Evaluation of the Unsteady Flamelet Progress Variable approach in Large Eddy Simulation of the ECN Spray A

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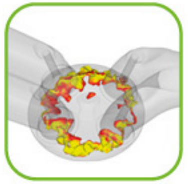
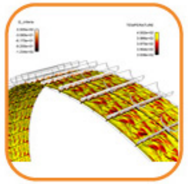

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State of the Art:

- Direct injection diesel engines for mid-term necessary for heavy duty application
- LES of spray combustion nowadays established as diagnostic tool
- Several combustion modeling strategies utilized in literature
- Focus here: Tabulated flame structures, i.e. UFPV approach
  - UFPV approach developed and applied for LES of gas-turbine model combustor [1]
  - Later extended and validated in 3D LES of lifted flame [2]
  - Reduced versions successfully applied in spray LES ([3], [4], [5])

Aim of this work:

- Validate the original UFPV [1] approach in LES of spray combustion
- Investigate flamelet parameter statistics
- Show influence of scalar dissipation rate on reaction progress

[1] H. Pitsch and M. Ihme, *43rd AIAA Aerosp. Sci. Meet. Exhib. - Meet. Pap.*, pp. 2593–2606, 2005. | [2] M. Ihme and Y. C. See, *Combust. Flame*, vol. 157, no. 10, pp. 1850–1862, 2010. | [3] C. Bekdemir, L. M. T. Somers, L. P. H. De Goey, J. Tillou, and C. Angelberger, *Proc. Combust. Inst.*, vol. 34, no. 2, pp. 3067–3074, 2013.| [4] A. Wehrfritz, O. Kaario, V. Vuorinen, and B. Somers, *Combust. Flame*, vol. 167, pp. 113–131, 2016. | [5] J. M. Desantes, J. M. García-Oliver, R. Novella, and E. J. Pérez-Sánchez, *Comput. Fluids*, vol. 200, p. 104419, 2020.

Description ECN Spray A

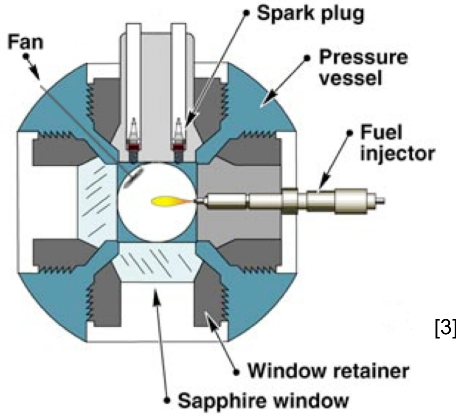
Experimental Setup

- **ECN Spray A** [1]:
  - Bosch single-hole injector
  - d_{nozzle}: 90 µm
  - Fuel: n-Dodecane
  - 6 ms injection duration
  - 1500 bar rail pressure
  - 60 bar chamber pressure
  - T_{fuel} = 363 K, $T_{chamber}$ = 900 K
  - $X_{O2,Chamber}$ = 0.15

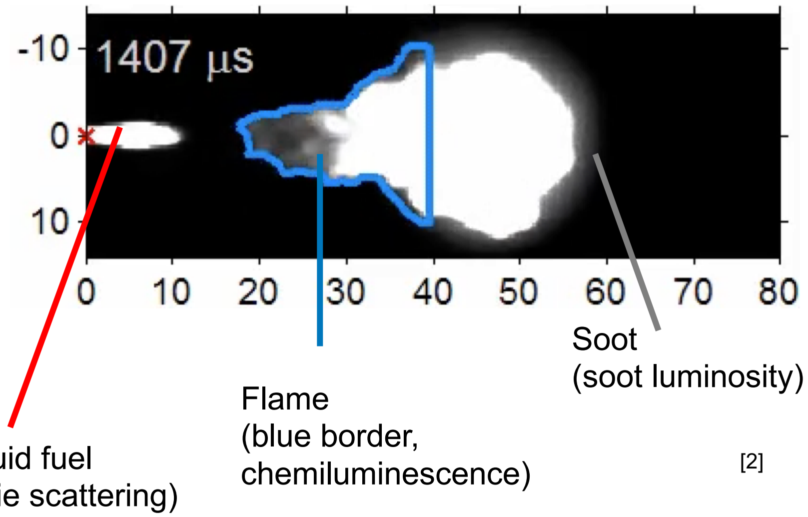
ECN Spray A injector

[1]

ECN Spray A setup



[3]



[2]

[1] ECN: https://ecn.sandia.gov/diesel-spray-combustion/target-condition/spray-ab/
[2] https://ecn.sandia.gov/data/high-speed-movies-at-spray-a/
[3] https://ecn.sandia.gov/diesel-spray-combustion/sandia-cv/combustion-vessel-geometry/1997-to-2009

Numerical Setup

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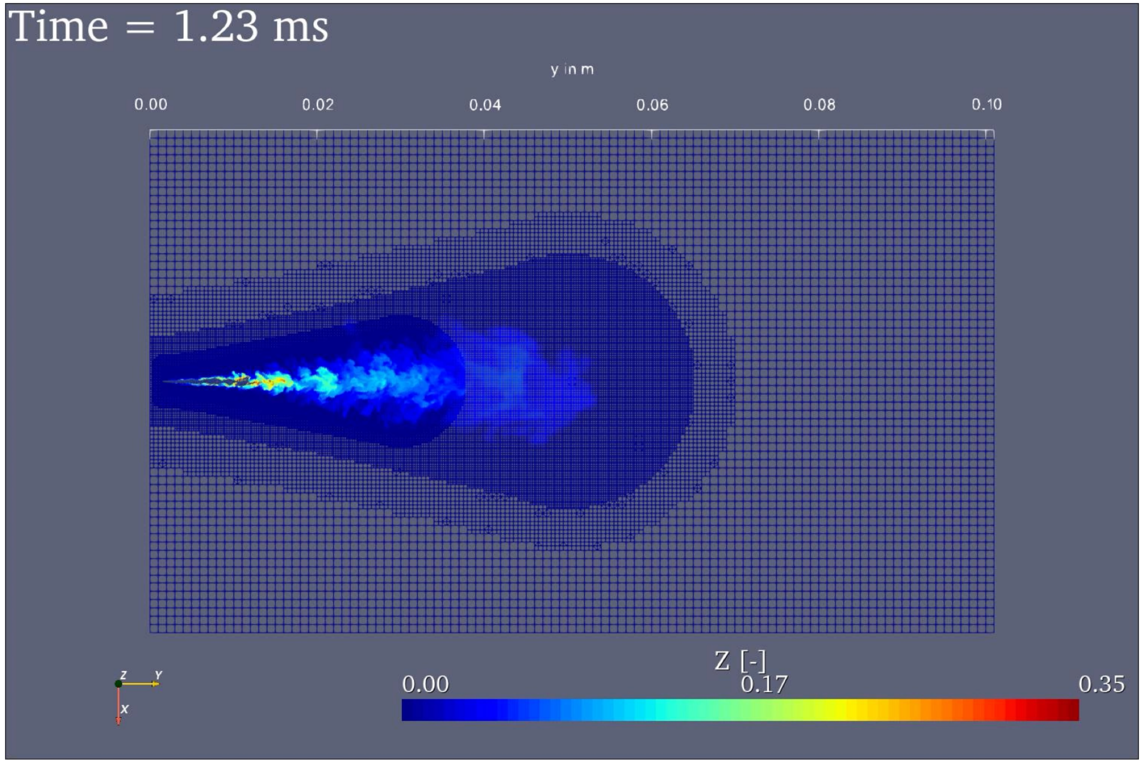
Software / Approach
OpenFOAM v2012
Euler / Lagrange

Discretization
X,Y,Z: 60x110x60 mm
Δx = 64.5 µm at nozzle [1]
4 refinement levels
#Cells: ~12.8 Mill.
Δt = 50 ns (Co < 0.5)
2nd order in space and time

Turbulence
σ-model [2], c_σ = 2.0



Spray
Injection + Breakup: Blob-Injection + KH-RT [1]
Forces: Sphere drag
Heat Transfer: Droplet Energy Balance
Evaporation: Frössling correlation [4]
Correlation: Ranz-Marshall correlation [5] for Sh and Nu Numbers
#Parcels: 7.5e5 / ms (avg. mass: 3.4e-12 kg/parcel)

