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

Fuel-effects in dual-swirl gas-turbine combustor

- LES modeling analysis
- Model development: Fidelity-adaptive combustion modeling
- Thermoacoustic network analysis

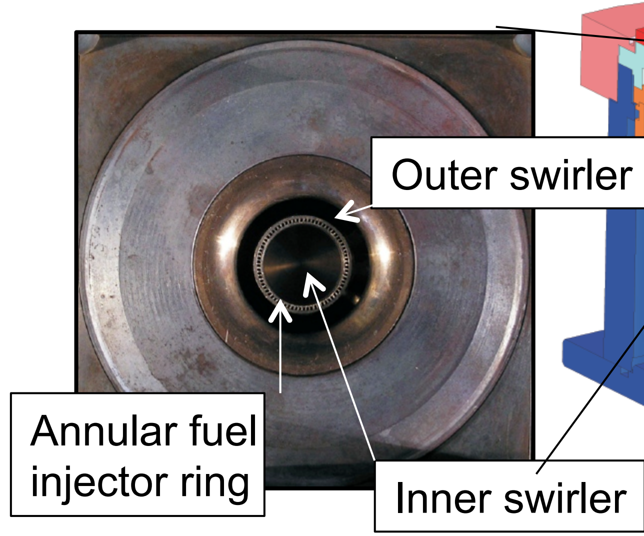
Facility-induced non-idealities

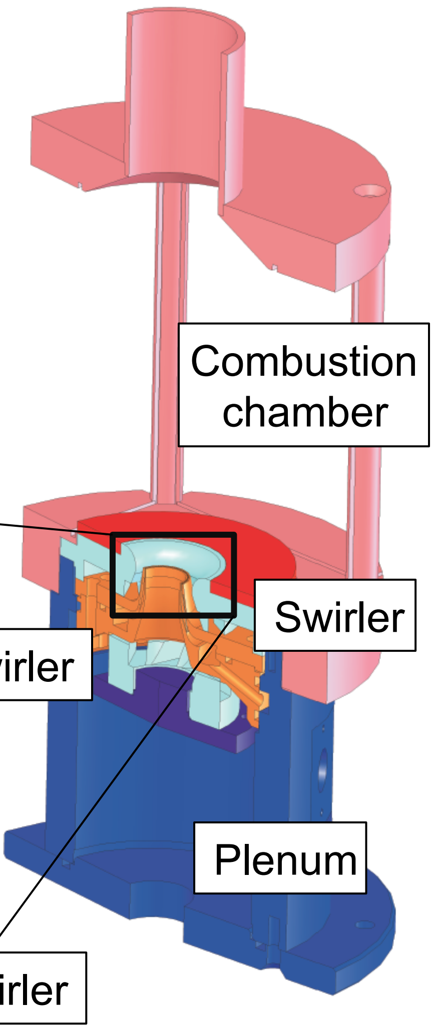
Conclusions

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]

