It's in ME

Computational Combustion and Energy Group

NUS National University of Singapore

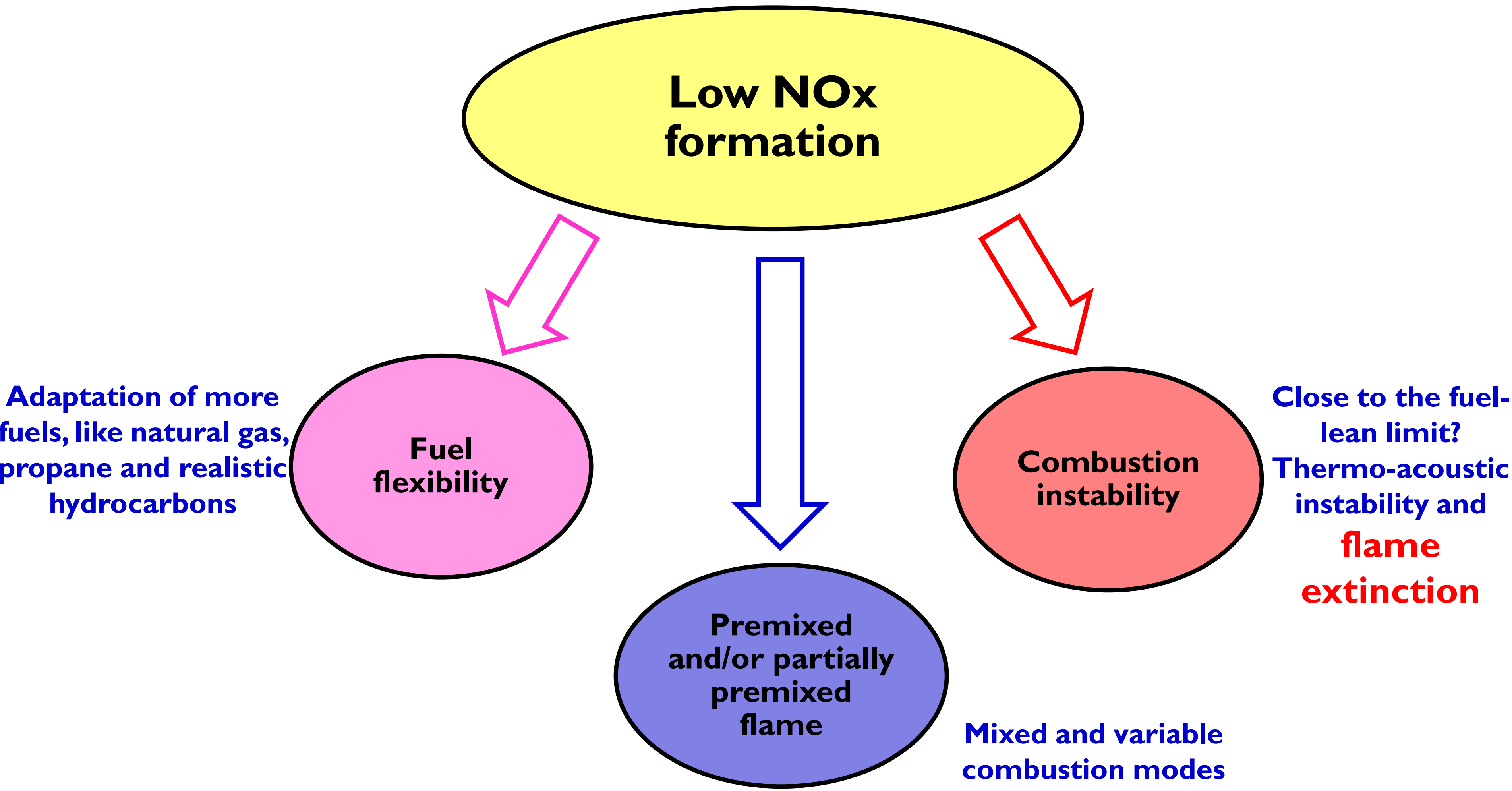
Department of Mechanical Engineering
Faculty of Engineering

Clean Combustion Technology

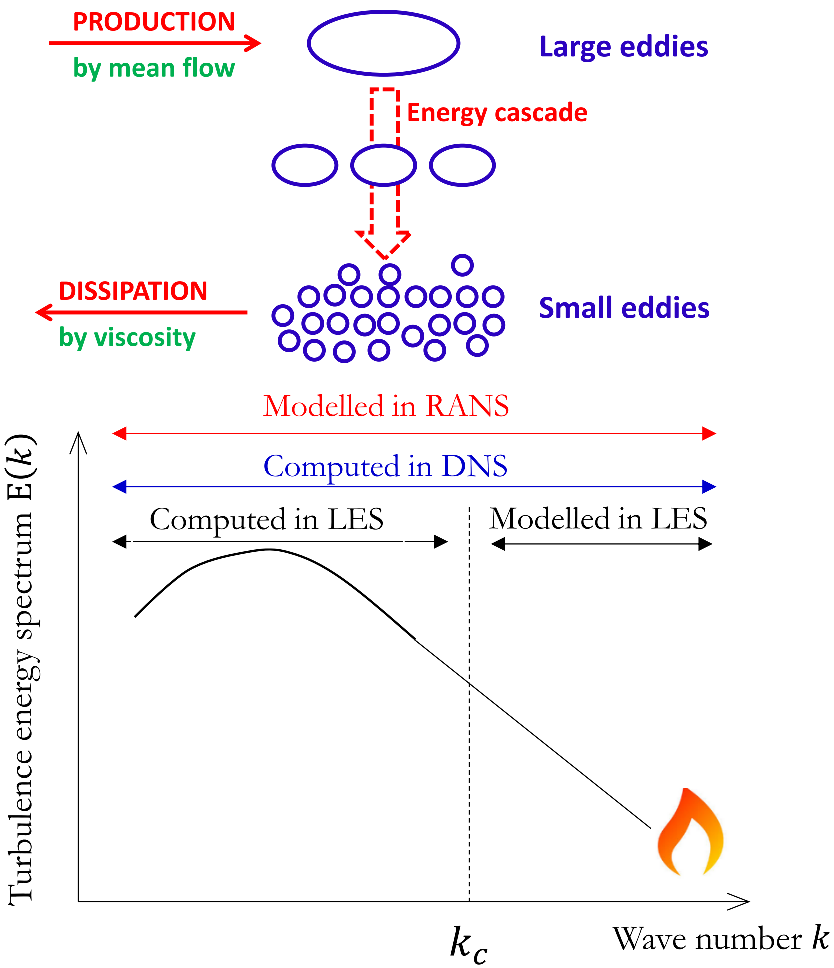
- **Decrease pollutant emission (mainly nitrogen oxides NOx)**
- **Increase combustion efficiency**

Innovative combustion Technologies ⇔ **Alternative Fuels**

❖ **low NOx (nitrogen oxide) emission ←→ Fuel lean combustion**



Multi-scale and nonlinearity in turbulence & combustion



Kolmogorov turbulence spectrum

A Hypothetical Chemical Mechanism

$$A + B \rightarrow C + F$$

$$B + F \rightarrow C + D$$

$$A + C \rightarrow E$$

$$B + D \rightarrow G$$

Nonlinearity in Arrhenius-type reaction rate:

$$\dot{\omega}_F = \dot{\omega}_F(Y_1 \dots Y_\alpha, T) = -AT^\beta Y_F Y_O exp\left(-\frac{T_A}{T}\right)$$

Is **Direct Numerical Simulation** of Turbulent Combustion Possible?

