27th International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS)

Large-Eddy Simulation (LES) of a Reactive Jet in Supersonic Cross Flow (JISCF) Based on a Hybrid Model of Turbulent Combustion

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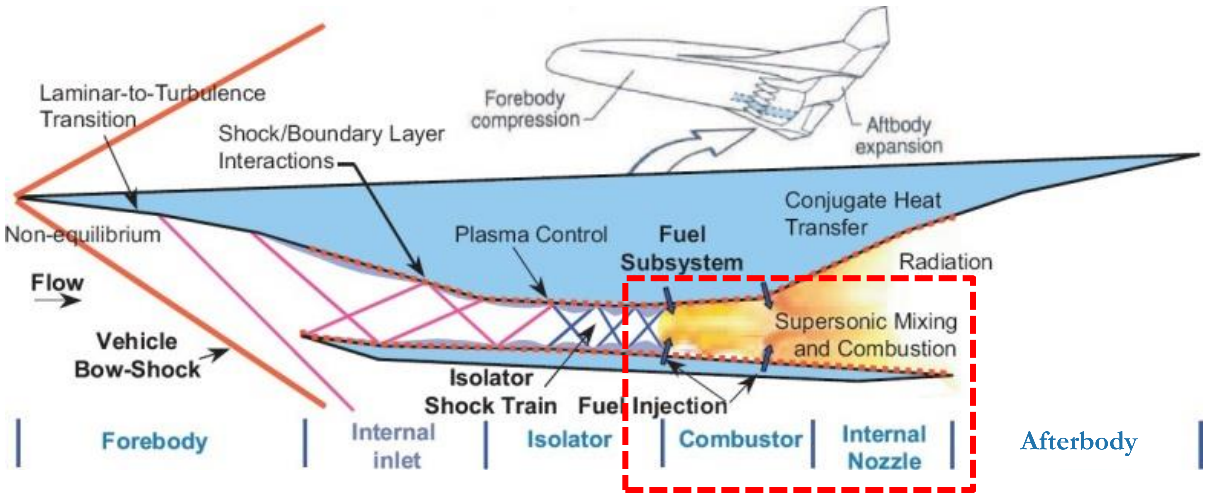
Contents

Introduction

- Supersonic combustion ramjets (scramjets)

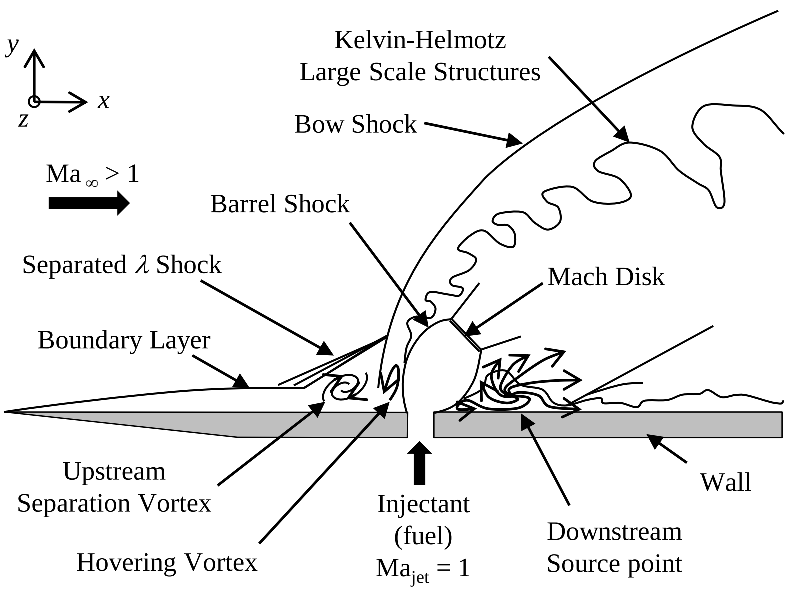


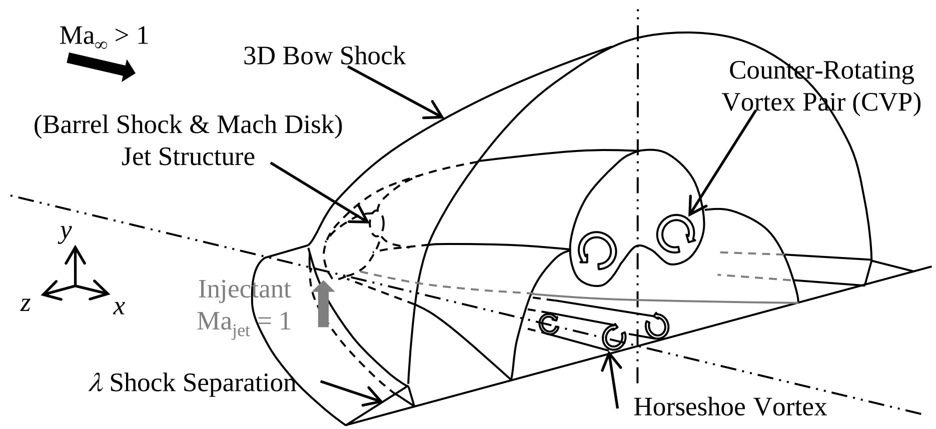
source : http://web.stanford.edu

- no mechanical moving part (external & internal compression)
- higher specific impulse I_{sp} than rocket engines
- extremely large flight Mach number values
- *Mixing and combustion in supersonic flow*

Introduction

- Application to supersonic combustion ramjets (scramjets)
  - Jet in supersonic cross-flows (JISCF) [1, 2]





+ realistic total temperature level ($T_0 \approx 1700$ K)
+ geometry relevant to scramjets

[1] A. Ben-Yakar, M Mungal and R Hanson, "Time evolution and mixing characteristics of hydrogen and ethylene transverse jets in supersonic crossflows", *Physics of Fluids*, 2006
[2] Techer, A., Moule, Y., Lehnasch, G. et Mura, A. "Mixing of a fuel jet in a supersonic crossflow: estimation of subgrid-scale scalar fluctuations". *AIAA Journal* (2017).

Introduction

- Current state of the art

Momentum flux ratio : $J = \frac{\left(\rho u^2\right)_{jet}}{\left(\rho u^2\right)_{\infty}}$

Non-exhaustive list

Authors	Expe.	Num. Sim.	Inert	Reactive	J
Santiago & Dutton (1997)	X		X		1.7
Lavante *et al.* (2001)		LES	X	X	2.50
Ben-Yakar *et al.* (2006)	X		X	X	1.4 +/- 0.1
Kawai & Lele (2010)		LES	X		1.7
Castagna & Sandham (2010)		DNS	X		1
Gamba *et al.* (2011)		RANS + LES		X	5
Crafton *et al.* (2011)	X		X		0.5 to 3.0
Larson *et al.* (2011)		LES	X	X	3.33
Ingenito & Cecere (2013)		LES	X	X	0.512
Vincent-Randonnier *et al.* (2014)	X	RANS	X	X	2.56
Chai *et al.* (2015)		LES	X		1.7
Gamba & Mungal (2015)	X			X	0.3, 2.7, 5.0
Fureby (2017)		LES		X	1.1

$T_0 \approx 1700$ K
$J \approx 2.56$

[1] A. Vincent-Randonnier, Y. Moule and M. Ferrier, "Combustion of hydrogen in hot air flows within ***LAPCAT-II* Dual Mode Ramjet combustor** at ONERA-LAERTE facility-Experimental and Numerical Investigation", *AIAA Technical conference*, 2014