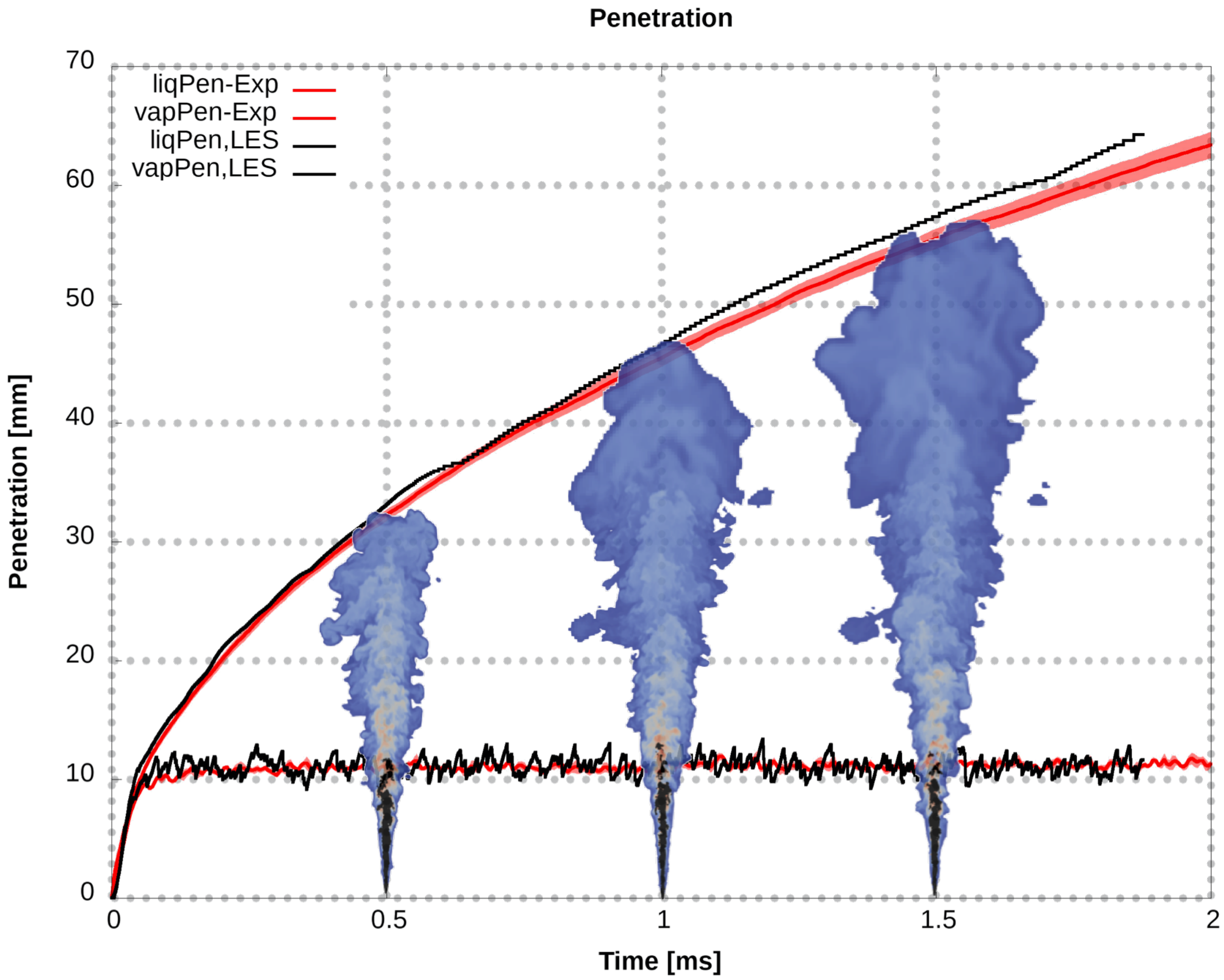
[1] Wehrfritz, Phd Thesis: "Large Eddy Simulation of Fuel Spray Combustion", 2016 | [2] F. Nicoud and F. Ducros, *Flow, Turbul. Combust.*, vol. 62, no. 3, pp. 183–200, Sep. 1999. | [3] R. D. Reitz, "Modeling atomization processes in high-pressure vaporizing sprays," *At. Spray Technol.*, vol. 3, pp. 309–337, 1987. | [4] N. Frössling, "Über die Verdunstung fallender Tropfen," *Gerlands Beiträge zur Geophys.*, vol. 52, pp. 170–216, 1938. | [5] W. Ranz and W. R. Marshall, "Evaporation from drops I–II," *Chem. Eng. Prog.*, vol. 48, pp. 141–146, 1952.

Penetration non-reactive

- Evaluation:
  - Vapor penetration:
    - Distance to nozzle, where fuel mass fraction fall below 0.1 %
  - Liquid penetration:
    - Distance to nozzle, where 99 % of liquid mass is incorporated