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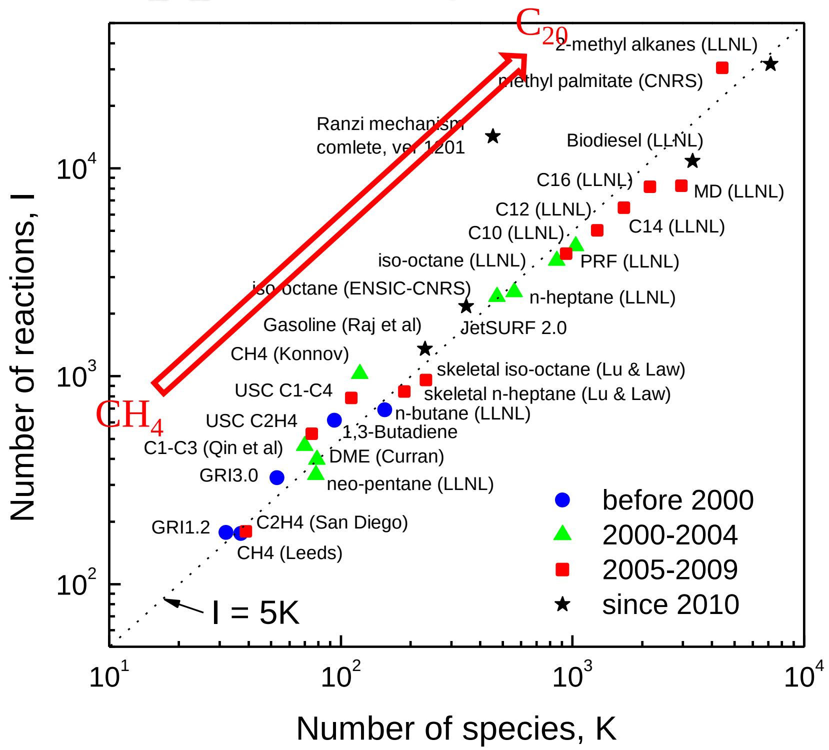
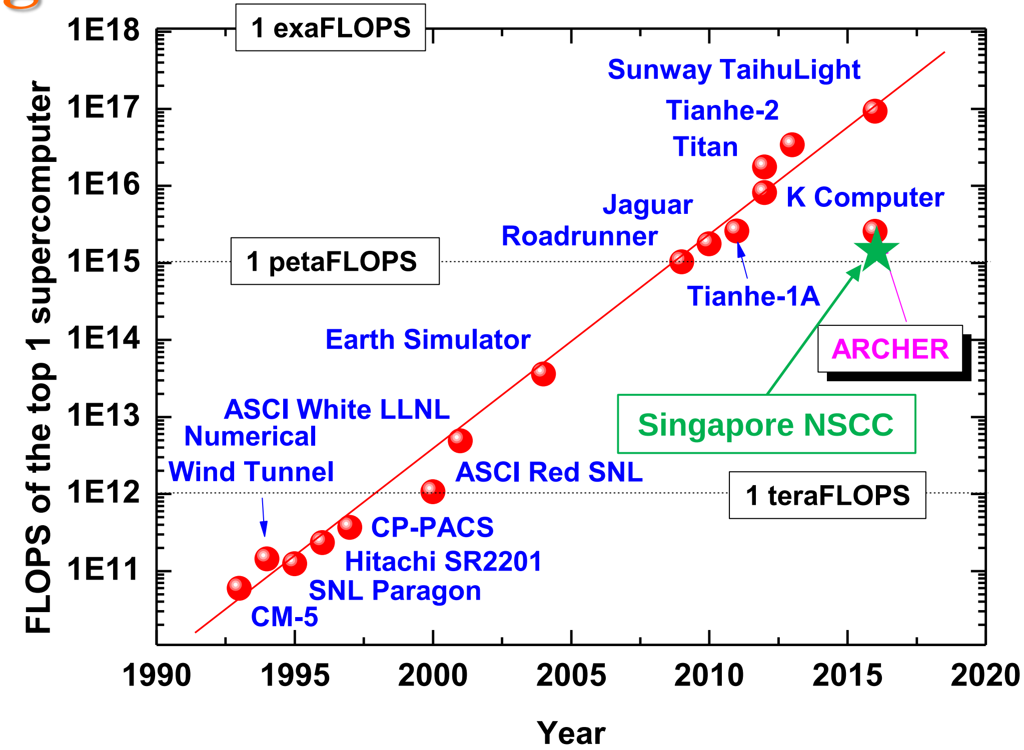
Opportunity and challenge in numerical combustion



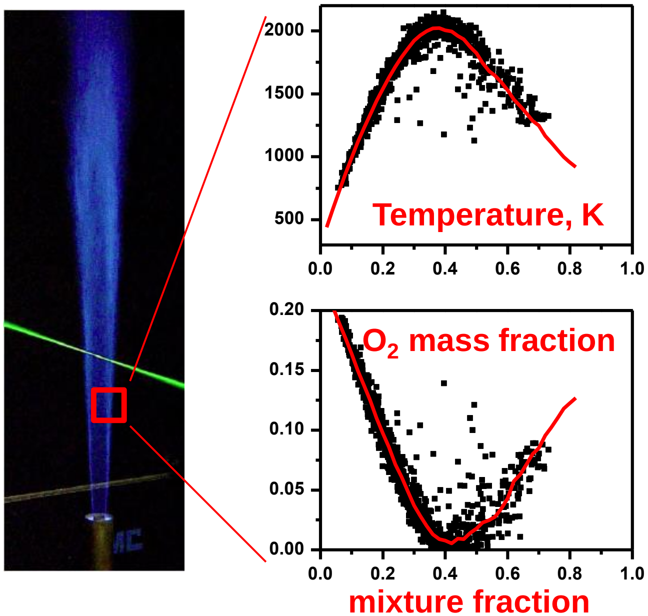
(Lu & Law, Prog. Energy Combust. Sci. 2009)



(Data source: Top 500 Supercomputer Website)

Is Direct Numerical Simulation of **Realistic** Turbulent Combustion with **Detailed** Chemistry Possible?

Conditional Moment Closure (CMC) Model



Sandia flame D
Barlow and Frank, Proc. Combust. Inst. 1998

$$\widetilde{\omega_\alpha} \neq \omega_\alpha\left(\tilde{Y}_1 \dots \tilde{Y}_n, \tilde{T}\right)$$

$$\widetilde{\omega_\alpha|\eta} \approx \widetilde{\omega_\alpha}\left(\widetilde{Y_1|\eta}, \dots, \widetilde{Y_n|\eta}, \widetilde{T|\eta}\right)$$

First-order CMC model

- **Five-dimensional Eqs. of species mass fraction ($\widetilde{Y_\alpha|\eta}$) and energy ($\widetilde{h|\eta}$):**

$$\underbrace{\int_{\Omega_{CMC}} \frac{\partial Q_\alpha}{\partial t} d\Omega}_{T_0} + \underbrace{\int_{\Omega_{CMC}} \nabla\cdot\left(\widetilde{\mathbf{U}|\eta} Q_\alpha\right) d\Omega}_{T_1} = \underbrace{\int_{\Omega_{CMC}} Q_\alpha \nabla\cdot\widetilde{\mathbf{U}|\eta}\, d\Omega}_{T_2} + \underbrace{\int_{\Omega_{CMC}} \widetilde{N|\eta}\,\frac{\partial^2 Q_\alpha}{\partial^2 \eta} d\Omega}_{T_3} + \underbrace{\int_{\Omega_{CMC}} \widetilde{\omega_\alpha|\eta}\, d\Omega}_{T_4} + \underbrace{\int_{\Omega_{CMC}} \nabla\cdot\left(D_t \nabla Q_\alpha\right) d\Omega}_{T_5}$$

T1: Convection; *T2*: Dilatation; *T3*: Micro-mixing;
T4: Chemistry; *T5*: Turbulent Scalar Flux