Contents

Numerical methods - Solver

- **CREAMS**: **C**ompressible **REA**ctive **M**ulti-**S**pecies solver (P' Institute)
  - Cartesian NS solver, compressible, unsteady, (non-)viscous, multi-species, **massively parallel** (MPI-OmpSs, up to 100 000 cores), 3D
  - **Numerical aspects**
    - Coupling
      - **EGLIB library**: detailed multi-species transport (Ern & Giovangigli) [2]
      - **DVODE/CVODE solver**: detailed chemistry (Brown *et al.*) [1]
    - Spatial discretizations
      - Convective flux (non viscous)
        - » combines non-linear weighting procedure of **WENO7 & high order FDS**
        - » shock sensor: modified **Adams & Shariff** [3] $|\rho_{i+1}-\rho_i|/\rho_i$ & $|p_{i+1}-p_i|/p_i$
      - Molecular flux: **CDS8**
    - Temporal integration
      - combines a **TVD RK3** scheme (non reactive contribution) & **CVODE** integrator (reactive contribution) by using **Strang's splitting** [4]

[1] P. N. Brown, G. D. Byrne and A. C. Hindmarsh. VODE, a variable-coefficient ODE solver. *SIAM J. Sci. Stat. Comput*. 10,1038–1051, (1989).
[2] A. Ern and V Giovangigli. Fast and accurate multicomponent transport property evaluation. *J. Comput. Physics*, 120, 105-116, (1995).
[3] N.A. Adams and K. Shariff. *Journal of Computational Physics*, 127 :27–51, 1996
[4] J. C. Strikwerda. Finite difference schemes and partial differential equations. Wadsworth, Belmont (1989).

Numerical methods - Equations

- LES formulation

Mass

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i} = 0$$

Ideal gas

$$\bar{p} \approx \frac{\bar{\rho} R \tilde{T}}{\tilde{W}}; \quad \frac{1}{\tilde{W}} = \sum_{\alpha=1,N} \frac{\tilde{Y}_\alpha}{W_\alpha}$$

SGS terms Negligible [1, 2]

Momentum

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \breve{\tau}_{ij}}{\partial x_j} - \boxed{\frac{\partial \tau_{ij}^{sgs}}{\partial x_j} + \cancel{\frac{\partial}{\partial x_j}\left(\bar{\tau}_{ij} - \breve{\tau}_{ij}\right)}}$$

Species

$$\frac{\partial \bar{\rho}\tilde{Y}_\alpha}{\partial t} + \frac{\partial \bar{\rho}\tilde{Y}_\alpha\tilde{u}_j}{\partial x_j} = -\frac{\partial \breve{J}_{\alpha i}}{\partial x_j} - \boxed{\frac{\partial J_{\alpha i}^{sgs}}{\partial x_j} - \cancel{\frac{\partial}{\partial x_j}\left(\bar{J}_{\alpha i} - \breve{J}_{\alpha i}\right)} + \bar{\rho}\tilde{\omega}_\alpha}$$

Total energy [2]

$$\bar{\rho}\breve{e}_t = \bar{\rho}\breve{e} + \frac{1}{2}\bar{\rho}\tilde{u}_i\tilde{u}_i$$

$$\frac{\partial \bar{\rho}\breve{e}_t}{\partial t} + \frac{\partial \bar{\rho}\breve{e}_t\tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}\tilde{u}_j}{\partial x_j} + \frac{\partial \tilde{u}_i\breve{\tau}_{ij}}{\partial x_j} - \frac{\partial \breve{q}_j}{\partial x_j} - \boxed{\left(B_1 + B_2 + B_3\right) + \left(\cancel{B_4} + \cancel{B_5} + \cancel{B_6}\right) - \cancel{B_7}}$$

[1] Ragab & Sreedhar, *"An investigation of finite-difference methods for large-eddy simulation of a mixing layer"*, AIAA Paper 92-0554 , 1992.

[2] Vreman, *Direct and Large-Eddy Simulation of the compressible turbulent mixing layer*, PhD Thesis, Univ. of Twente, 1995

Numerical methods – Formulation

- LES formulation
  - Molecular transport properties
    - Resolved shear stress tensors

$$\breve{\tau}_{ij} = \tau_{ij}\left(\tilde{\mathbf{u}},\tilde{T}\right) = 2\tilde{\mu}\left(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{kk}\delta_{ij}\right) \qquad \tilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right)$$

    - Resolved mass flux (Hirschfelder & Curtiss approximation [1])

$$\breve{J}_{\alpha i} = J_{\alpha i}\left(\bar{\rho},\tilde{\mathbf{Y}},\tilde{T}\right) = \bar{\rho}\tilde{Y}_\alpha \tilde{V}_{\alpha j} = -\bar{\rho}\tilde{D}_{\alpha m}\frac{W_\alpha}{\tilde{W}}\frac{\partial \tilde{X}_\alpha}{\partial x_j} + \bar{\rho}\tilde{Y}_\alpha \underbrace{\sum_{\beta=1,N}\tilde{D}_{\beta m}\frac{W_\beta}{\tilde{W}}\frac{\partial \tilde{X}_\beta}{\partial x_j}}_{\breve{V}_{ci}}$$

    - Resolved heat flux [1]

$$\breve{q}_j = q_j\left(\bar{\rho},\tilde{\mathbf{Y}},\tilde{T}\right) = -\tilde{\lambda}\frac{\partial \tilde{T}}{\partial x_j} + \sum_{\alpha=1,N}\breve{J}_{\alpha u}\tilde{h}_\alpha$$

    - Transport coefficients

$$\tilde{\mu} = \mu\left(\tilde{\mathbf{Y}},\tilde{T}\right) \qquad \tilde{D}_{\alpha m} = D_{\alpha m}\left(\bar{\rho},\tilde{\mathbf{Y}},\tilde{T}\right) \qquad \tilde{\lambda} = \lambda\left(\tilde{\mathbf{Y}},\tilde{T}\right)$$

[1] Hirschfelder J. O. and Curtiss C. F., Molecular theory of gases and liquids, *John Wiley & Sons*, New York, 1969

Numerical method – SGS closures

- LES formulation
  - SGS terms closures
    - SGS stress tensor (Boussinesq hypothesis) $\boxed{\tau_{ij}^{\mathrm{sgs}}} = -2\mu_{\mathrm{sgs}}\left(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{kk}\delta_{ij}\right) + \frac{1}{3}\tau_{kk}^{\mathrm{sgs}}\delta_{ij}$
    - SGS mass flux $\boxed{J_{\alpha i}^{\mathrm{sgs}} = -\bar{\rho}D_{\mathrm{sgs}}\frac{\partial \tilde{Y}_\alpha}{\partial x_j}}$
    - SGS heat flux [2]

$$\boxed{B_1 + B_2 + B_3} = \underbrace{\frac{\partial}{\partial x_j}(\overline{\rho e u_j} - \bar{\rho}\tilde{e}\tilde{u}_j) + \frac{\partial}{\partial x_j}(\overline{p u_{j,j}} - \bar{p}\tilde{u}_{j,j})}_{q_j^{\mathrm{sgs}}} + \frac{\partial}{\partial x_j}(\tau_{ij}^{\mathrm{sgs}}\tilde{u}_j)$$

    - WALE (Wall Adaptative Local Eddy) model [3]

$$\boxed{\mu_{\mathrm{sgs}}} = \bar{\rho}(C_w\Delta)^2 \frac{\left(\tilde{S}_{ij}^d\tilde{S}_{ij}^d\right)^{3/2}}{\left(\tilde{S}_{ij}\tilde{S}_{ij}\right)^{5/2} + \left(\tilde{S}_{ij}^d\tilde{S}_{ij}^d\right)^{5/4}}; \quad C_w = C_s\sqrt{10.6}$$

    - Isotropic part of the SGS stress tensor (Yoshizawa [4]) $\boxed{\tau_{kk}^{\mathrm{sgs}}} = 2C_I\bar{\rho}\Delta^2\left|\tilde{S}\right|^2$

[1] Daly B. J. and Harlow F. H., Transport Equations in Turbulence., *Physics of Fluids*, 1970

