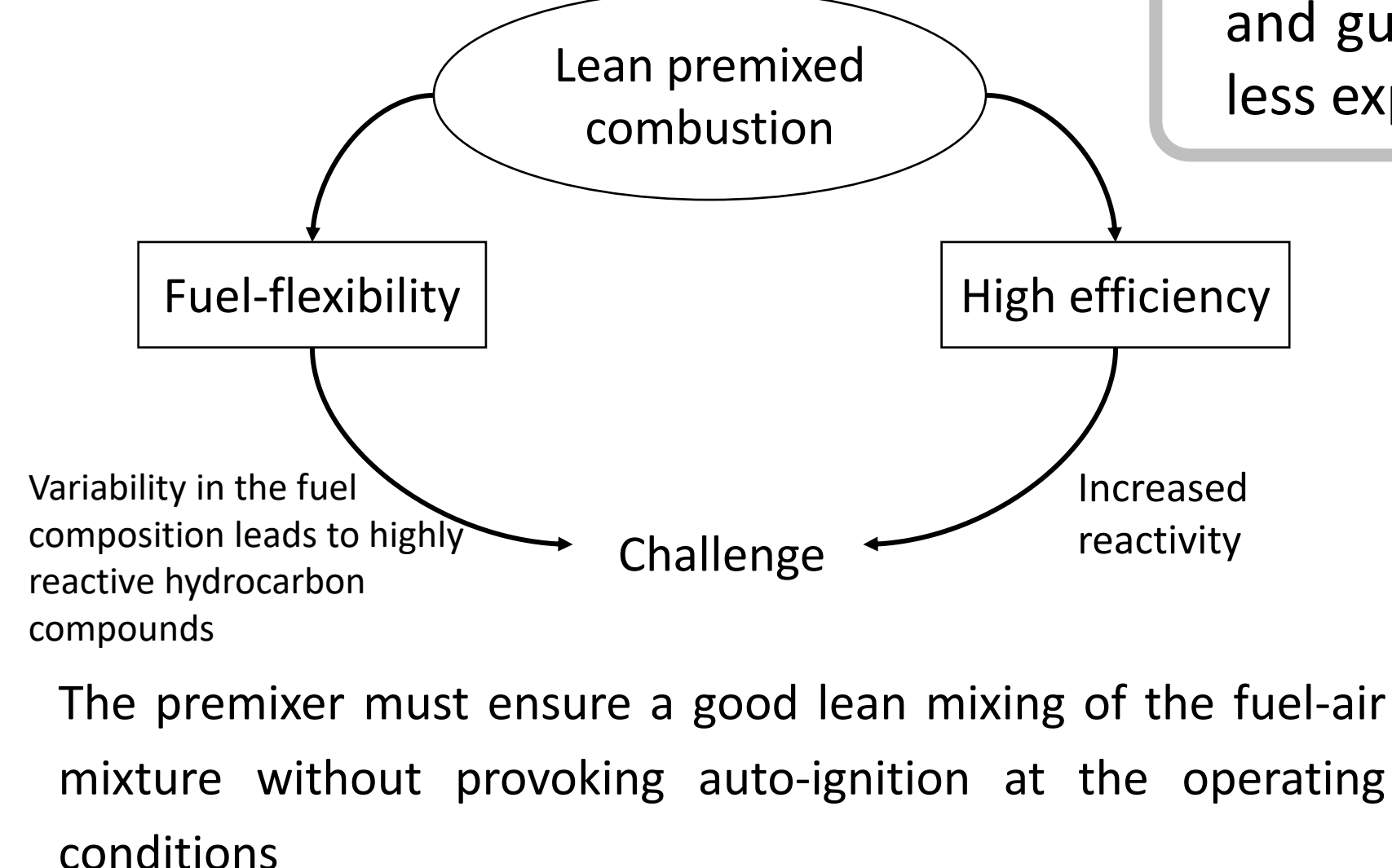


Context

Reducing pollutant emissions (CO, CO₂, NO_x, ...)

