CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

Supercritical combustion

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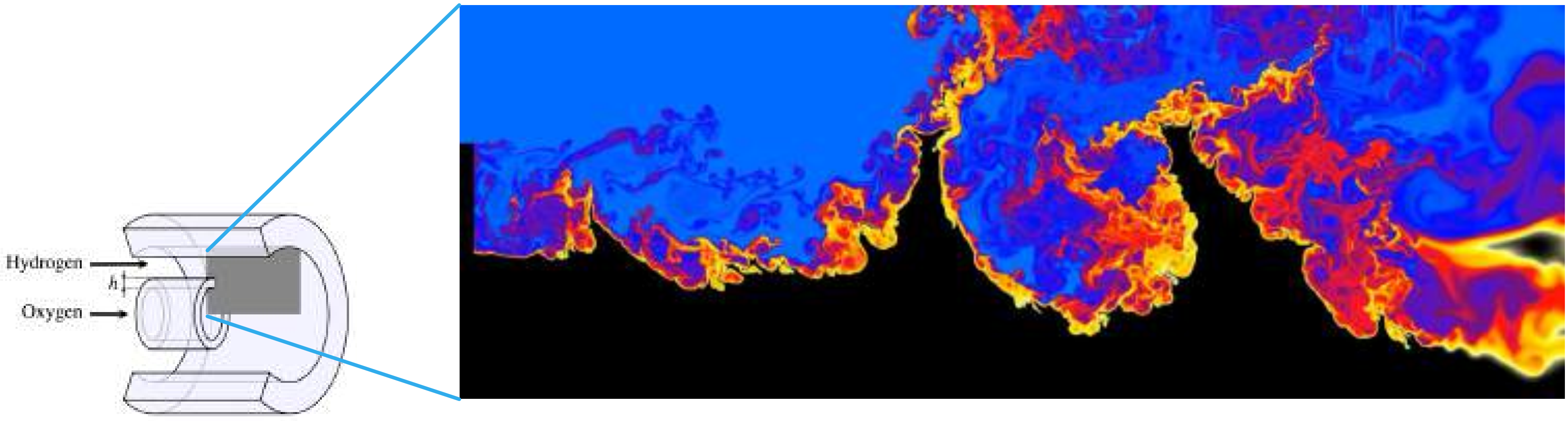
Supercritical injection



Ruiz et al., 2015

- **<u>High density</u>**, velocity, temperature **<u>gradients</u>**
- Pure **<u>diffusion flame</u>**

<u>Requires:</u>
- A dedicated **equation of state**
- To numerically handle sharp gradients

Supercritical combustion

Challenges:

- Fuel injection
- Chemistry / combustion
- Walls
- Instabilities

Supercritical combustion

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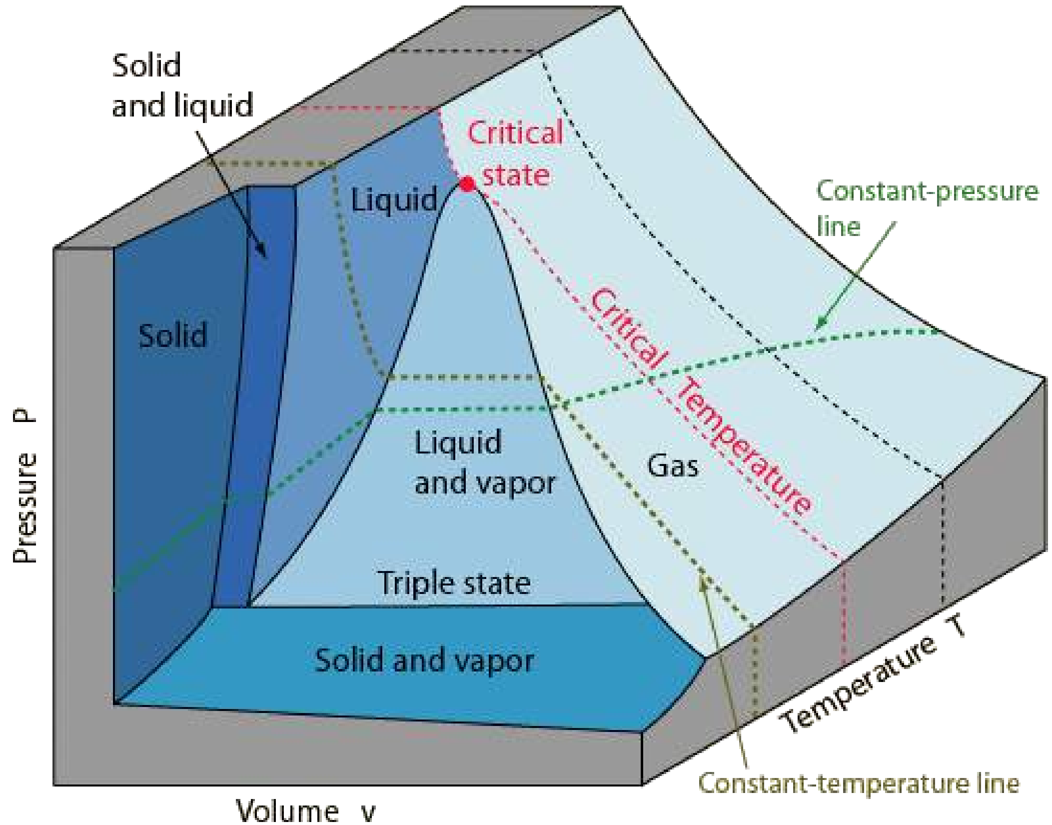
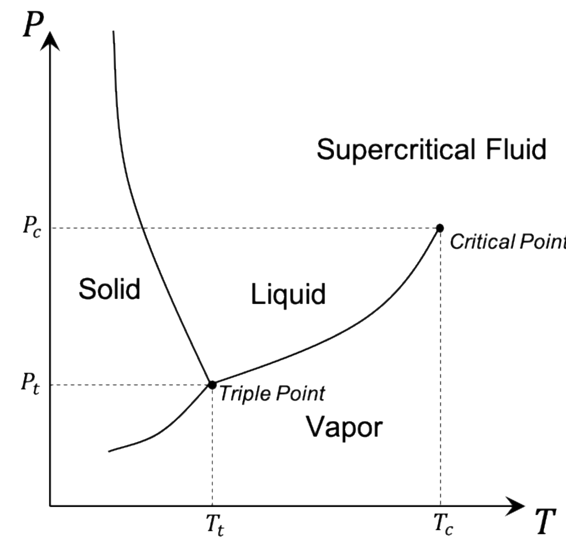
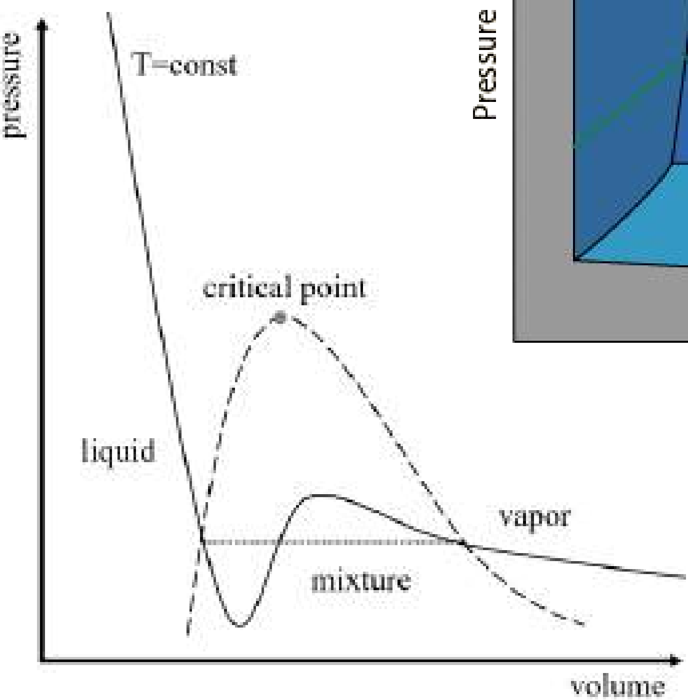
PTV diagram