[2] Vreman, Direct and Large-Eddy Simulation of the compressible turbulent mixing layer, PhD Thesis, Univ. of Twente, 1995

[3] Nicoud F. and Ducros F., Subgrid-Scale Stress Modelling Based on the Square of the Velocity Gradient Tensor, *Flow, Turbulence and Combustion*, 1999

[4] Yoshizawa A., Statistical theory for compressible turbulent shear flows with the application to subgrid modeling, *Physics of Fluids*, 1986

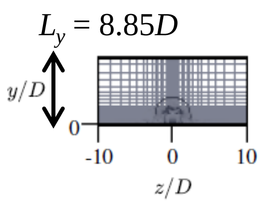
Numerical setup – Configuration

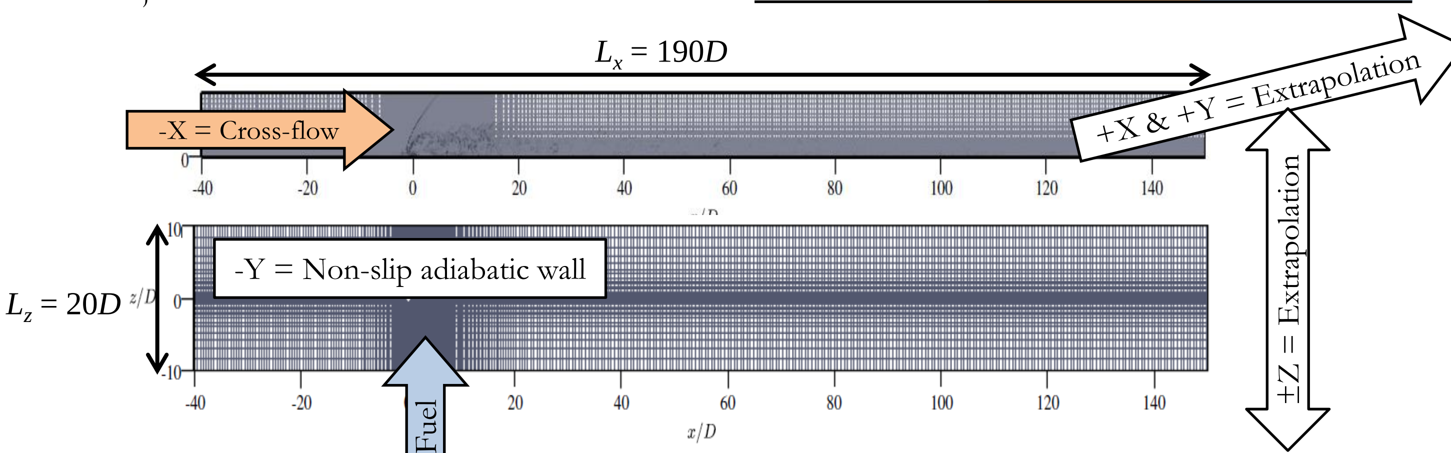
- Computational domain and boundary conditions

Direction		x	y	z
Length L_x/D		190	8.85	20
Number of points N_x		2253	196	193
Stretching (%)		0.35 to 0.55	2 to 3	1.7 to 3.15
Mesh size	$\Delta x_i/D$	0.03 to 0.1	0.003 to 0.25	0.03 to 0.3
	Δx_i^+	13 to 30	0.4 to 1.2	10 to 40

$N_{total} \approx$ 85,000,000 points
D = 2 mm, 50 points in the injection diameter

	Cross-flow	Fuel
Ma	2	1
T_0 (K)	1700	300
p_0 (kPa)	409	960
Mass fractions	O_2 = 0.2527 H_2O =0.1631 N_2 = 0.5842	H_2 = 1
Mixture frac. ξ	0	1





$$J = \frac{(\rho u^2)_{jet}}{(\rho u^2)_\infty} \approx 2.56$$

$$NPR = \frac{p_{0,jet}}{p_\infty} \approx 17$$

$$\Phi \approx 0.4$$

(Mesh is displayed with every 6^{th} grid point)

Numerical setup – Chemical mechanism

- Boivin *et al.* reduced mechanisms [1, 2, 3]
  - based on the San Diego mechanism
    - 12 reactions + 8 species

Rate coefficients in Arrhenius form $k = AT^n \exp(-E/R^o T)$, for the skeletal (12s) mechanism.

	Reaction		A^a	n	E^a		A^a	n	E^a
1	$H + O_2 \rightleftharpoons OH + O$	k_f	3.52×10^{16}	−0.7	71.42	k_b	7.04×10^{13}	−0.26	0.60
2	$H_2 + O \rightleftharpoons OH + H$	k_f	5.06×10^{4}	2.67	26.32	k_b	3.03×10^{4}	2.63	20.23
3	$H_2 + OH \rightleftharpoons H_2O + H$	k_f	1.17×10^{9}	1.3	15.21	k_b	1.28×10^{10}	1.19	78.25
4	$H + O_2 + M \rightharpoonup HO_2 + M$ [b]	k_0	5.75×10^{19}	−1.4	0.0	k_∞	4.65×10^{12}	0.44	0.0
5	$HO_2 + H \rightharpoonup 2OH$		7.08×10^{13}	0.0	1.23				
6	$HO_2 + H \rightleftharpoons H_2 + O_2$	k_f	1.66×10^{13}	0.0	3.44	k_b	2.69×10^{12}	0.36	231.86
7	$HO_2 + OH \rightharpoonup H_2O + O_2$		2.89×10^{13}	0.0	−2.08				
8	$H + OH + M \rightleftharpoons H_2O + M$ [c]	k_f	4.00×10^{22}	−2.0	0.0	k_b	1.03×10^{23}	−1.75	496.14
9	$2H + M \rightleftharpoons H_2 + M$ [c]	k_f	1.30×10^{18}	−1.0	0.0	k_b	3.04×10^{17}	−0.65	433.09
10	$2HO_2 \rightharpoonup H_2O_2 + O_2$		3.02×10^{12}	0.0	5.8				
11	$HO_2 + H_2 \rightharpoonup H_2O_2 + H$		1.62×10^{11}	0.61	100.14				
12	$H_2O_2 + M \rightharpoonup 2OH + M$ [d]	k_0	8.15×10^{23}	−1.9	207.62	k_∞	2.62×10^{19}	−1.39	214.74

	4 steps [3]
Elementary steps	(I) $3H_2 + O_2 = 2H_2O + 2H$ (II) $2H + M = H_2 + M$ (III) $H_2 + O_2 = HO_2 + H$ (IV) $H_2 + O_2 = H_2O_2$
Transported species	**7 species** H_2 O_2 H_2O H HO_2 H_2O_2 + N_2
Steady species	**2 species** OH O
Comments	• Extended to $T < T_c$ • Successful convergence of the CFD solver.

$$
\begin{aligned}
\omega_{\mathrm{I}} &= \omega_1 + \omega_{5f} + \omega_{12f}, \\
\omega_{\mathrm{II}} &= \omega_{4f} + \omega_8 + \omega_9 - \omega_{10f} - \omega_{11f}, \\
\omega_{\mathrm{III}} &= \omega_{4f} - \omega_{5f} - \omega_6 - \omega_{7f} - 2\omega_{10f} - \omega_{11f}, \\
\omega_{\mathrm{IV}} &= \omega_{10f} + \omega_{11f} - \omega_{12f}.
\end{aligned}
$$

$$
C_{\mathrm{OH}} = \frac{\sqrt{A_1^2 + 4A_0A_2} - A_1}{2A_2},
$$

$$
C_{\mathrm{O}} = \frac{k_{1f} C_{\mathrm{H}} C_{\mathrm{O_2}} + k_2 C_{\mathrm{OH}} C_{\mathrm{H}}}{k_{1b} C_{\mathrm{OH}} + k_{2f} C_{\mathrm{H_2}}}.
$$