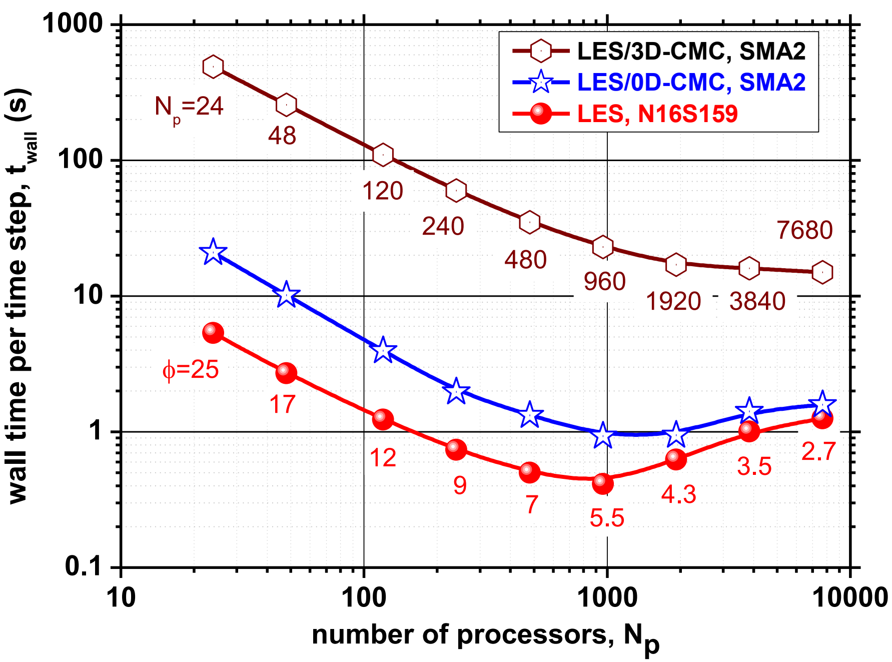
Modeled Terms

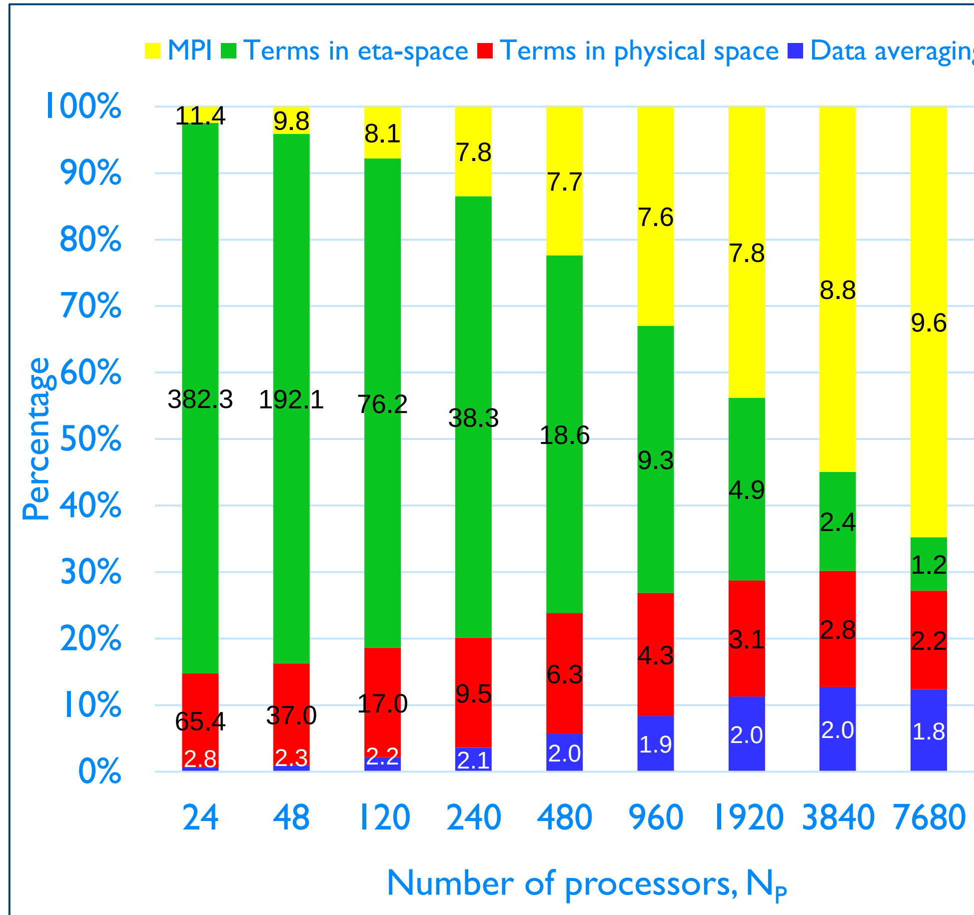
- ✓ $\widetilde{\mathrm{U}|\eta} = \tilde{\mathrm{U}}$
- ✓ $\widetilde{N|\eta}$: amplitude mapping closure (AMC)
- ✓ $\tilde{P}(\eta)$: presumed beta-function
- ✓ $\widetilde{\omega_\alpha|\eta}$: **first order CMC closure, detailed chemistry, ARM2 mechanism**
- ✓ a gradient model used for sub-grid scale scalar flux

Zhang et al., Proc. Combust. Inst. 2015.
Zhang and Mastorakos, Flow Turb Combust 2016.
Garmory and Mastorakos, Proc. Combust Inst 2015.

Sung et al., Proc. Combust. Inst. 1998.
Klimenko and Bilger, Prog. Combust. Energy Sci. 1999.

Parallelization and computational cost





- Perfect loading balancing for parallelized CMC solver: round-robin parallel algorithm $p=mod(n-1, Np)+1$,
- Good scaling for O(10^3) processors on ARCHER Cluster of UK National Supercomputer

Zhang, PhD Thesis, University of Cambridge, Cambridge, UK, 2015.

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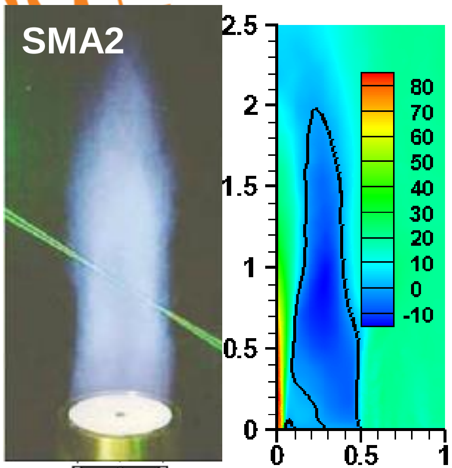
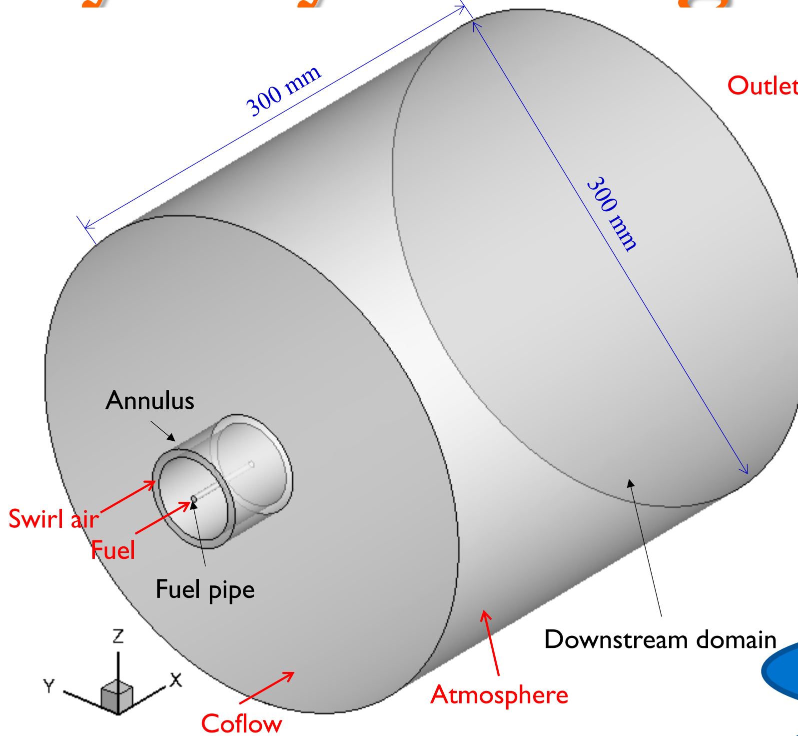
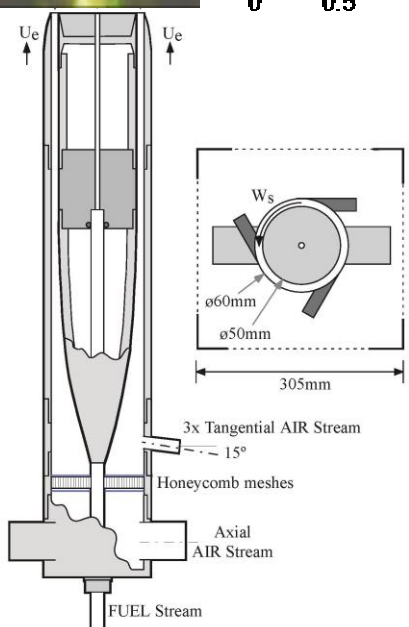
Sydney swirling flames