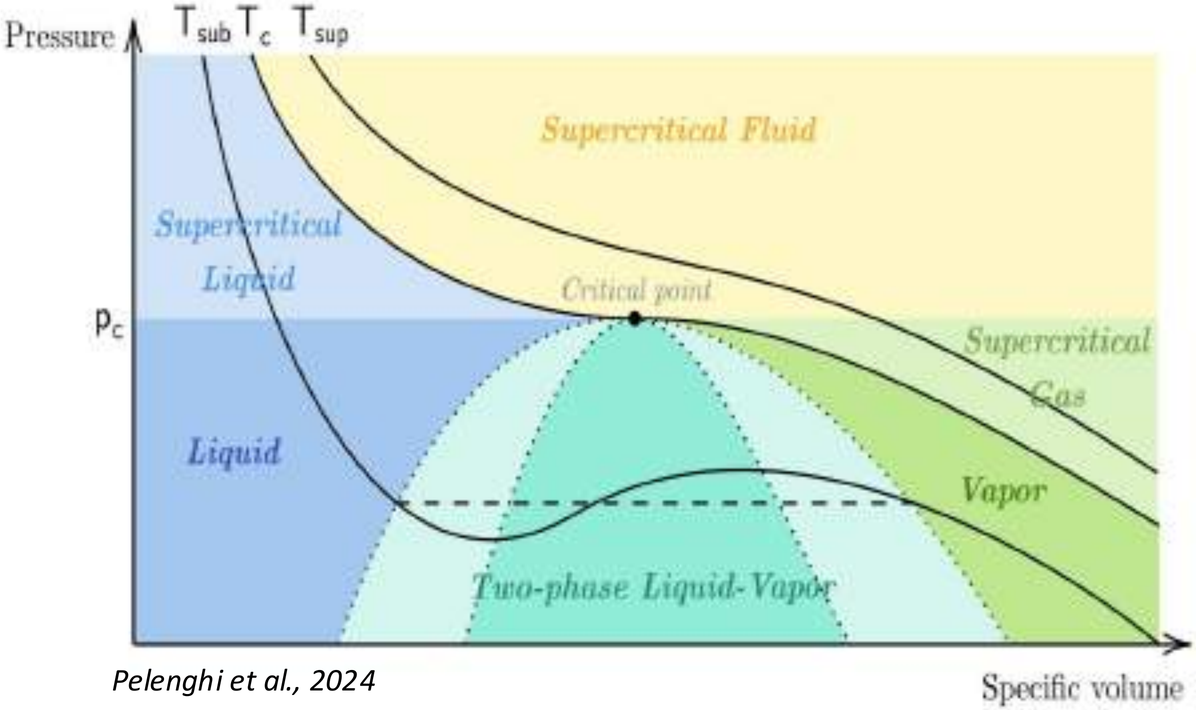




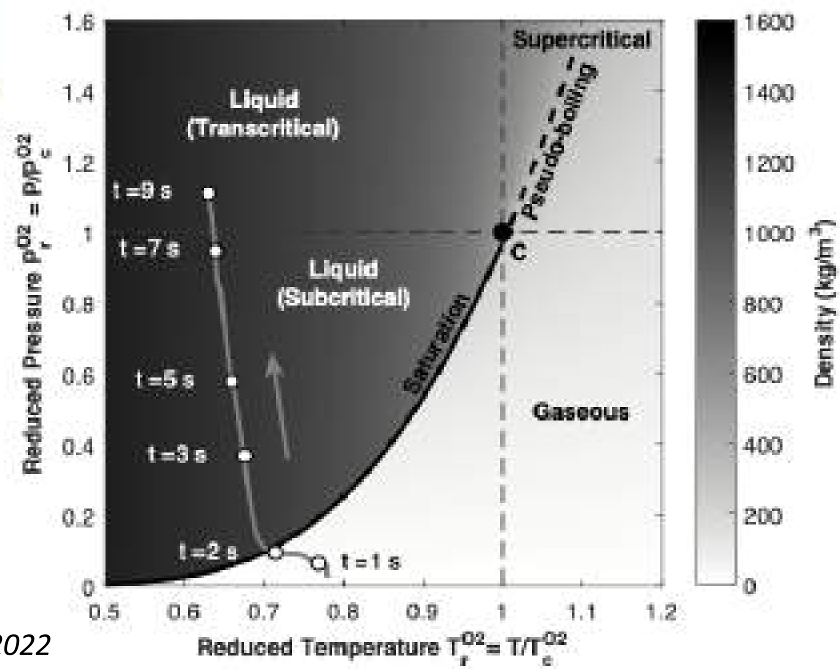


Pure component diagram

PTV diagram

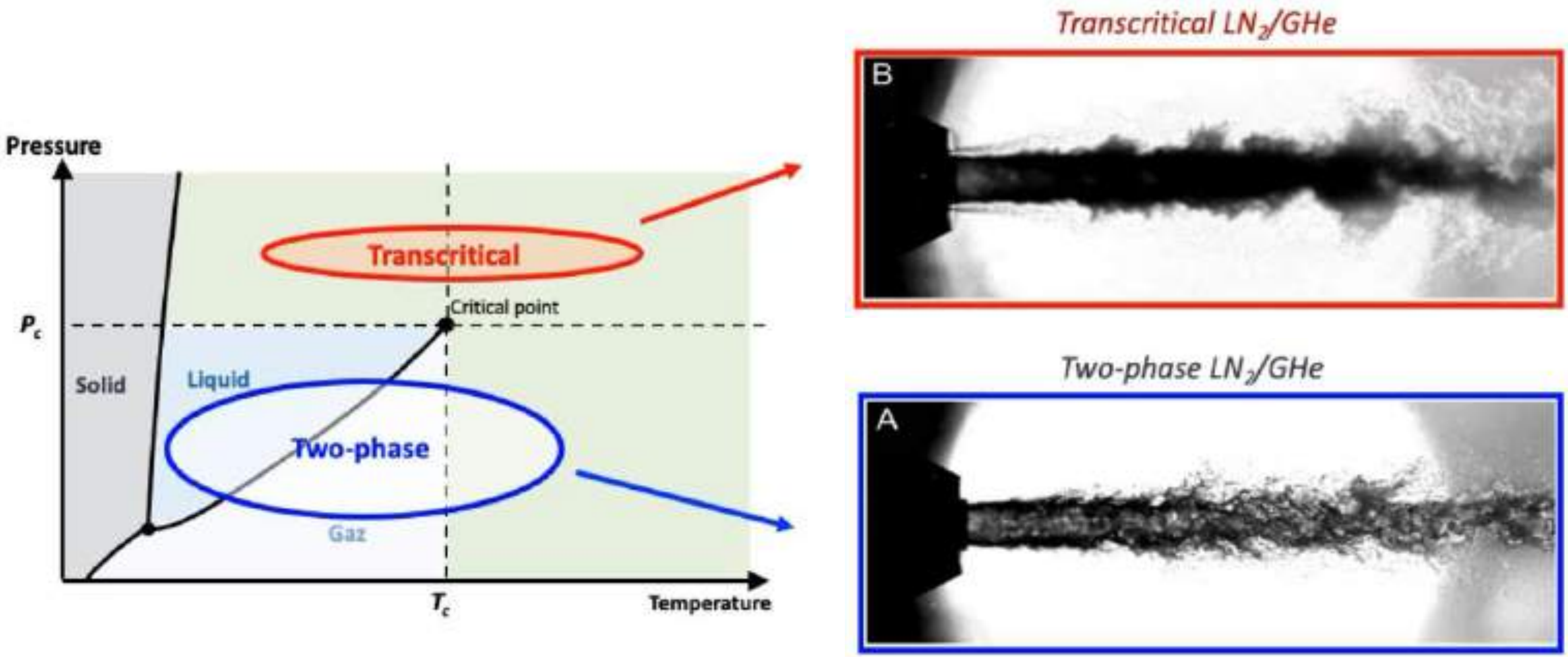


Pelenghi et al., 2024



Boulal et al, C&F, 2022

Injection regimes



Real-gas equations of state

- Dedicated EoS is mandatory to get the accurate mass flow rate

Perfect gaz

$$P = \rho r T$$

Significant errors for large density flows

Van der Waals (1873):

Molecular attraction effects

Thermal agitation

$$P_{VDW} = \frac{\rho r T}{1 - b\rho} - a\rho^2$$

Short distance repulsion

Molecular attraction

a Constant
b Covolume

Soave Redlich Kong (SRK, 1972)

$$P_{SRK} = \frac{\rho r T}{1 - b\rho} - \frac{a(T)\rho^2}{1 + b\rho}$$

Peng-Robinson, 1976

$$P_{PR} = \frac{\rho r T}{1 - b\rho} - \frac{a(T)\rho^2}{1 + 2b\rho - \rho^2}$$

➔ Allow prediction of **liquid-gas mixture**
➔ Allow a **large range of density**

