Development and Experimental Validation of LES Techniques for the Prediction of Combustion-Dynamic Processes in Syngas Combustion

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Research Objectives

Joint computational and experimental research program to develop simulation techniques for

- Prediction of autoignition and unstable combustion processes, at GT-relevant operating conditions
- Perform analysis of facility effects in flow-reactors and rapid compression machines to reconcile observed discrepancies between measurements and simulations

Overview

Research objectives

Computational research effort

- Characterization of facility effects in flow reactors
- LES modeling of dual-swirl gas-turbine model combustor

Conclusions

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Background

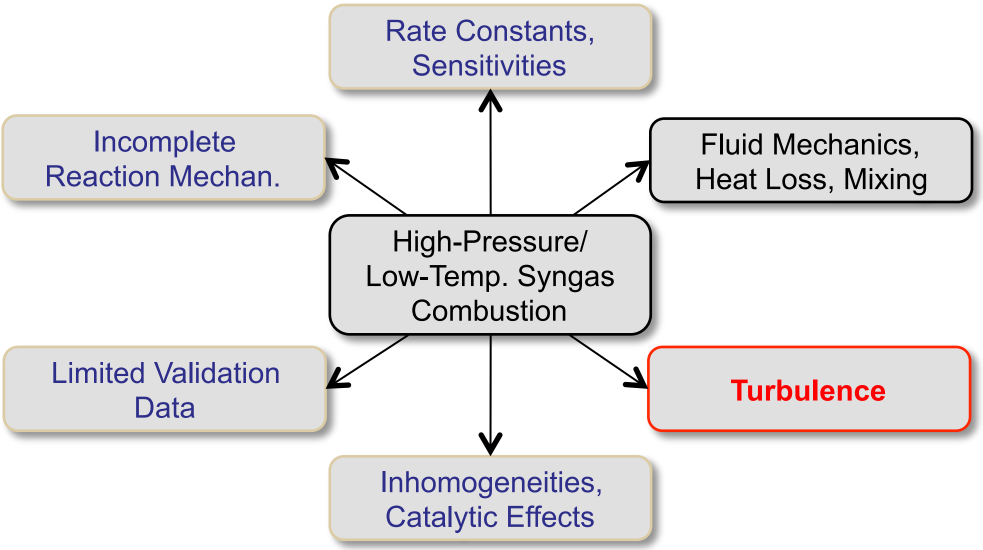
Facility-induced non-idealities can play critical role in affecting chemical kinetics and combustion

- Ignition delay
- Combustion transients
- Flame-speed

Sources of experimentally-observed discrepancies are facility-dependent

- Rapid compression engines, Flow reactors, Shock tube

Uncertainties introduce systematic and stochastic uncertainties → require quantitative understanding



Motivation

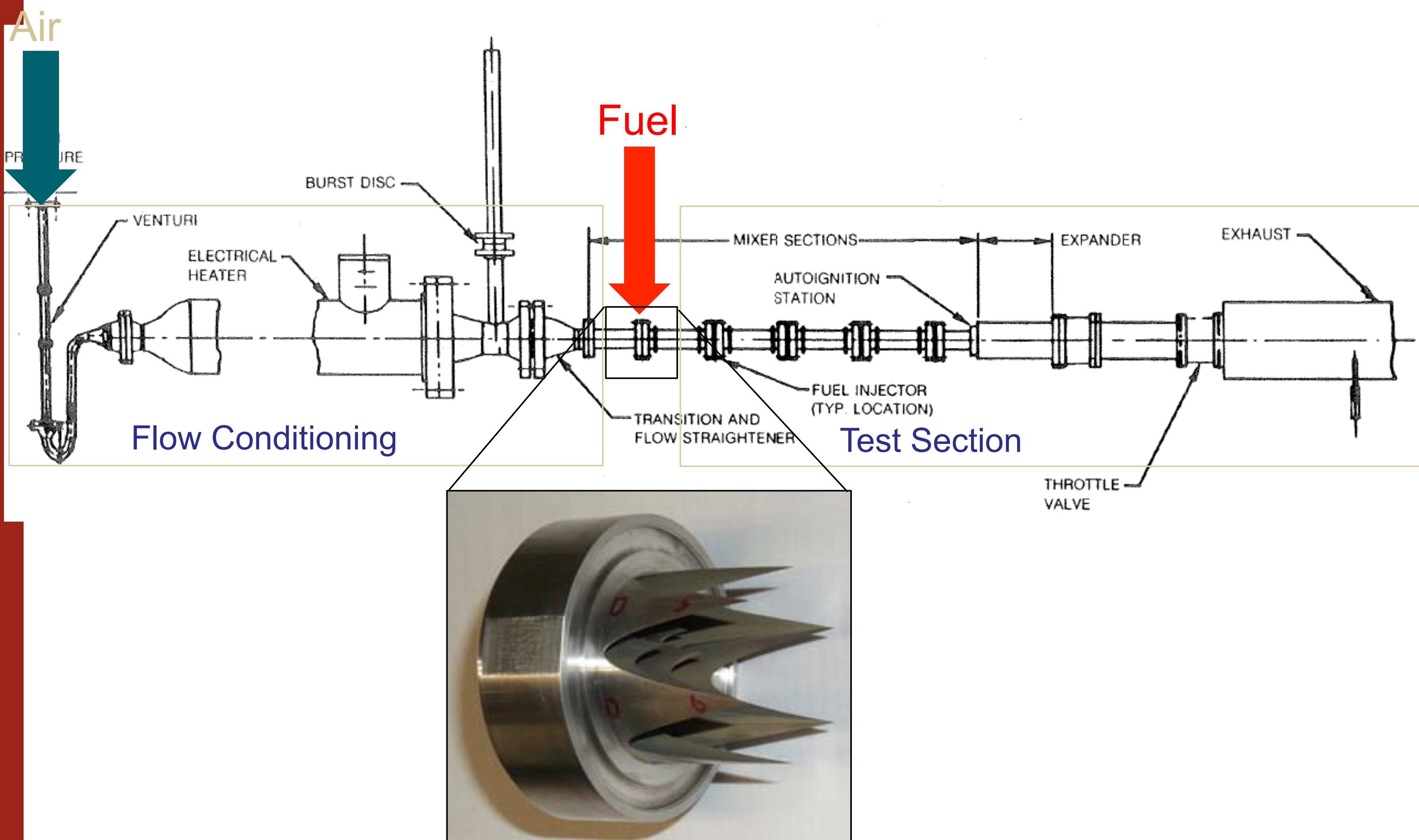
Objectives

- Develop model to quantify effects of mean-flow and inhomogeneities of temperature and mixture composition on ignition dynamics

Approach

- Employ particle method; enables consideration of
  - Detailed chemistry effects
  - Turbulent mixing
  - Reduces to classical homogeneous reactor model under idealized conditions

Flow-Reactor Facility



Peschke & Spadaccini, (1985); Santoro (2009)

Parametric Analysis

Develop Eulerian parabolized formulation to describe ignition and combustion dynamics

Stationary flow-field:

Mixture Fraction: $$\overline{\rho}\widetilde{u}\partial_x\widetilde{Z} = \frac{1}{r}\partial_r\left(r\alpha_T\partial_r\widetilde{Z}\right),$$

Progress Variable: $$\overline{\rho}\widetilde{u}\partial_x\widetilde{C} = \frac{1}{r}\partial_r\left(r\alpha_T\partial_r\widetilde{C}\right) + \overline{\rho}\widetilde{\omega_C},$$

Enthalpy: $$\overline{\rho}\widetilde{u}\partial_x\widetilde{h} = \frac{1}{r}\partial_r\left(r\alpha_T\partial_r\widetilde{h}\right),$$

Mixture Fraction Variance: $$\overline{\rho}\widetilde{u}\partial_x\widetilde{Z''^2} = \frac{1}{r}\partial_r\left(r\alpha_T\partial_r\widetilde{Z''^2}\right) + 2\alpha_T\left(\partial_r\widetilde{Z}\right)^2 - C_\phi\frac{\mu_T}{\Delta^2}\widetilde{Z''^2},$$

Progress Variable Variance: $$\overline{\rho}\widetilde{u}\partial_x\widetilde{C''^2} = \frac{1}{r}\partial_r\left(r\alpha_T\partial_r\widetilde{C''^2}\right) + 2\alpha_T\left(\partial_r\widetilde{C}\right)^2 - C_\phi\frac{\mu_T}{\Delta^2}\widetilde{C''^2} + 2\overline{\rho}\widetilde{\omega''_C C''},$$

Enthalpy Variance: $$\overline{\rho}\widetilde{u}\partial_x\widetilde{h''^2} = \frac{1}{r}\partial_r\left(r\alpha_T\partial_r\widetilde{h''^2}\right) + 2\alpha_T\left(\partial_r\widetilde{h}\right)^2 - C_\phi\frac{\mu_T}{\Delta^2}\widetilde{h''^2},$$

Results: Mixture/Temperature Inhomogeneities

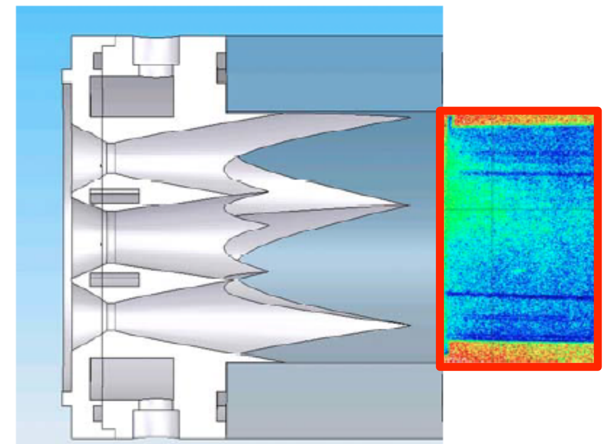
Experimentally observed stochastic ignition suggests sensitivity to initial conditions

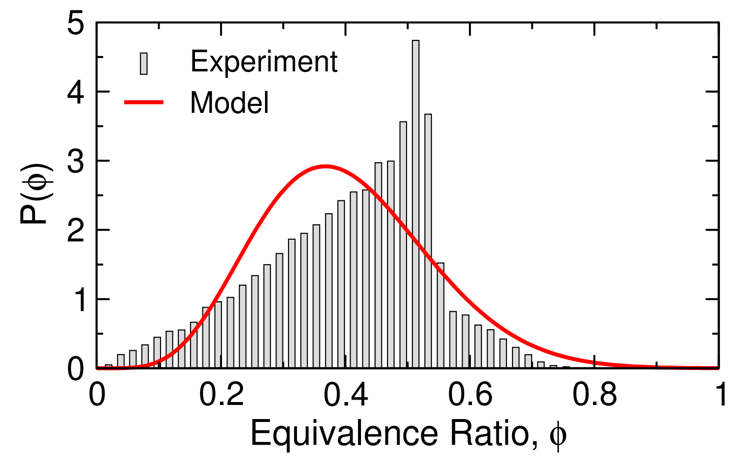
- Mixture composition
- Temperature
  - Unsteady heating
  - Wall-heat losses
  - Temp-difference btw. fuel and oxidizer

Consider inhomogeneities

- Equivalence ratio: sample from experimentally determined beta-distribution
- Temperature fluctuations: Sample from Gaussian with specified T'