- One of the target flames in **TNF workshop**, measured by researchers from University of Sydney and Sandia
- Swirl number $S_N = W_S/U_S = 1.59$
- Oxidizer: swirling air; fuel: non-swirling **CH_4/air** (1:2)
- Approximately **8,400,000** tetrahedral LES cells, About **120,000** polyhedral CMC cells

Strong turbulence, increased local extinction



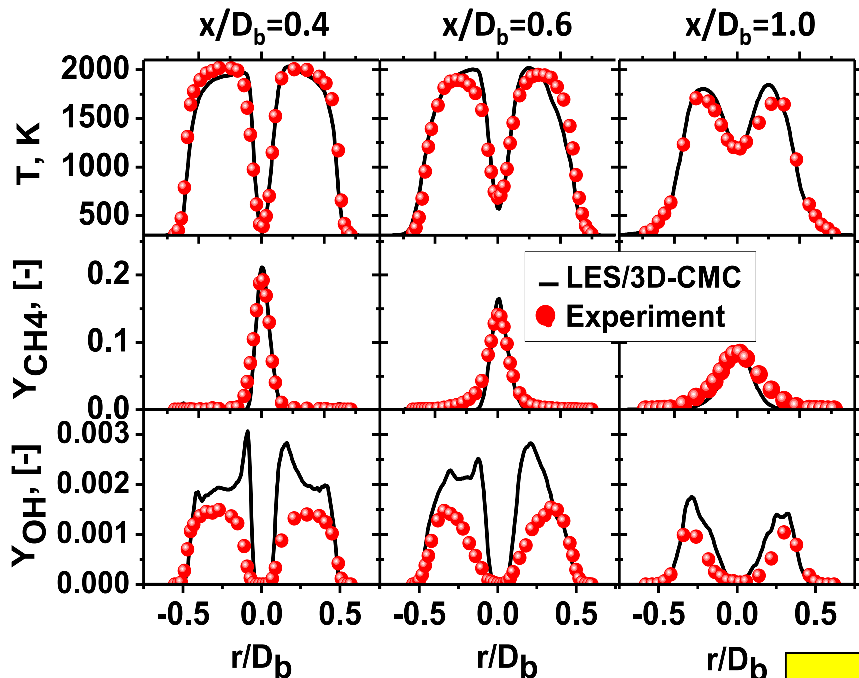
Cases	U_S (m/s)	W_S (m/s)	U_j (m/s)	$U_j / U_{j,SL}$	$\dot{W}$ (kW)	Re_j
SMA2	16.3	25.9	66.3	31%	11.5	15,400
SMA3			132.6	62%	23.0	30,800
SMA4			225.0	104%	39.0	52,300

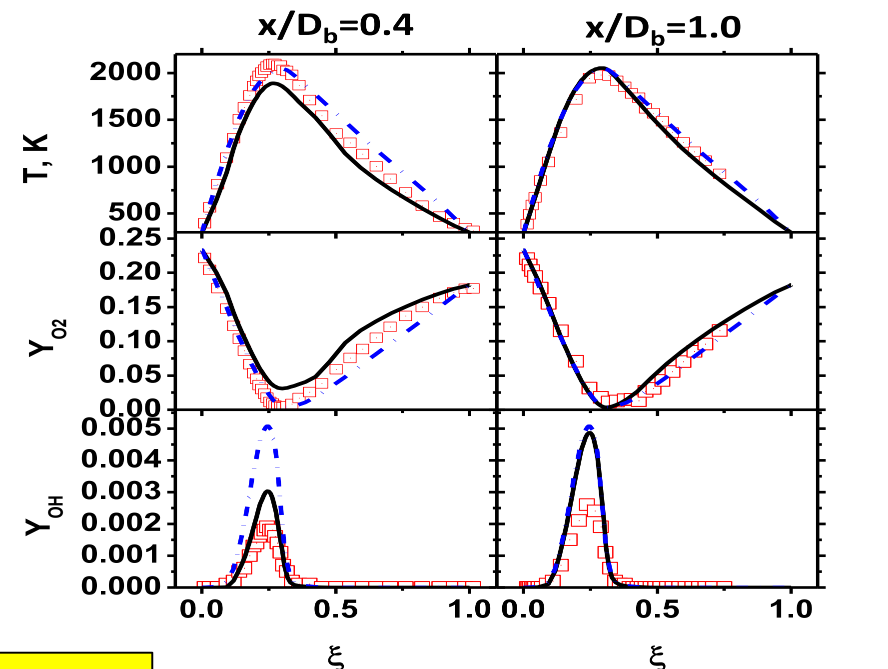
Sydney swirl burner

Masri et al, Combust. Theor. Model. 2007.
Masri et al, Combust. Flame 2004.
Al-Abdeli and Masri, Combust. Theor. Model. 2003.

Reactive scalars

Symbols : Experimental data (Masri et al. CNF 2004)
Solid lines : LES
Dashed lines: 0D-CMC calculation with low scalar dissipation



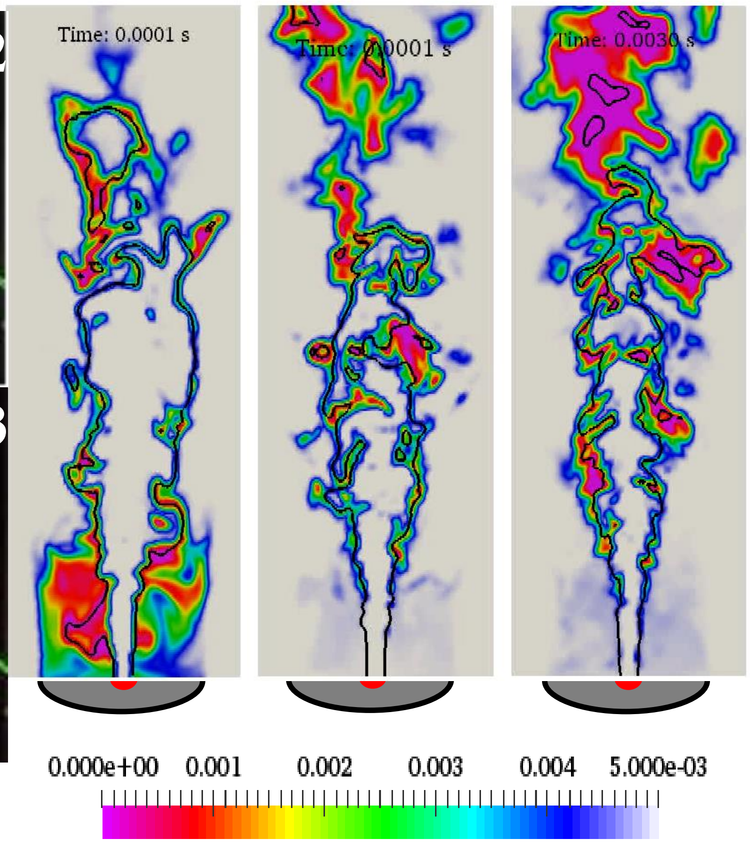


Unconditional scalars $\langle \tilde{f} \rangle$ ⟸ $\tilde{f} = \int_0^1 \widetilde{f|\eta} P(\eta) d\eta$ ⟸ Conditional scalars $\langle \widetilde{f|\eta} \rangle$

1. Unconditional means of temperature and methane mass fraction agree well with experimental data.
2. The conditional temperature and O2 mass fraction are computed well, which are close to the equilibrium flame structures, but the OH is over-predicted in LES.
3. Overall, the current LES/CMC solver demonstrates good accuracy in predicting the reactive scalars of this simulated flame.