Supercritical combustion

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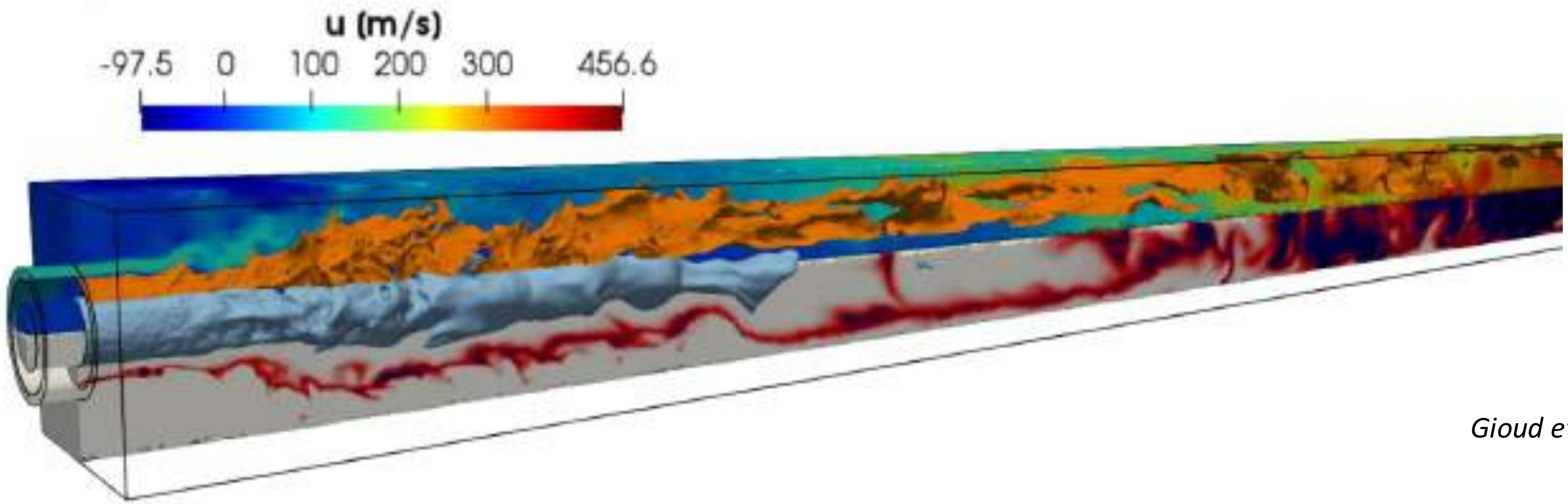
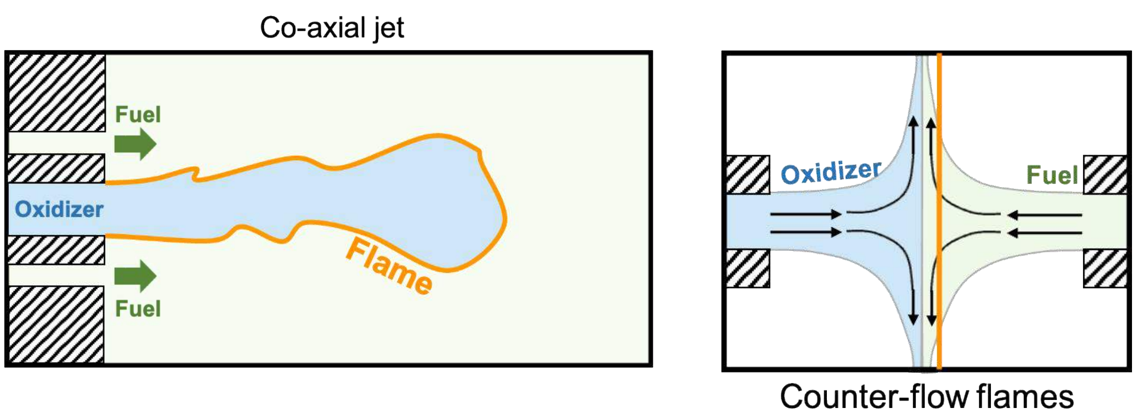
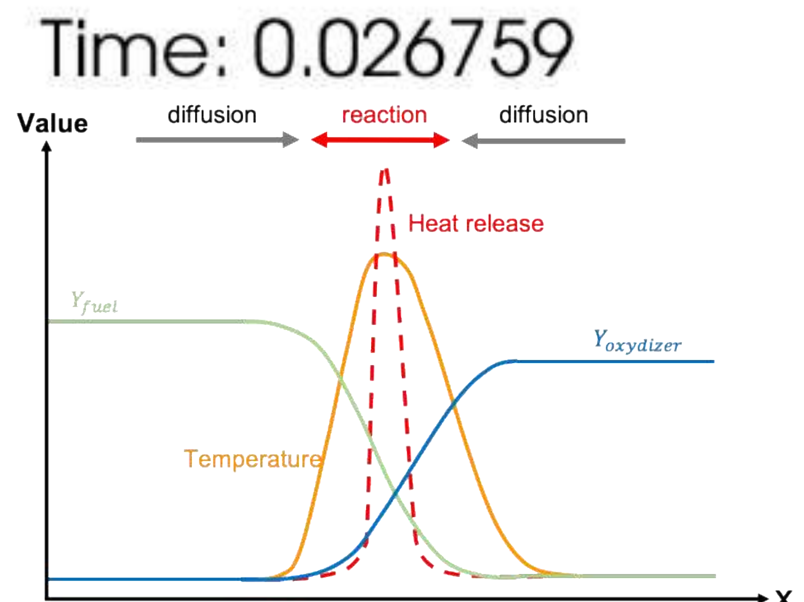
Diffusion flame



Gioud et al, FTAC 2025

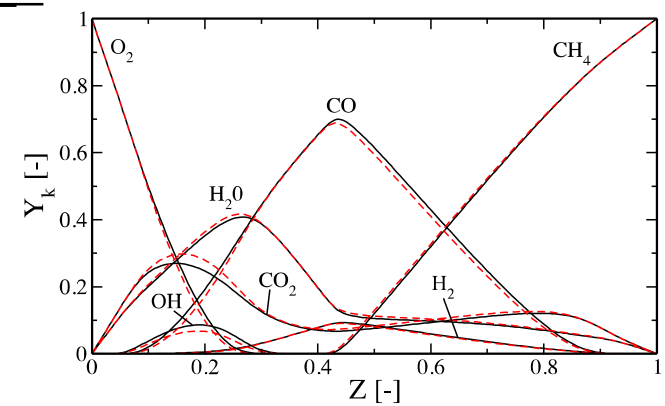




Infinitely fast combustion model

Reasonable hypothesis for **High pressure**, or **oxy-combustion.**

$$\rho\frac{\partial Y_k}{\partial t} = \dot{\omega}_k + \frac{1}{2}\rho\chi\frac{\partial^2 Y_k}{\partial z^2} \qquad \widetilde{\dot{\omega}_k} = \bar{\rho}\frac{\tilde{Y}_k\left(\widetilde{Z}, \widetilde{Z''^2}\right) - \widetilde{Y_k}}{C\Delta t}$$



- **Tabulated mass fractions** at equilibrium:

$$\widetilde{Y_k}(\widetilde{Z}, \widetilde{Z"^2}) = \int_0^1 Y_k(Z^*)P(Z^*, x, t)dZ^*$$

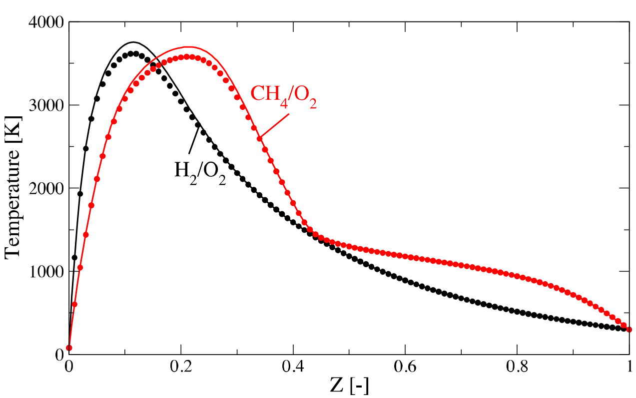
$$Z = \frac{sY_F - Y_O + Y_O^0}{sY_F^0 + Y_O^0}$$

$$\widetilde{Z''} = C\Delta^2|\nabla(\widetilde{Z})^2|$$

- Additional transport equations

$$\frac{\partial\bar{\rho}\widetilde{Z}}{\partial t} + \nabla\cdot(\bar{\rho}\widetilde{Z}\widetilde{u}) = \nabla\cdot\left(\bar{\rho}\left(D + D_t\right)\nabla\widetilde{Z}\right)$$

$$\frac{\partial\bar{\rho}\widetilde{Z''2}}{\partial t} + \nabla\cdot\left(\bar{\rho}\widetilde{Z}''^2\widetilde{u}\right) = \nabla\cdot\left(\bar{\rho}\left(\mathcal{D} + \mathcal{D}_t\right)\nabla\widetilde{Z''^2}\right) + 2\bar{\rho}\mathcal{D}_t|\nabla\widetilde{Z}|^2 - 2\bar{\rho}\mathcal{D}_t\frac{\widetilde{Z''}}{\Delta_x^2}$$