[1] Boivin, Jimenez, Sanchez & Williams, Proceeding of the Combustion Institute, 33 (2011) 517-523
[2] Boivin, Dauptain, Jimenez & Cuenot, Combustion and Flame, 159 (2012) 1779-1790
[3] Boivin, Sanchez & Williams, Combustion and Flame, 160 (2013) 76-82

Numerical setup – Chemical mechanism

- Boivin *et al.* reduced mechanisms
  - **4 reactions + 7 species (+ 2 "steady-state" species)**
  - Reaction rates correction due to QSSA applied to O and OH
    - **Steady-state parameter** on HO_2 and H

$$SS_\alpha = \left(\frac{\text{Prod. rate - Consum. rate}}{\text{Prod. rate}} \right)_\alpha \tag{4.4}$$

    - **Reactivity** λ (s^{-1})

$$\lambda = \frac{\sqrt{l_1^2 + 4 l_0 l_2} - l_1}{2 l_2} \propto \frac{1}{\tau_{\mathrm{igni}}} \quad \text{with} \quad \begin{cases} l_2 = k_1 C_{O_2} + k_2 C_{H_2} + k_4 C_{O_2} C_M \\ l_1 = k_2 k_3 C_{H_2}^2 + (k_2 + k_3) k_4 C_{H_2} C_{O_2} C_M \\ l_0 = (2 k_1 C_{O_2} - k_4 C_{O_2} C_M) k_2 k_3 C_{H_2}^2 \end{cases} \tag{4.5}$$

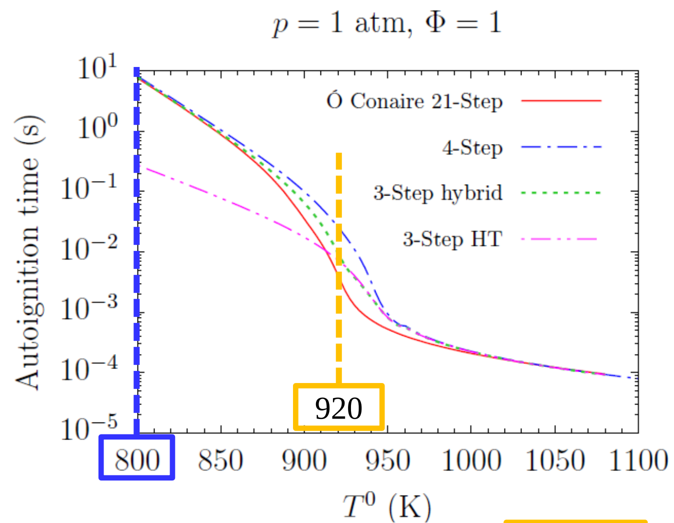
    - **Scale factor** Λ (adim.)

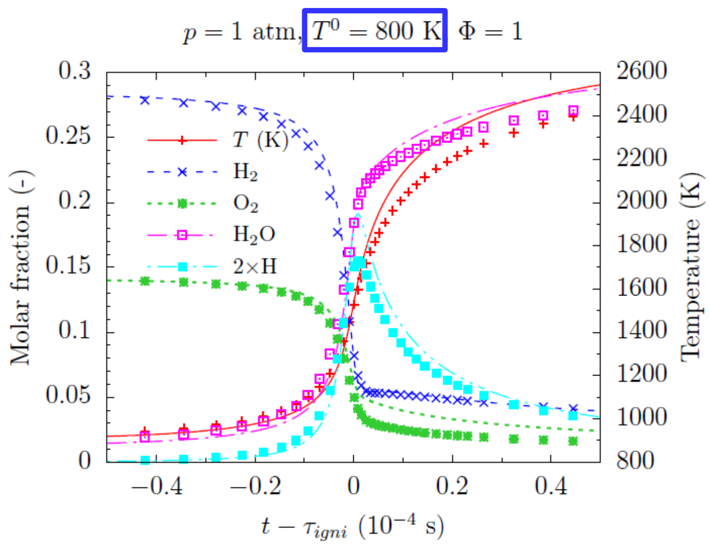
$$\Lambda = \begin{cases} \dfrac{\lambda}{(2k_1 - k_4) C_{O_2}} & \text{if } SS_{HO_2} \text{ and } SS_H < \varepsilon \\ 1 & \text{otherwise} \end{cases} \tag{4.6}$$

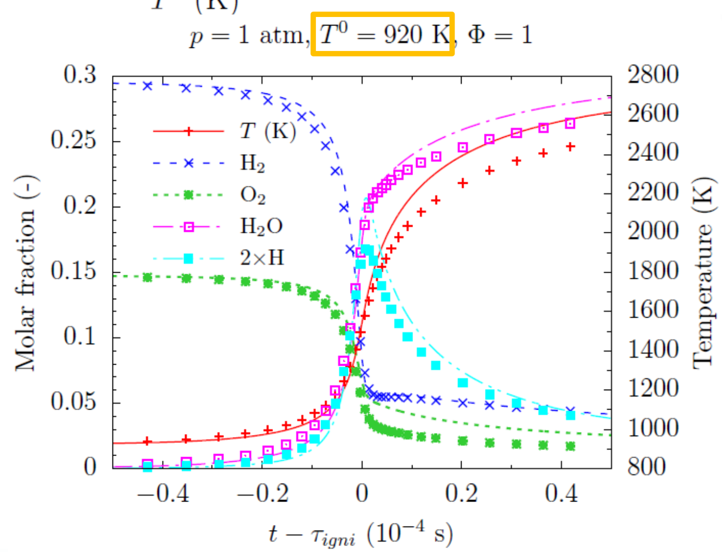
$$\omega_n^* = \Lambda \omega_n, \quad \forall n \in \{\mathrm{I, II, III, IV}\} \tag{4.7}$$

Numerical setup – Chemical mechanism

- Some implementation verifications







Lines = 4-Steps
Symbols = 21-Steps

Contents

Implicit reactive LES of the JISCF

- **Implicit model**: PSR / quasi-laminar / Arrhenius / ILES [1, 2, 3]
  - assumes species are **perfectly stirred** inside the computational mesh ⇔ **homogeneous composition and temperature** at the SGS level

$$\tilde{\dot{\omega}}_\alpha(\rho, T, \boldsymbol{Y}) = \breve{\dot{\omega}}_\alpha = \dot{\omega}_\alpha(\bar{\rho}, \tilde{T}, \tilde{\boldsymbol{Y}})$$

  - validity [1]: negligible SGS fluctuations, Damköhler number $\mathrm{Da}_{\mathrm{sgs}} = \tau_{\mathrm{sgs}}/\tau_c$ <<1