Use fully-developed turbulent pipe-flow at Re = 104

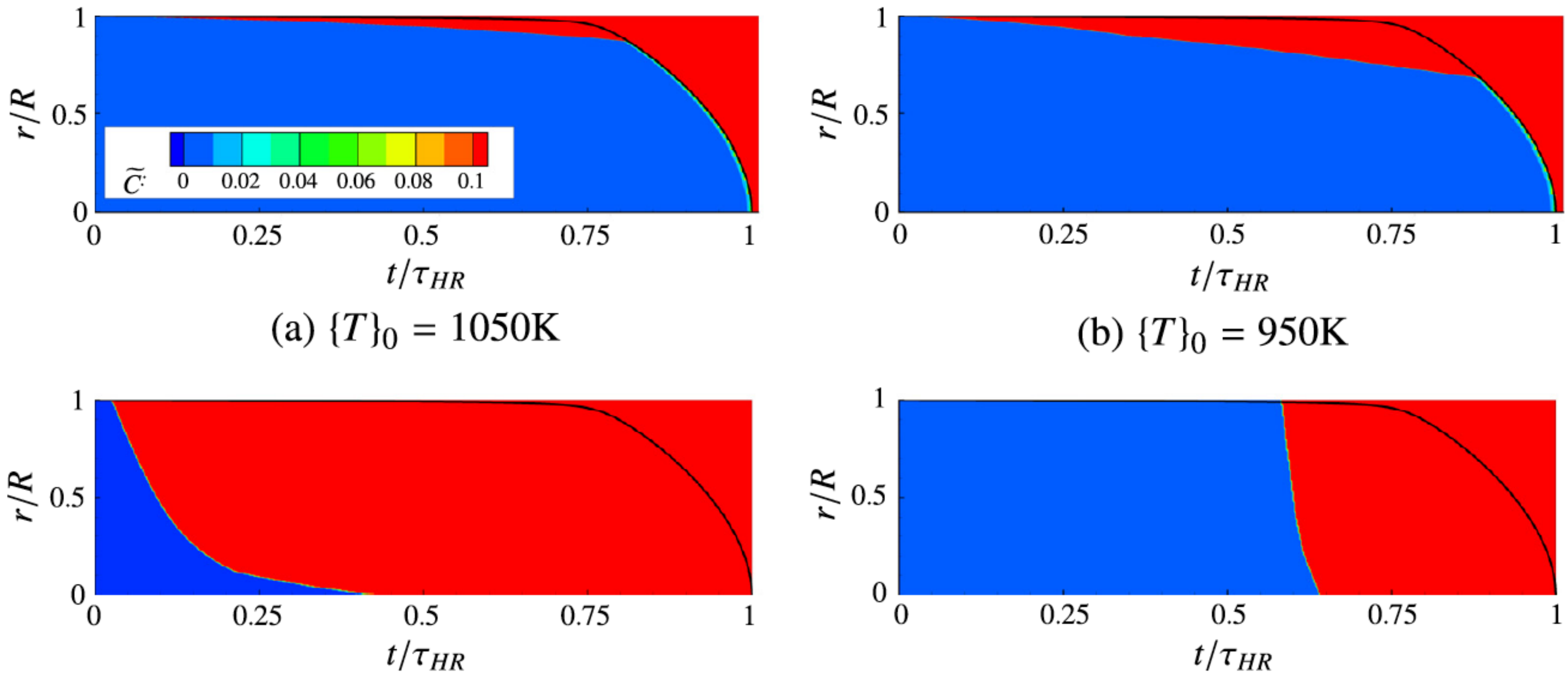




1 Santoro (2009)
2 Samuelsen et al. (2003)

Parametric Analysis

Temperature effects



(a) $\{T\}_0$ = 1050K

(b) $\{T\}_0$ = 950K

(c) $\{T\}_0$ = 850K

(d) $\{T\}_0$ = 750K

Results: Mixture/Temperature Inhomogeneities

Mixture variation: $\phi=0.4$; $\phi'=0.135$

Temperature variation: $T=850$ K; $T' = \{0, 25, 50, 75\}$ K

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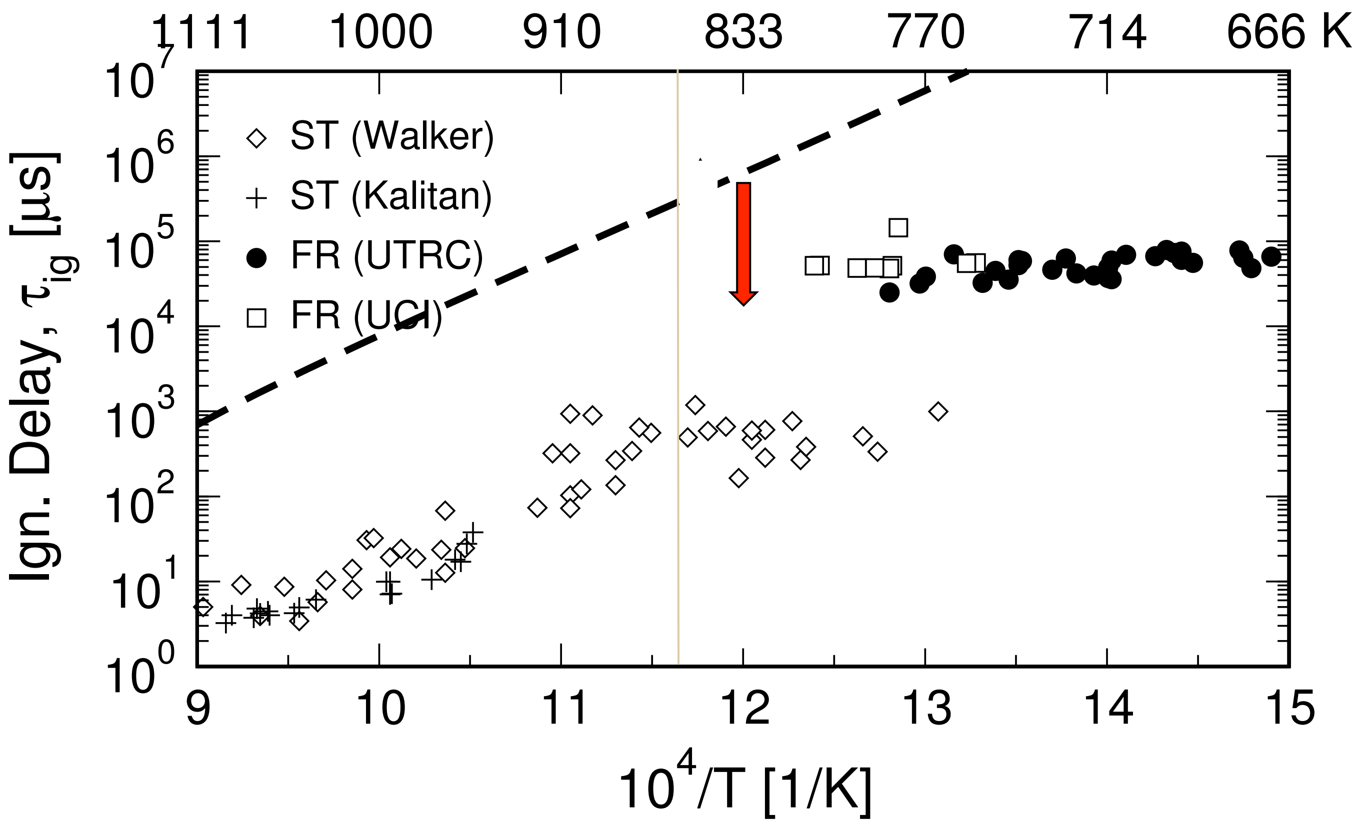
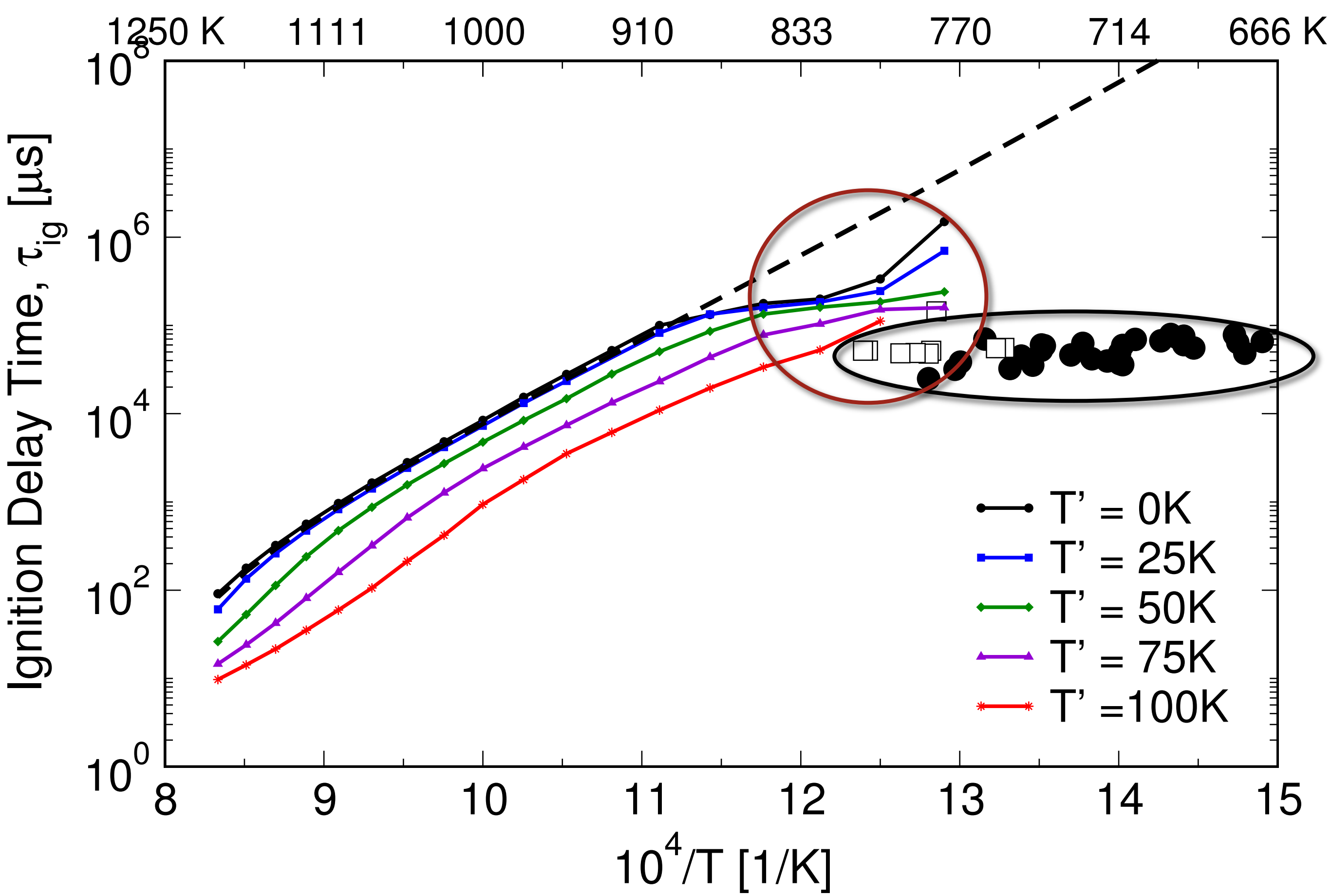


Results: Effect of Mean Temperature Variation

Instantaneous particle field



Results: Time-scale analysis

- Ignition delay of homogeneous reactor

$$\tau_{\mathrm{HR}} = \mathrm{argmin}_t (T_{\mathrm{HR}}(t) \geq T_{\mathrm{ig}})$$

- Characteristic diffusion time scale

$$\tau_{\mathrm{diff}} \propto \delta^2 / \nu_T$$

- Consumption rate

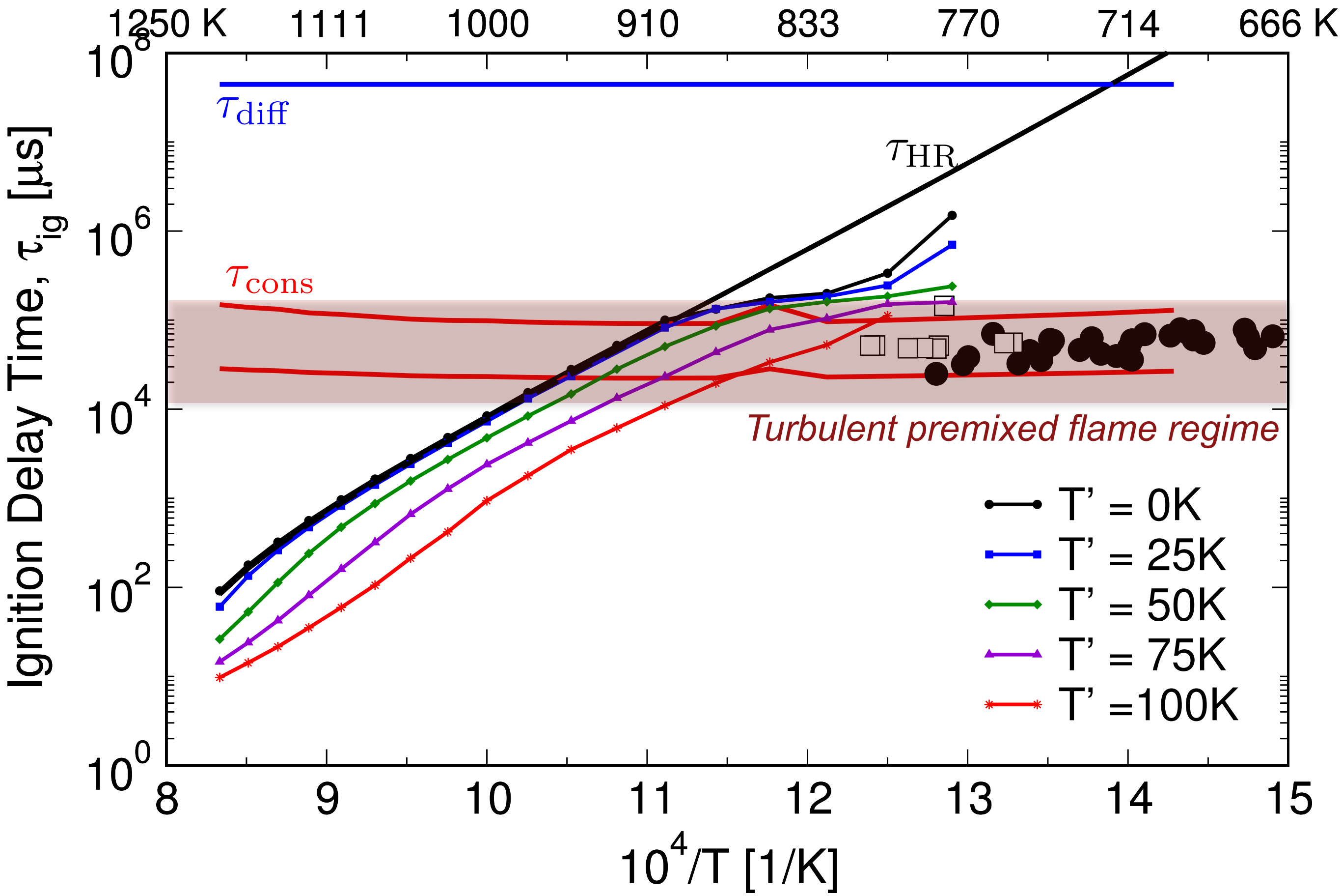
$$\tau_{\mathrm{cons}} \propto R / s_T$$

  - Turbulent burning speed is evaluated from thin-reaction zones regime/ corrugated flamelet regime

$$\frac{s_T^{\mathrm{TRZ}}}{s_L} \approx \left(\frac{\alpha_T}{\alpha}\right)^{1/2} \qquad \frac{s_T^{\mathrm{CFR}}}{s_L} \approx 1 + \left(\frac{u'}{s_L}\right)^{1/2}$$

Results: Time-scale analysis

Time-scale analysis



Flow Reactor
Summary and Conclusions

Main findings

- Velocity field has negligible effect on ignition time
- Rapid mixing minimizes effects of local equivalence fluctuations
- Temperature inhomogeneities have leading order effect on ignition delay
- Ignition initiated from hot particles in region of low mixing intensity
- Time-scale analysis suggests competition between *volumetric* and *deflagrative* ignition modes

Recommendations

- Spatio-temperature measurements of temperature field after injector
- Consider presence of deflagration-combustion transition at low-temperature conditions

Guibert et al., FTC, 84:79-95, 2010.