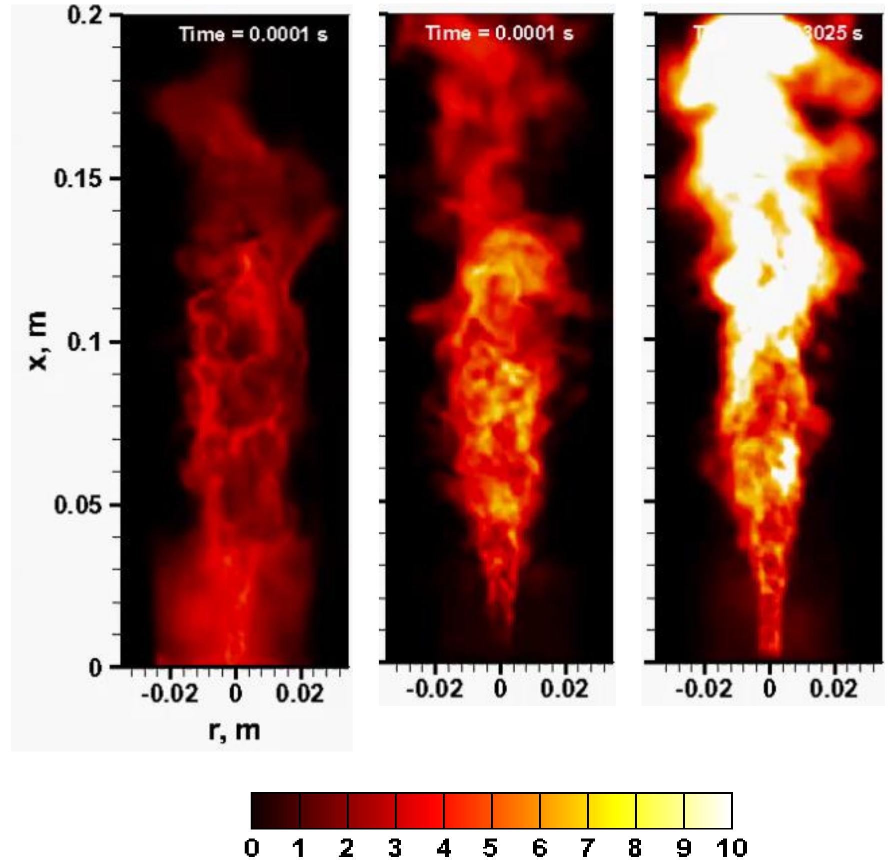
Time evolutions of OH and heat release rate

SMA2 SMA3 SMA4



Resolved **OH** mass fraction (OH-PLIF-like)
(black iso-lines: stoi. mixture fraction 0.25)

SMA2 SMA3 SMA4



Line-of-sight **integrated heat release rate** (MJ/m^2s)
(OH* chemiluminescence-like)

Experimental flame photos from: http://sydney.edu.au/engineering/aeromech/thermofluids/swirl.htm

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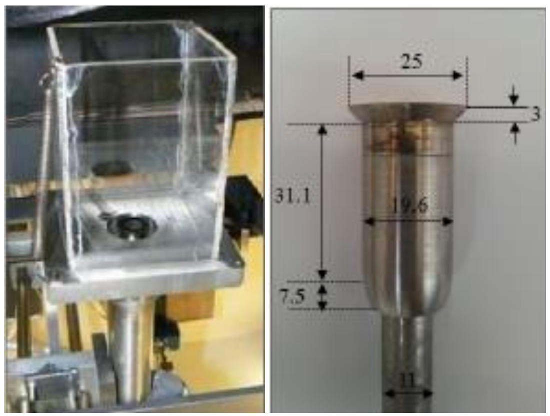
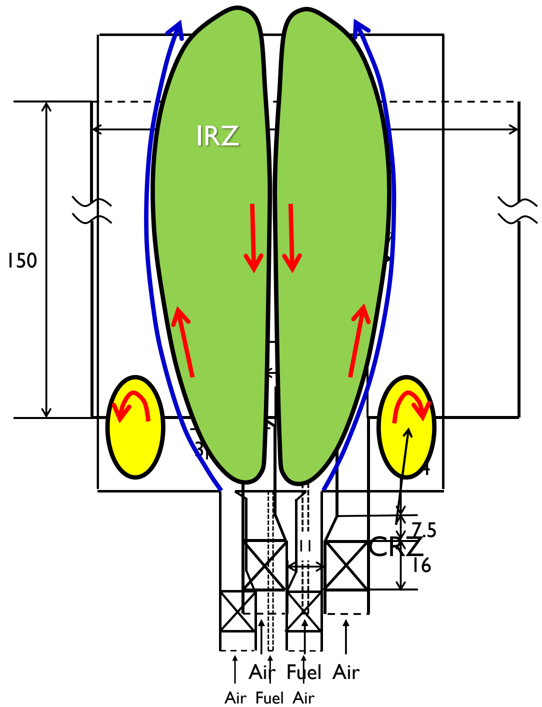
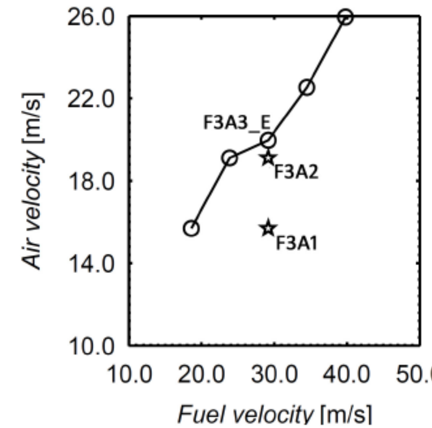
Cambridge swirling flames



(a) Chamber *(b) Bluff body*

Schematic of experimental setup

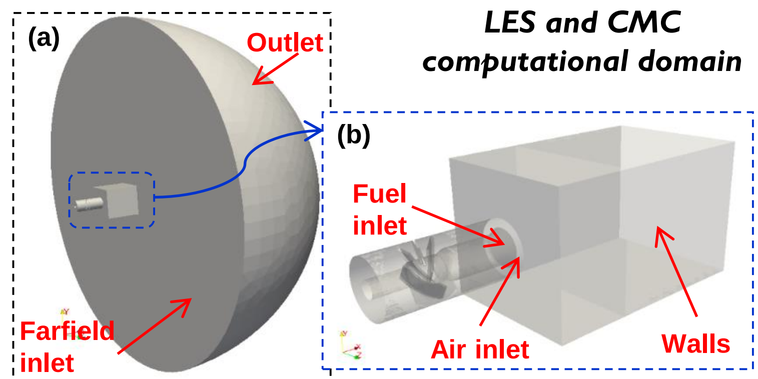




Blow-off curve

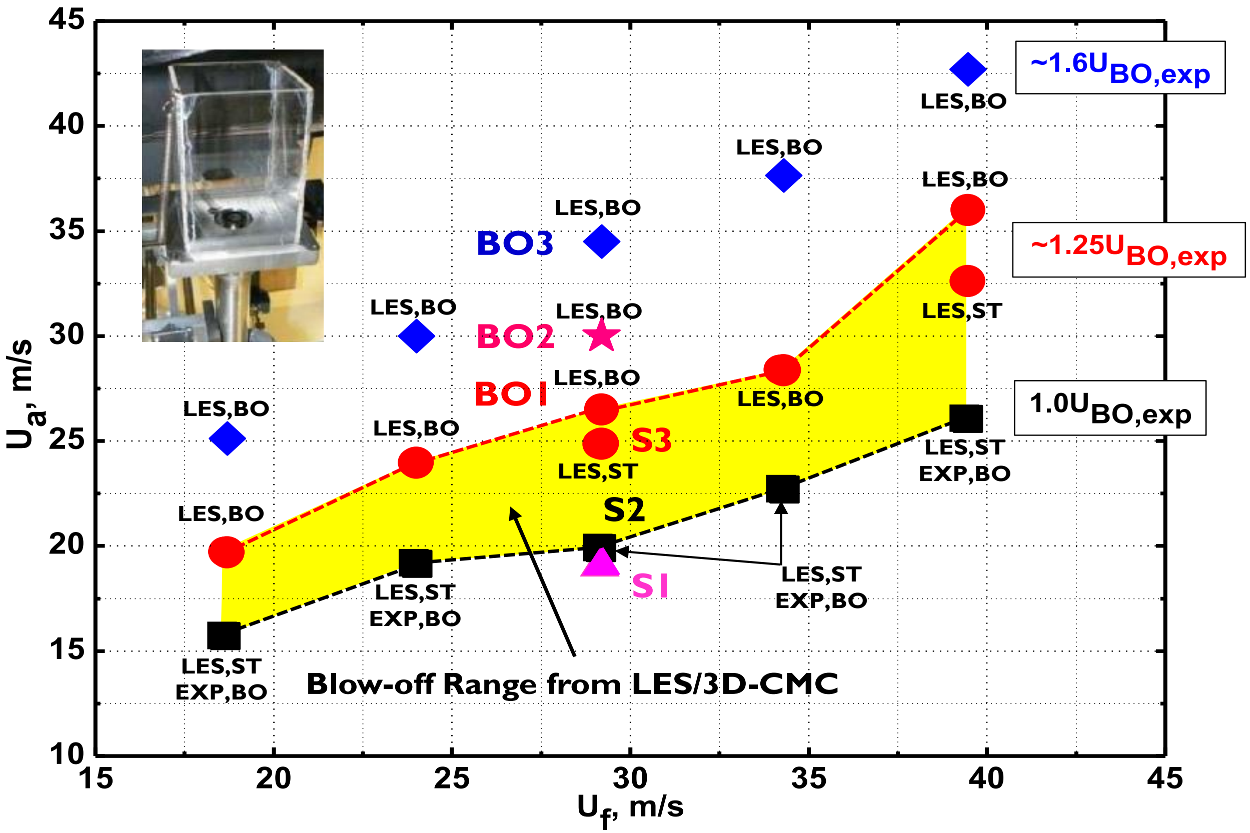
- Fuel/oxizider: pure methane (non-swirling) and air (swirling)
- The swirl number S_N is calculated following Beer and Chigier's method (Applied Science 1972):