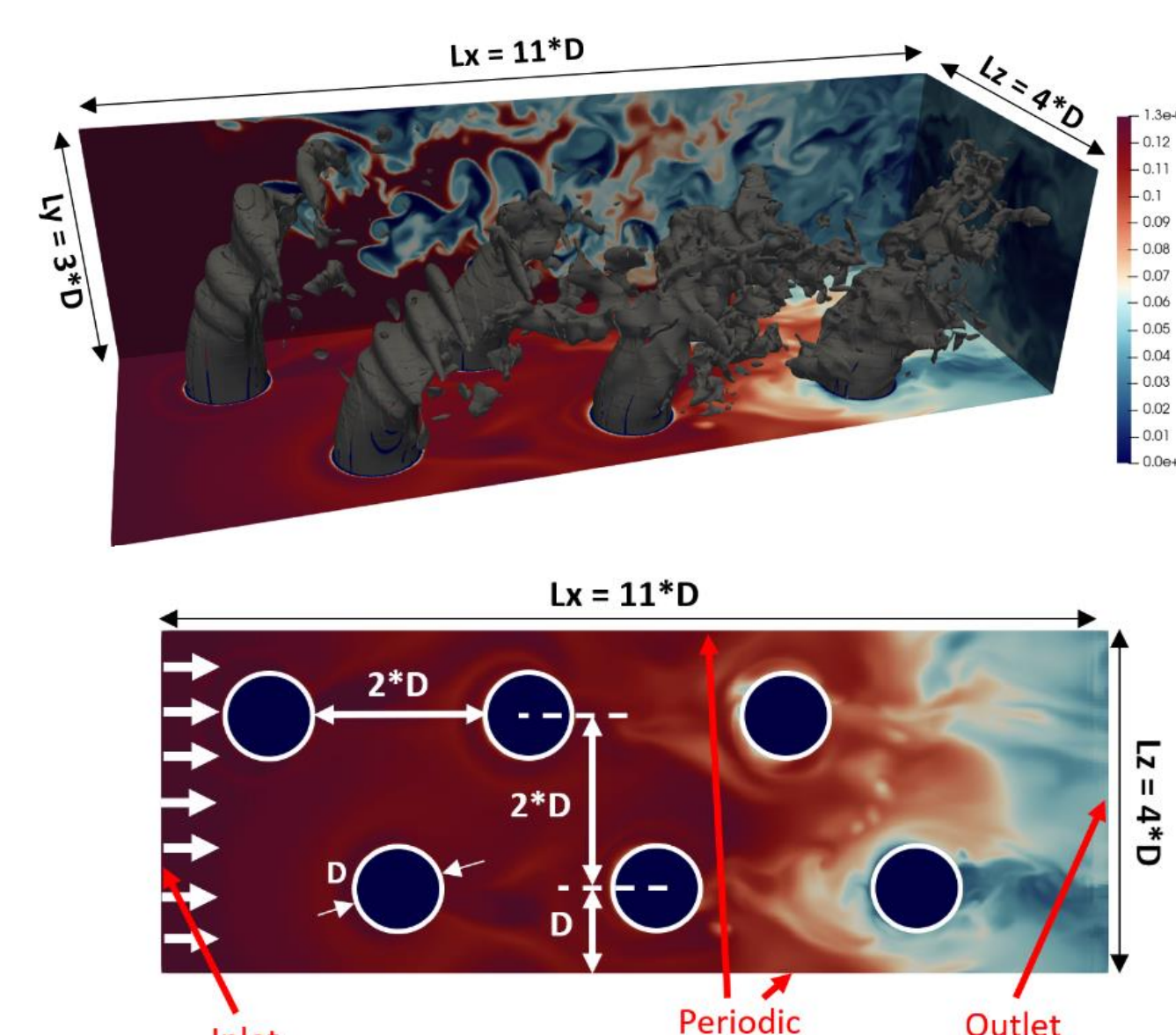
With the increasing need for fuel-flexibility, an understanding of auto-ignition inside gas turbine premixers is crucial. Direct numerical simulation (DNS) is a great tool to reveal the fine grain details of physics inside the premixer and guide the choice of the models to use for less expensive simulations.