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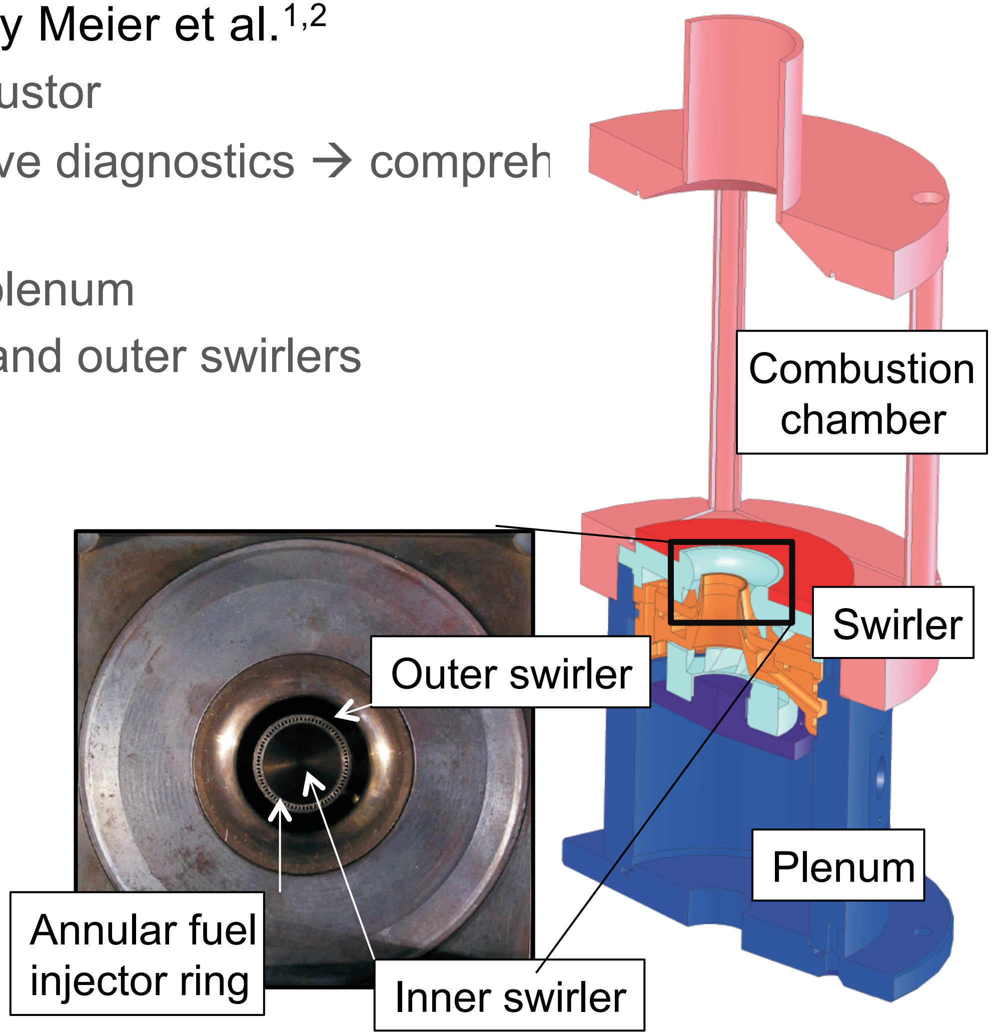
Conclusions

Experimental Setup

Gas-turbine model combustor by Meier et al.[1,2]

- Aero-derived dual-swirl combustor
- Optical access for non-intrusive diagnostics → compreh experimental database
- Common air-supply through plenum
- Fuel injection between inner and outer swirlers



1. Weigand et al. Combust. Flame, 144, 205 (2006)
2. Meier et al. Combust. Flame, 144, 225 (2006)

Experimental Setup

Gas-turbine model combustor by Meier et al.[1,2]

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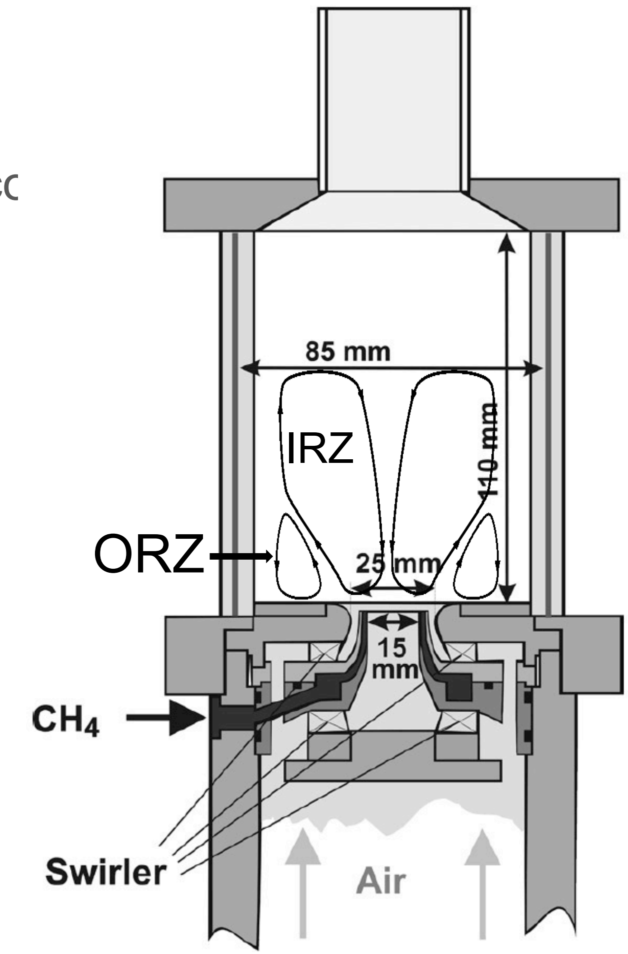
Operating Conditions

- Consider stable operating point “flame A”
- Power: 35kW, Air: 18 g/s, Methane: 0.7 g/s

Flow field features

- Inner recirculation zone (IRZ)
- Outer recirculation zone (ORZ)

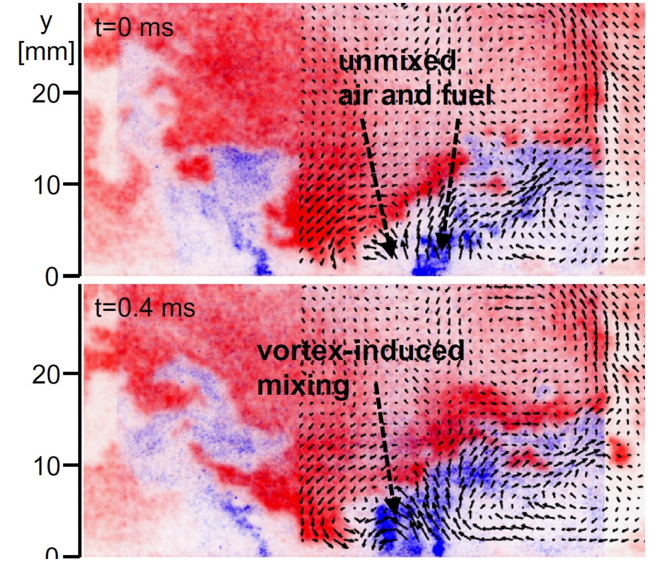


1. Weigand et al. Combust. Flame, 144, 205 (2006)
2. Meier et al. Combust. Flame, 144, 225 (2006)

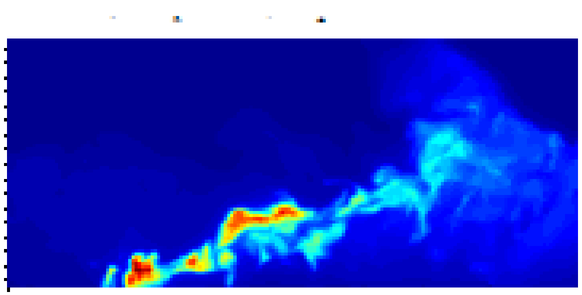
Flame Structure in Experiment

Comprehensive experimental investigations

- General characteristics of flame structure[1,2]
  - Evidence of local flame extinction
- Flame dynamic and stabilization
  - PVC and flame interaction[3,4]
  - Flame kernel analysis[5]
    - Auto-ignition is not dominant
  - Flame regime analysis[6]
    - Fuel is mostly aligned with oxidizer



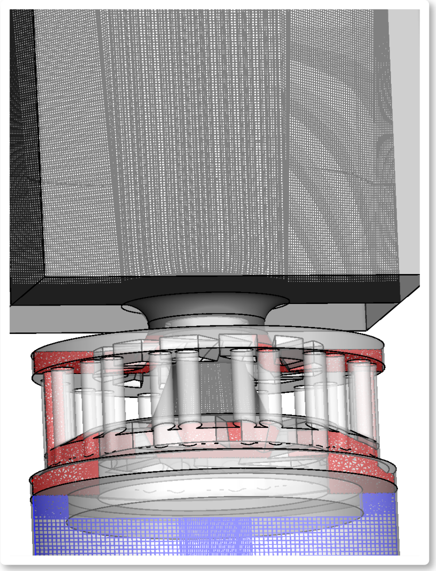
Stoehr et al. PCI 2014



Rosenberg et al. AIAA 2013-1181

1. Weigand et al. Combust. Flame, 144, 205 (2006)
2. Meier et al. Combust. Flame, 144, 225 (2006)
3. Steinberg et al. Combust. Flame 157 (2010)
4. Stohr et al. Combust. Flame 159 (2012)
5. Boxx et al. Exp. Fluids 54 (2013)
6. Rosenberg PhD Thesis 2013

Methodology



Computational Setup

Numerical scheme[1]

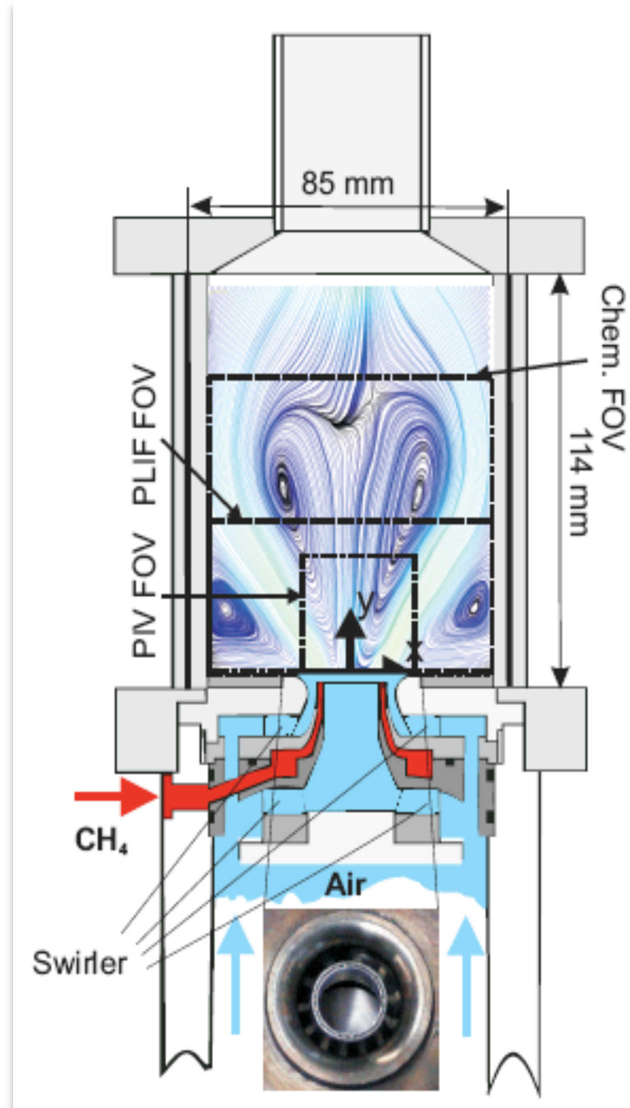
- Fully unstructured LES-solver
- Spatial discretization: Low dissipation scheme
- Temporal discretization
  - Predictor-corrector
  - Pressure-Poisson solver in both stages

Sub-grid Scale Models

- Standard Smagorinsky model
- Dynamic Smagorinsky model (DSM)
- Vreman[2]
- WALE[3]

Mesh

- Refined block-structured mesh: 18m CVs
- Element breakdown
  - Plenum: 2 million
  - Swirlers: 9 million
  - Combustion chamber: 7 million



Computational Setup

COMPREHENSIVE PARAMETRIC ANALYSIS FOR NON-REACTING AND REACTING CONDITIONS[1,2,3]

- Mesh resolution and mesh topology
- Subgrid-scale models

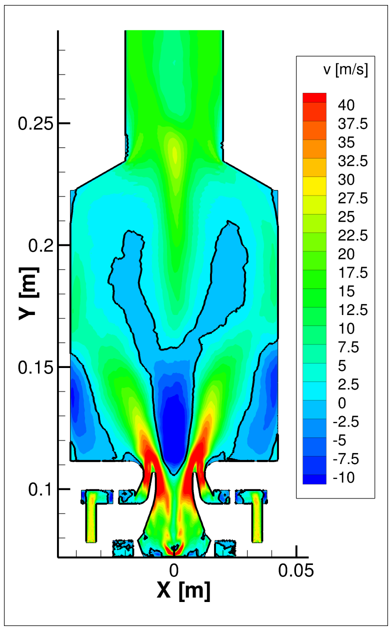
Number of Elements	Mesh Type	Subgrid Scale Model
7 million	Hex+Tet	Vreman
7 million	Hex+Tet	DSM
20 million	Hex+Tet	Vreman
8 million	Hex	Vreman
18 million	Hex	Vreman
18 million	Hex	Smagorinsky
40 million	Hex	Vreman

1. See, PhD thesis, University of Michigan, 2014.
2. See and Ihme, AIAA 2014-0621, 2014.
3. See and Ihme, AIAA 2013-0172, 2013.