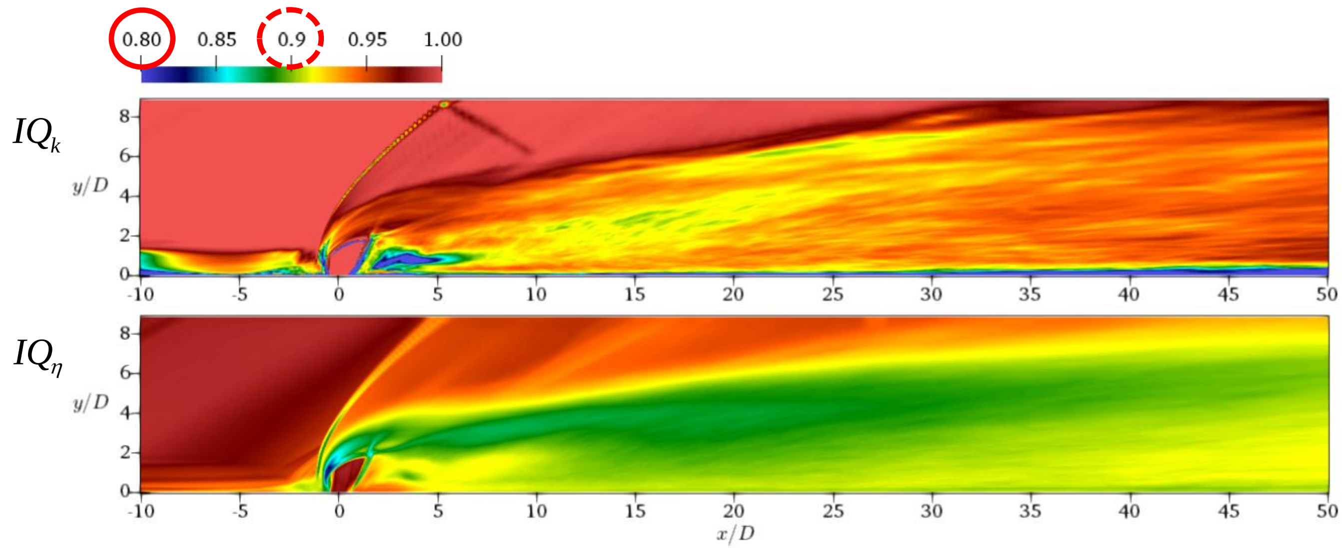
  Where $\tau_c = \left|\left\{\tilde{\dot{\omega}}_\alpha\right\}\right|^{-1}$ and $\tau_{\mathrm{sgs}} = \Delta^2/D_{\mathrm{sgs}}$

- Numerical setup
  - *Initial condition*: established non-reactive flow
  - *Simulated physical time*: t = 170 D/u_∞ = 260 µs
  - *CPU time:* 3.6 millions hours

[1] C. Duwig *et al.*, "Large Eddy Simulations of a piloted lean premix jet flame using finite-rate chemistry.," *Combustion Theory and Modelling*, 2011
[2] M. Karaca *et al.*, "Implicit LES of high-speed non-reacting and reacting air/H2 jets with a 5th order WENO scheme.," *Computers & Fluids*, 2012
[3] P. Boivin *et al.*, "Simulation of a supersonic hydrogen–air autoignition-stabilized flame using reduced chemistry.," *Combustion and Flame*, 2012

Implicit reactive LES of the JISCF

- Time-averaged flowfields – resolution criteria in LES



Pope index quality [1, 2]

$$IQ_k = \frac{k}{k + \{k_{sgs}\}}$$

$$IQ_k \geq 0.8 \Leftrightarrow \text{Good resolution}$$

Celik *et al.* index quality [3]

$$IQ_\eta = \frac{1}{1 + \alpha_\eta \left(\Delta / L_\eta\right)^m}$$

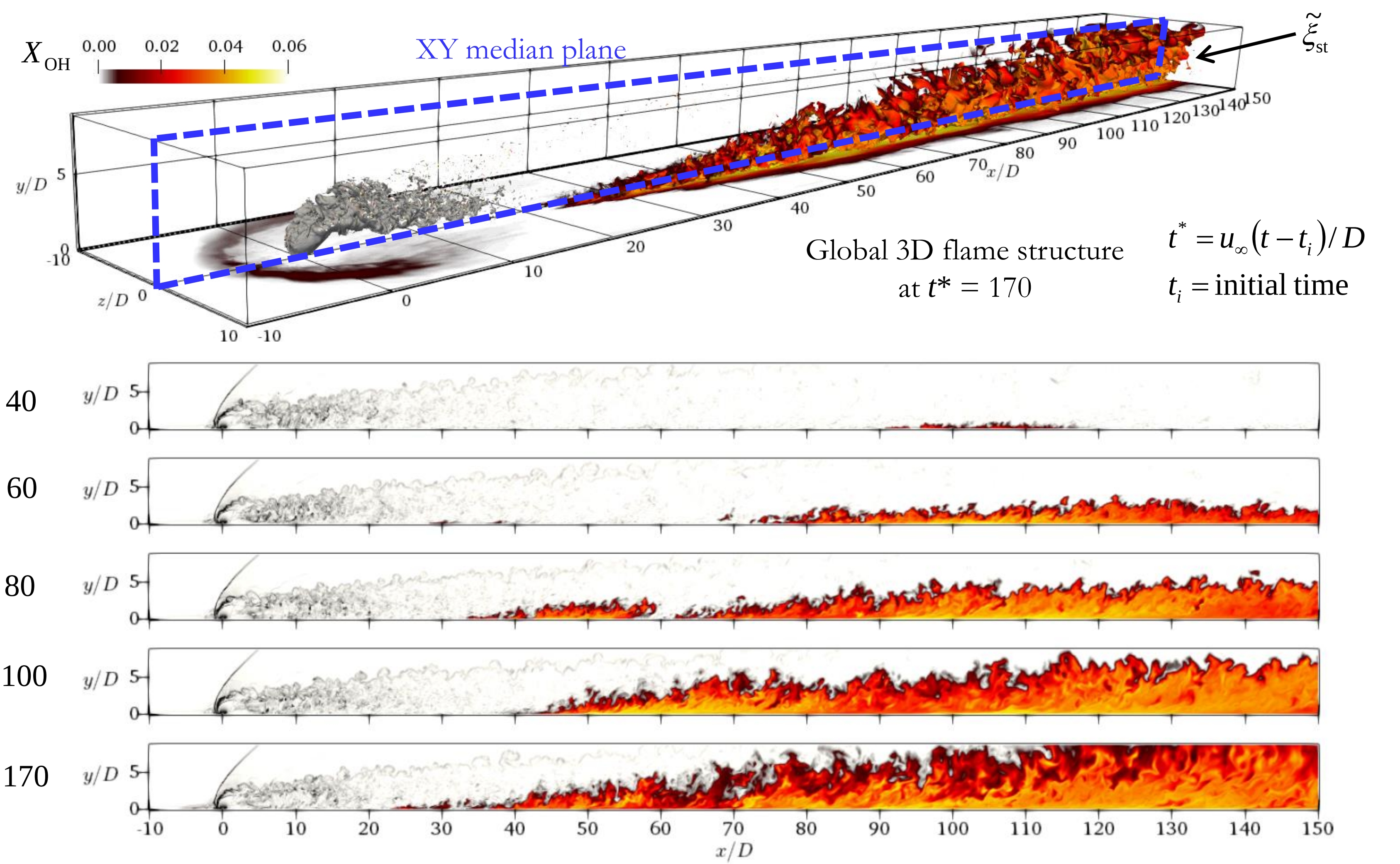
$$(\alpha_\eta, m) = (0.05, 0.5)$$

$$IQ_\eta \geq 0.97 \Leftrightarrow \text{DNS}$$

[1] S. Pope, Ten questions concerning the large-eddy simulation of turbulent flows, *New journal of physics*. 2004
[2] Yoshizawa A., Statistical theory for compressible turbulent shear flows with the application to subgrid modeling, *Physics of Fluids*, 1986
[3] I.B. Celik, Z.N. Cehreli, I. Yavuz, Index of resolution quality for large eddy simulations, *J. Fluids Eng.*, 2005

(results with Smagorinsky model & mesh 1)

Implicit reactive LES of the JISCF



Global 3D flame structure at $t^* = 170$

$t^* = u_\infty (t - t_i)/D$

t_i = initial time

Implicit reactive LES of the JISCF – Reactive flow structure

- Comparison with similar cases in literature (simulation)

Parameters	Ingenito et al. [1]	Present simulation
J	0.5	2.56
Φ	0.426	0.4
Ma_∞	2.79	2
T_∞ / T_0 (K)	1229 / 3140	1100 / 1700
p_∞ (kPa)	82	56
Wall	adiabatic	adiabatic