Objectives

- Observe the mechanisms leading to auto-ignition
- Identify the flame formation and stabilization process
- Analyze the combustion modes and the flame propagation

Methodology



Top : 3D view of the premixer configuration with mixture fraction background contours
Bottom : Top view of the bottom face

Premixer characteristics

- Simplified and downscaled configuration of the premixer from Jella et al. [2]
- Multiple air jets in rich fuel crossflow
- Intense fuel-air mixing
- Autoignitive fuel-air mixture
- Flame-turbulence interaction

Boundary conditions

- Bottom wall : no slip adiabatic wall and jet inlets
- Top wall : slip adiabatic wall

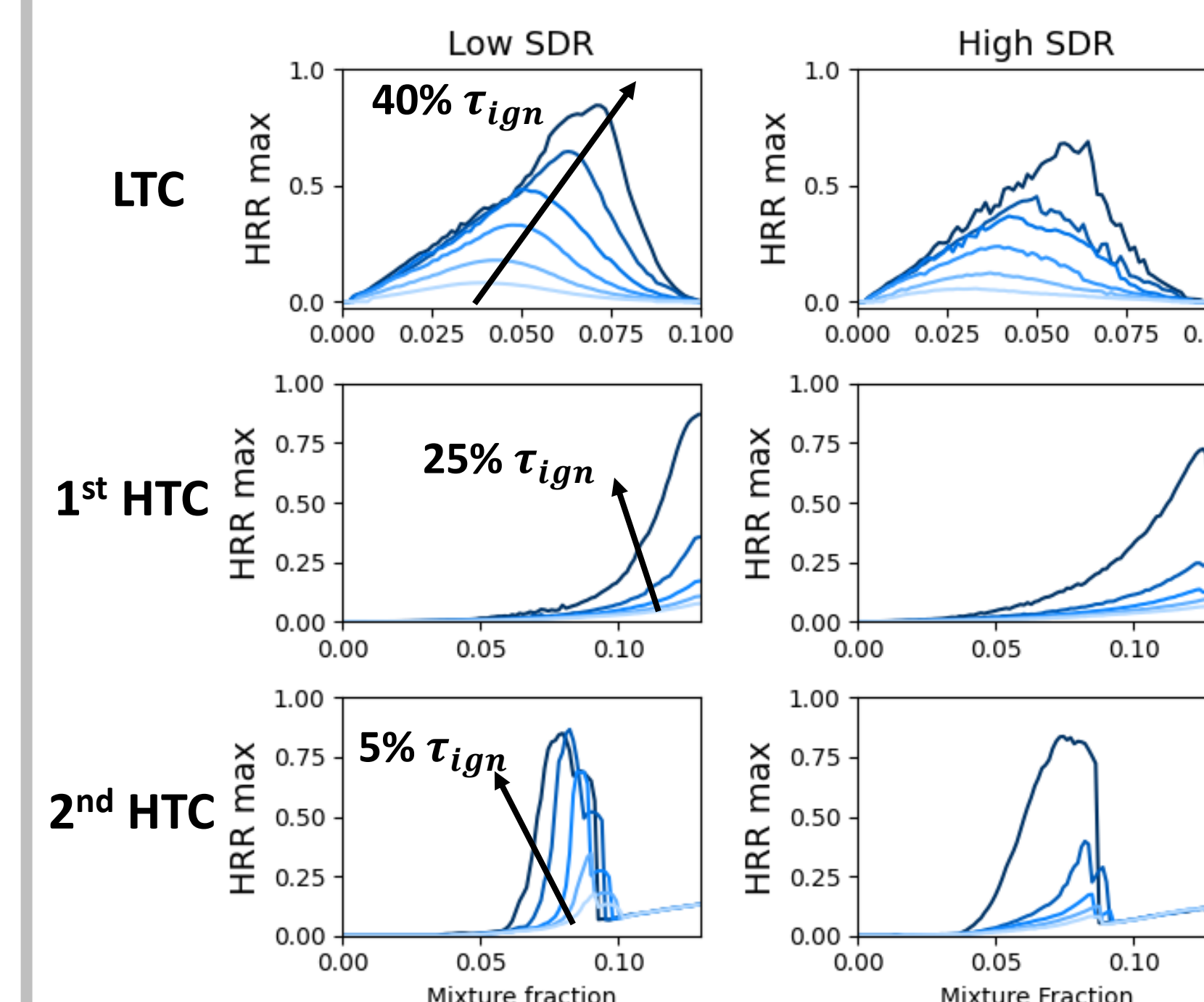
Numerical strategy

- Software PeleLM [3] for DNS of low-Mach turbulent combustion