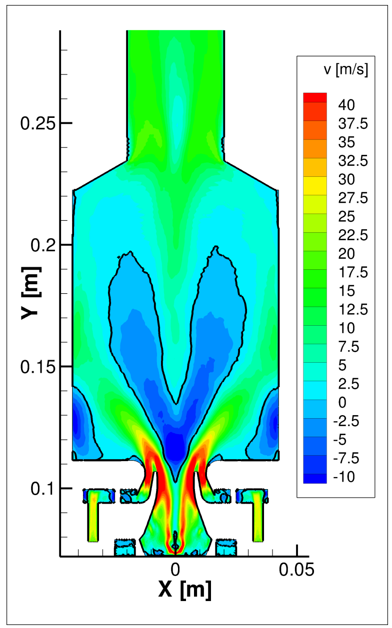
Mesh Sensitivity

Conduction systematic mesh-refinement studies

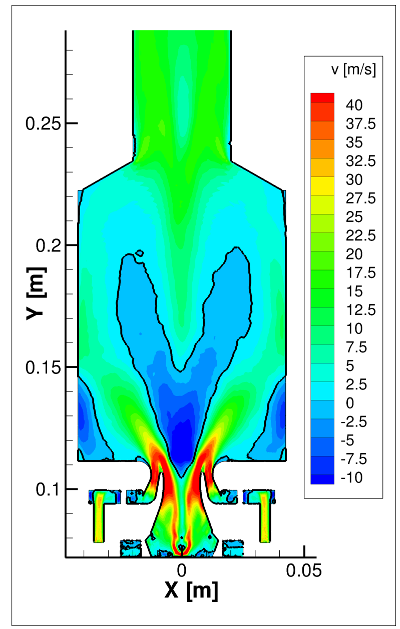
- Considered mesh-refinement cases with different mesh-characteristics



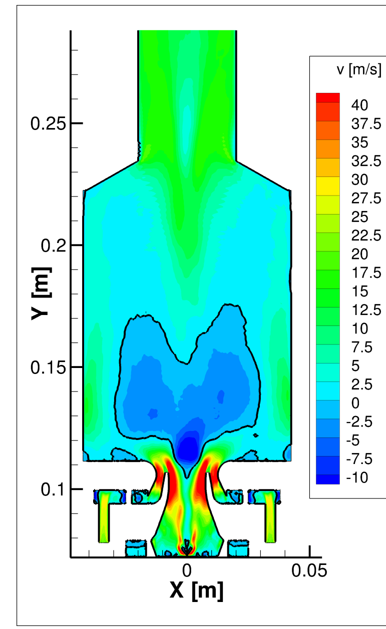
Hex (8m)



Hex (16m)



Hex (40m)

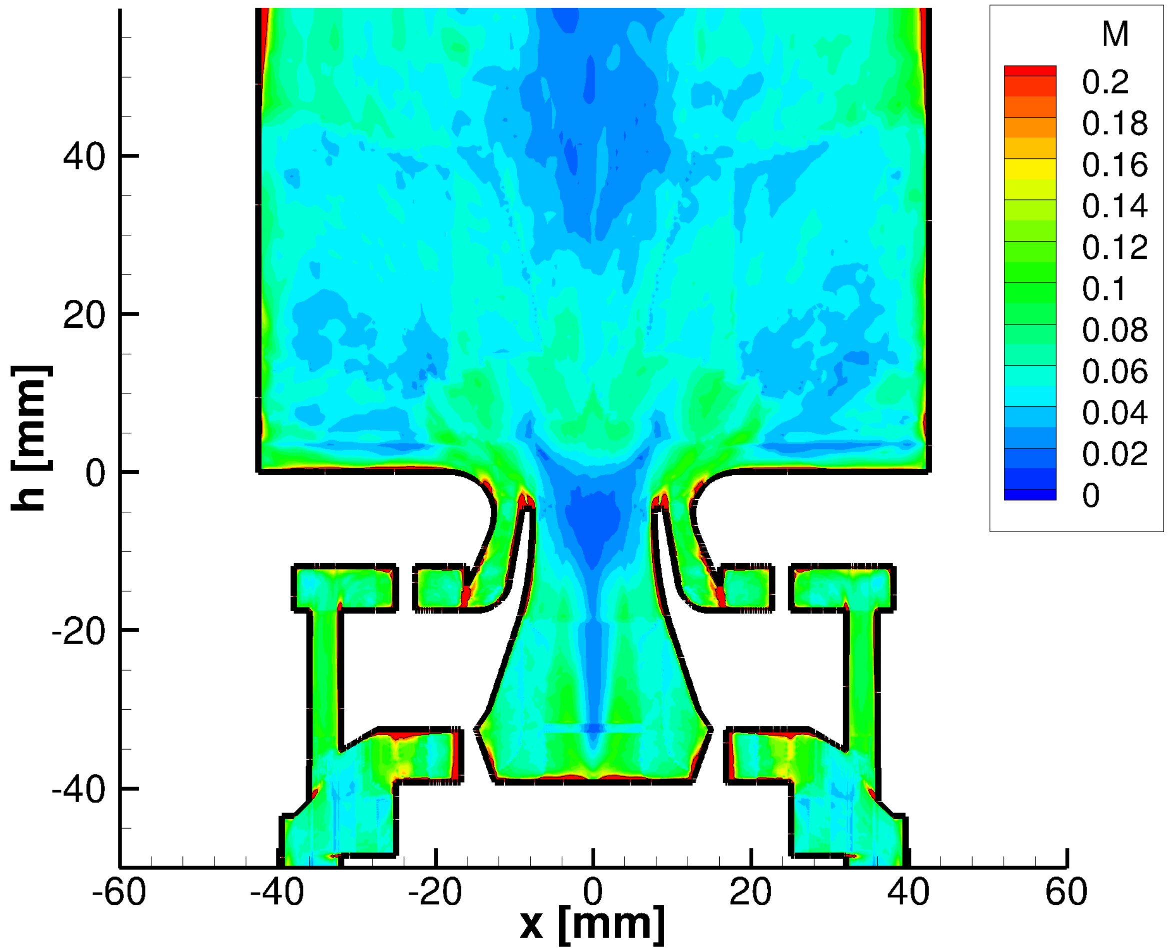


Hex/Tet (40m)

Mesh Quality

Assess mesh-resolution using Pope Criterion

$$M = \frac{k_{\mathrm{res}}}{k_{\mathrm{res}} + k_{\mathrm{rslvd}}}$$



1. Pope, New J. Physics, 6:1–24, 2004.

Combustion Models

Models	Flamelet Progress Variable (FPV)[1]	FPV with Progress Variable (FPV-Cvar)[2]	Filtered Tabulated Chemistry for LES (F-TACLES)[3]
Flamelet regime	Non-premixed	Non-premixed	Premixed
Tab. variables	$\widetilde{Z}, \widetilde{Z''^2}, \widetilde{C}$	$\widetilde{Z}, \widetilde{Z''^2}, \widetilde{C}, \widetilde{C''^2}$	$\widetilde{Z}, \widetilde{Z''^2}, \widetilde{C}$
Z model	Beta PDF	Beta PDF	Beta PDF
C model	Dirac PDF	Beta PDF	Pre-filtering and efficiency function[4]

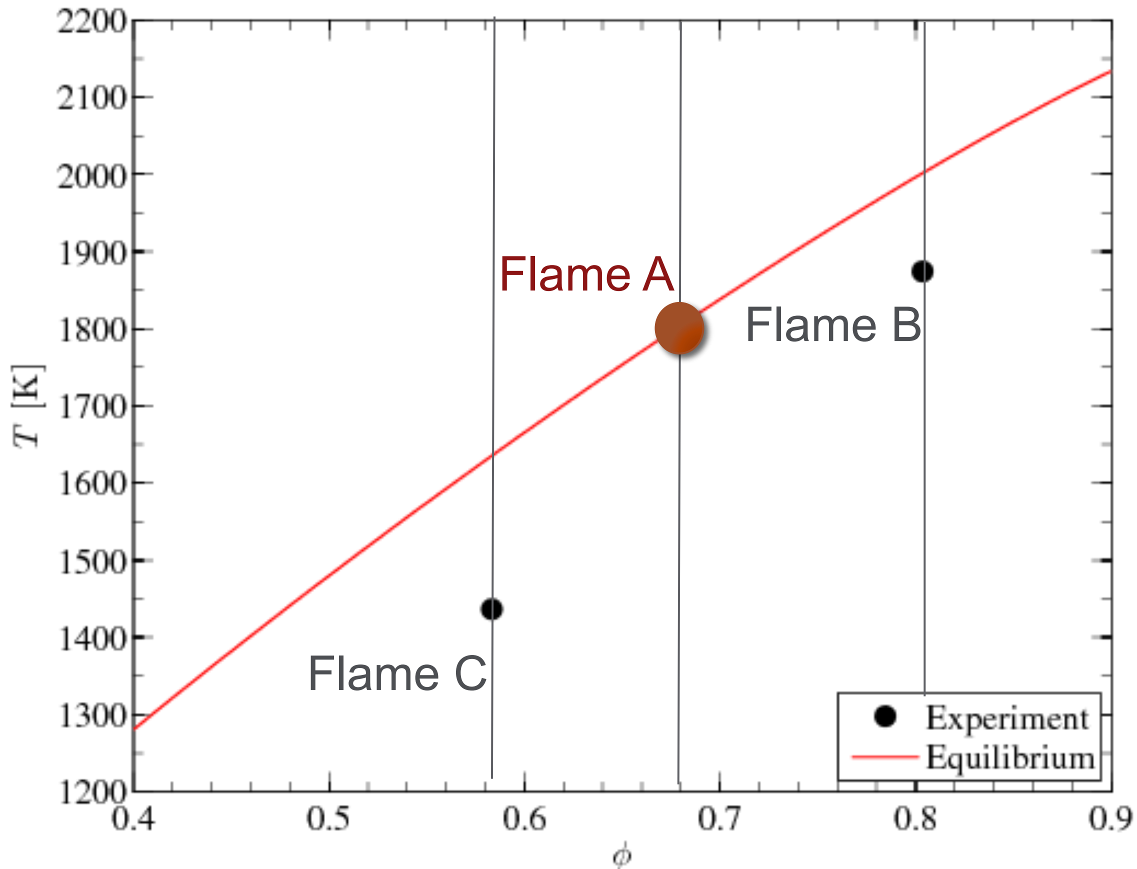
Chemistry library generation

- GRI-2.11 detailed chemistry kinetics
- Unity Lewis number is assumed for flamelet calculations
- Progress variable, $C = Y_{H2O} + Y_{H2} + Y_{CO2} + Y_{CO}$
- Adiabatic combustion models

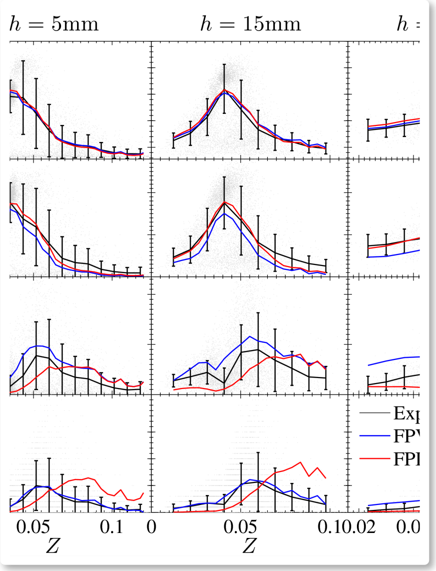
1. Pierce and Moin, JFM (2004)
2. Ihme, Cha, and Pitsch, PCI, 30 (2005)
3. Fiorina et al. Combust. Flame 157 (2010)
4. Charlette et al. Combust. Flame 131 (2002)

Significance of Wall Heat-loss Effects

Estimate wall-heat loss from mean-temperature at Farthest down-stream measurement location (h = 90mm) and comparison with equilibrium calculation



Prior Model Evalation



Prior Model Examination

Experimental Raman single shot measurements Φ_{EXP}

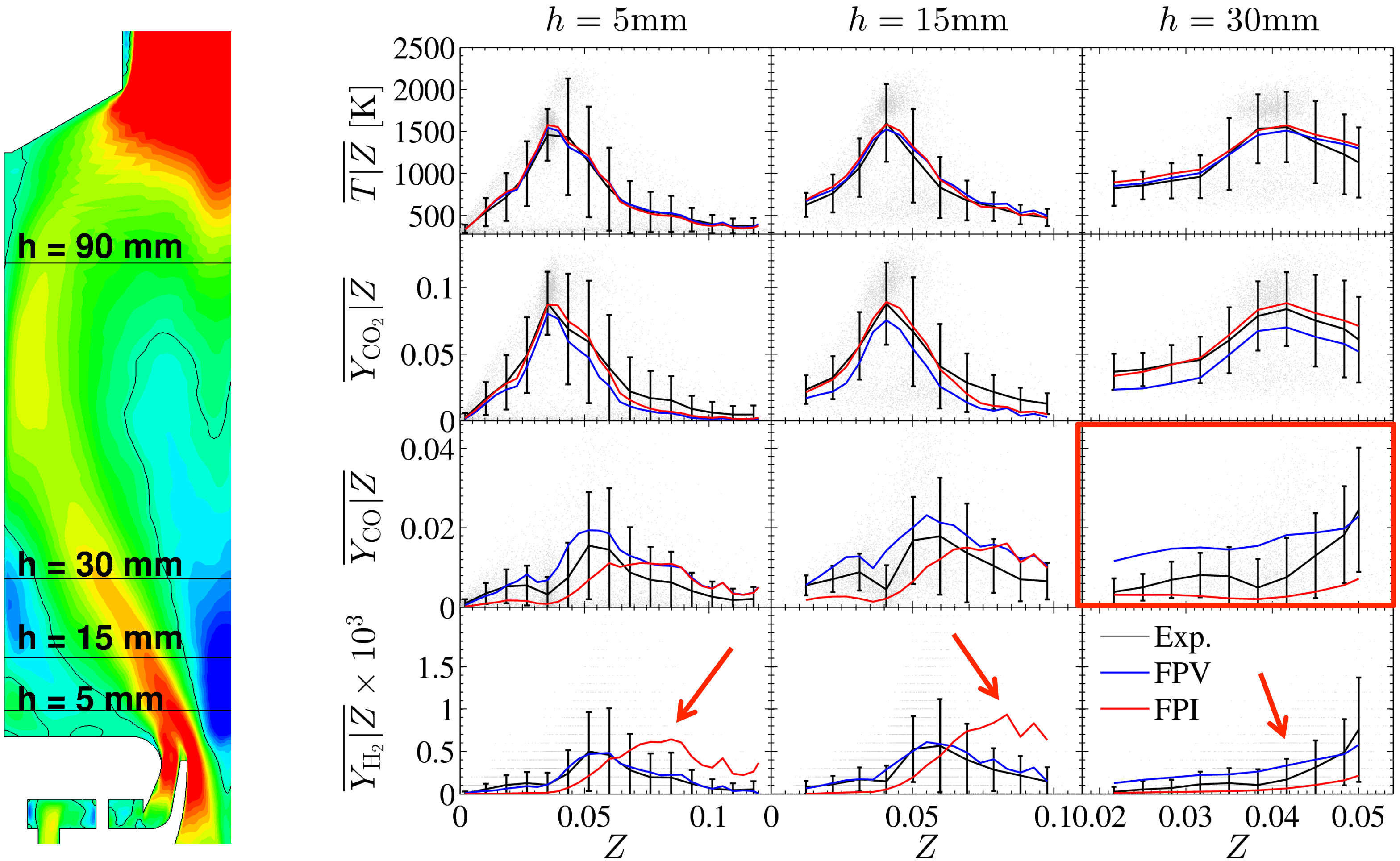
- Mixture fraction, Z_{exp} computed following Bilger's definition[1]
- Progress variable, $C_{exp} = Y_{H2O} + Y_{H2} + Y_{CO2} + Y_{CO}$
- Direct evaluation of thermo-chemical variables from flamelet manifold using (Z_{exp}, C_{exp}) from measurements
  - Unfiltered flamelets and assume zero variance of Z,C
  - $\Phi_{FPV/FPI} = F_{FPV/FPI}(Z_{exp}, C_{exp})$