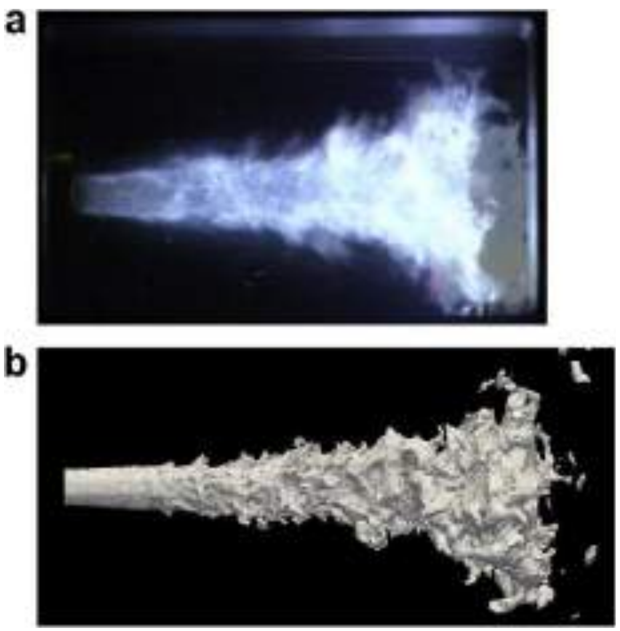


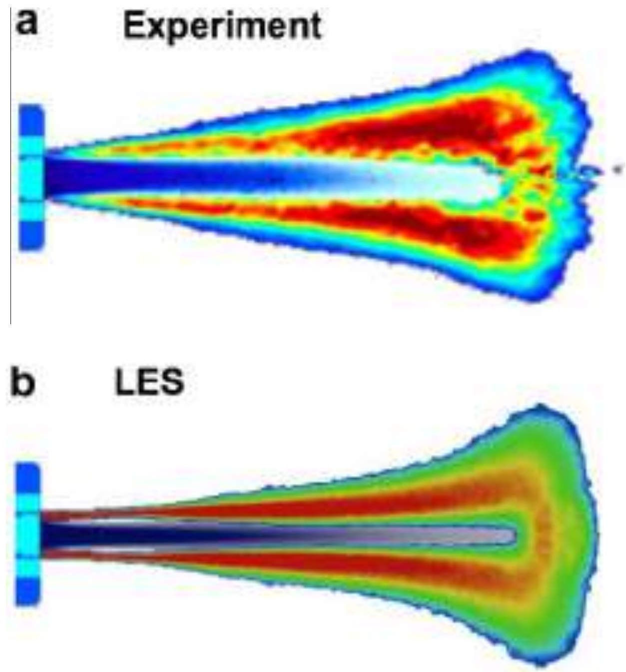
➔ **Allows to save CPU cost**

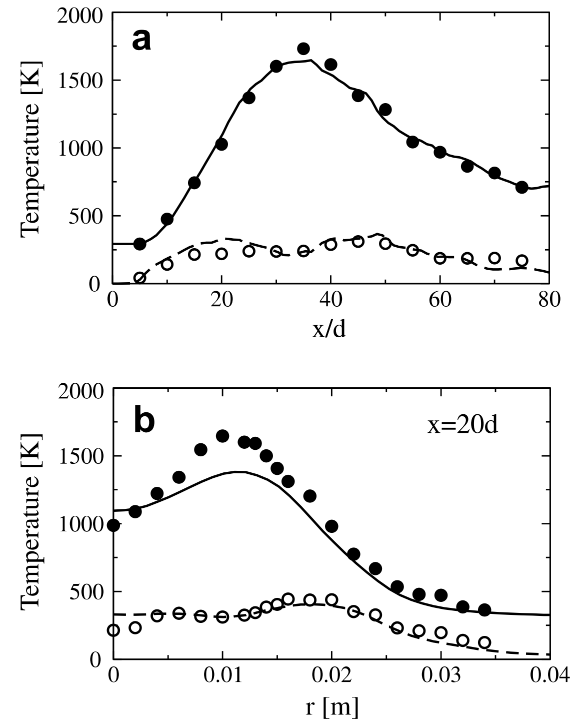
Schmitt, FTAC 2020

Injection + infinitely fast combustion

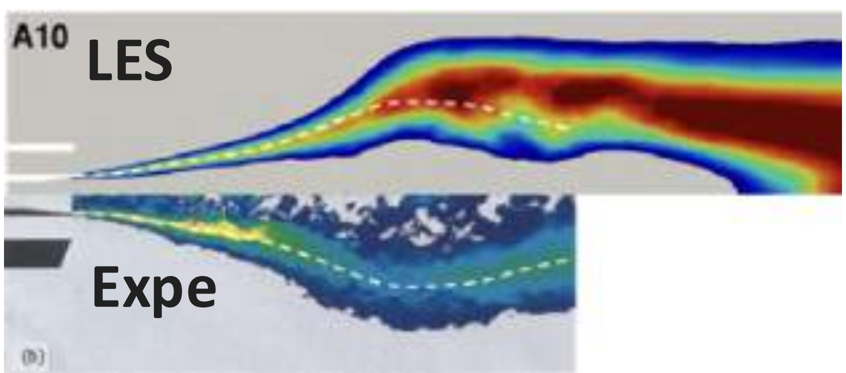
Transcritical LO2/CH4







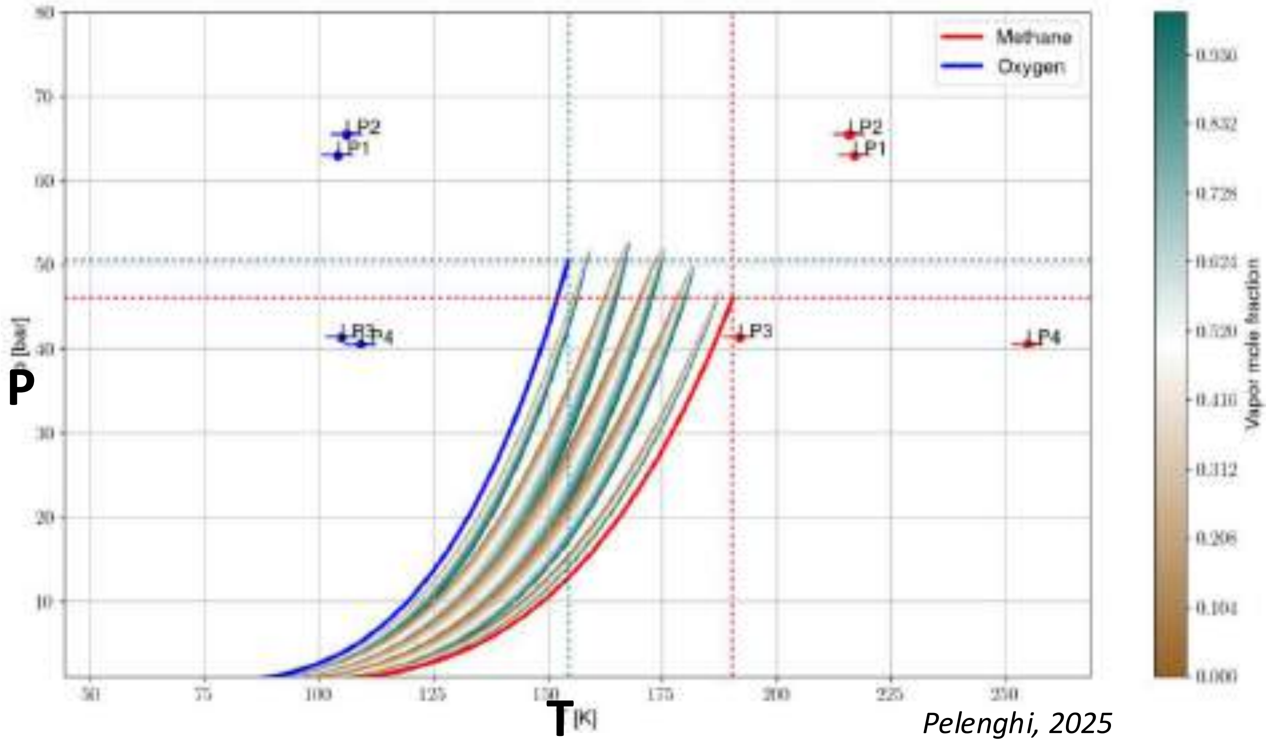
Schmitt et al. PCI 2011



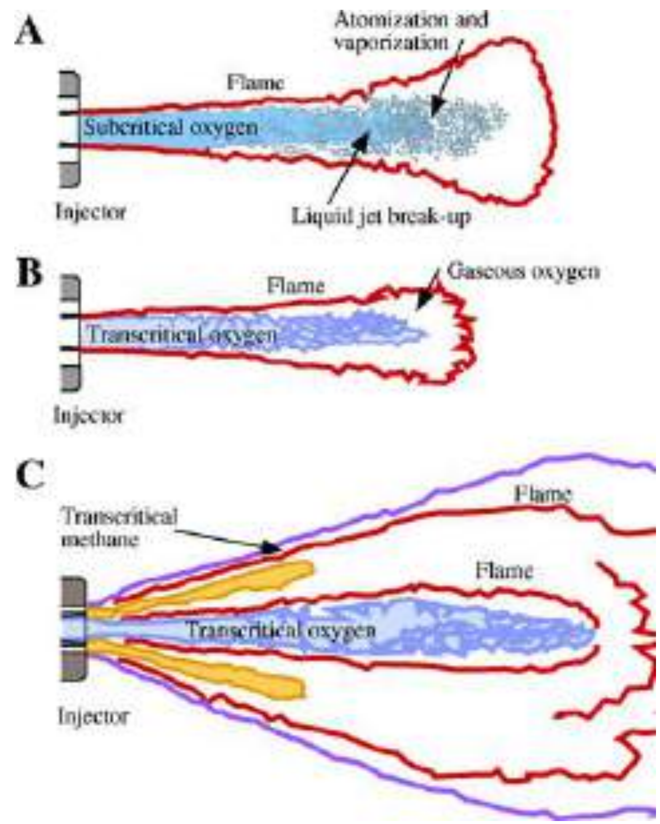
Schmitt 2023

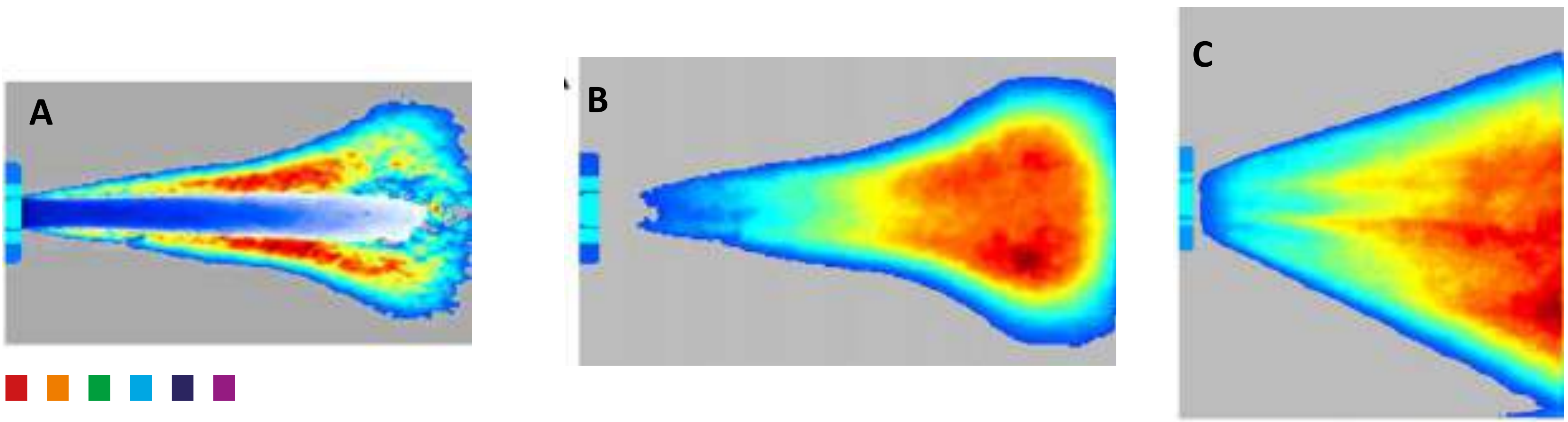
Multicomponent injection

Complex multi-component regimes !



