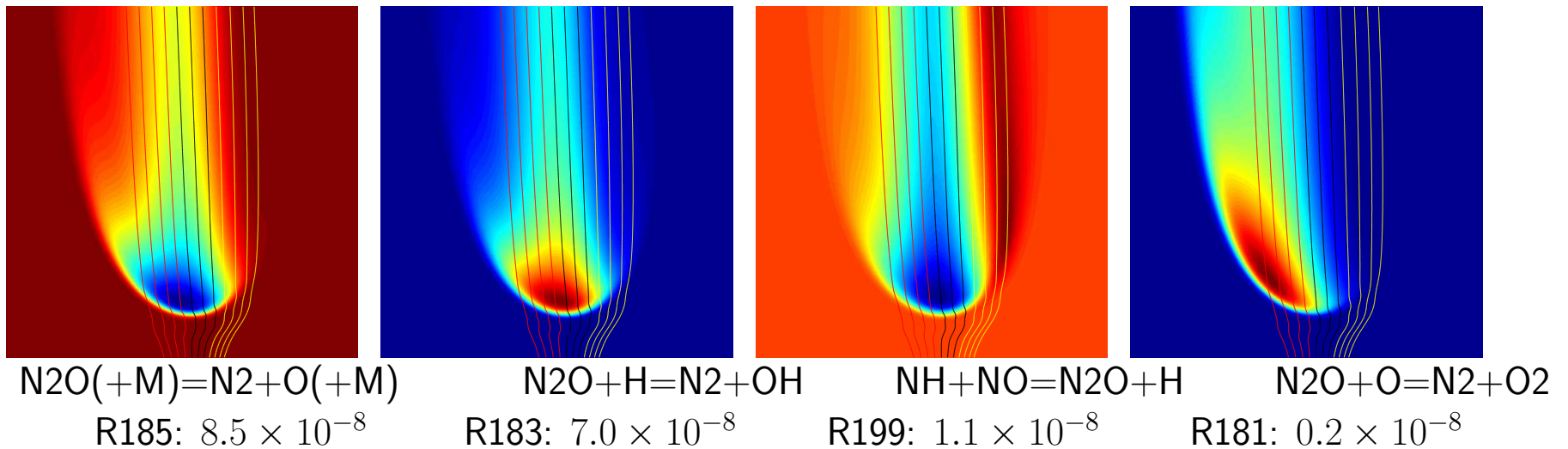
N_2O



$w_{\text{N}_2\text{O}}$

- N_2O is a greenhouse gas
- Important intermediate for NO production

Basic Edge Flame Structure — N₂O Reactions



- Reactions with Large positive Importance to N₂O
 - R185 : $\text{N}_2\text{O}(+\text{M})=\text{N}_2+\text{O}(+\text{M})$ all ξ (prem for $\xi = 0.075$)
 - R199 : $\text{NH}+\text{NO}=\text{N}_2\text{O}+\text{H}$ $\xi = 0.075$ ($\lesssim 0$ for $\xi = \xi_{st}$)
 - R184 : $\text{N}_2\text{O}+\text{OH} \leftarrow \text{N}_2+\text{HO}_2$ $\xi = 0.075$ (prem)
 - R38 : $\text{H}+\text{O}_2 \rightarrow \text{O}+\text{OH}$ $\xi = 0.075$ (diff)
- Reactions with Large negative Importance to N₂O
 - R183 : $\text{N}_2\text{O}+\text{H}=\text{N}_2+\text{OH}$ all ξ ($\rightarrow$ for $\xi = 0.075$)

Conclusions

- Used CSP analysis to explore internal structure of hydrocarbon and nitrogen chemistry in a methane-air edge flame
- Large number of modes exhausted behind the premixed flame front
- Larger separation between low-T and primary reactive layers on the rich side of the edge flame
 - Slower low-T active process on the rich side
- Identified important NO, N₂O, and NO₂ reactions in different regions of the edge flame