Φ_{EXP} , Φ_{FPV} and Φ_{FPI} are conditioned on mixture fraction space for each measurement station

Similar methodology was used to evaluate the feasibility of flamelet models[1,2,3]

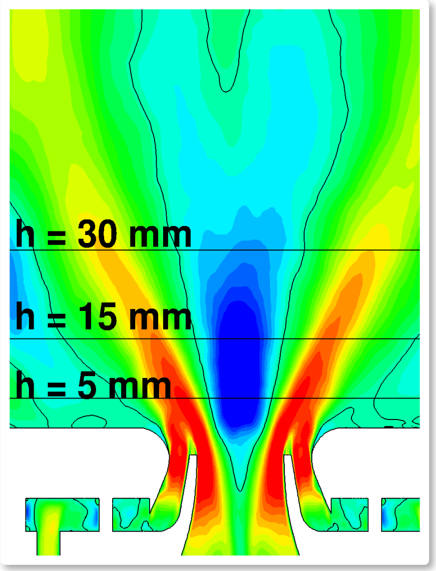
1. Bilger et al., Combust. Flame (1990)
2. Sutherland et al., Combust. Theory Modeling (2007)
3. Ramaekers et al., Flow Turbulence Combust. (2010)
4. Chen and Ihme, Combust. Flame (2013)

Prior Model Examination

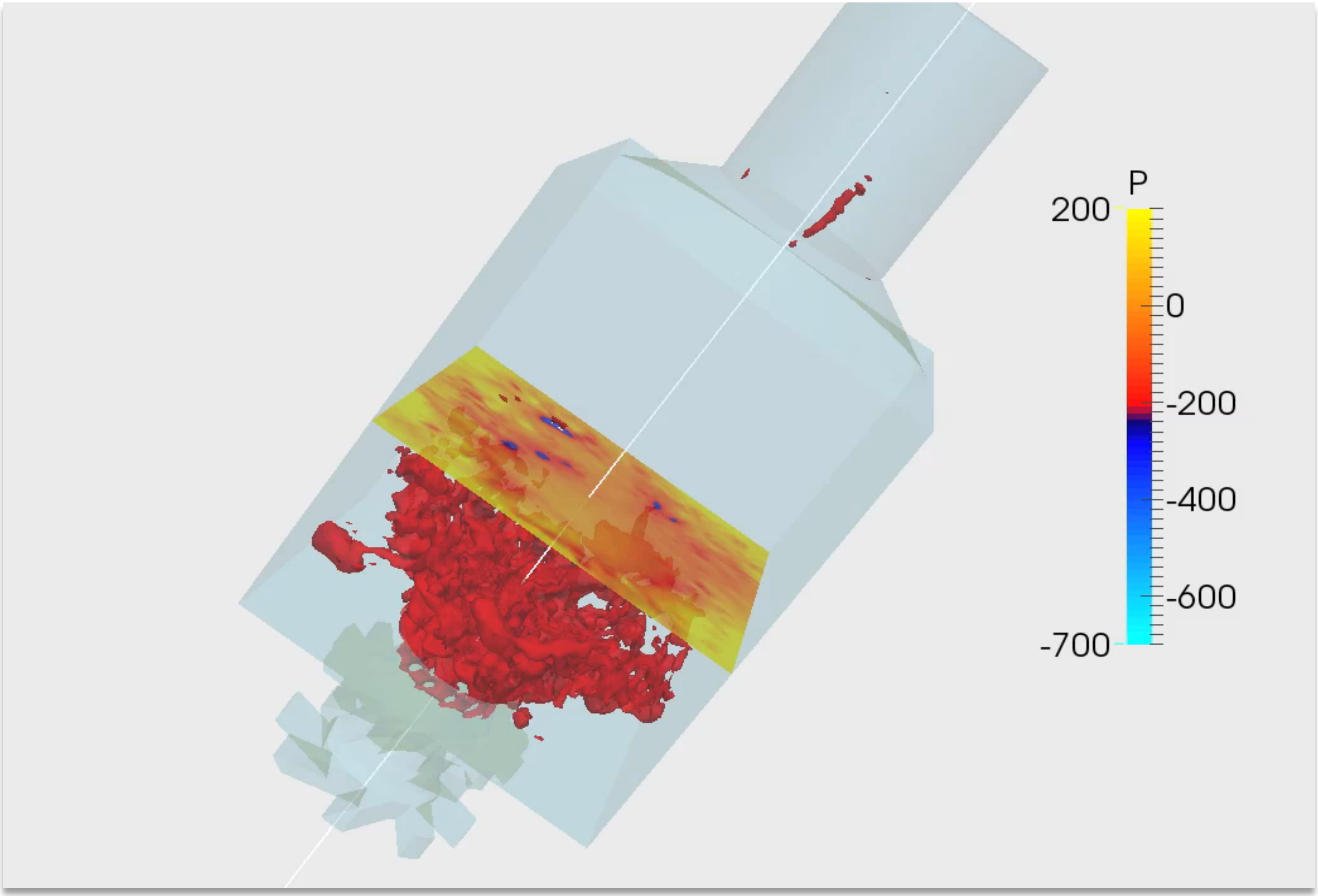


- Flamelet manifolds provide good representation of temperature and major species
- Discrepancies for CO and H2

Simulation Results



Unstable Combustion Processes
Flow Field Results

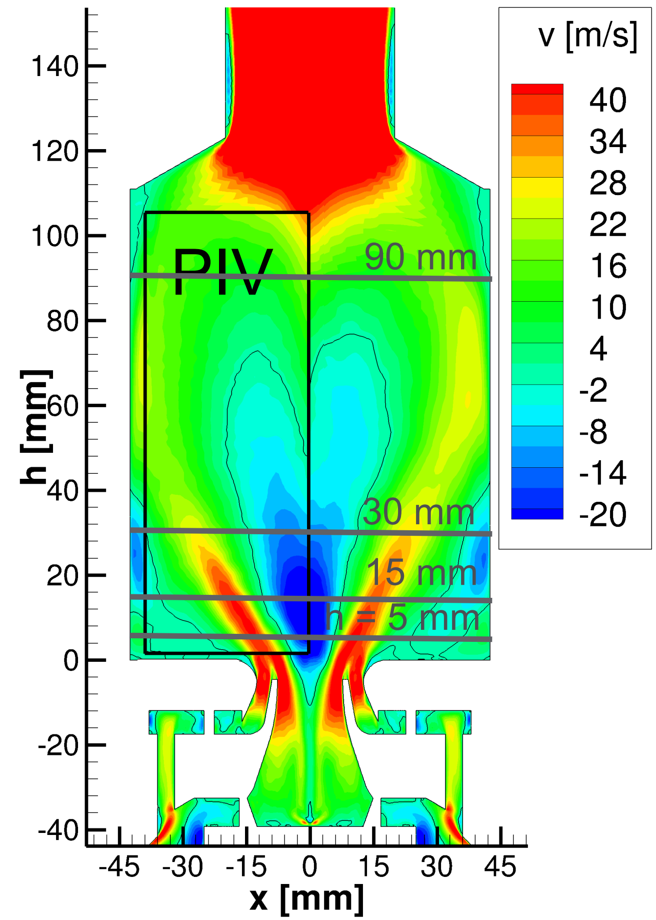


Simulation Results: Mean Flow Field

Flow-field structure

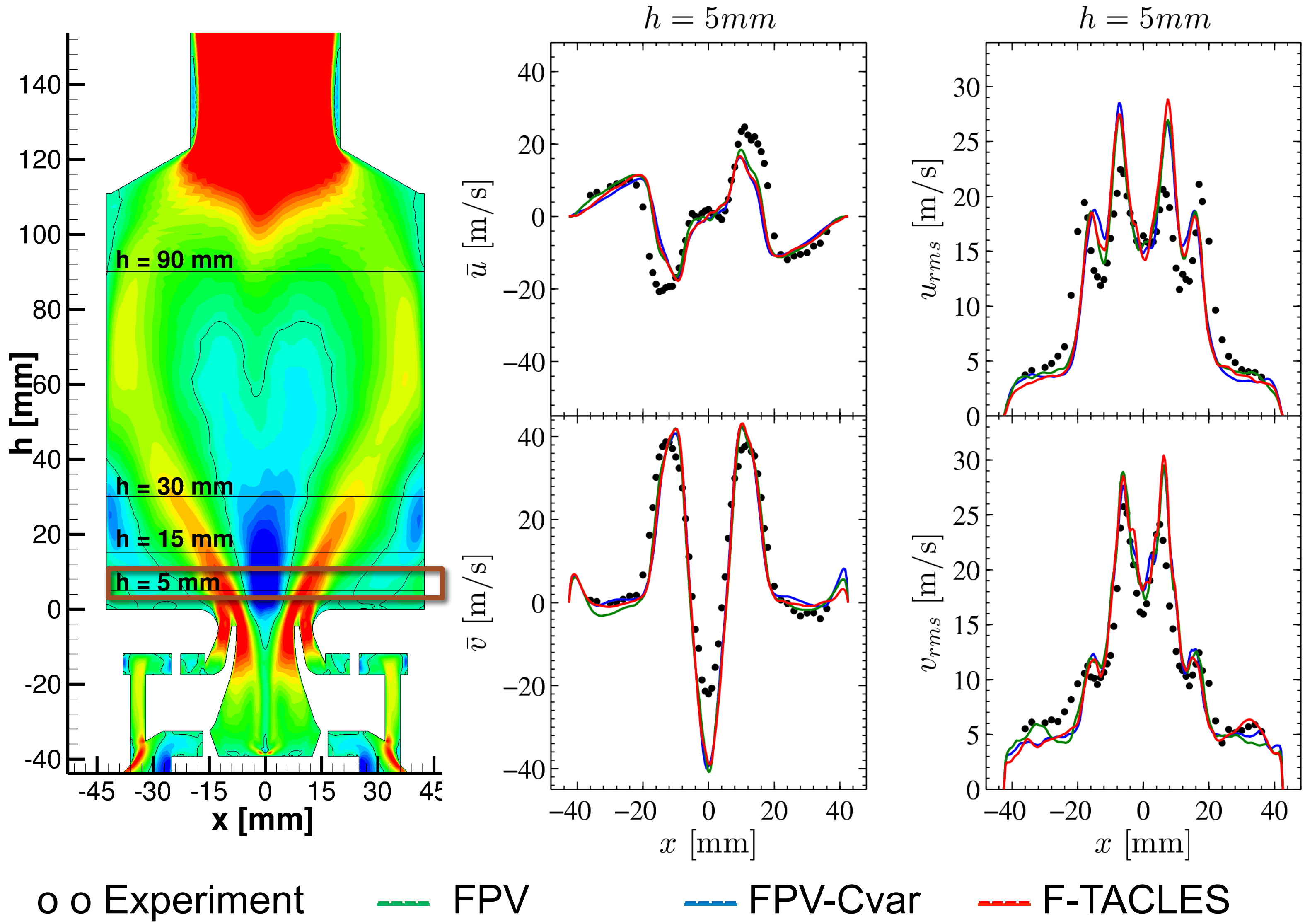
- General mean flow-field structure
- Y-shaped internal recirculation zone
- Corner vortices
- Opening angle of the injector stream is well captured
- Elongated inner recirculation zone

Comparison with PIV measurements[1] are in good agreement



1. Stohr, et al. Combust. Flame 159 (2012)

Simulation Results: Mean and RMS Velocities (h=5mm)