- Penetration lengths met well

- Small overestimation of vapor penetration due to grid coarsening

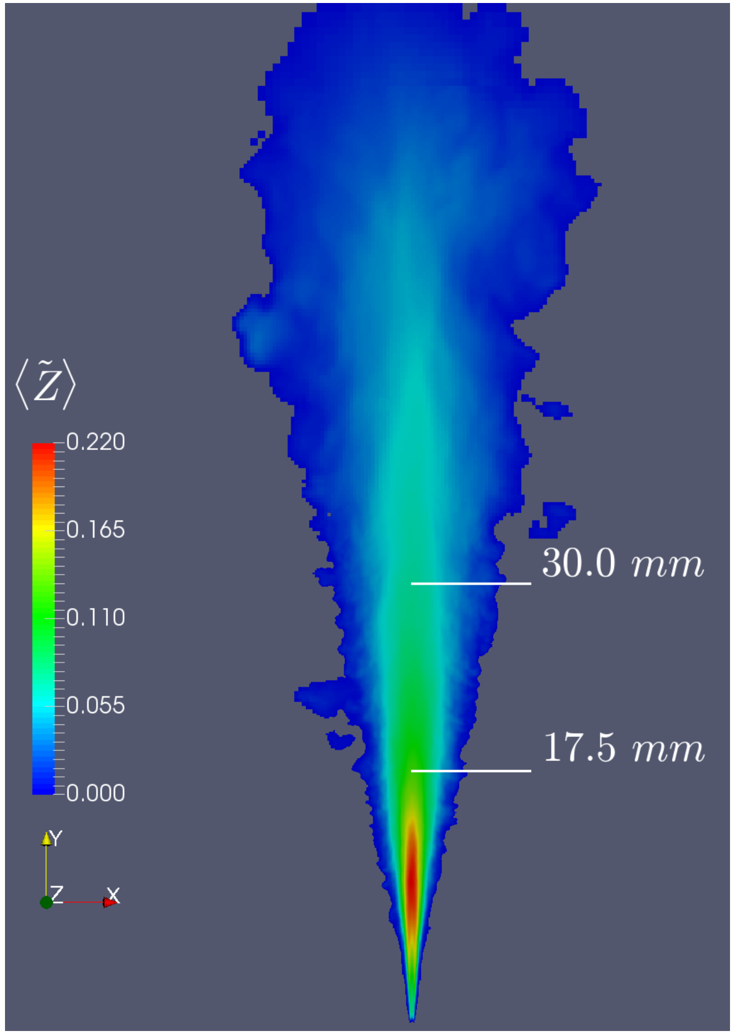


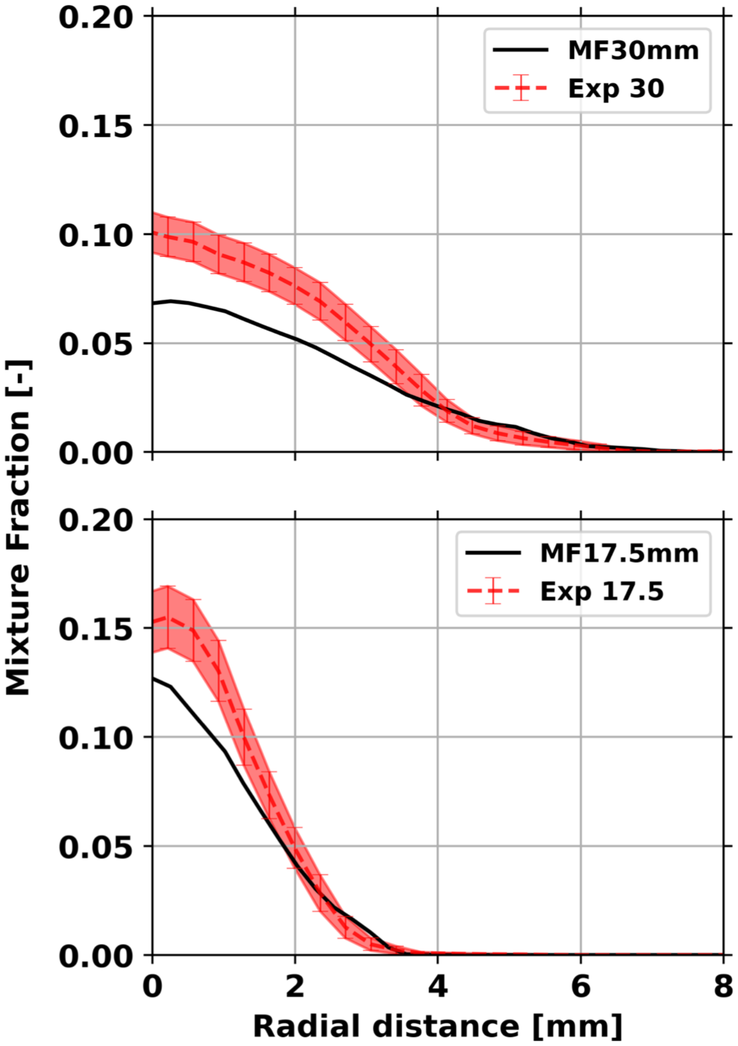
Mixture fraction distribution non-reactive

- Evaluation:
  - Time average 1.5 ... 2.5 ms
  - Circumferential average

- Simulation shows underprediction of Mixture fraction near centerline

- Results are within the range of other works in literature [1,2] using similar simulation strategy

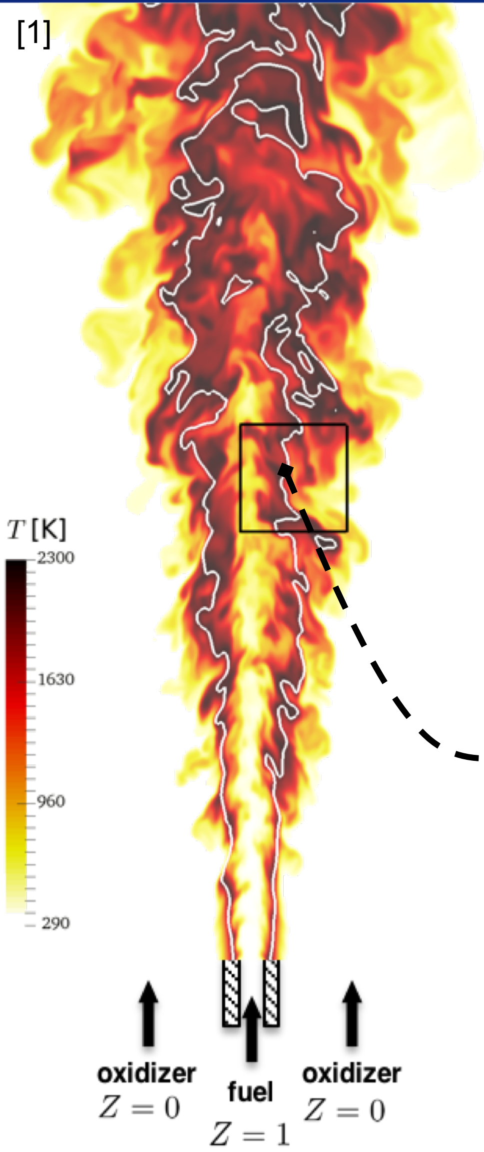




[1] A. Wehrfritz, O. Kaario, V. Vuorinen, and B. Somers, *Combust. Flame*, vol. 167, pp. 113–131, 2016.
[2] M. Davidovic, T. Falkenstein, M. Bode, L. Cai, S. Kang, J. Hinrichs, and H. Pitsch, *Oil Gas Sci. Technol.*, vol. 72, no. 5, 2017.

Flamelet Concept - Phemomenology

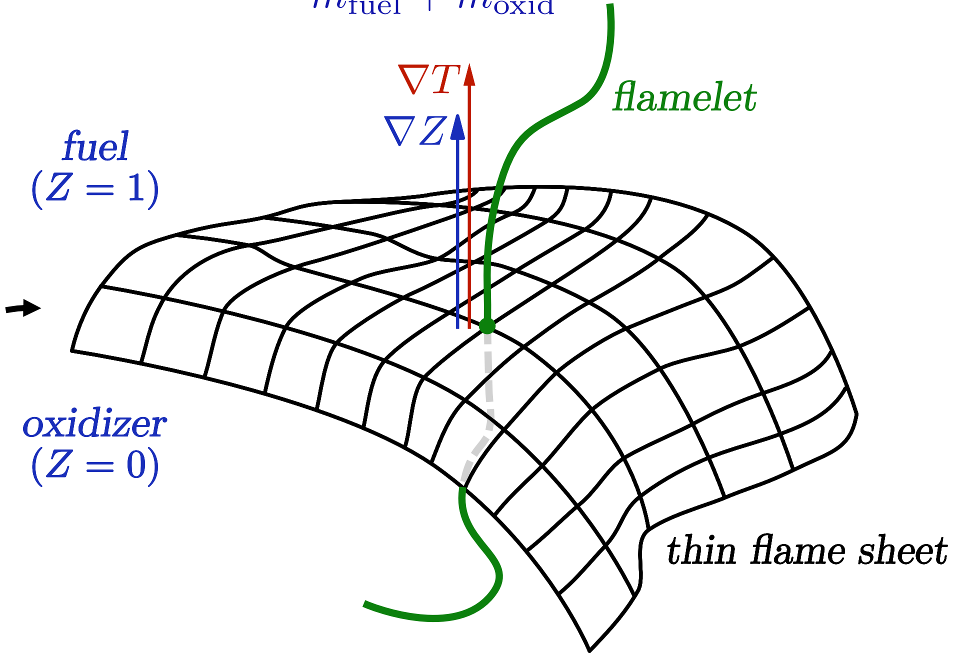
[1]



Theoretical basis of the flamelet concept:

- combustion chemistry is fast
- **thin flame sheet** assumption
- **gradient alignment** at flame sheet
- important physics along **flame-normal** direction

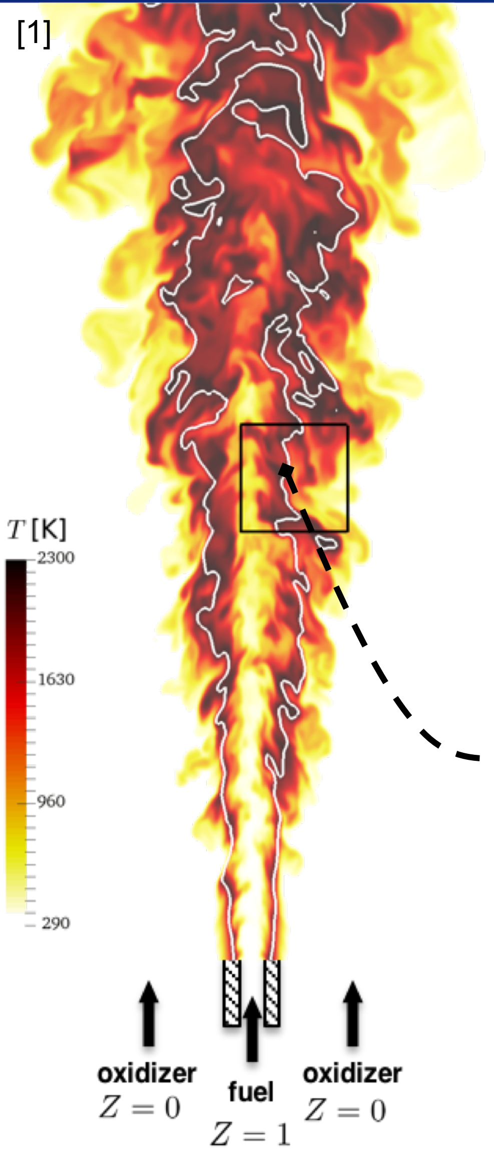
Definition: $Z = \dfrac{m_{\mathrm{fuel}}}{m_{\mathrm{fuel}} + m_{\mathrm{oxid}}}$