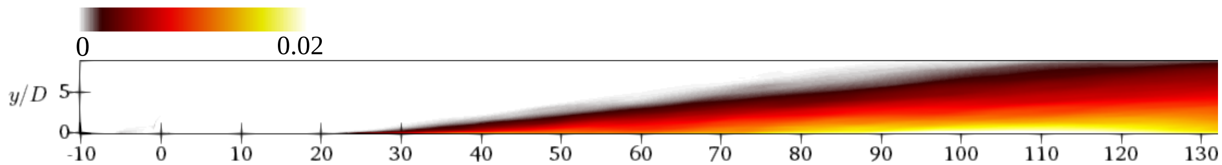
[1] Ingenito, A., Cecere, D. and Giacomazzi, E. "Large-Eddy Simulation of turbulent hydrogen fuelled supersonic combustion in an air cross-flow". *Shock Waves* 23 (2013), pp. 481–494

Implicit reactive LES of the JISCF

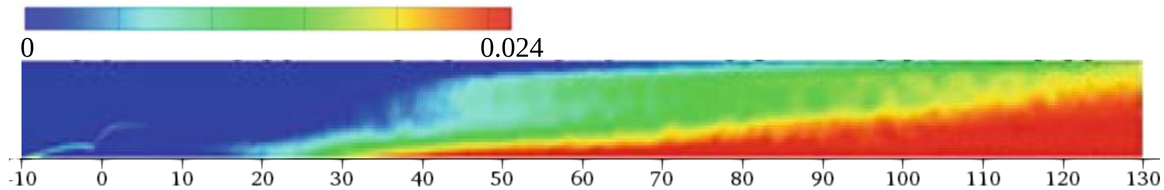
- Comparison with similar cases in literature (simulation)

Present simulation

XY plane at $z/D = 0$

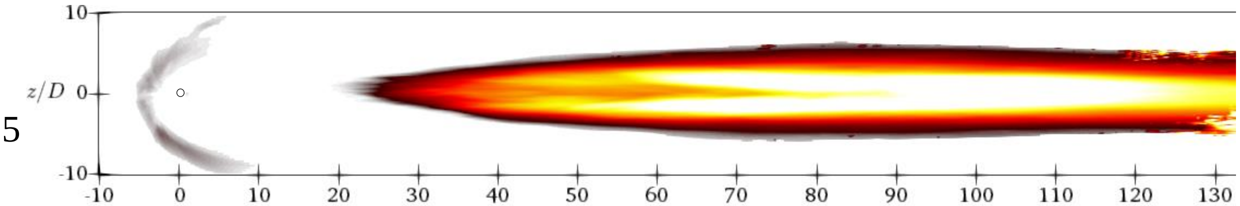


Ingenito *et al.*[1]



Present simulation

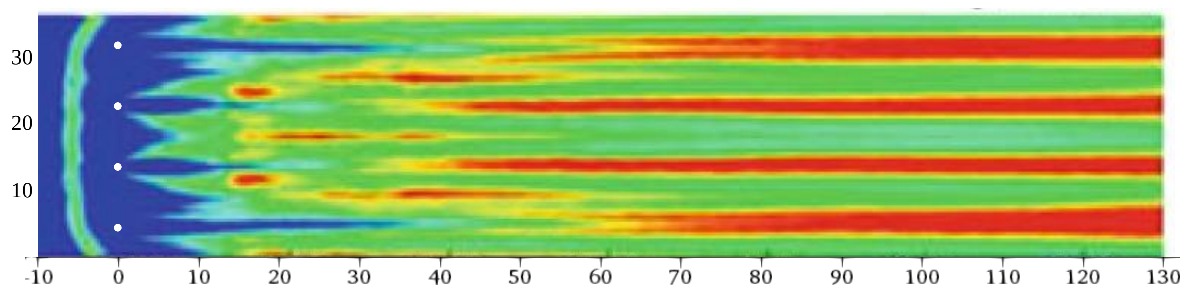
XZ plane at $y/D = 0.25$



Ingenito *et al.*[1]

(multiple injection)

XZ plane at $y/D = 0.25$



[1] Ingenito, A., Cecere, D. and Giacomazzi, E. “Large-Eddy Simulation of turbulent hydrogen fuelled supersonic combustion in an air cross-flow”. *Shock Waves* 23 (2013), pp. 481–494

Contents

Explicit reactive LES of the JISCF

- **Main issue in turbulent (SGS) combustion modeling**

$$\widetilde{\dot{\omega}}_\alpha = \underbrace{\breve{\dot{\omega}}_\alpha}_{\text{Resolved}} + \underbrace{\left(\widetilde{\dot{\omega}}_\alpha - \breve{\dot{\omega}}_\alpha\right)}_{\text{Subgrid scale}}$$

  – 2 solutions:
    1. model directly $\widetilde{\dot{\omega}}_\alpha$ from physical consideration
    2. model the SGS part

- **Implicit model**: PSR / quasi-laminar / Arrhenius / ILES [1, 2, 3]
  – assume species are **perfectly stirred** inside the computational mesh
  ⬄ **homogeneous composition and temperature**

$$\widetilde{\dot{\omega}}_\alpha(\rho,T,\boldsymbol{Y}) = \breve{\dot{\omega}}_\alpha = \dot{\omega}_\alpha(\overline{\rho},\widetilde{T},\widetilde{\boldsymbol{Y}})$$

  – validity [1]: negligible SGS fluctuations, Da < 1 (fast mixing / slow chemistry)

[1] C. Duwig *et al.*, "Large Eddy Simulations of a piloted lean premix jet flame using finite-rate chemistry.," *Combustion Theory and Modelling*, 2011
[2] M. Karaca *et al.,* "Implicit LES of high-speed non-reacting and reacting air/H2 jets with a 5th order WENO scheme.," *Computers & Fluids*, 2012
[3] P. Boivin *et al.*, "Simulation of a supersonic hydrogen–air autoignition-stabilized flame using reduced chemistry.," *Combustion and Flame*, 2012

Explicit reactive LES of the JISCF

- **Taylor series development of the reaction rate** [1]
  - for one-step mechanism

$$\tilde{\dot{\omega}}_F = -A\tilde{T}^b \tilde{Y}_F \tilde{Y}_O \exp(-T_a/\tilde{T})\left(1+\alpha_{\text{sgs}}+\ldots\right) \quad \text{with} \quad \underbrace{\alpha_{\text{sgs}} = \frac{\widetilde{Y_F Y_O} - \tilde{Y}_F \tilde{Y}_O}{\tilde{Y}_F \tilde{Y}_O}}_{\text{Segregation rate}} \quad \text{(0 well mixed)} \qquad (6.3)$$

  - in the small Da limit

$$\tilde{\dot{\omega}}_F \underset{\text{Da}<1}{=} \underbrace{\breve{\dot{\omega}}_F}_{\text{Resolved}} + \underbrace{\alpha_{\text{sgs}} \breve{\dot{\omega}}_F}_{\text{SGS}}$$

- ***New proposal*** **: hybrid turbulent combustion model**

SGS variance to model…

$$\tilde{\dot{\omega}}_\alpha(\rho,T,\mathbf{Y}) = \underbrace{(1-S_\xi)\dot{\omega}_\alpha(\bar{\rho},\tilde{T},\tilde{\mathbf{Y}})}_{\substack{\text{Resolved} \\ \text{(laminar chemistry)}}} + \underbrace{S_\xi \tilde{\dot{\omega}}_\alpha^{\text{sgs}}}_{\text{SGS}} \quad \text{with} \quad \underbrace{S_\xi = \frac{\tilde{V}_\xi}{\tilde{\xi}(1-\tilde{\xi})}}_{\text{Segregation rate}} \in \begin{cases} 0 & \text{well mixed} \\ 1 & \text{otherwise} \end{cases} \qquad (6.4)$$