- Adaptive mesh refinement (AMR) based on heat release rate, species mass fraction, vorticity magnitude and wall distance
- 4000 cores run on the Niagara cluster for several days
- Finite rate chemistry is used with a 38 species / 238 reactions mechanism [2]

LTC	HTC
Base level + 3 AMR levels	Base level + 3 AMR levels
100 million grid cells	150 million grid cells
1 million CPU-h	2 million CPU-h
$\Delta x = D/250$	$\Delta x = D/200$

Results (continued)

Auto-ignition



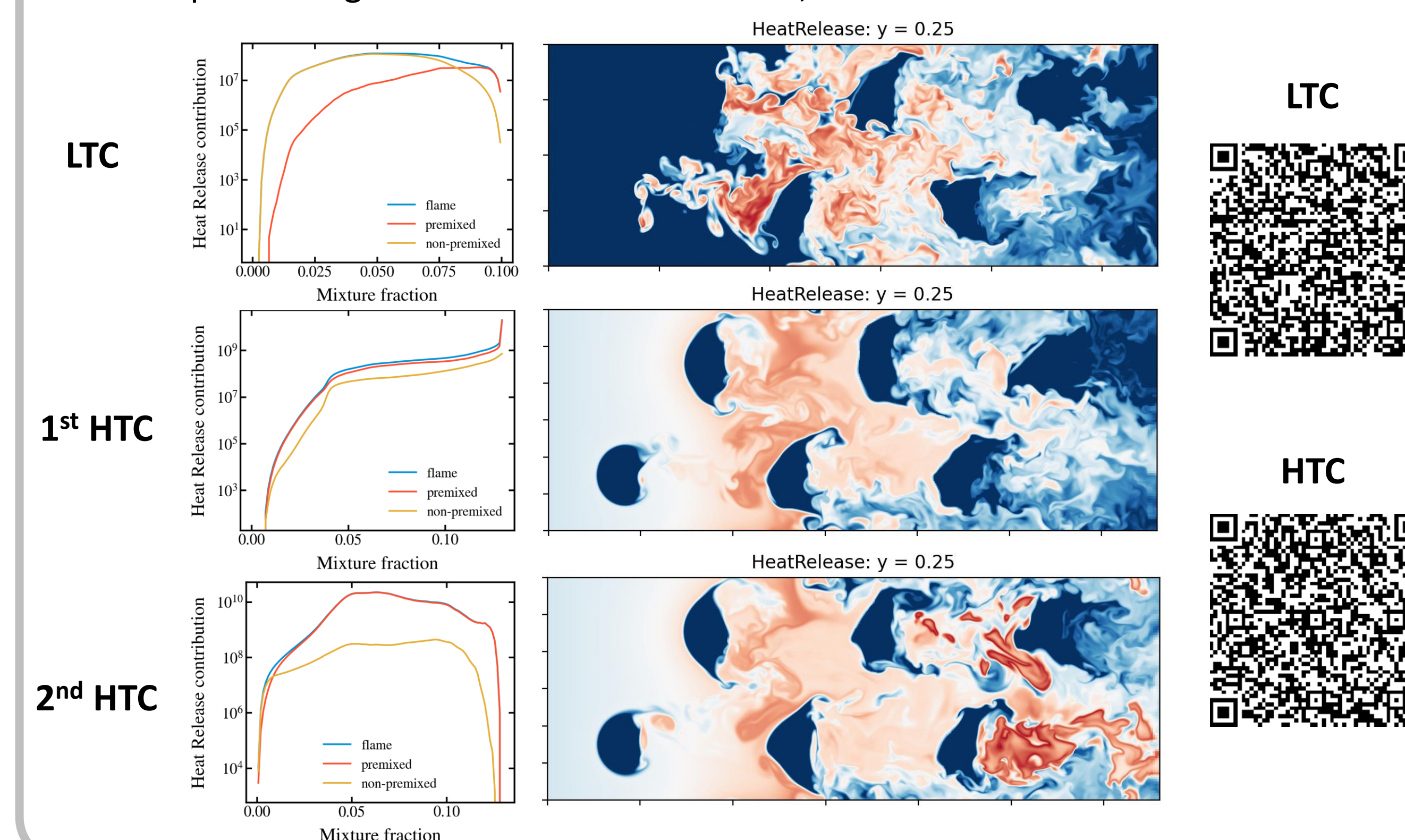
- LTC : ignition initiates in lean mixtures and propagates slowly to richer mixtures
- HTC : ignition initiates in rich mixtures and propagates to leaner mixtures in both substages.
- The second substage forms ignition kernels that expand very quickly and fuse
- In all cases, the impact of SDR is very moderate compared to the results in the literature [1]