Turbulent flames ≈ Ensembles of 1D flamelets

[1] Popp, STFS, 2015

Flamelet Concept - Phemomenology



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- important physics along **flame-normal** direction

Definition: $Z = \dfrac{m_{\text{fuel}}}{m_{\text{fuel}} + m_{\text{oxid}}}$

$$\rho \frac{\partial Y_i}{\partial \tau} = \frac{\rho\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i$$

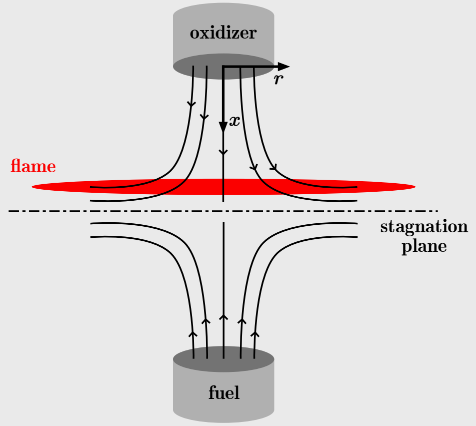
$$\rho \frac{\partial T}{\partial \tau} = \frac{\rho\chi}{2}\frac{\partial^2 T}{\partial Z^2} + \dot{\omega}_T$$

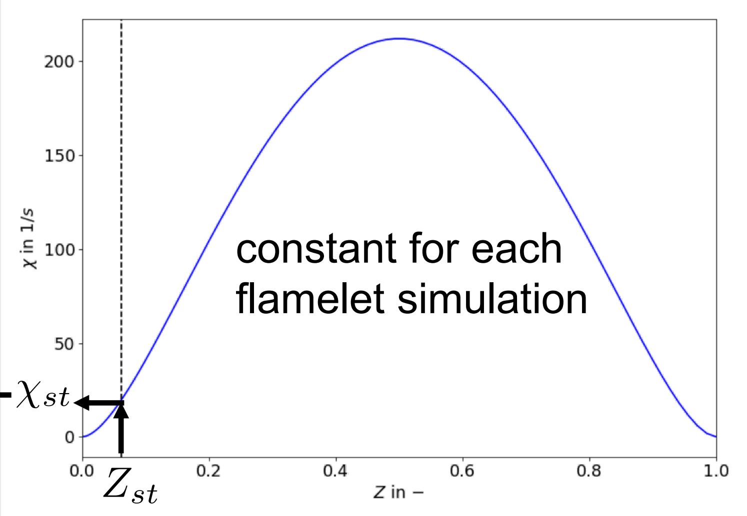
$$\chi = 2D|\nabla Z|^2$$

$$\chi(Z) = \chi_{\text{st}} \exp(2[\text{erfc}^{-1}(2Z_{\text{st}})]^2 - 2[\text{erfc}^{-1}(2Z)]^2)$$

free parameter

Canonical configuration

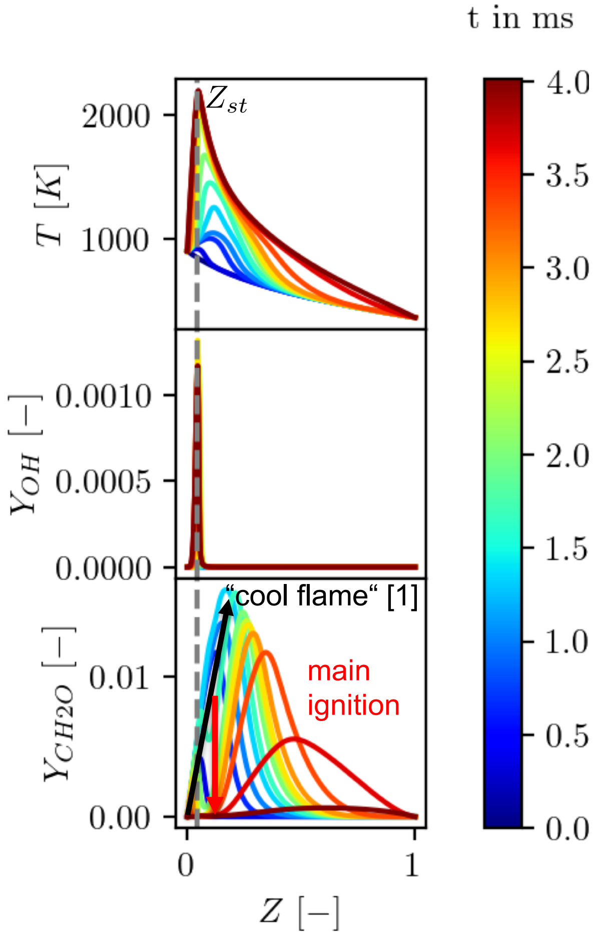




[1] Popp, STFS, 2015

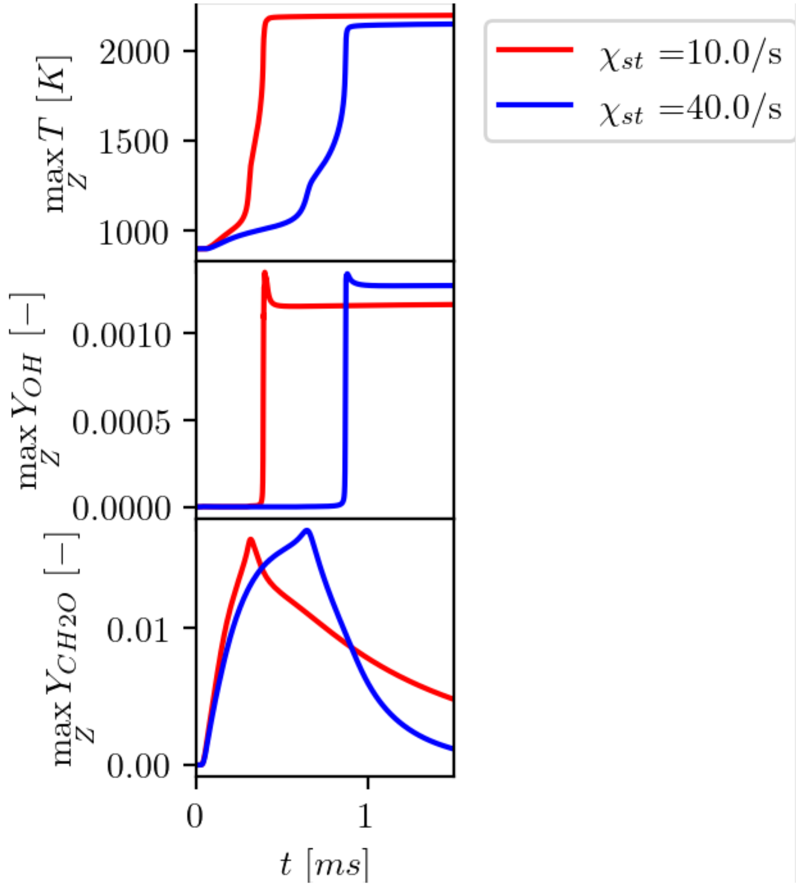
Ignition of single flamelets for long chained hydrocarbon fuels

- Flamelet with χ_{st} = 10 1/s:



- Qualitative behavior similar for each flamelet at const. χ_{st}

- Maximum of variables over time:

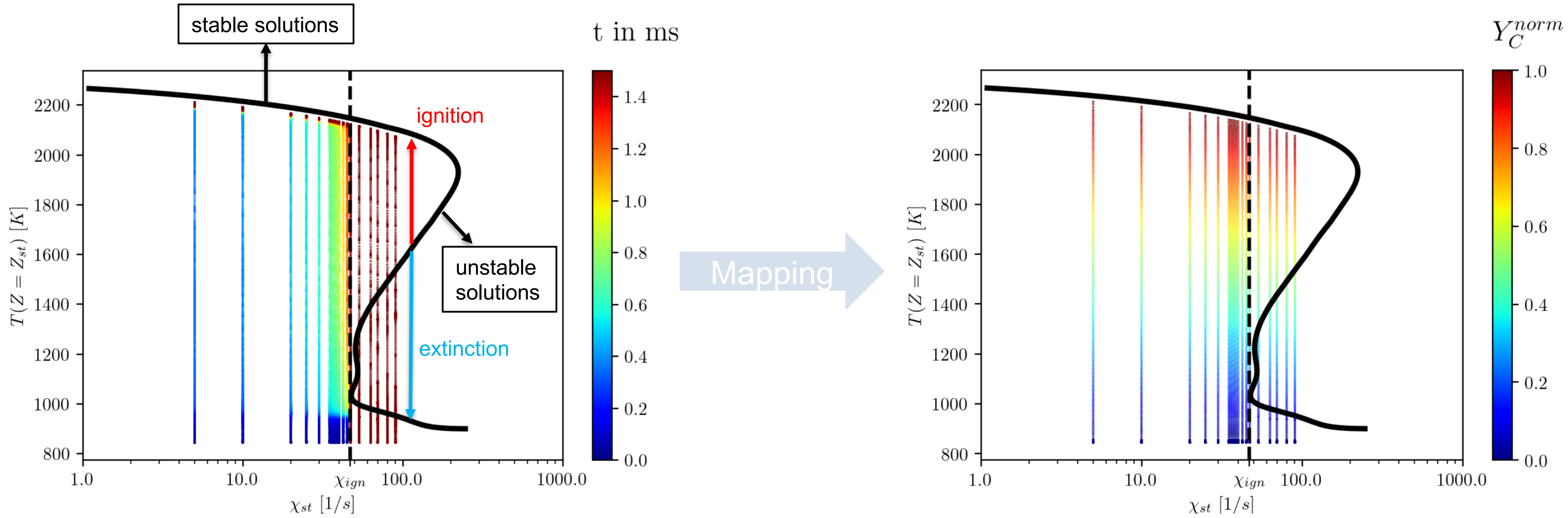


- Time-scales and maximum temperature depending on χ_{st}
- **Variation of χ_{st} has to be taken into account**

[1] R. N. Dahms, G. A. Paczko, S. A. Skeen, and L. M. Pickett, "Understanding the ignition mechanism of high-pressure spray flames," *Proc. Combust. Inst.*, vol. 36, no. 2, pp. 2615–2623, 2017.

Steady flamelet Solutions, S-shaped curve, and UFPV model

- Unsteady flamelet progress variable (UFPV) approach [1]:



Reduced-order Model

$$\psi = \psi\left(Z, \chi_{st}, Y_C^{norm}\right)$$

[1] H. Pitsch and M. Ihme, "An unsteady/flamelet progress variable method for les of nonpremixed turbulent combustion," *43rd AIAA Aerosp. Sci. Meet. Exhib. - Meet. Pap.*, pp. 2593–2606, 2005.

Coupling to CFD code for spray flame simulation

CFD Code

$\widetilde{T}\left(x_i, t\right)$

$\widetilde{h}(x_i; t)$

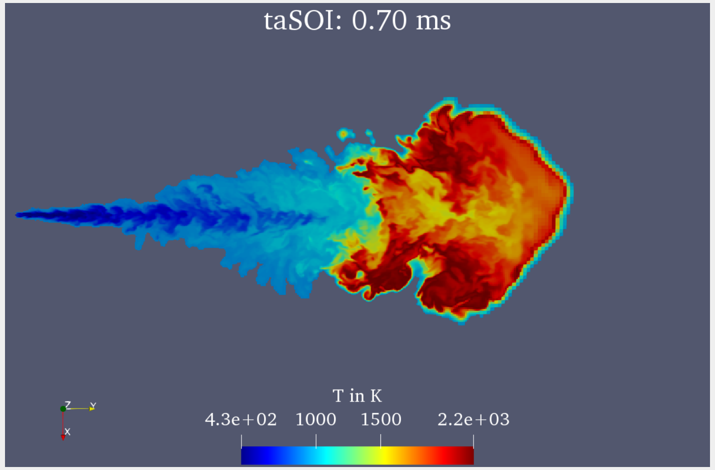
$$\widetilde{h}\left(x_i, t\right) = \sum_{k=1}^{n_s} h_k(T)\widetilde{Y}_k$$

$\widetilde{\dot{\omega}}_{Y_C}\left(x_i, t\right)$

$\widetilde{Y}_k(x_i, t)$

$\widetilde{Z}, \widetilde{Z''^2}, \widetilde{\chi}_{st}, \widetilde{Y}_C$

Database



CFD coupling

1D Flamelets

tabulation
+ β-pdf integration

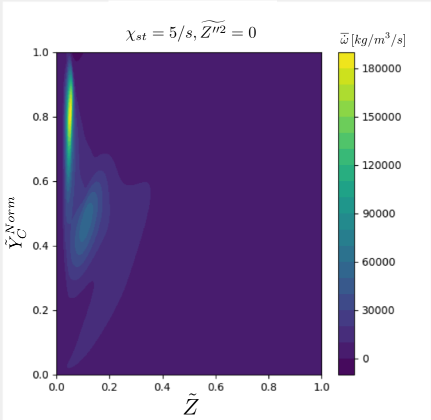
Database

Thermochemical State

$$\psi = [T, Y_1, Y_2, \ldots, Y_{n_s}]$$

Reduced-order Model

$$\widetilde{\psi} = \widetilde{\psi}\left(\widetilde{Z}, \widetilde{Z''^2}, \widetilde{\chi}_{st}, \widetilde{Y}_C^{norm}\right)$$