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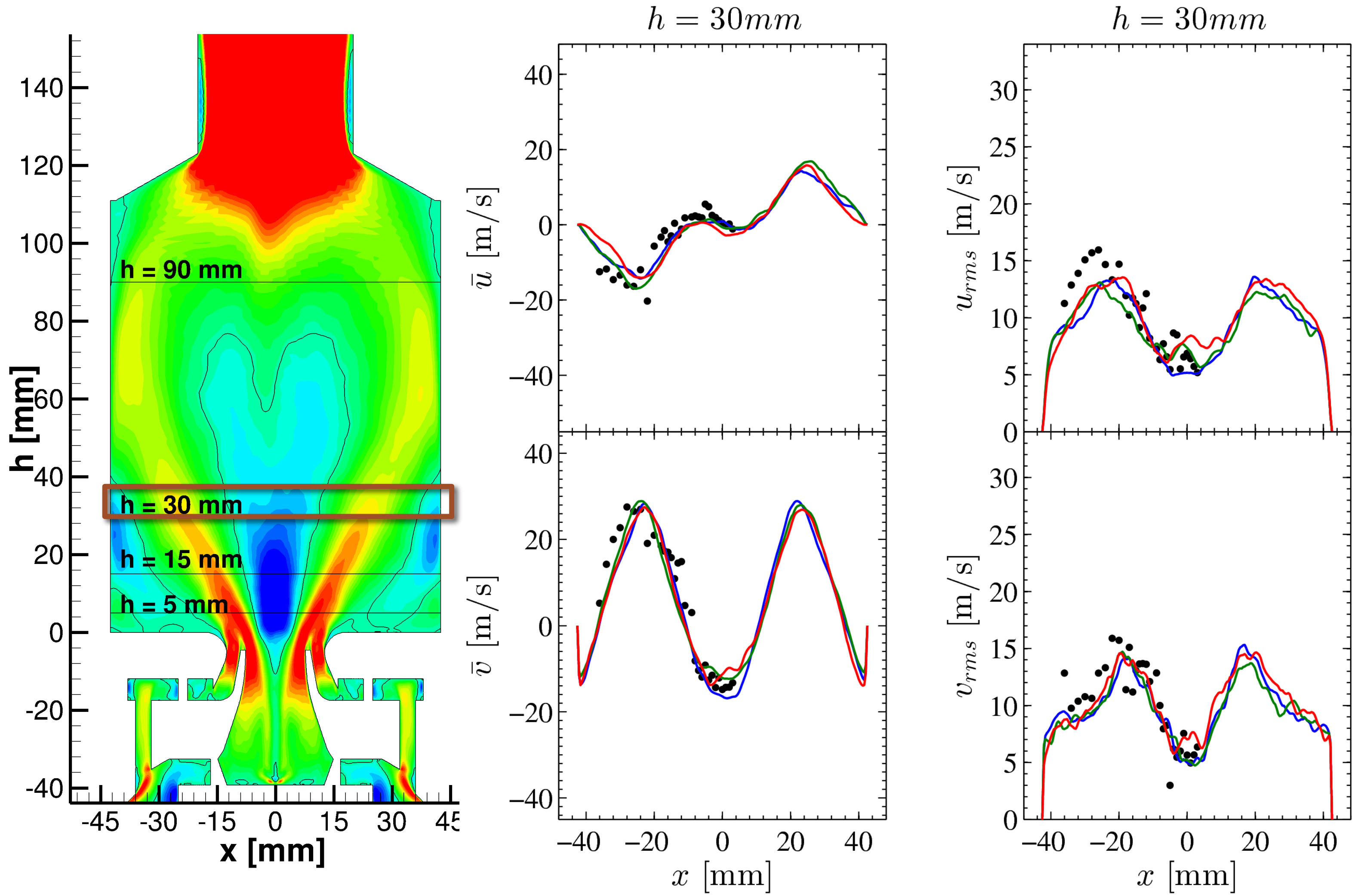
Simulation Results: Mean and RMS Velocities (h=30mm)



o o Experiment   FPV   FPV-Cvar   F-TACLES

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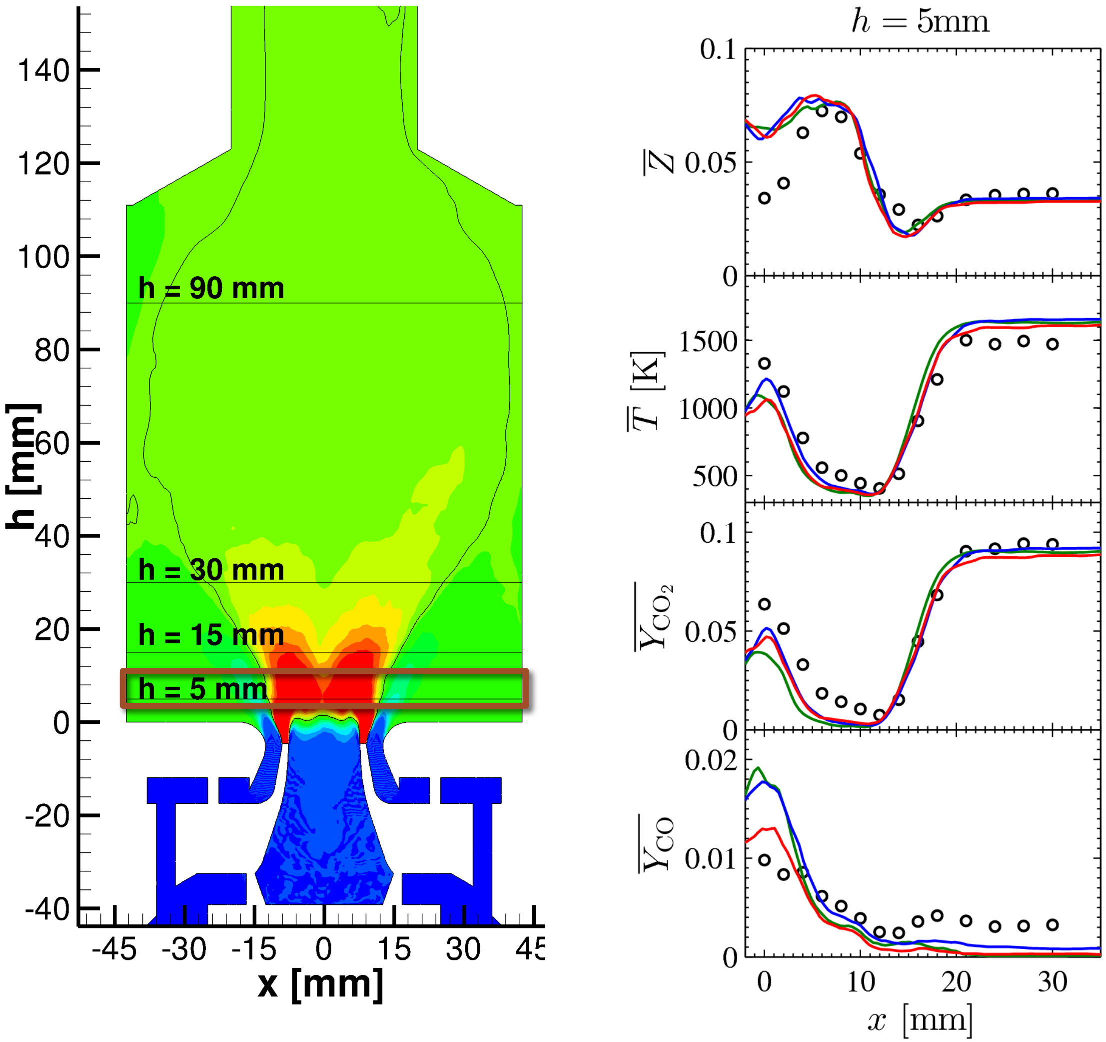
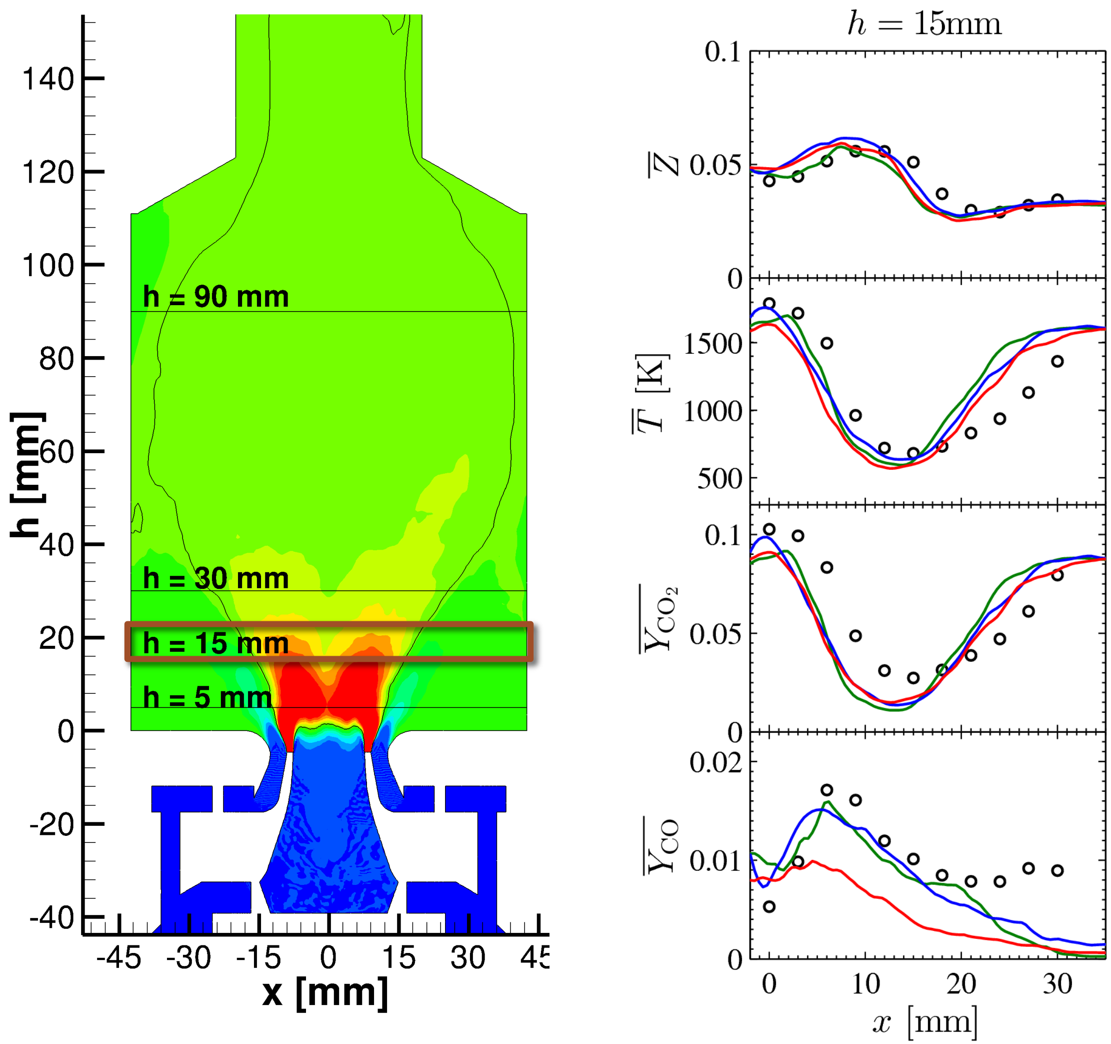
Simulation Results: Temperature and Species (h=5mm)



o o Experiment ---- FPV ---- FPV-Cvar ---- F-TACLES

Simulation Results: Temperature and Species (h=15mm)