  - inspired from the bridging type model for SDR [2]
  - if $S_\xi \rightarrow 0$: **laminar chemistry = PSR** (consistent with DNS limit)
  - otherwise: **SGS contribution** = **Intermittent Lagrangian Model (MIL) [3]** $\tilde{\dot{\omega}}_\alpha^{\text{sgs}} = \tilde{\dot{\omega}}_\alpha^{\text{MIL}}$

↳ *1st application for LES*

[1] Borghi R., *Réactions chimiques en milieu turbulent*. Thèse d'état, Université Pierre et Marie Curie, 1978

[2] Mura A., Robin V. and Champion M. "Modeling of scalar dissipation in partially premixed turbulent flames". *Combustion and Flame* (2007)

[3] Mura A. & Demoulin F.X., "Lagrangian intermittent modelling of turbulent lifted flames", *Combustion Theory and Modelling* (2007)

Explicit reactive LES of the JISCF

- **Intermittent Lagrangian Model (MIL)** [1, 2, 3]
  - *hypothesis*: **sudden chemistry**
    - based on a **PaSR** behavior
    - **statistical dependence** between progress variable Y_O and mixing variable ξ
  - based on the competition between
    - *flow mechanism*: large eddies **convection** (residence time), **SGS mixing** (micro-mixing)
    - *chemical mechanism*: flame (**diffusion/reaction**), **ignition**
  - **Instantaneous** chemical reaction rate
    - **Interaction by Exchange with the Mean (IEM)**

$$\left\{ \frac{d\xi}{dt} = \frac{\tilde{\xi} - \xi}{\tau_\xi} ; \quad \frac{dY_\alpha}{dt} = \frac{\tilde{Y}_\alpha - Y_\alpha}{\tau_{Y_\alpha}} + \omega_\alpha \right\}$$

    - **Sudden chemistry hypothesis** ➔ $\boxed{Y_\alpha = Y_\alpha^{\mathrm{MIL}}(\xi) \text{ MIL trajectory in compositions space}}$

$$\omega_\alpha = \omega_{O_2}^{\mathrm{MIL}}(\tau, Y_O^{\mathrm{MIL}}, \xi) = \frac{1}{\tau}\left[\frac{d\boxed{Y_O^{\mathrm{MIL}}(\xi)}}{d\xi}\left(\tilde{\xi} - \xi\right) - \left(\tilde{Y}_O - \boxed{Y_O^{\mathrm{MIL}}(\xi)}\right) \right]$$

[1] Borghi & Gonzalez, *Combustion and Flame*, 1986

[2] A. Mura & F.X. Demoulin, *Combustion Theory and Modelling* Vol. 11 pp. 227-257, 2007

[3] L. Gomet, V. Robin & A. Mura, *Combustion Science and Technology*, 2012

Explicit reactive LES of the JISCF

- Numerical setup
  - same as the previous reactive simulation
  - *Hybrid turbulent combustion model*

$$\tilde{\dot{\omega}}_\alpha(\rho,T,\boldsymbol{Y}) = (1-S_\xi)\dot{\omega}_\alpha^{\mathrm{PSR}}(\bar{\rho},\tilde{T},\tilde{\boldsymbol{Y}}) + S_\xi \tilde{\dot{\omega}}_\alpha^{\mathrm{MIL}}$$

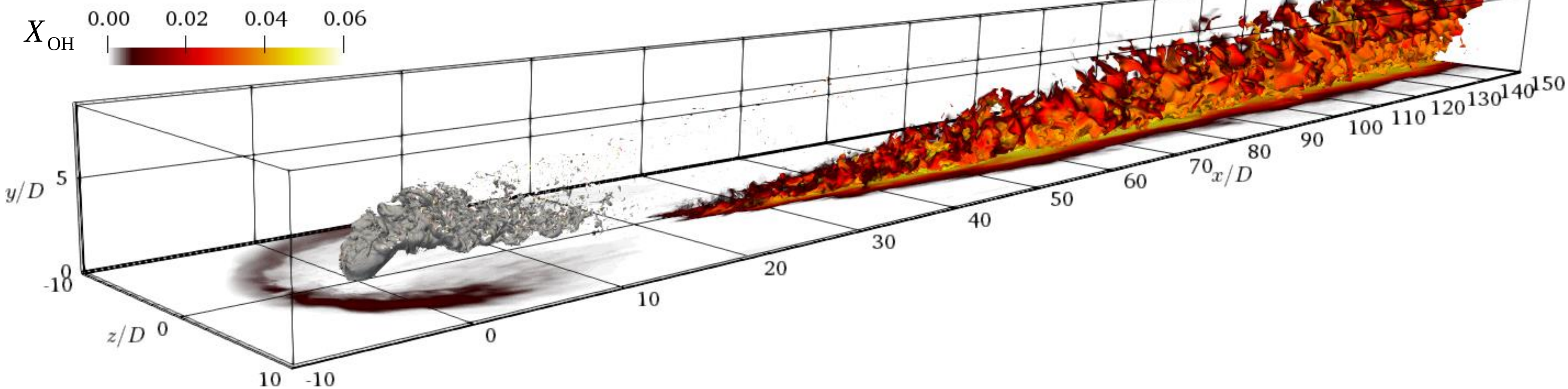
    - *MIL chemical time scale tabulation*
      - replaced by *analytical calculation*, using reactivity $\lambda \sim t_{igni}^{-1}$
      - from local concentration & temperature
      - compare to classical pre-tabulation save 14 % computational time [2]
  - *Simulated physical time*: $t = 170\ D/u_\infty = 260\ \mu s$

[1] Gomet, L., Robin, V. & Mura, A. "Influence of Residence and Scalar Mixing Time Scales in Non-Premixed Combustion in Supersonic Turbulent Flows". *Combustion Science and Technology* 184 (2012)

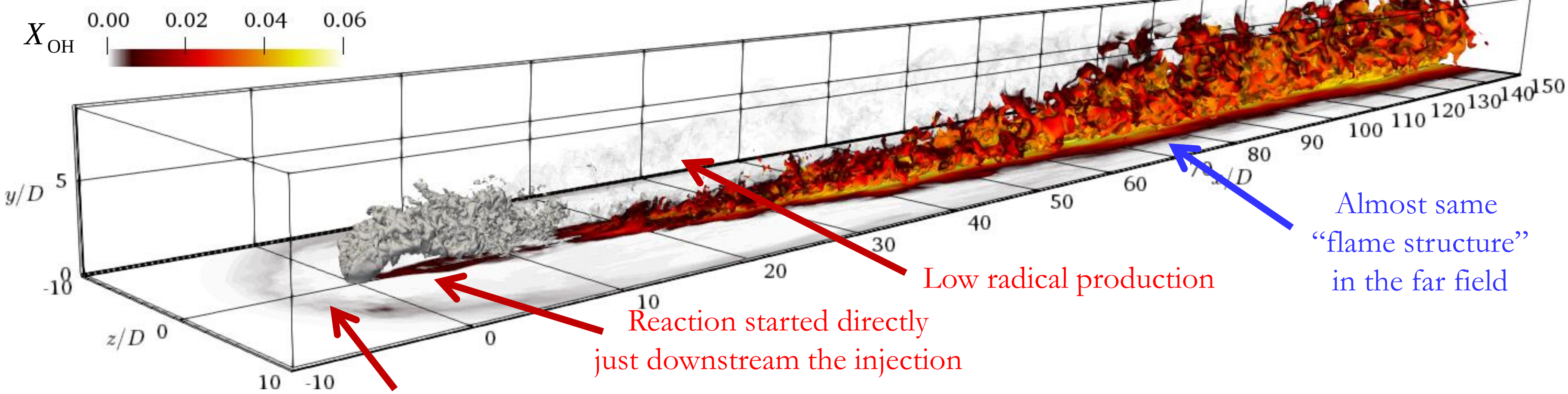
[2] Bridel-Bertomeu T., & Boivin P.. "Explicit Chemical Timescale as a Substitute for Tabulated Chemistry in a H_2–O_2 Turbulent Flame Simulation". *Combustion Science and Technology* 187 (2015),