$$S_N = \frac{2}{3}\frac{1-(D_{hub}/D_{sw})^3}{1-(D_{hub}/D_{sw})^2}\tan\theta = 1.23$$



LES and CMC computational domain

Prediction of global extinction (blow-off) condition in Cambridge burner



- Prediction of the full blow-off curve is still one of the targets of combustion CFD.
- Capturing the blow-off condition with LES has not been demonstrated yet.

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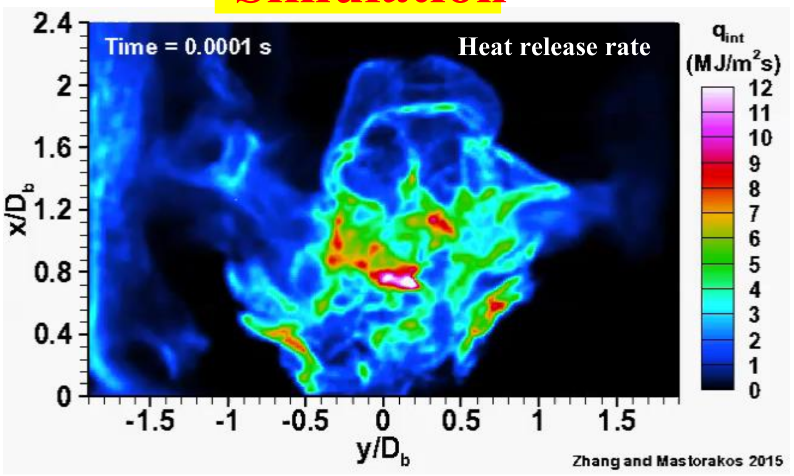
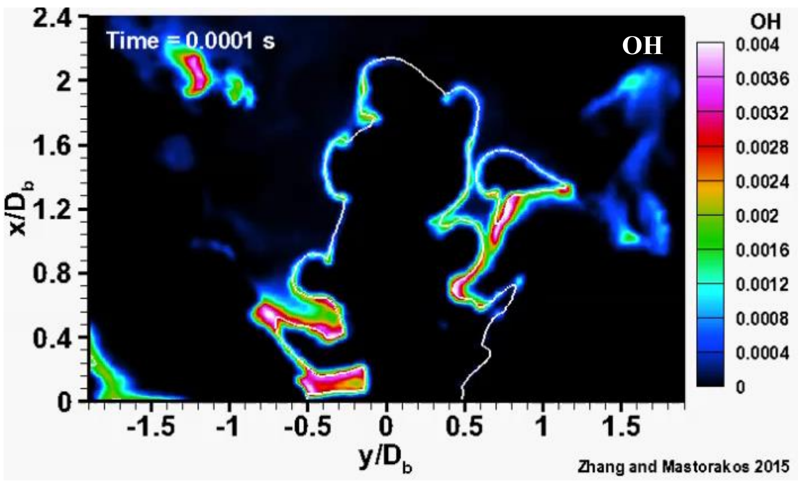
Blow-off transient: LES vs. experiment