o o Experiment ---- FPV ---- FPV-Cvar ---- F-TACLES

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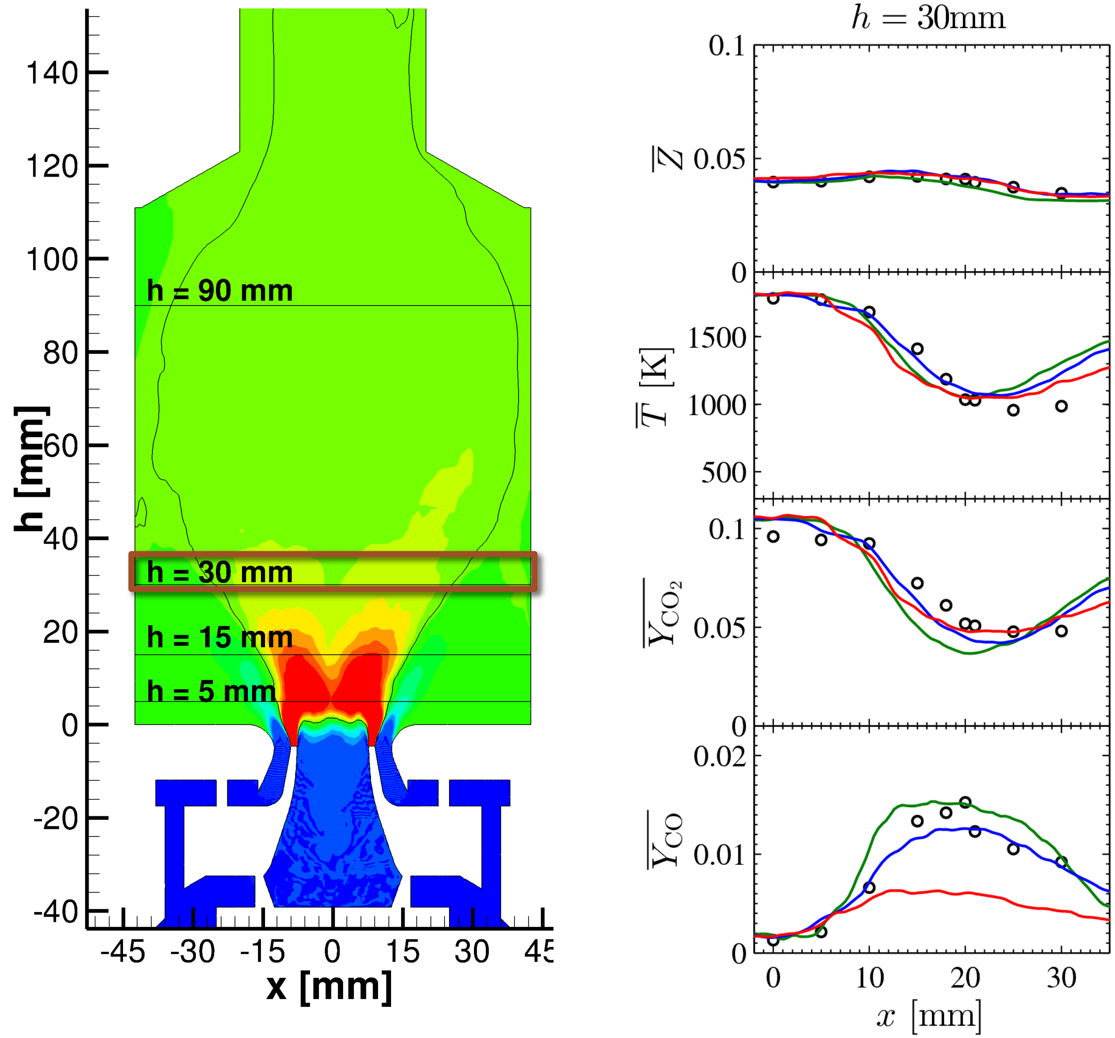
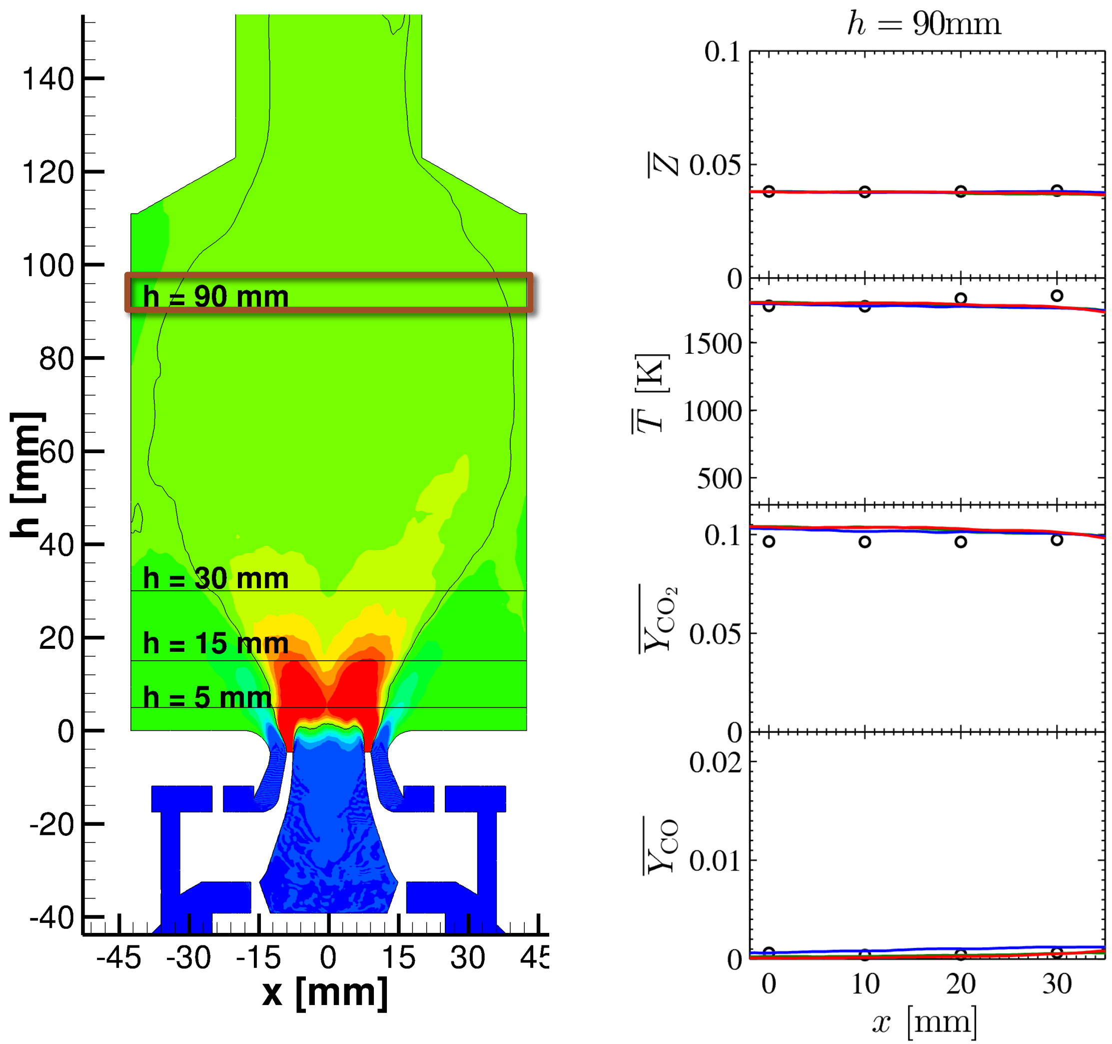
Simulation Results: Temperature and Species (h=30mm)



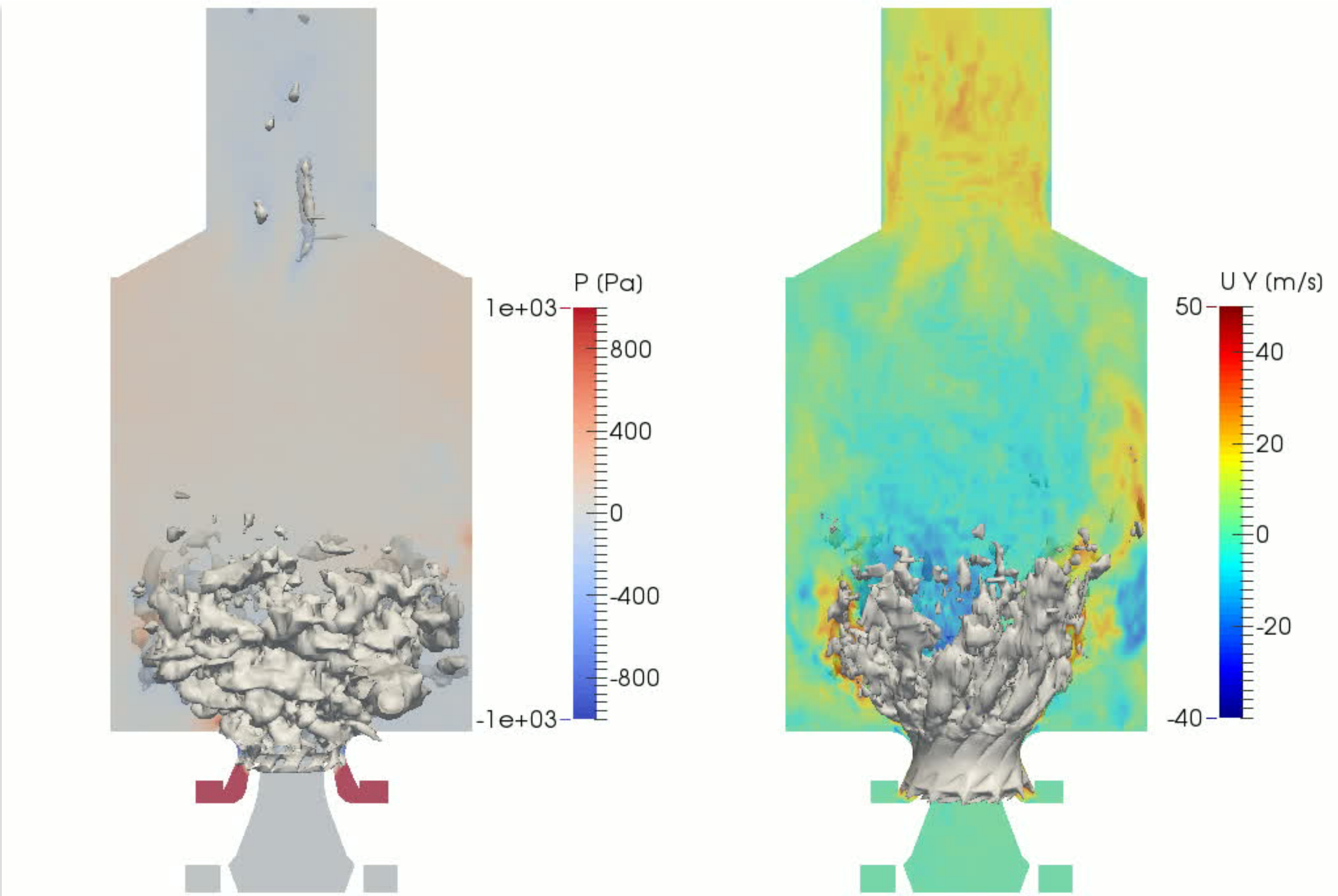
o o Experiment — FPV — FPV-Cvar — F-TACLES

Simulation Results: Temperature and Species (h=90mm)