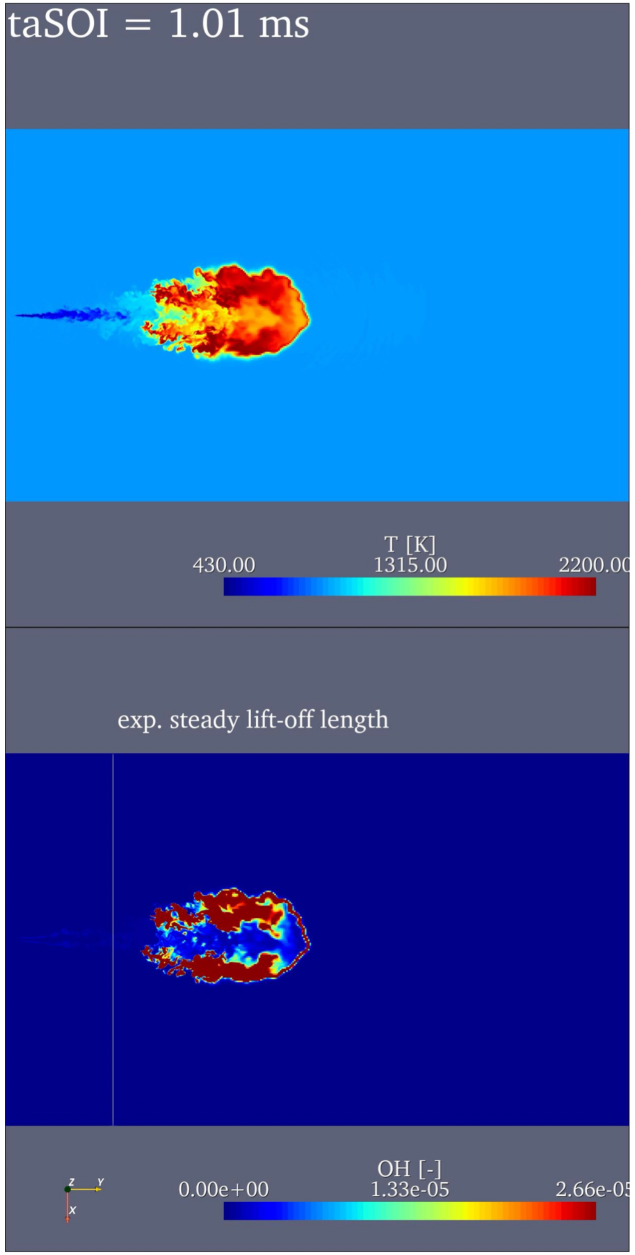


Database generation

Validation ignition

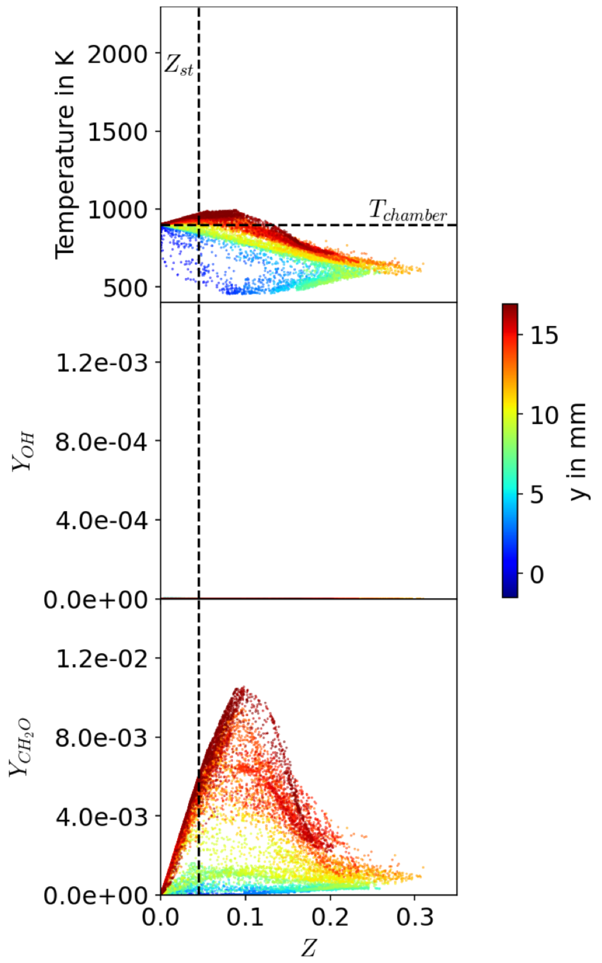
- Qualitative ignition behavior reasonable predicted
- Quantitative comparison:
  - Ignition delay:
    - First time, at which 2% of max Y_{OH} observed
  - Flame lift-off:
    - Smallest distance to nozzle, at which 2% of max Y_{OH} observed

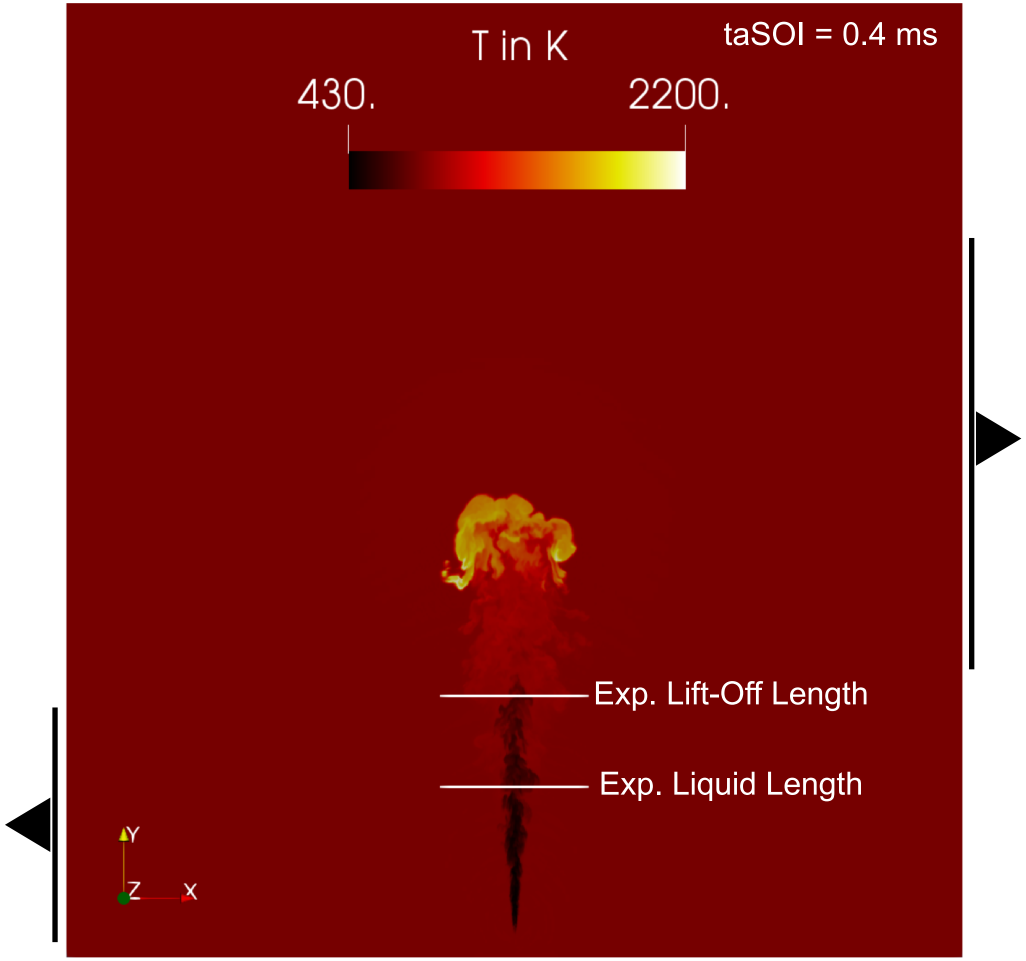
Quantity	Exp.	Sim.	Deviation
Ignition delay time	0.40 ms	0.366 ms	8 %
Steady lift-off Length	16.10 mm	16.97 mm	5 %

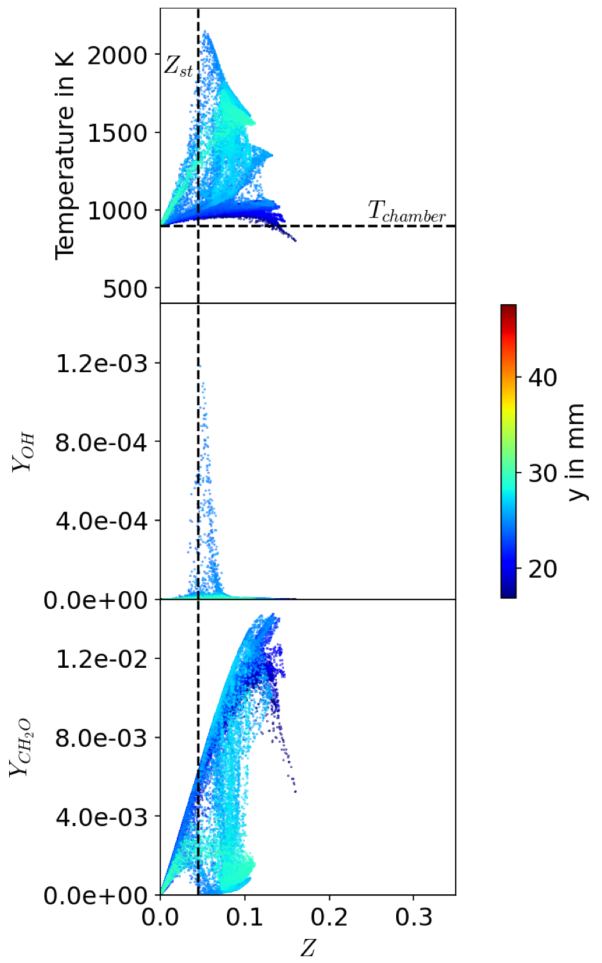


Flame structure analysis

- Flame structure can be distinguished by distance from nozzle (~residence time)