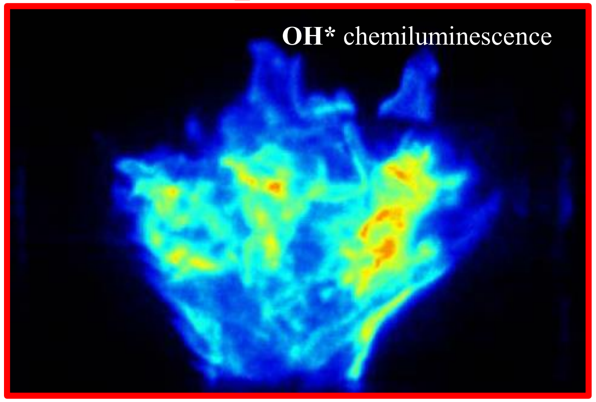
Simulation

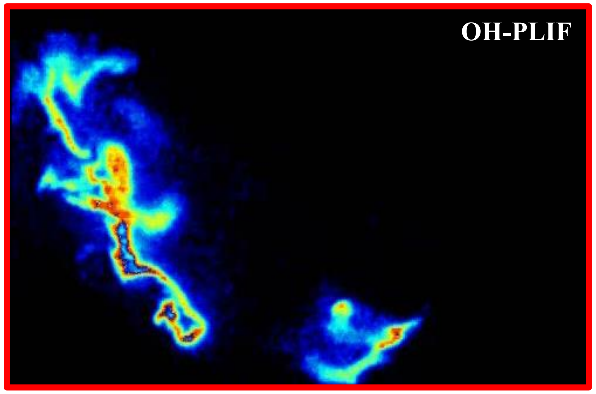




Swirling air | non-swirling CH_4 | Swirling air

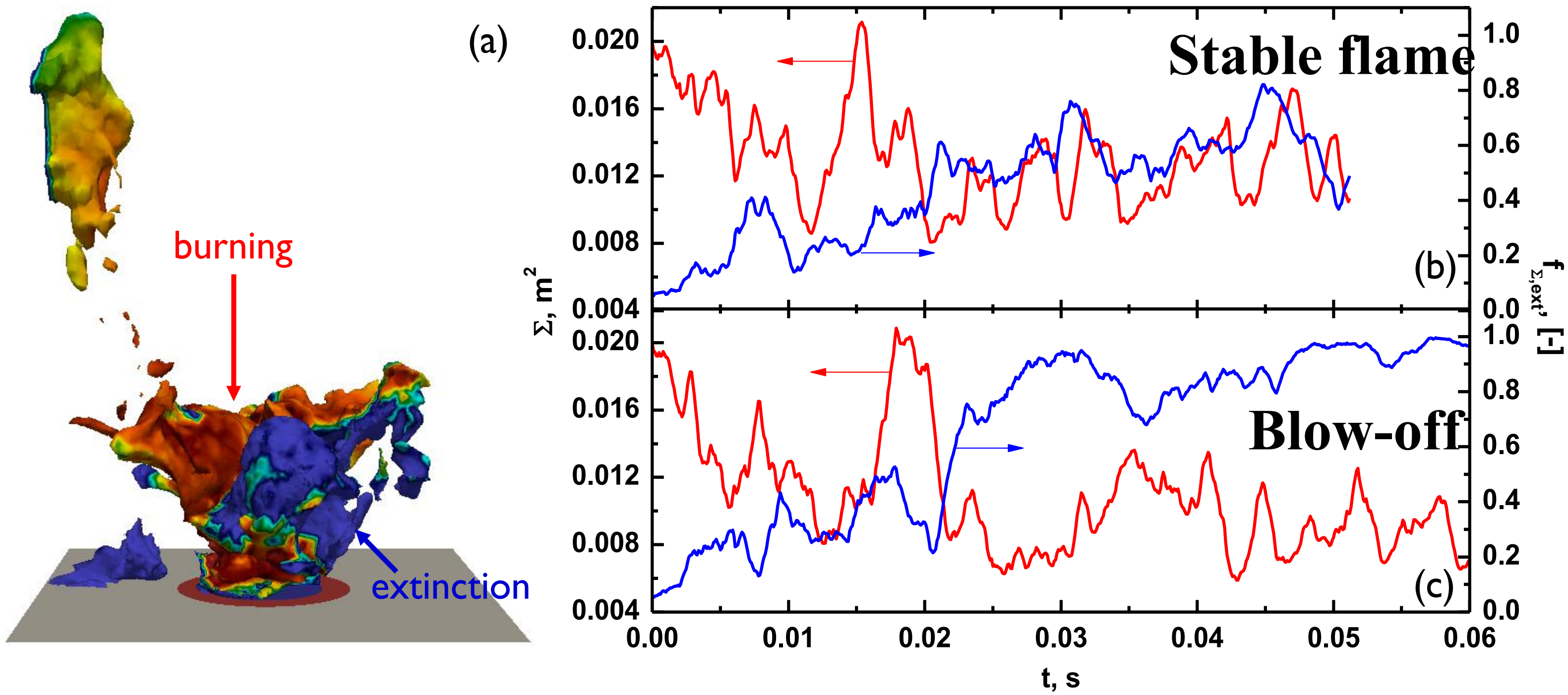
Experiment





(Cavaliere et al. Flow Turb. Combust. 2013)

Localized extinction during blow-off

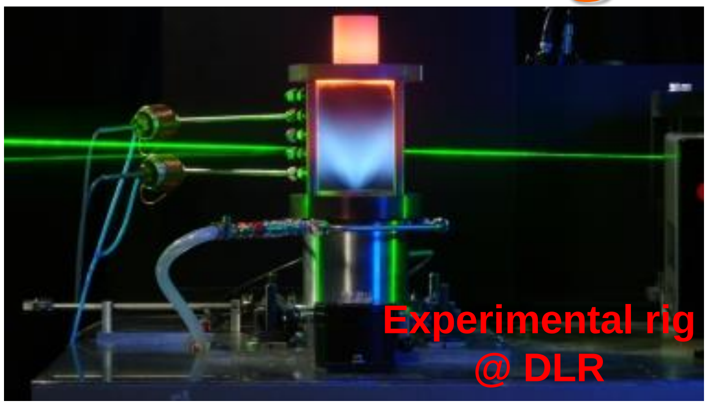


Metrics for quantifying flame extinction:

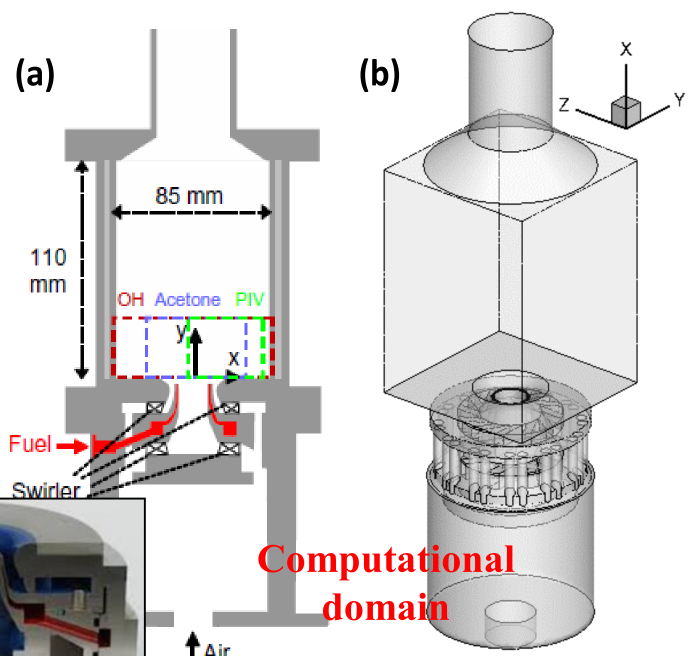
- ❖ **Area of the stoichiometric mixture fraction iso-surface Σ**
- ❖ **Extinguished fraction $f_{\Sigma,ext}$**

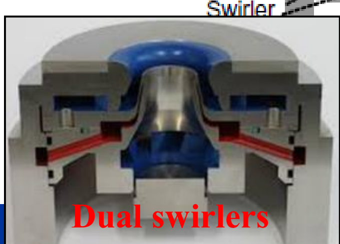
$$f_{\Sigma,ext} = \frac{extingsuihed\ area}{total\ stiochiometric\ area}$$

DLR (German Aerospace Center) model gas turbine combustor

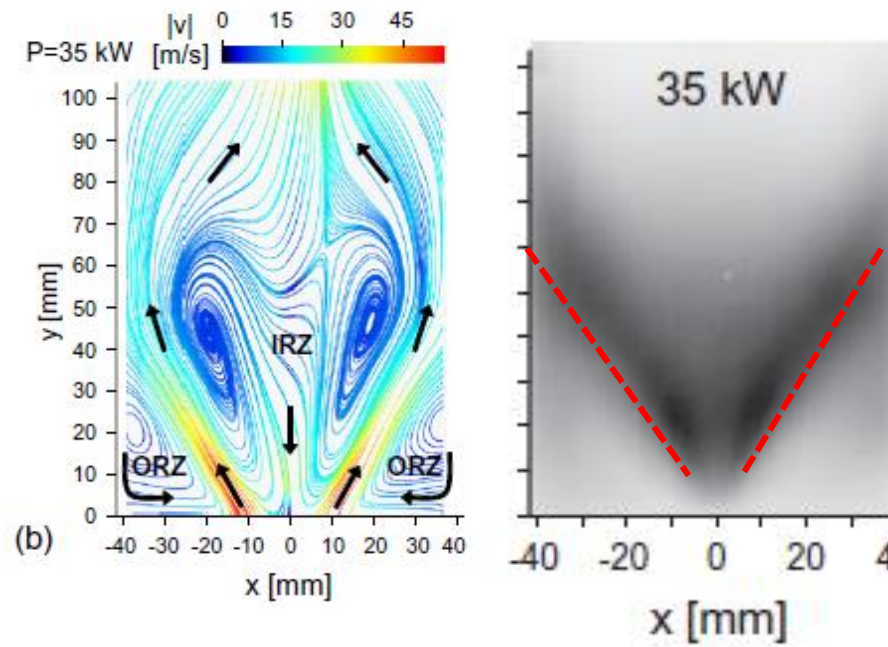


Case	Fuel mass flow rate (kg/s)	Air mass flow rate (kg/s)	Swirl number	Thermal power (kW)	Global equivalence ratio
A	0.000697	0.018	0.9	34.9	0.65
C	0.00015	0.0047	0.55	7.6	0.55