Explicit reactive LES of the JISCF

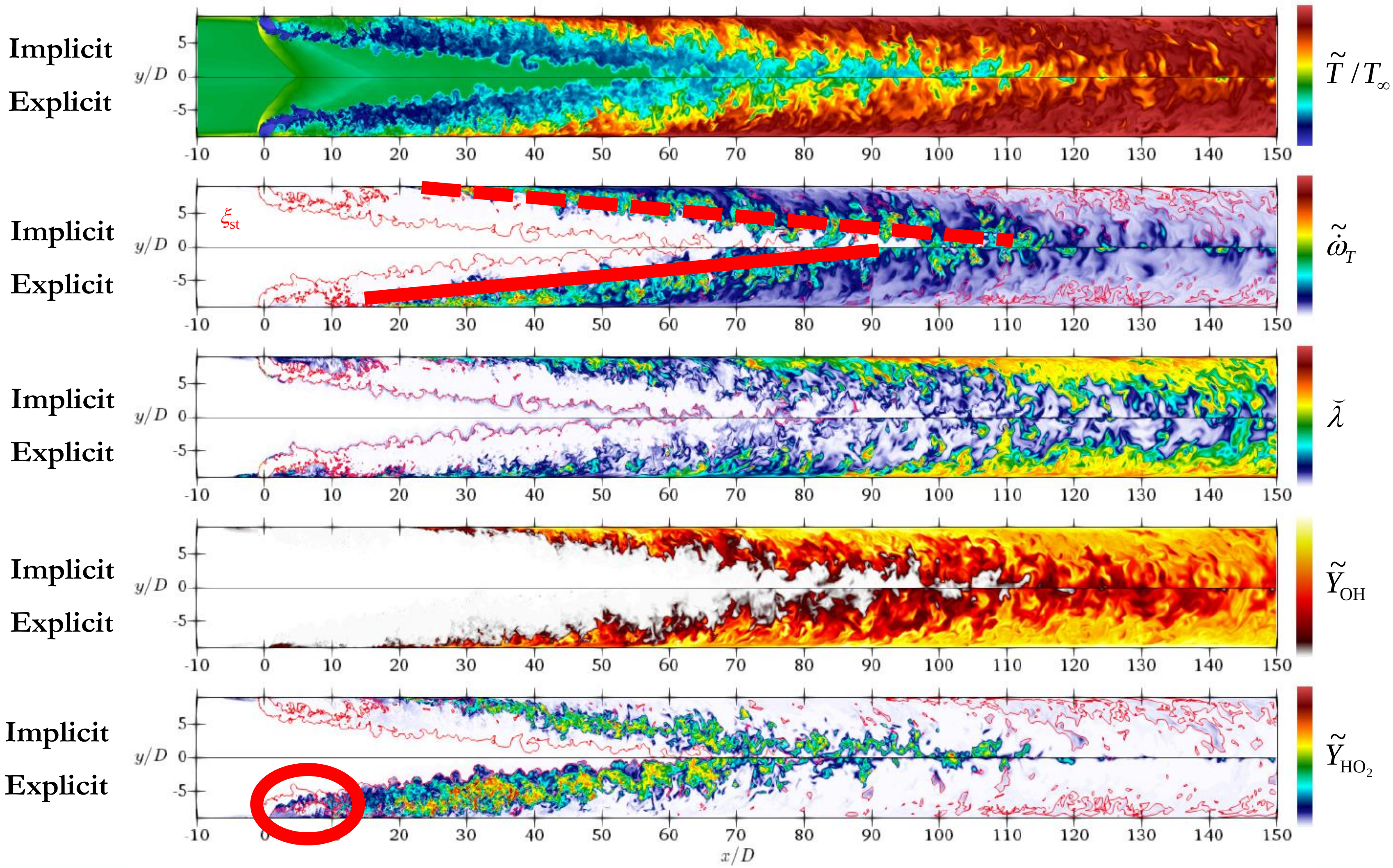
Implicit (PSR model)



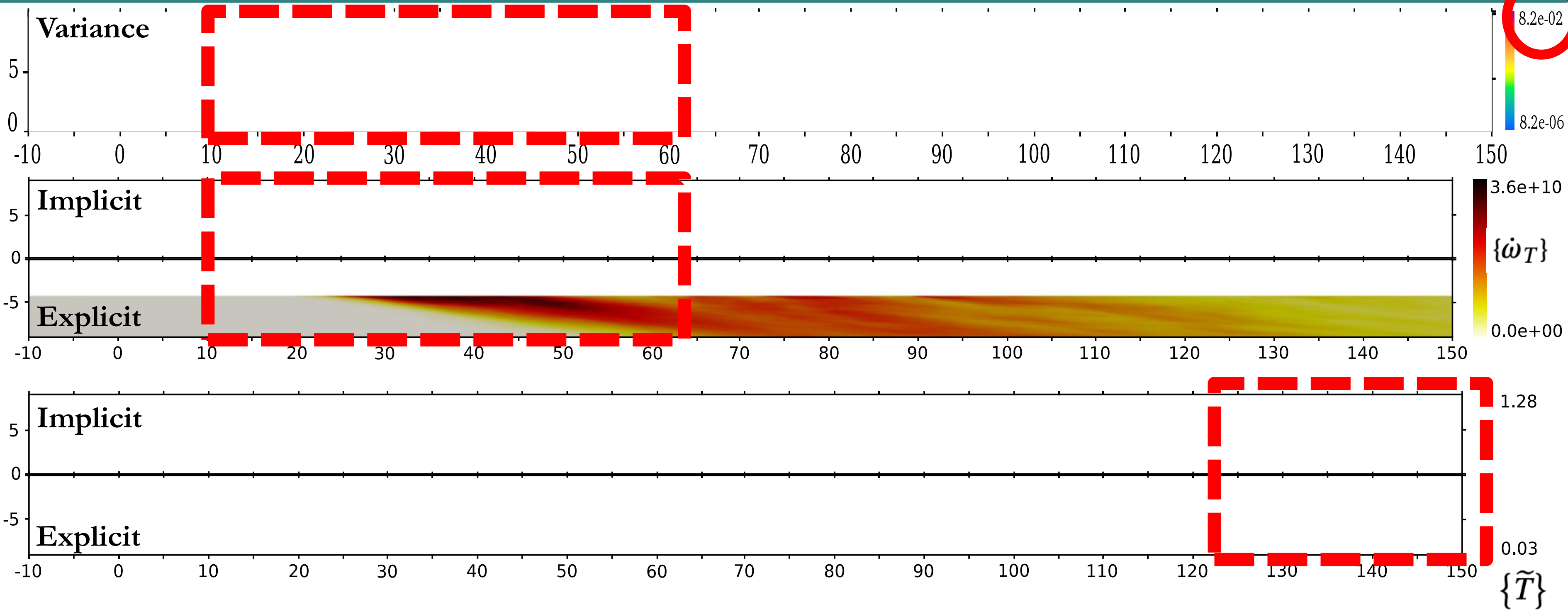
Explicit (hybrid turbulent combustion model)



Explicit reactive LES of the JISCF



Explicit reactive LES of the JISCF



- Hybrid model
  - The stabilization of the reactive zone takes place rather close to the injection port with the Hybrid model
  - The width of the development of the reactive zone is larger
  - Thermal expansion is less important in the far field

Contents

Conclusions and prospects

- Conclusions
  - Introduction of a new LES closure to describe the departure from PSR limit in supersonic reactive flows
  - Most striking differences are obtained in the near field of the Hydrogen injection
    - ✓ The impact of residual SGS fluctuations of composition may indeed be non-negligible

- Prospects
  - More quantitively inspection is in progress (especially complementary statistical analysis)
  - should be validated in simpler cases
  - should be tested for various resolution levels