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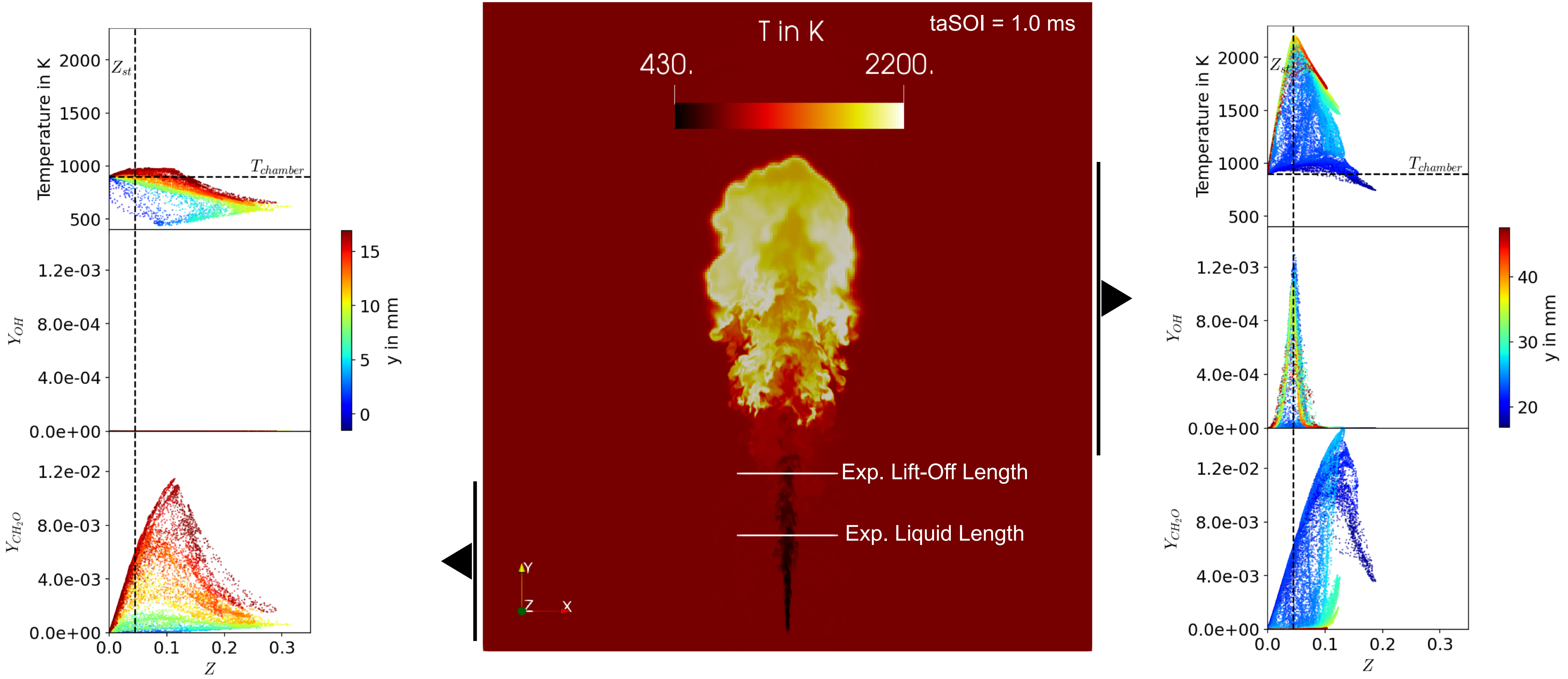
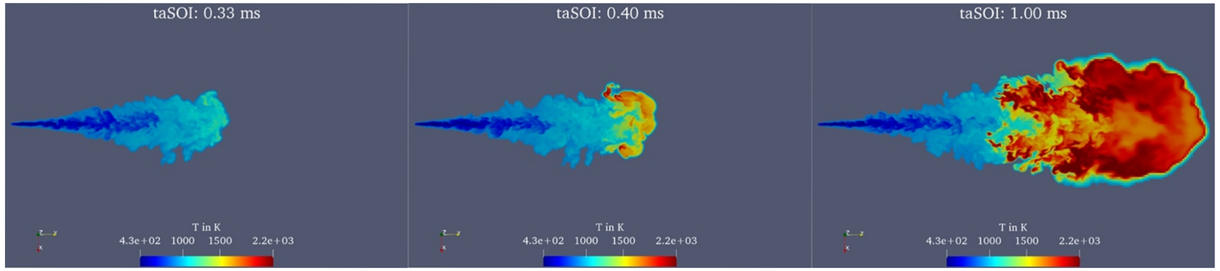
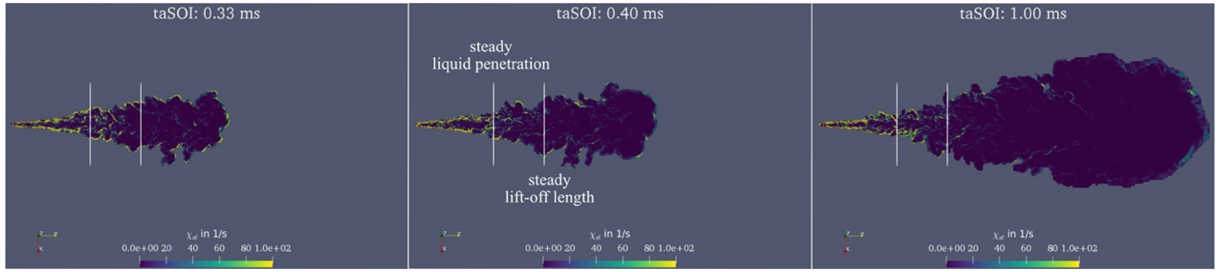
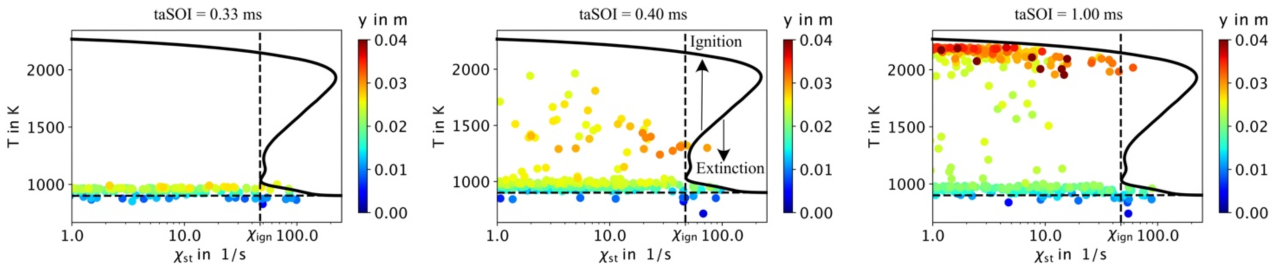


- Influence of scalar dissipation rate on ignition process in spray flame





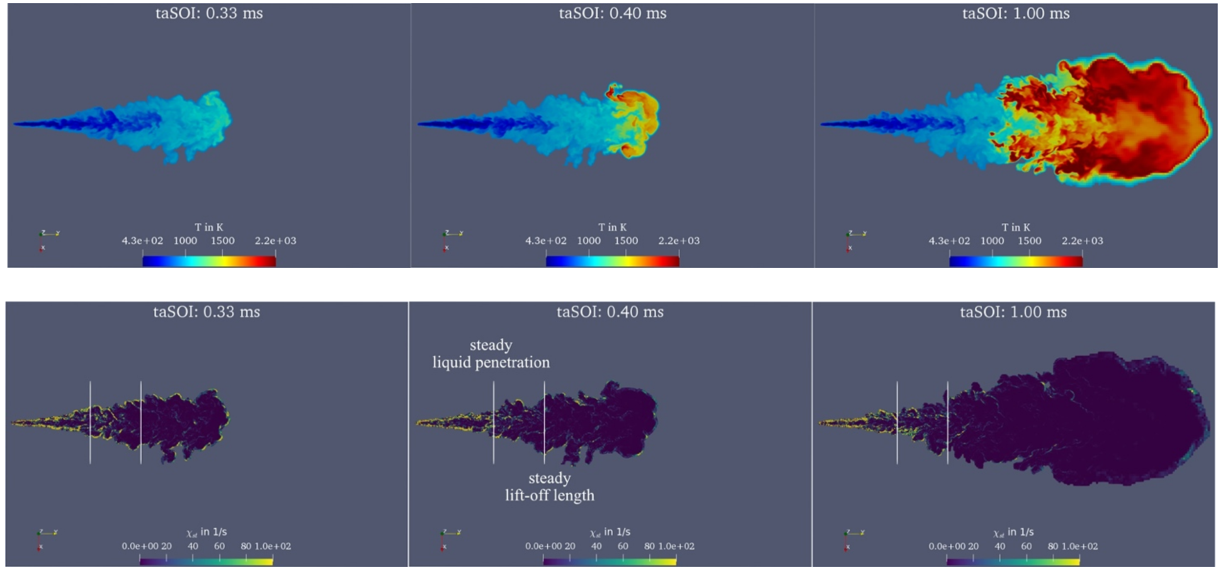


- Spatial χ_{st} distribution:
  - High values of χ_{st} mainly near the nozzle
  - Strong decrease between liquid penetration and lift-off length
  - Afterwards, high values near spray border