Flame stabilization

The flame index [4] **FI** is used to determine locally if a mixture is burning in premixed or non-premixed mode:

$$FI = \frac{\nabla Y_{fuel} \cdot \nabla Y_{O_2}}{|\nabla Y_{fuel}| \cdot |\nabla Y_{O_2}|}$$

- For LTC, heat release contribution is dominated by non-premixed flames in lean mixtures, and premixed in rich mixtures
- For both HTC stages, heat release contribution is dominated by premixed flames
- Strong flames are stabilized in the premixer and the second stage HTC flame is propagating upstream
- Independent ignition kernels are observed, even when the flame is formed



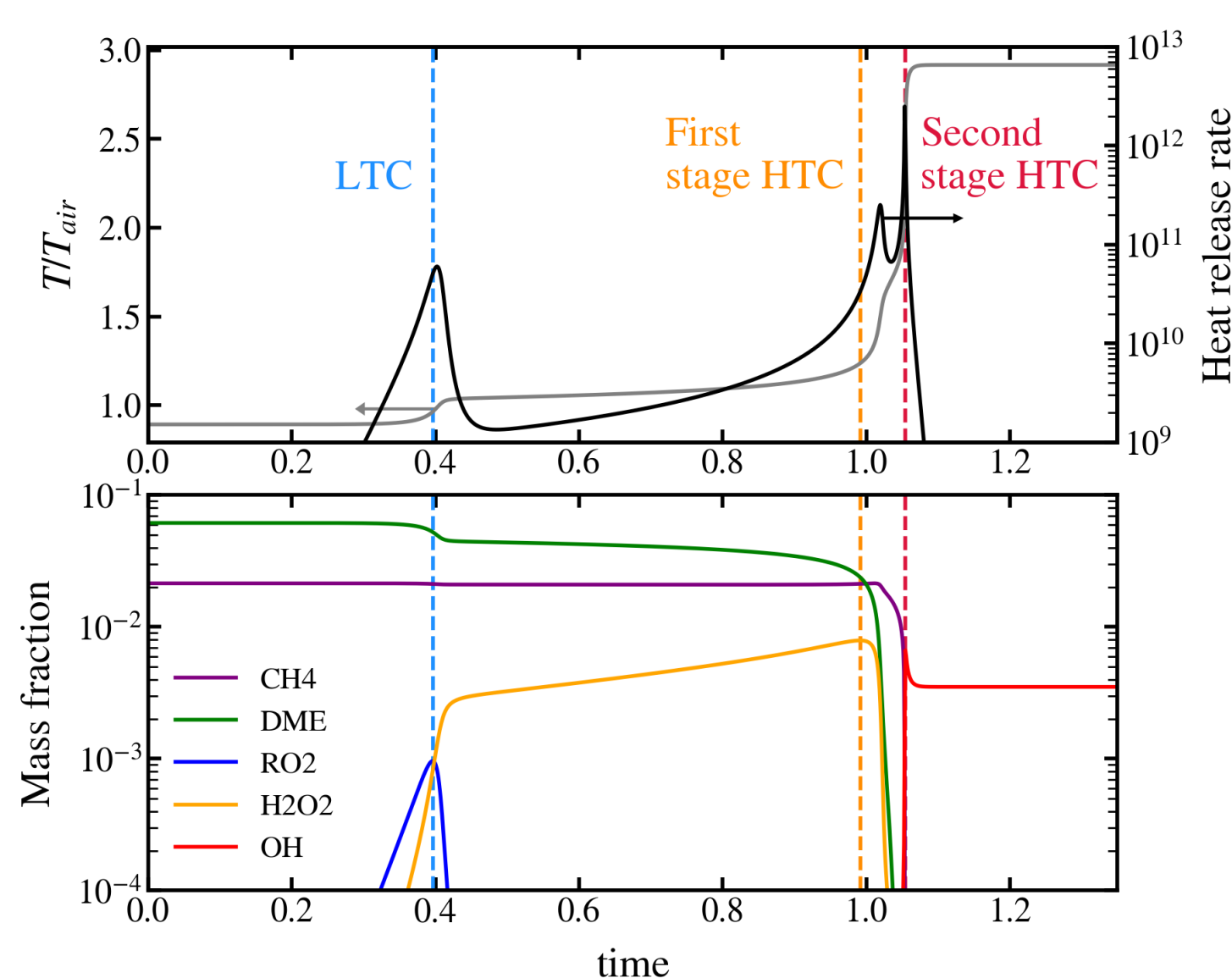
Chemistry of Auto-ignition

Operating conditions

- High pressure
- High air temperature
- 50% DME (CH₃OCH₃)/50% CH₄ fuel blend

Fuel characteristics

- Representative of highly reactive components of natural gas
- Two-stage ignition behaviour :
 - Low Temperature chemistry (LTC) ignition
 - High Temperature chemistry (HTC) ignition divided in two substages



Homogeneous reactor evolution of a stoichiometric mixture at the operating conditions