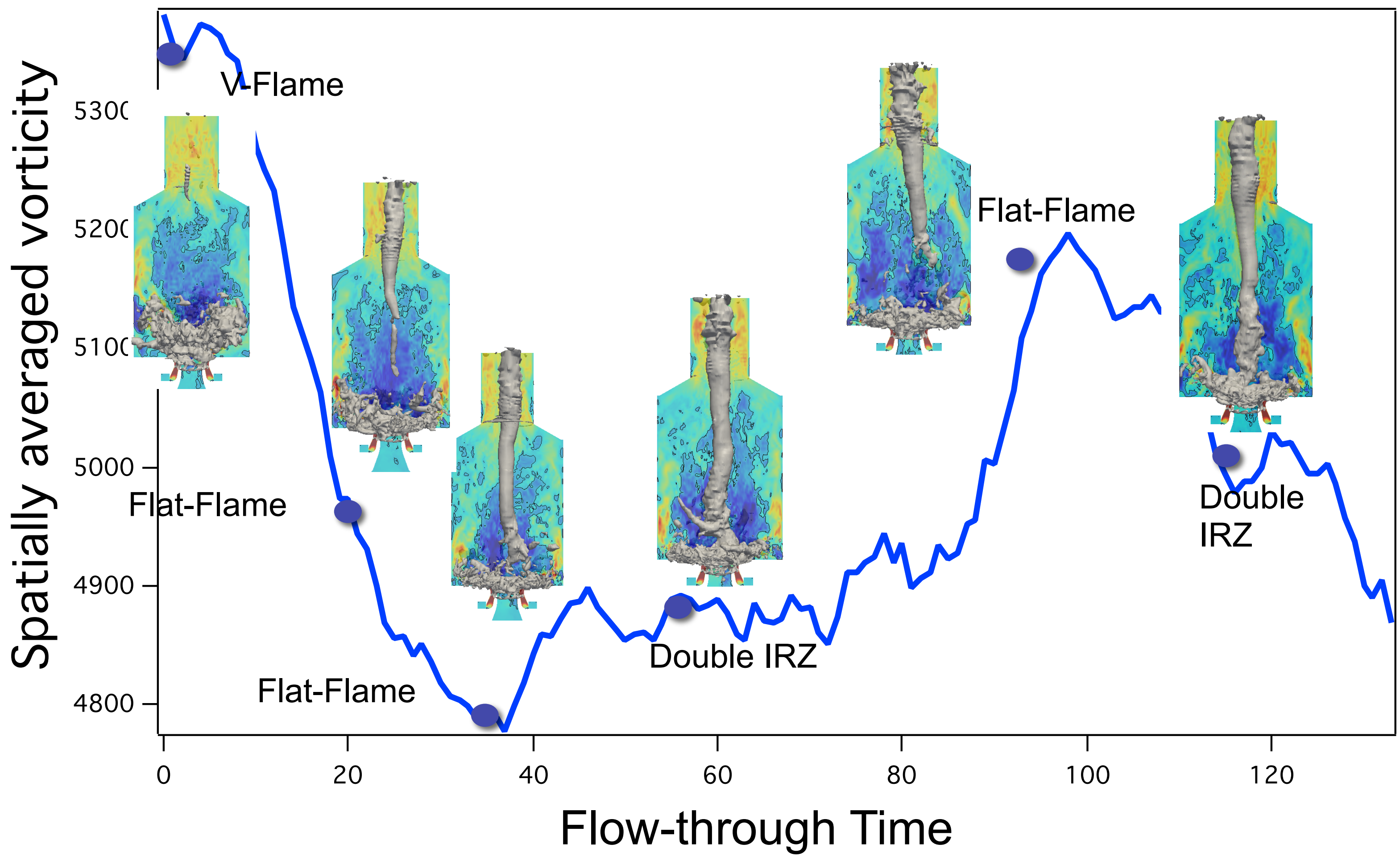


o o Experiment ---- FPV ---- FPV-Cvar ---- F-TACLES

Transient Combustion Dynamics

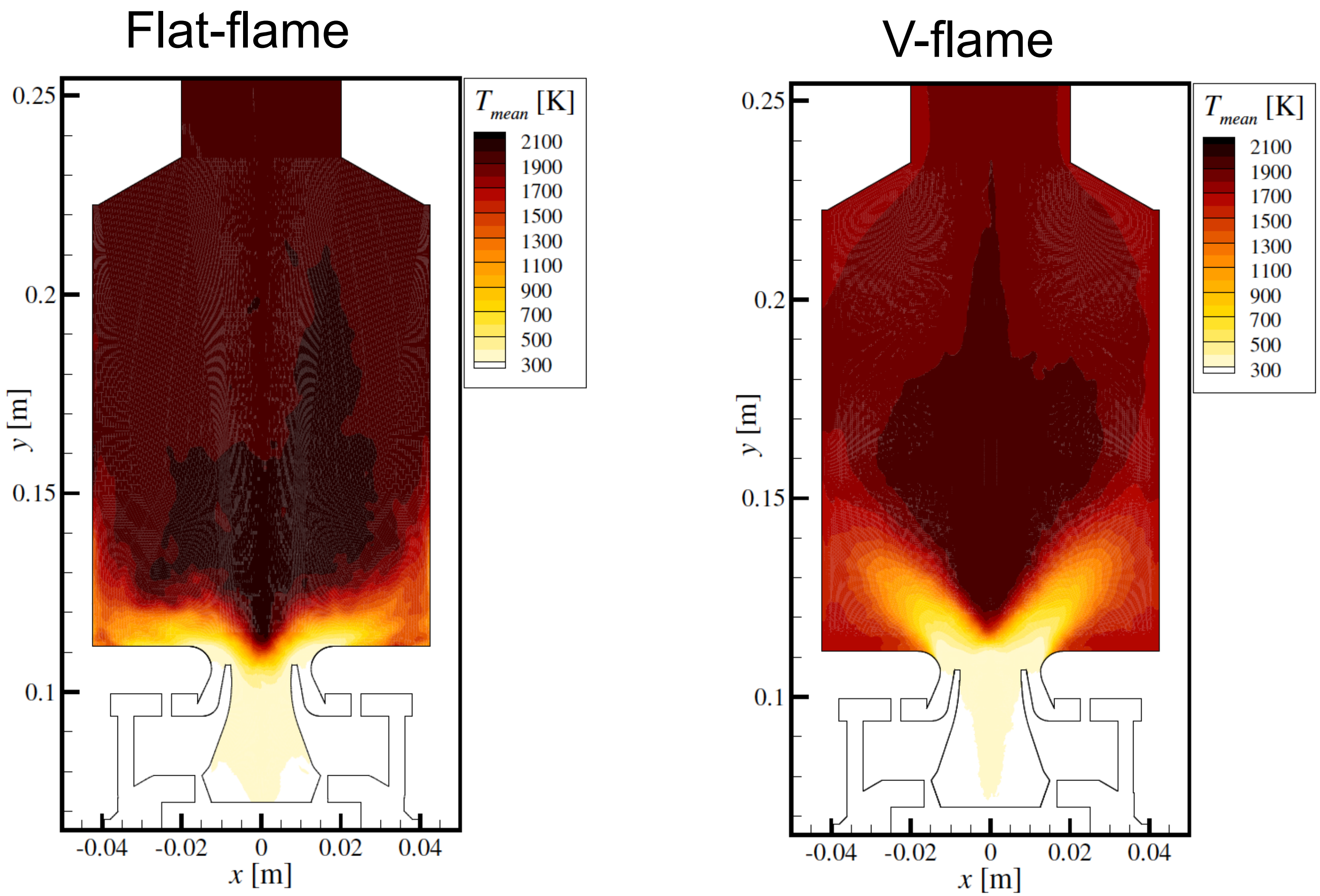


Transient Combustion Dynamics



Transient Combustion Dynamics

Simulation results predict presence of flame switching mode



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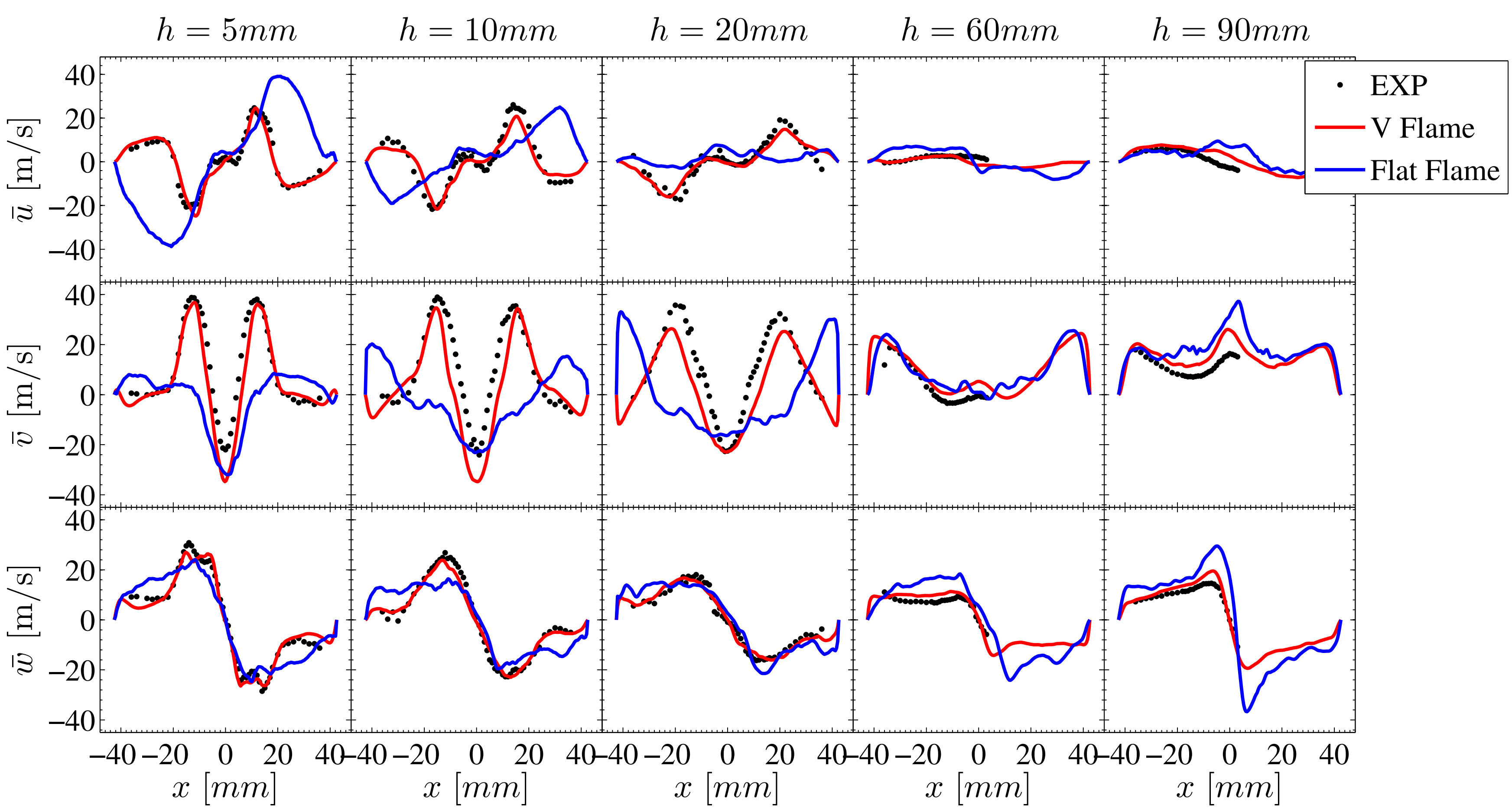
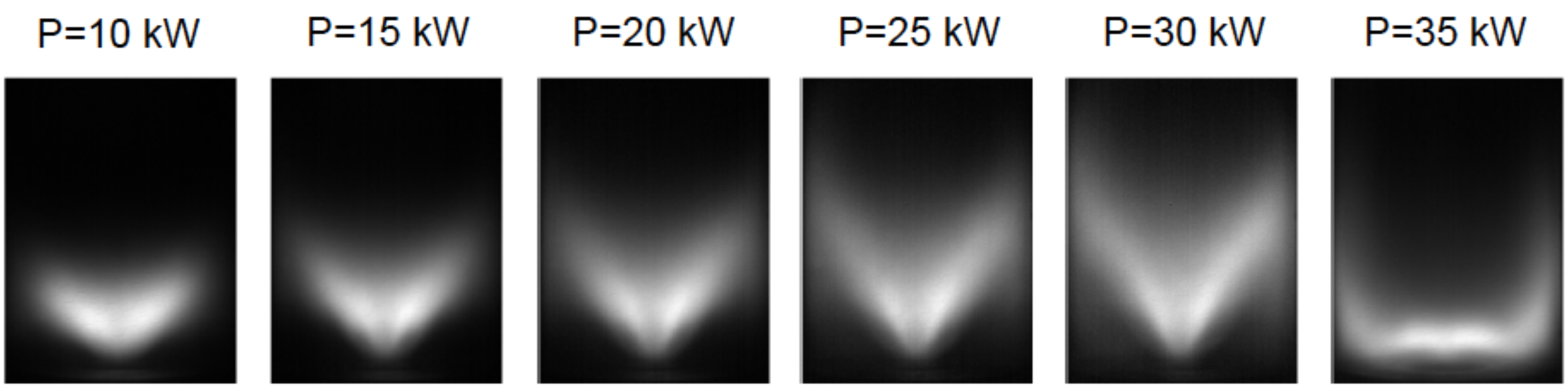
Transient Combustion Dynamics



Transient Combustion Dynamics

Wolfgang Meier (DLR): "The bifurcation of the flame behavior has often been observed by us. It is a quite difficult matter, because the reproducibility of such operating points is subject to many influences. Slight changes in temperature, pressure, flow meters etc. can lead to different results at different days."



Flame shapes (OH chemiluminescence)

M, Stoehr, private communication, 2014

Transient Combustion Dynamics

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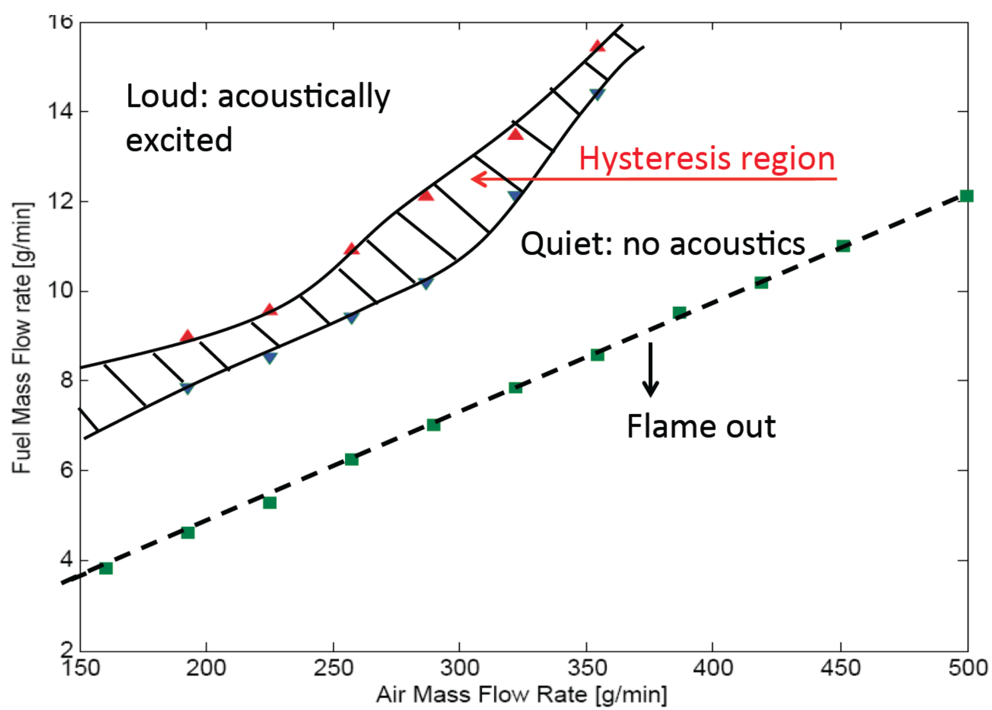

Allison, Driscoll, Ihme, PCI, 34, 2013

Stanford University

Conclusions

Performance evaluation of different topology-based flamelet models in GTMC

- Velocities are insensitive to combustion models
- Similar predictions for major species for both models
- All simulation results shows an elongated IRZ

Main Observations from LES computations of GTMC

- Simulation results exhibit dependence on
  - Mesh resolution and mesh type
  - Subgrid closure
  - Wall-resolution in swirler
- Global modification of flame topology and dependence on flow field require more investigation

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Computational research effort

- Characterization of facility effects in flow reactors
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Summary and Conclusions

Summary and Conclusions

Modeling and analysis of dual-swirl gas-turbine model combustor

- Prior model evaluation showed that premixed and diffusion-based combustion models provide comparable representation of flame-structure in absence of turbulence/chemistry interaction
- Flame-shape and major-species profiles are well captured with FPV and F-TACLES; FPV provides better prediction of minor species profiles (H2, CO)
- In agreement with experimental observation, LES captures bifurcation dynamics (sensitivity to SGS-closure, mesh-resolution, and boundary conditions)

Publications

- See, Y. C. and Ihme, M., "Large eddy simulation of a partially-premixed gas turbine model combustor." Proceedings of the Combustion Institute, 35, 2014, in press
- Allison, P. M., Chen, Y., Ihme, M., and Driscoll, J. F., "Coupling of flame geometry and combustion instabilities based on kilohertz formaldehyde PLIF measurements." Proceedings of the Combustion Institute, 35, 2014, in press.
- See, Y. C. and Ihme, M., "Investigation of flow field sensitivity in a gas turbine model combustor." Paper presented at the AIAA Science and Technology Forum and Exposition (SciTech2014), AIAA 2014-0621, Washington, DC, 2014.
- See, Y. C. and Ihme, M., "Large Eddy Simulation of a Gas Turbine Model Combustor." Paper presented at the 51st AIAA Aerospace Sciences Meeting and Exhibit, AIAA 2013-0172, Grapevine TX, 2013.

Summary and Conclusions

Analysis of facility effects in flow reactors

- Developed Eulerian parabolized model to describe ignition and combustion dynamics in flow reactors
- Performed comprehensive analysis of facility specific sensitivities: velocity field, temperature, species
- Scaling analysis revealed presence of relevant time-scales associated with
  - Diffusion
  - Homogeneous ignition
  - Deflagration in thin-reaction zones regime and in corrugated reaction zones regime
- Recommendation:
  - Measurements of temperature field after injector
  - Consider competition of HR-ignition and deflagration at low-temp. conditions

Publications

- Wu, H. and Ihme, M., "Effects of flow-field and mixture inhomogeneities on the ignition dynamics in continuous flow reactors." *Combust. Flame,* 161, 9, 2317-2326, 2014.
- Ihme, M., "The known unknowns: Detailed simulations and low-order modeling to characterize facility-induced non-idealities in chemical-kinetics experiments." Invited Talk, Meeting of the American Physical Society - Division of Fluid Dynamics, Pittsburgh, PA, 2013.