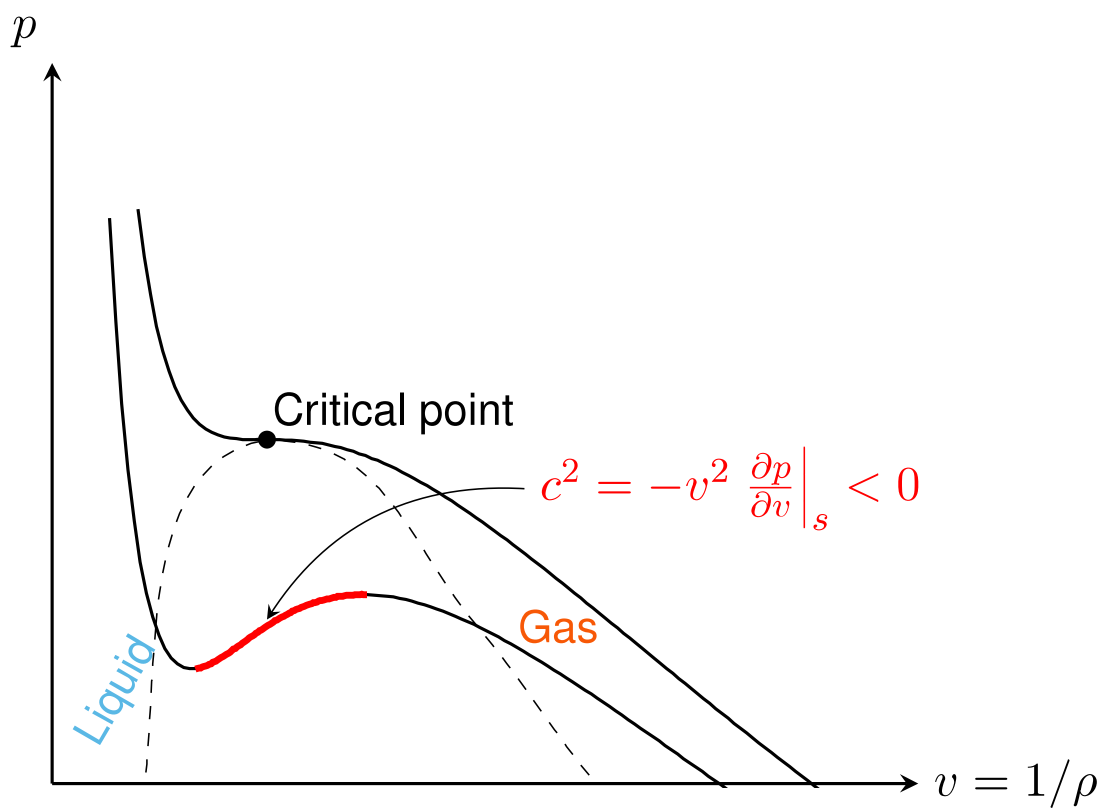
Pelenghi, 2025





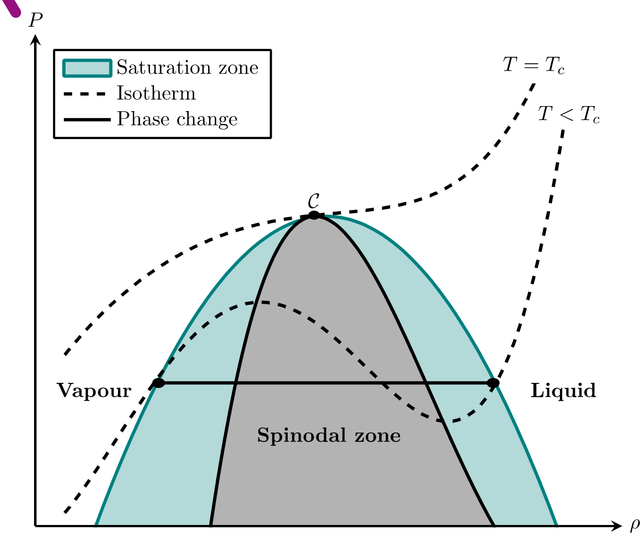
Singla et al., PCI 2005

Subcritical injection



- Cubic equation of state **cannot be used in the liquid-gas mixture region**
- A **dedicated equilibrium computation** must be conducted

Subcritical injection



Tabulated, normalized saturation curve

(ρ^n, e_s^n) → Stability test

- Stable: single-phase
- Instable:

(T, P, μ) **equilibrium computation**:
➔ Provides α_l

Need to account for surface tension:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u} + P \underline{\underline{I}} - \underline{\underline{\tau}}) = \vec{F}_{ST}$$

$$\frac{\partial \rho e_t}{\partial t} + \vec{\nabla} \cdot ((e_t + P)\vec{u} - \underline{\underline{\tau}} \cdot \vec{u}) = \vec{u} \cdot \vec{F}_{ST}$$

$$\mathbf{F}_s = \sigma \kappa \nabla \alpha_l$$

Surface tension coefficient

curvature

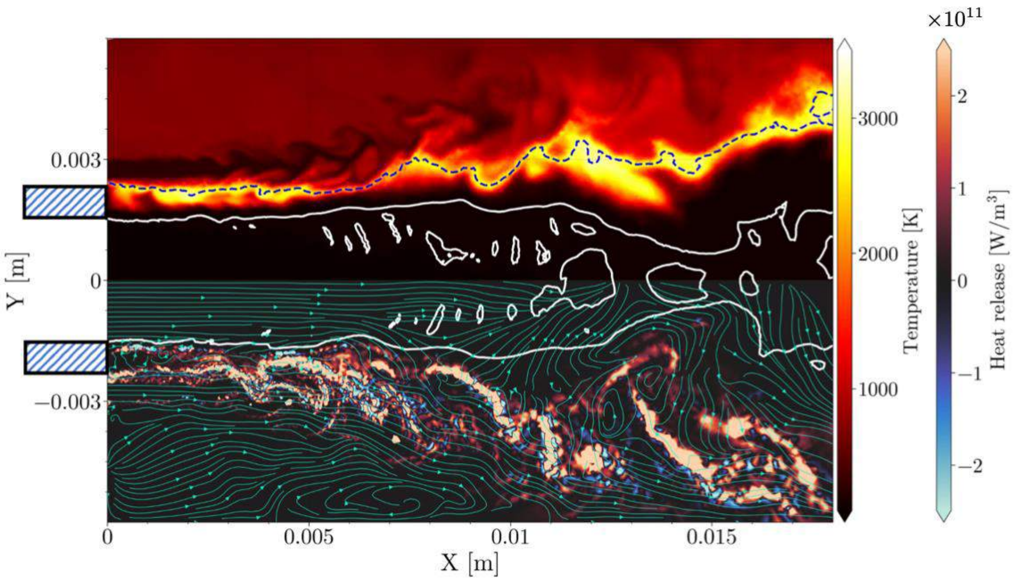
For multi-components mixture:

Let's assume:

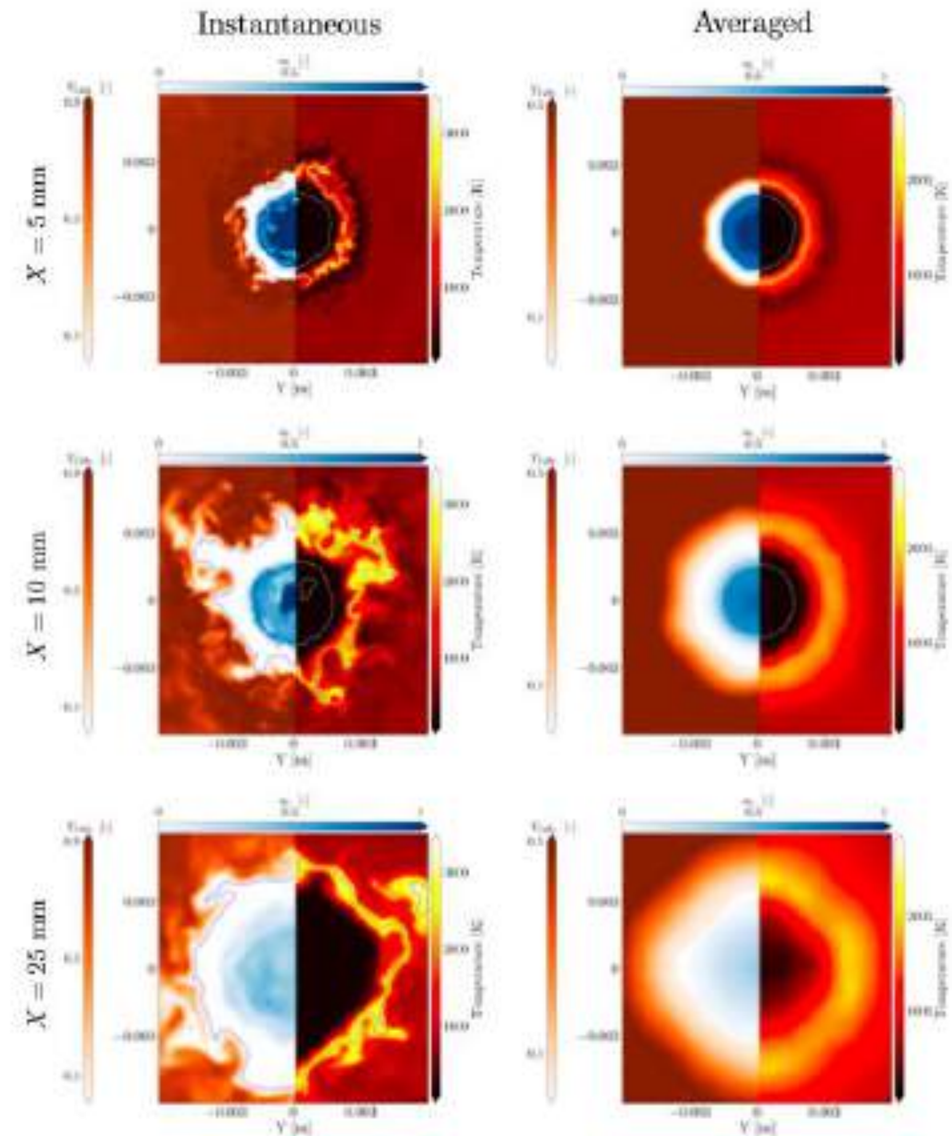
$$Y_{k,l} = Y_{k,v} = Y_k$$

Pelletier et al., 2020
Gioud et al., 2025

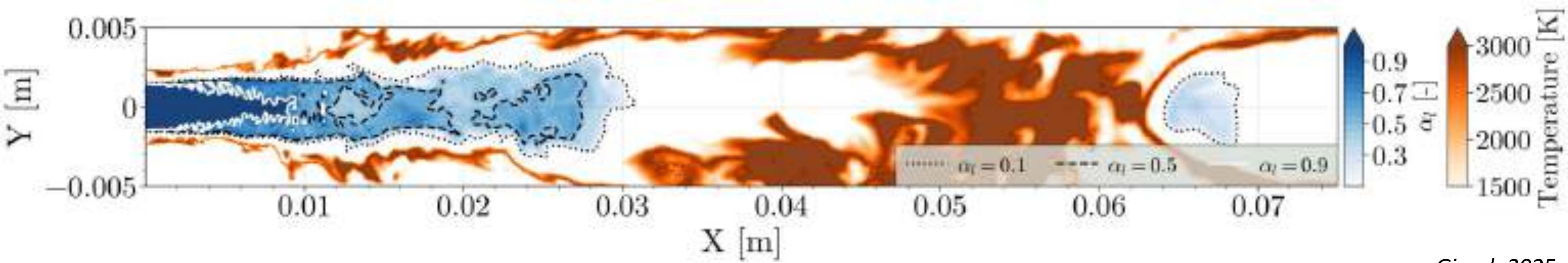
Liquid / Flame interaction



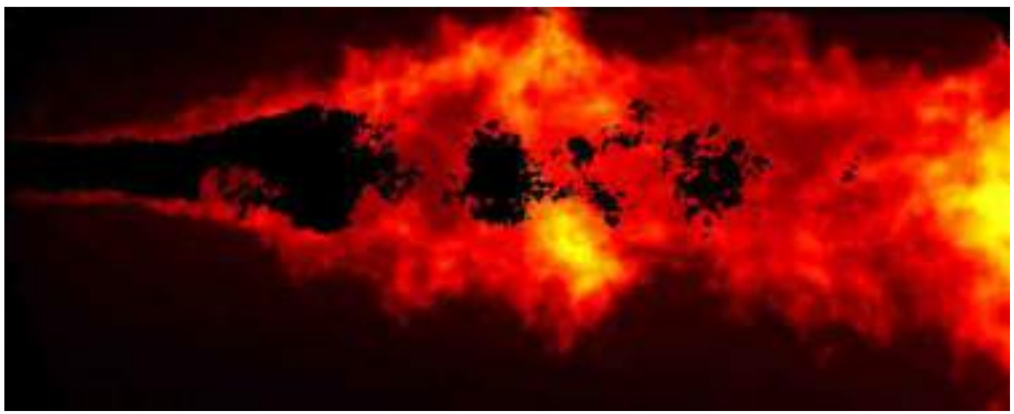
Gioud et al, FTAC, 2025



Spray unsteadiness



Gioud, 2025



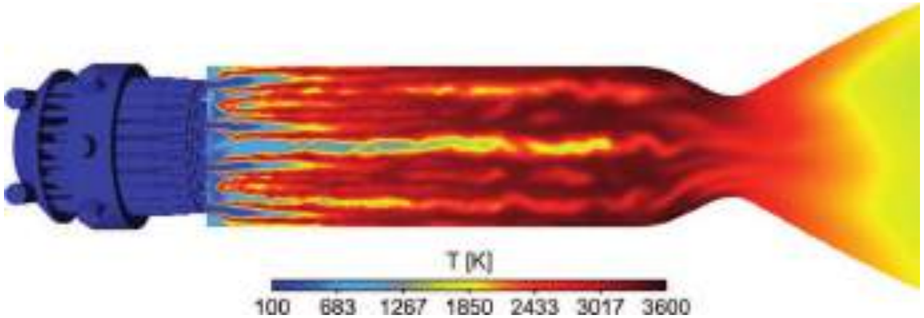
LOx/ CH4

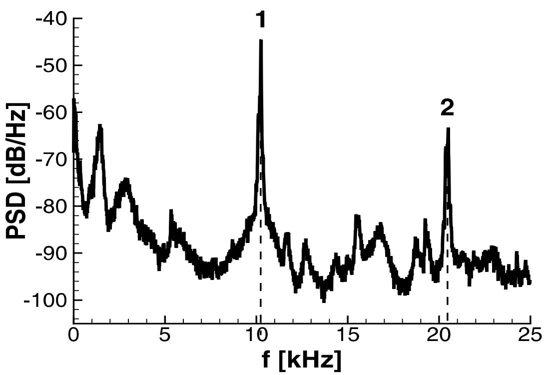
Fdida, Eucass 2019

- Release of **large spray packets**
- Still requires physical investigation

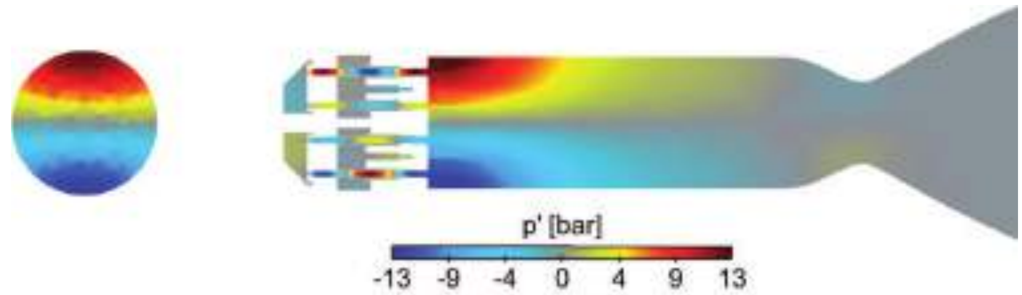
Thermo-acoustic Instabilities

Urbano et al., CnF 2016

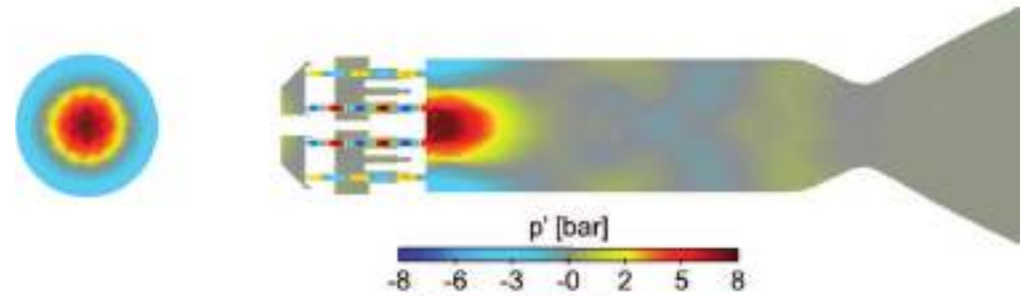




(d) LP4-experiment: $f_1 = 10,260$ Hz, $f_2 = 20,500$ Hz.

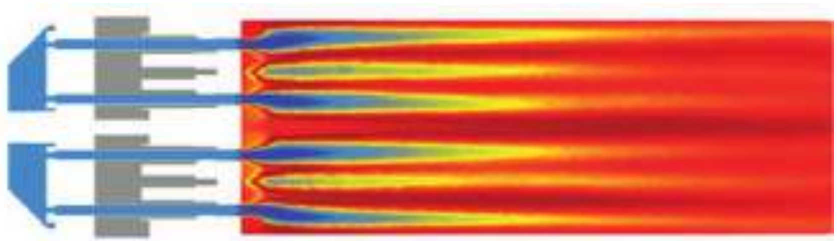


(a) $f_1 = 10,700$ Hz.

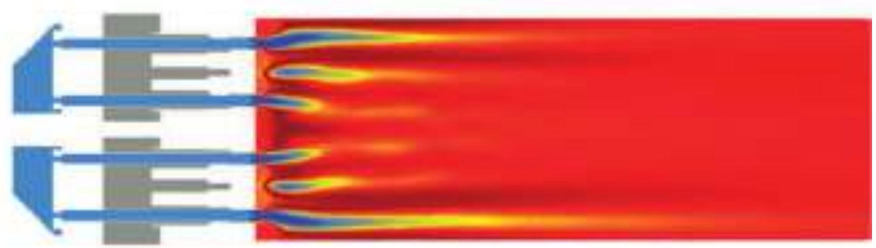


(b) $f_2 = 21,400$ Hz.

→ Significant **sound speed gradients:** 239 m/s → 2000 m/s !!