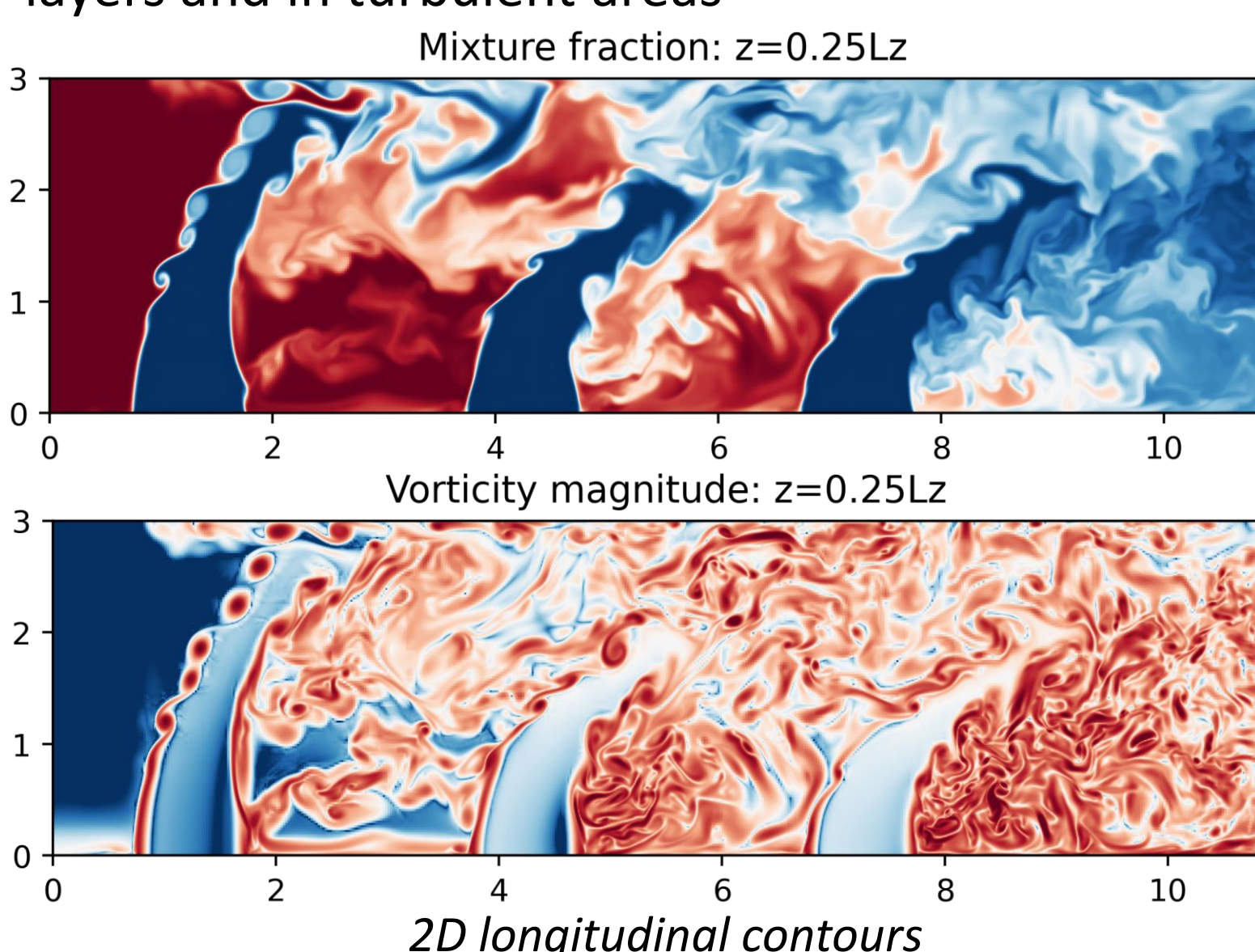
Two simulations

- Two different simulations were performed to independently study LTC and HTC ignition and the resulting flames
- The mixtures in both simulations have different ignition and flame properties
- Non-dimensional turbulent combustion numbers were kept in the same order of magnitude

Results

Visualization of the flow

- The flow is accelerated both by the jets and the combustion
- Turbulence develops rapidly, and is highest behind the jet base and at the end of the domain
- Mixing happens almost everywhere, especially in the jet-crossflow shear layers and in turbulent areas



Animation of the flow

Important literature results

- Important parameters for auto-ignition are the mixture fraction Z (related to the fuel/air ratio) and the scalar dissipation rate (SDR) χ (rate of mixing)
- Auto-ignition happens in homogeneous turbulence first at a most-reactive mixture fraction Z_{MR} and low SDR [1]

$$\chi = 2D(\nabla Z)^2$$

D : mixture diffusivity

$$\tau_{ign} = \min(t_{ign}(Z))$$

$$Z_{MR} = \operatorname{argmin}(t_{ign}(Z))$$

References

[1] E. Mastorakos, "Ignition of turbulent non-premixed flames," Progress in Energy and Combustion Science, vol. 35, pp. 57–97, feb 2009.
[2] Jella et al., "Analysis of Auto-ignition Chemistry in Aeroderivative Premixers at Engine Conditions," Journal of Engineering for Gas Turbines and Power, vol. 143, nov 2021.

[3] M. Day et al., "Pele: An Exascale-Ready Suite of Combustion Codes", 18th Numerical Combustion Conference, San Diego, CA, May 2022.
[4] Yamashita et al., "A numerical study on flame stability at the transition point of jet diffusion flames", Symposium (International) on Combustion, vol. 26, no. 1, pp. 27–34, 1996.