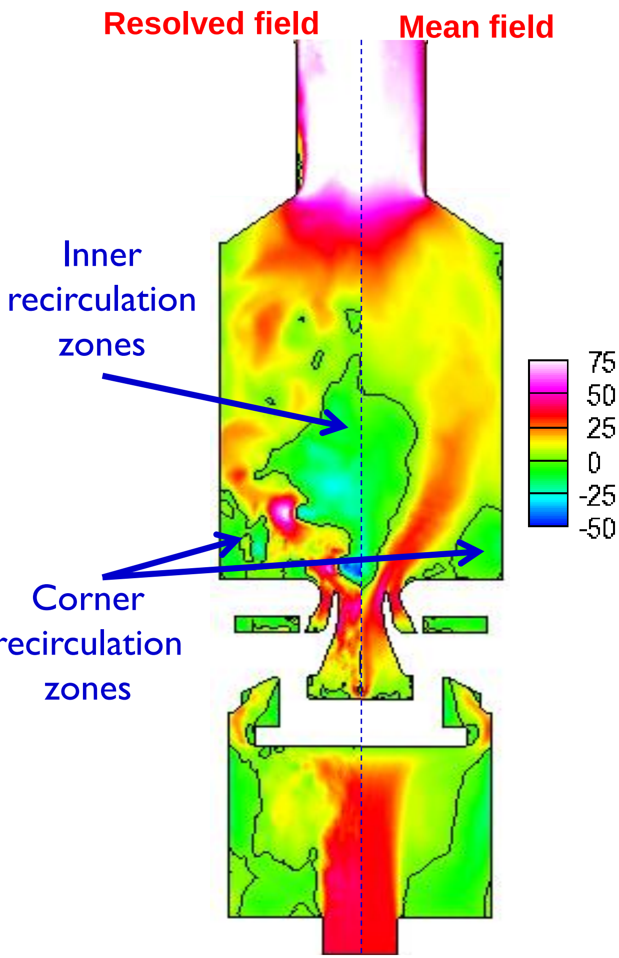
Computational domain



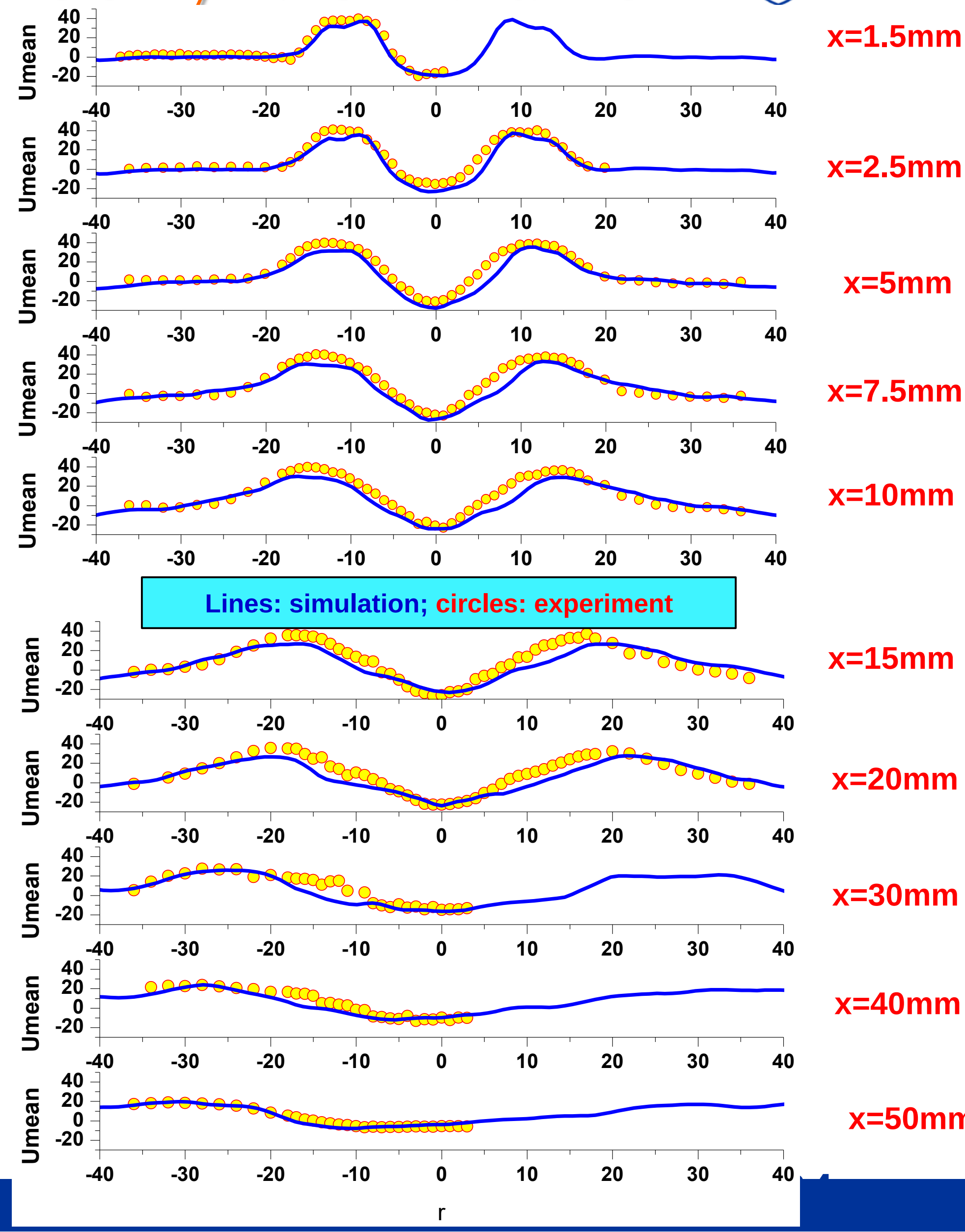
Experimental visualizations of flow pattern and reaction zone of Flame A case

Weigand et al. Combust Flame 2006.
Stohr et al. Combust. Flame 2012.

Axial mean velocity distribution

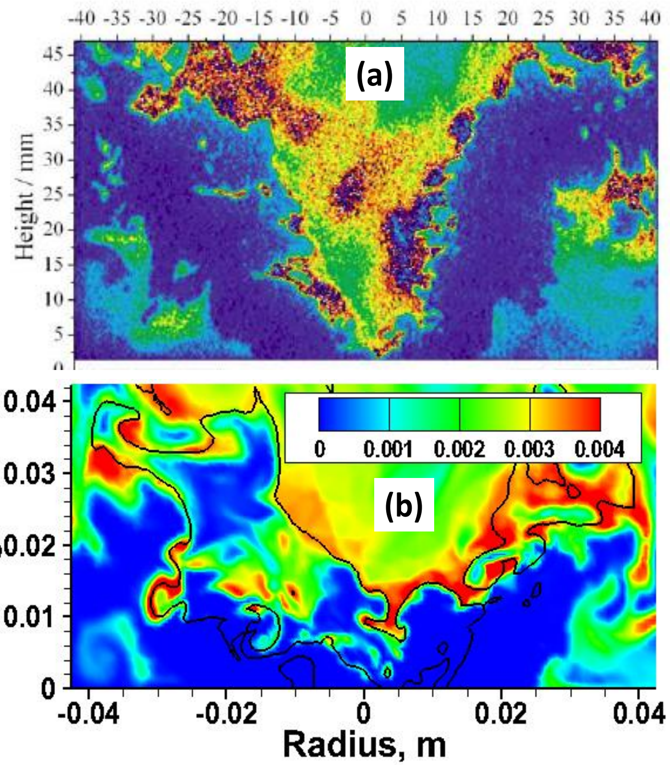


Contours of resolved (left) and mean (right) axial velocity for Flame A case.



OH mass fraction vs. OH-PLIF

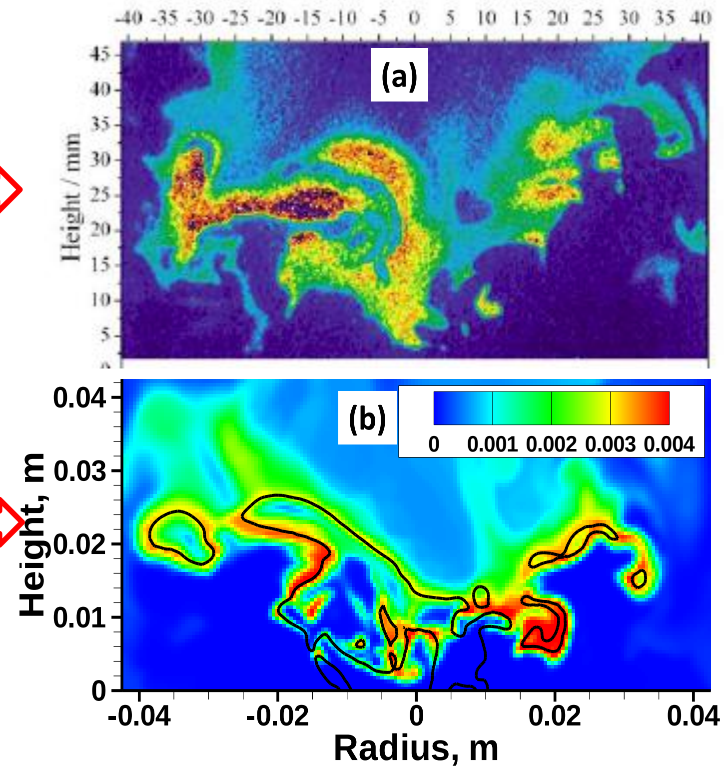
Flame A



Experiment
(Weigand et al. Combust. Flame 2006)

Simulation

Flame C



- ✓ **Localized extinction?**
- ✓ **Lean blowout?**
- ✓ **Partially premixed?**