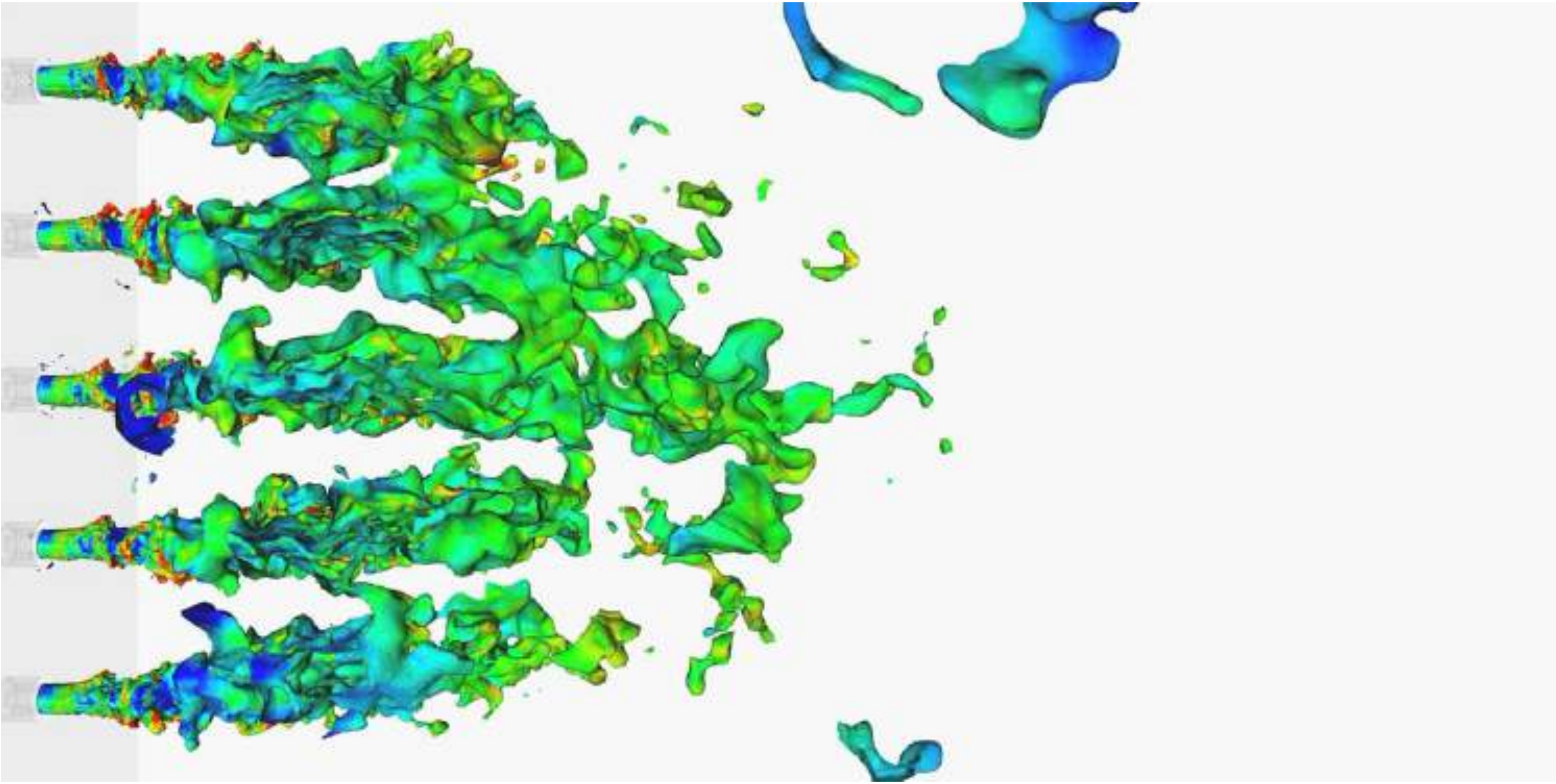


(a) Stable.



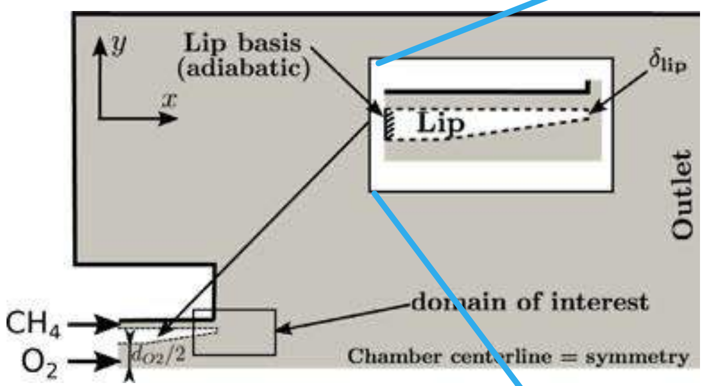
(b) Unstable.

Thermo-acoustic Instabilities

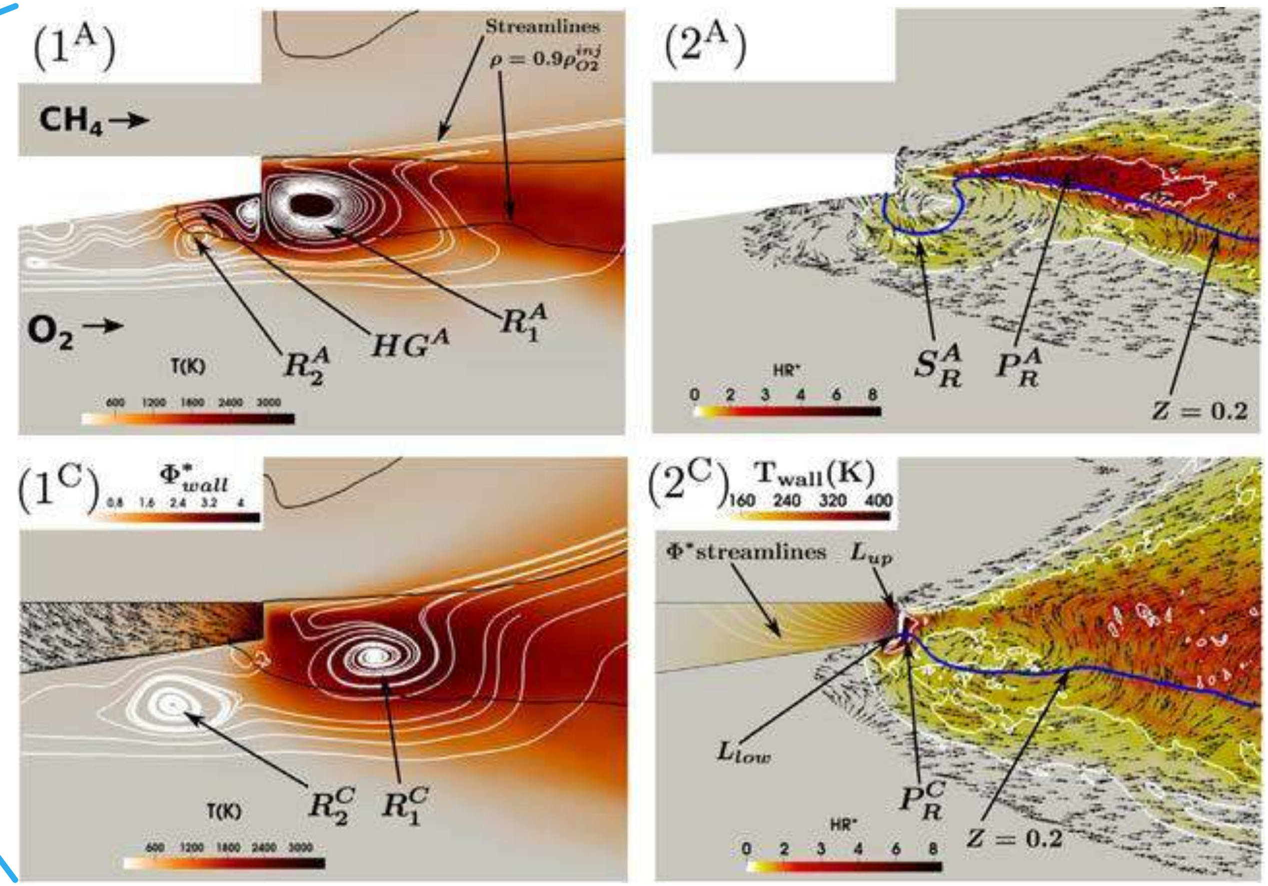


Hakim et al., PCI 2015

Effect of solid conduction



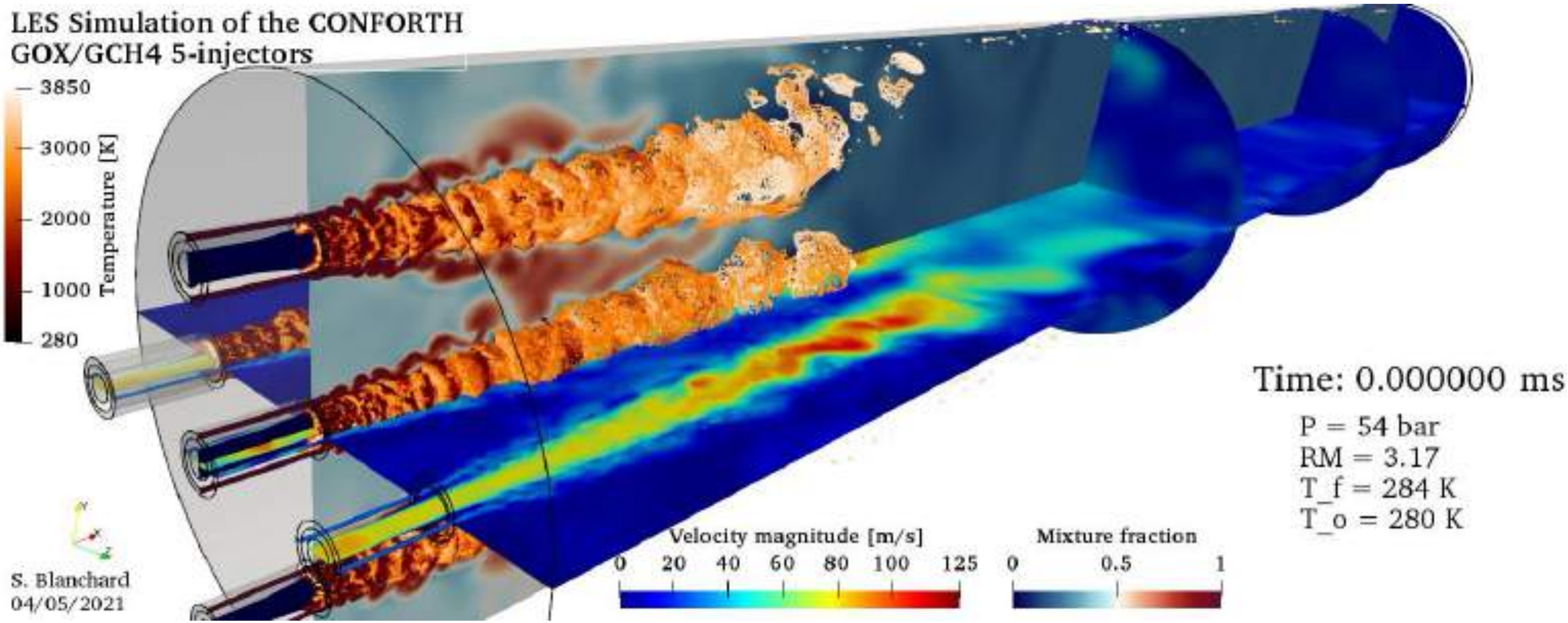
	Injection conditions		
	$\dot{m}_{inj}/\dot{m}^{O2}_{inj}$	T^{inj}_R	P^{inj}_R
O_2	1.0	0.55	1.49
CH_4	3.59	0.62	1.64
HG		–	



Laurent et al., PCI 2019

➔ May change the **mean heat Release**, and **the unsteady dynamics** !