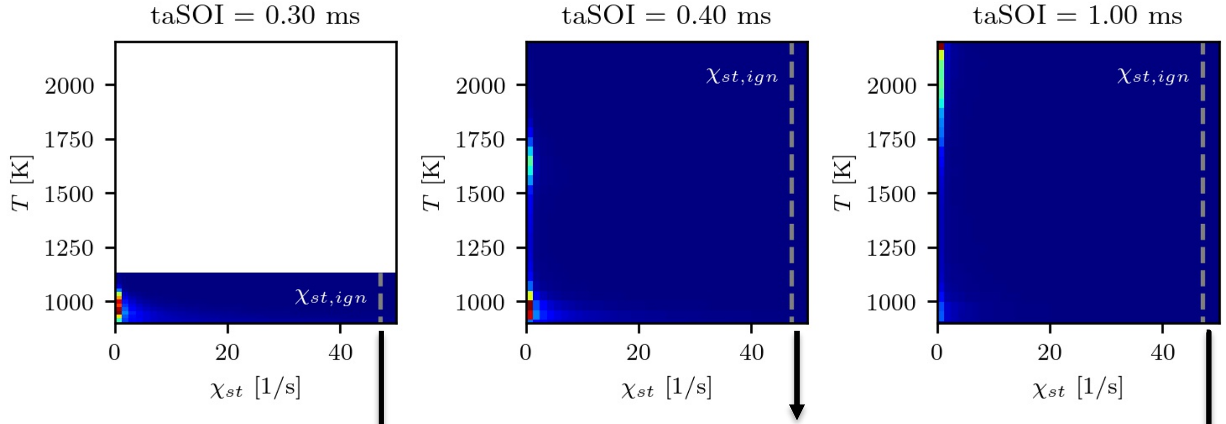
- Influence on ignition behavior:
  - For early times: No ignition
  - At ignition delay time:
    - Ignition over wide range of χ_{st}
    - Entering unstable branch with extinction possible
  - Later times: Fully ignited states over wide range of χ_{st} influencing steady temperature

Analysis flamelet parameter

- Influence of scalar dissipation rate on ignition process spray flame



$\boxed{P(T,\chi_{st})}$

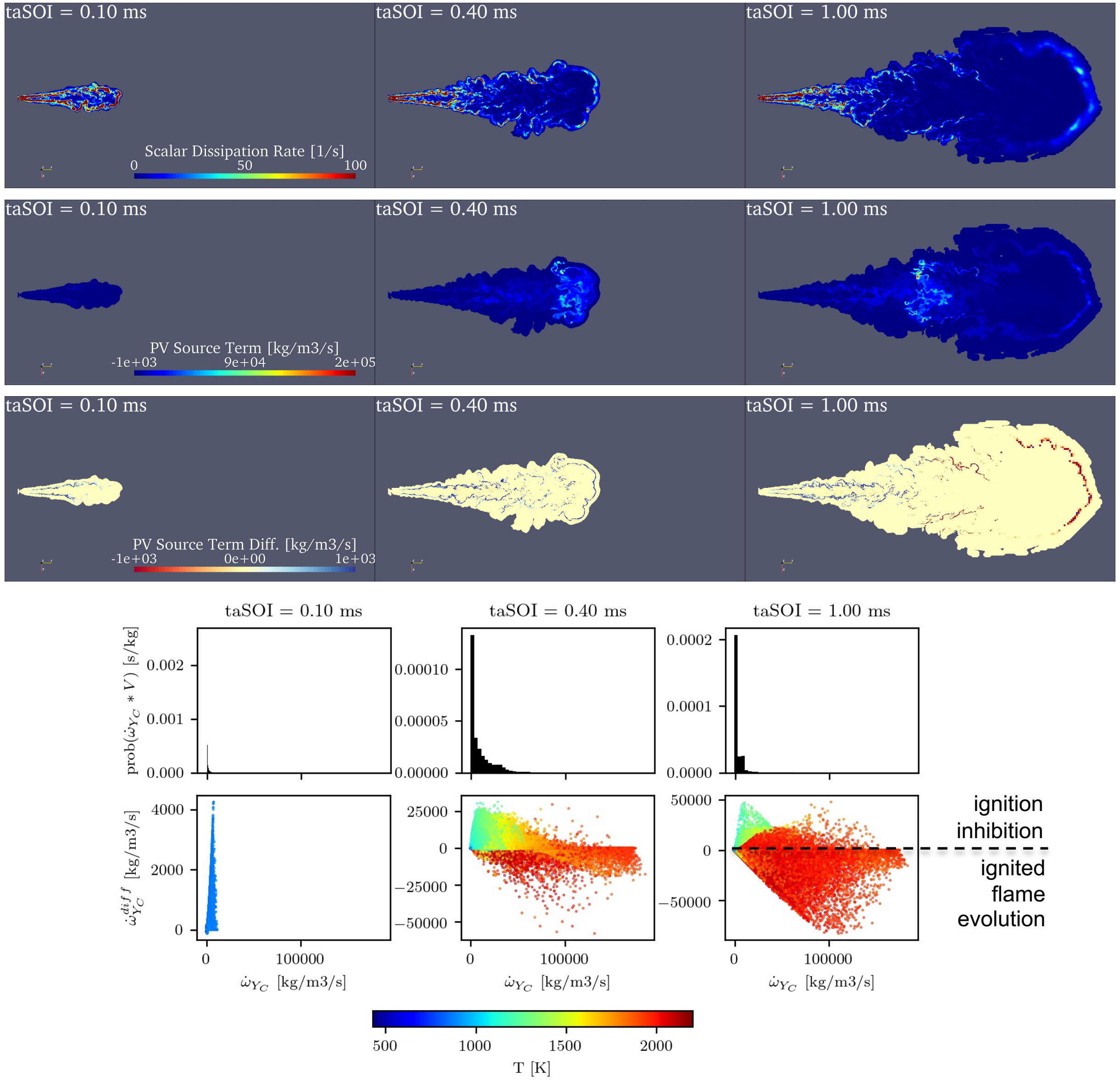


small probability

- Spatial χ_{st} distribution:
  - High values of χ_{st} mainly near the nozzle
  - Strong decrease between liquid penetration and lift-off length
  - Afterwards, high values near spray border

- Influence on ignition behavior:
  - For early times: No ignition
  - At ignition delay time:
    - Ignition over wide range of χ_{st}
    - Entering unstable branch with extinction possible (**with small probability**)
  - Latter times: Fully ignited states over wide range of χ_{st} influencing steady temperature

- Influence of χ_{st} on reaction progress:



- Comparison of progress variable source term based on $\chi_{st} = const. = \ 5/s$ with CFD result:

$$\dot{\omega}_{Y_C}^{diff} = \boxed{\dot{\omega}_{Y_C}}(\widetilde{Z}, \widetilde{Y}_C^{norm}, \widetilde{Z''^2}^{norm}, \boxed{\widetilde{\chi}_{st} = 5/s}) - \dot{\omega}_{Y_C}^{CFD}$$

- Source term difference visible in all jet regions
- At early times after injection:
  - $\dot{\omega}_{Y_C}^{diff} > 0$: ignition inhibition due to variable χ_{st}
- For high temperature downstream of high source term region
  - $\dot{\omega}_{Y_C}^{diff} < 0$: Enhancement of ignited flame evolution due to variable χ_{st}
  - Probability low

Summary and Conclusion

- Coupling of the complete UFPV approach to spray LES described
- UFPV approach able to capture ignition characteristics properly in ECN Spray A
- Influence of scalar dissipation rate:
  - Ignition takes place over wide range of χ_{st}
  - Largest values of scalar dissipation rate found at jet border
  - Points between stable and unstable branch in S-curve present
    - They can lead to further ignition but also to extinction
    - However, probability of entering unstable branch small for this operating condition
  - Compared to single (small) χ_{st} value used for table look-up, complete UFPV approach shows increased ignition inhibition near nozzle
  - When using only one χ_{st} for ignition, care must be chosen to chose an appropriate value

Thank you for your attention

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