Wall heat transfer



Blanchard, 2021

Thermal Law-of-the-wall

- A logarithmic relation can be derived for **thermal flux**:

$$\begin{cases} T^+ = \frac{P_{r_t}}{\kappa}\ln(y^+) + \beta(P_r) \\ u^+ = \frac{1}{\kappa}\ln(y^+) + C_{vd} \end{cases}$$

➔ Provides q_w

➔ Provides τ_w

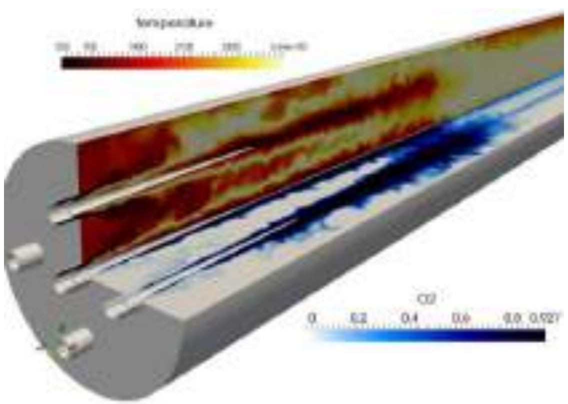
$$T^+ = \frac{\overline{T_w} - \overline{T}}{T_\tau}$$

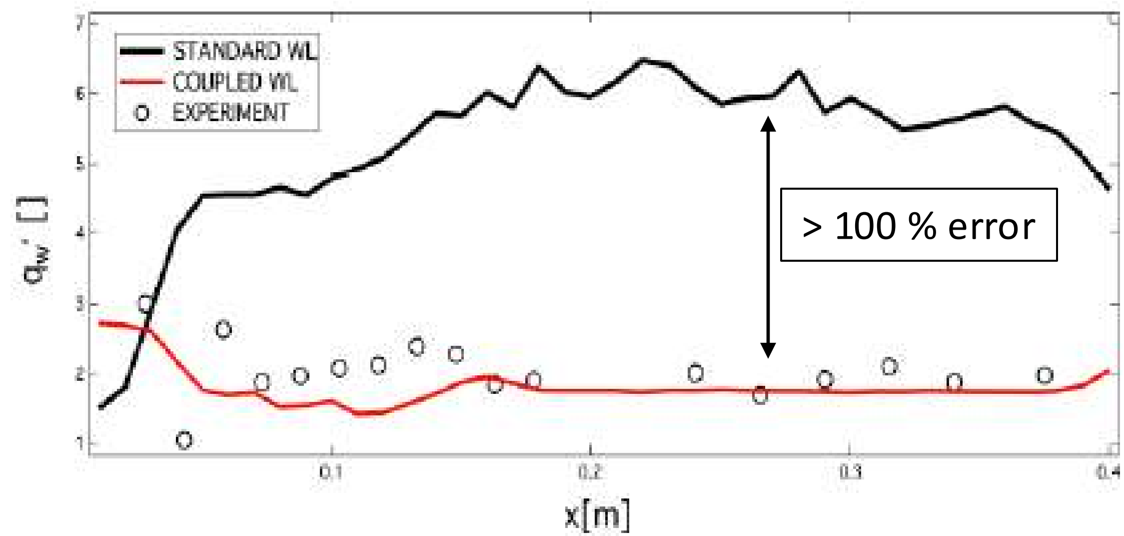
$$T_\tau = \frac{\overline{q_w}}{\rho_w C_{p,w} u_\tau}$$

- <u>**Cabrit, 2009**</u>: **Coupled velocity-temperature** analytical wall model

$$\begin{cases} \frac{2}{P_{r_t} B_q}\left(\sqrt{1 - KB_q} - \sqrt{\frac{T}{T_w}}\right) = \frac{1}{\kappa}\ln y^+ + C_{vd} \\ T^+ = P_{r_t} u^+ + K \end{cases}$$

Strong improvement for **large temperature gradients** (rocket engines) :



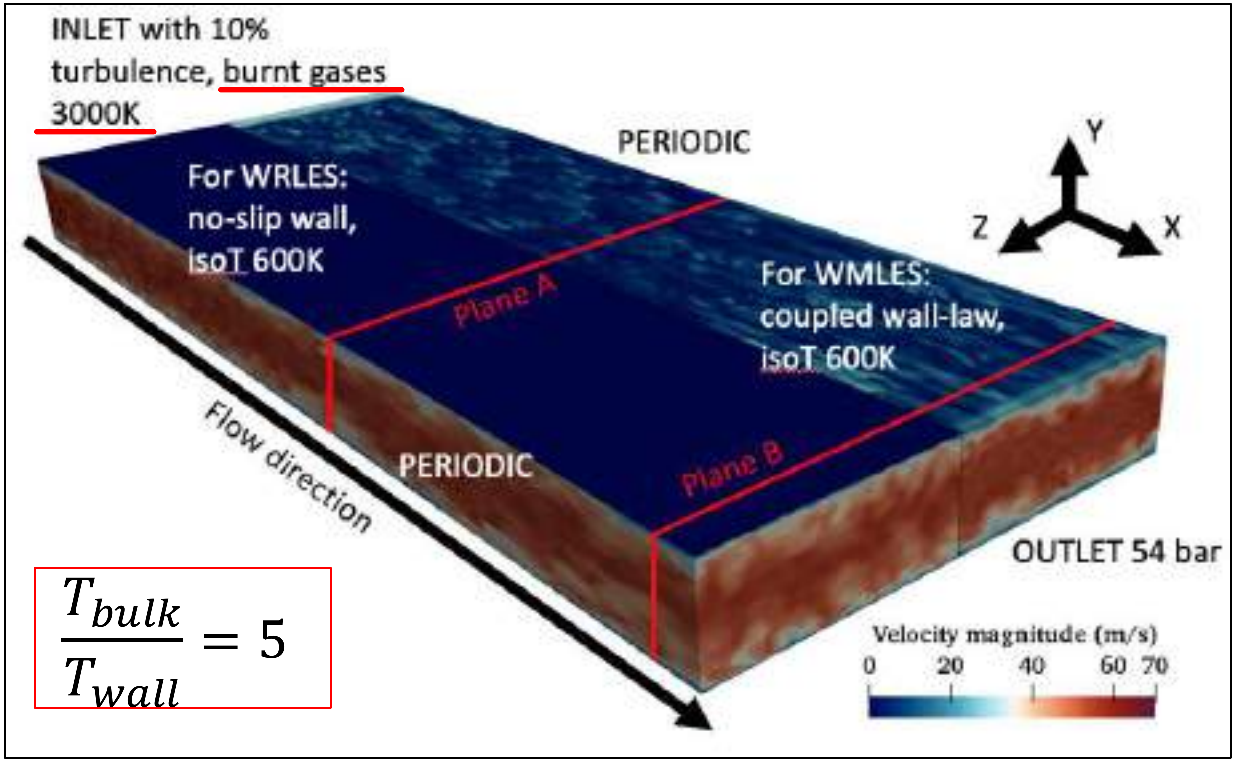


Impact of wall chemistry

PhD Blanchard, 2021

$$\overline{q_{tot}} \approx \underbrace{\bar{\rho}\widetilde{v''h''_s}}_{\substack{1\\ \text{turbulent}}} + \underbrace{\bar{\rho}\sum_k \widetilde{v''Y''_k}\Delta h^0_{f,k}}_{\substack{2\\ \text{chemical}}} - \underbrace{\overline{\lambda\frac{dT}{dy}}}_{\substack{3\\ \text{laminar}}} + \underbrace{\bar{\rho}\sum_k \overline{h_k Y_k V_{k,y}}}_{\substack{4\\ \text{Species diffusion}}}$$

Reactive / non reactive case comparisons



$$\boxed{\frac{T_{bulk}}{T_{wall}} = 5}$$

WRLES	Plane A	Plane B
q_w	-10.2%	-9.2%

WMLES	Plane A	Plane B
q_w	-3.9%	-6.4%

- **Wall modelled LES is missing the chemical activity**
- Dedicated work is still required…

Short conclusions

Supercritical combustion:

Thermodynamics / two-phase + chemistry + turbulence
+ acoustic + heat transfer + wall-bounded

= Complex topic !

Still open questions:

- Dedicated chemistry for high-pressure, combustion models
- Dedicated wall-modelling, including chemical activity
- Spray-flame interaction, impact on instabilities

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THANK YOU

Credits

All this work, and gained knowledge, have benefited from constant support along the years from :

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