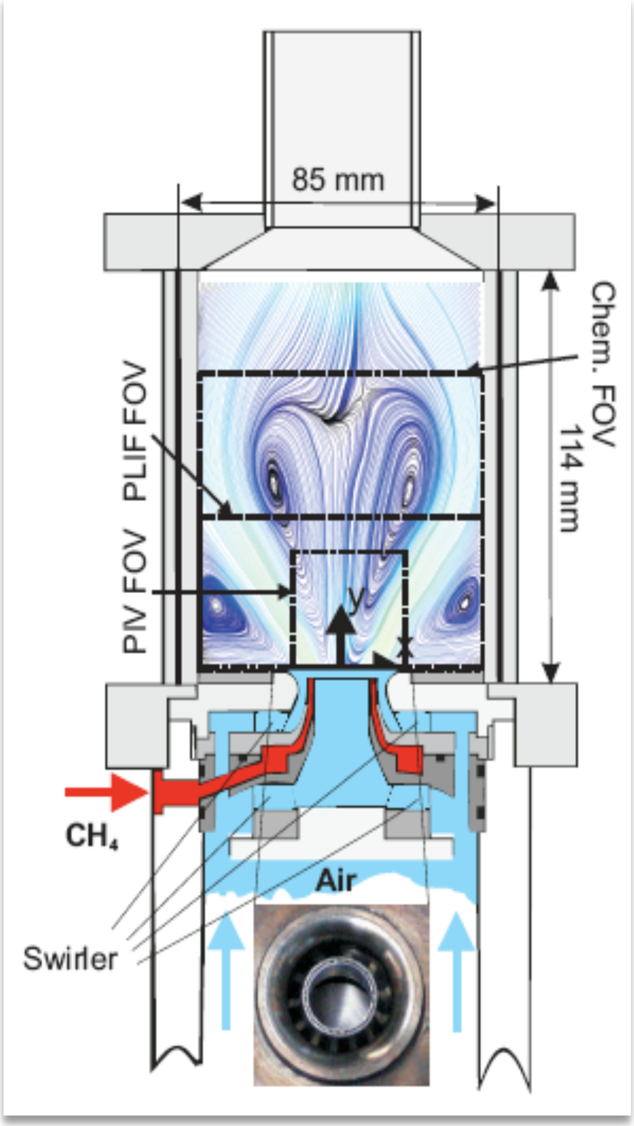
- Aero-derived dual-swirl combustor
- Optical access for non-intrusive diagnostics
- Common air-supply through plenum
- Fuel injection between inner and outer swirlers

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)

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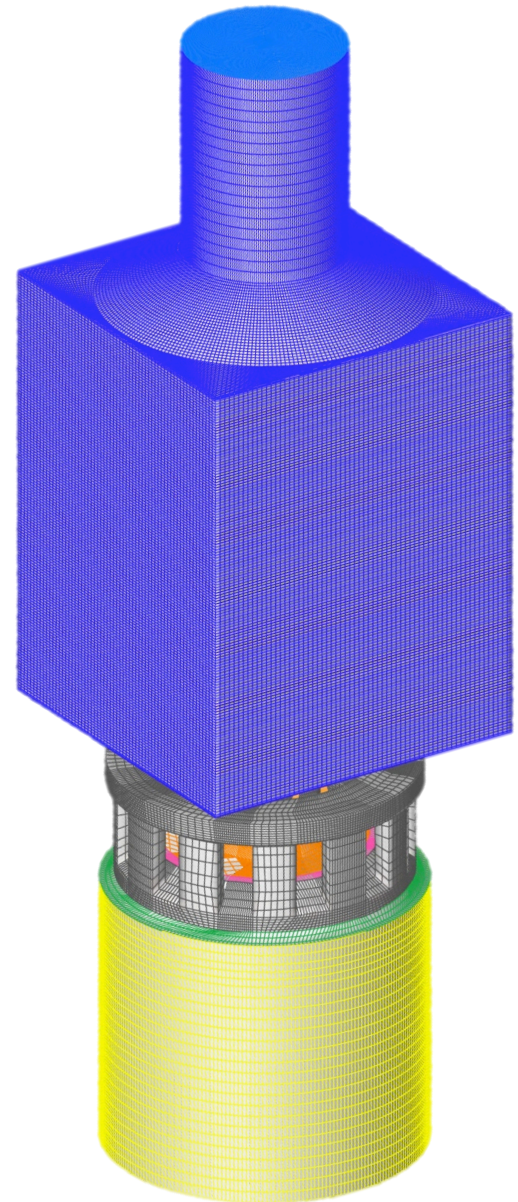
Computational Setup

Computational mesh

- Mesh-types
  - Fully block-structured hex-mesh
  - Hybrid hex/tet meshes
- Wall-resolved mesh in swirler and base of combustion chamber

Mesh-investigation

	Numer of Elements (millions)			
Mesh	**Plunum**	**Swirler**	**Comb. Chamber**	**Total**
Hex1	0.5	6	1.5	**8**
Hex2	2.0	10	5	**17**
Hex3	2.0	20	21	**43**
Hyb1	0.5	2	4.5	**7**
Hyb2	2	10	8	**20**
Hyb3	5	75	20	**100**



Combustion Models

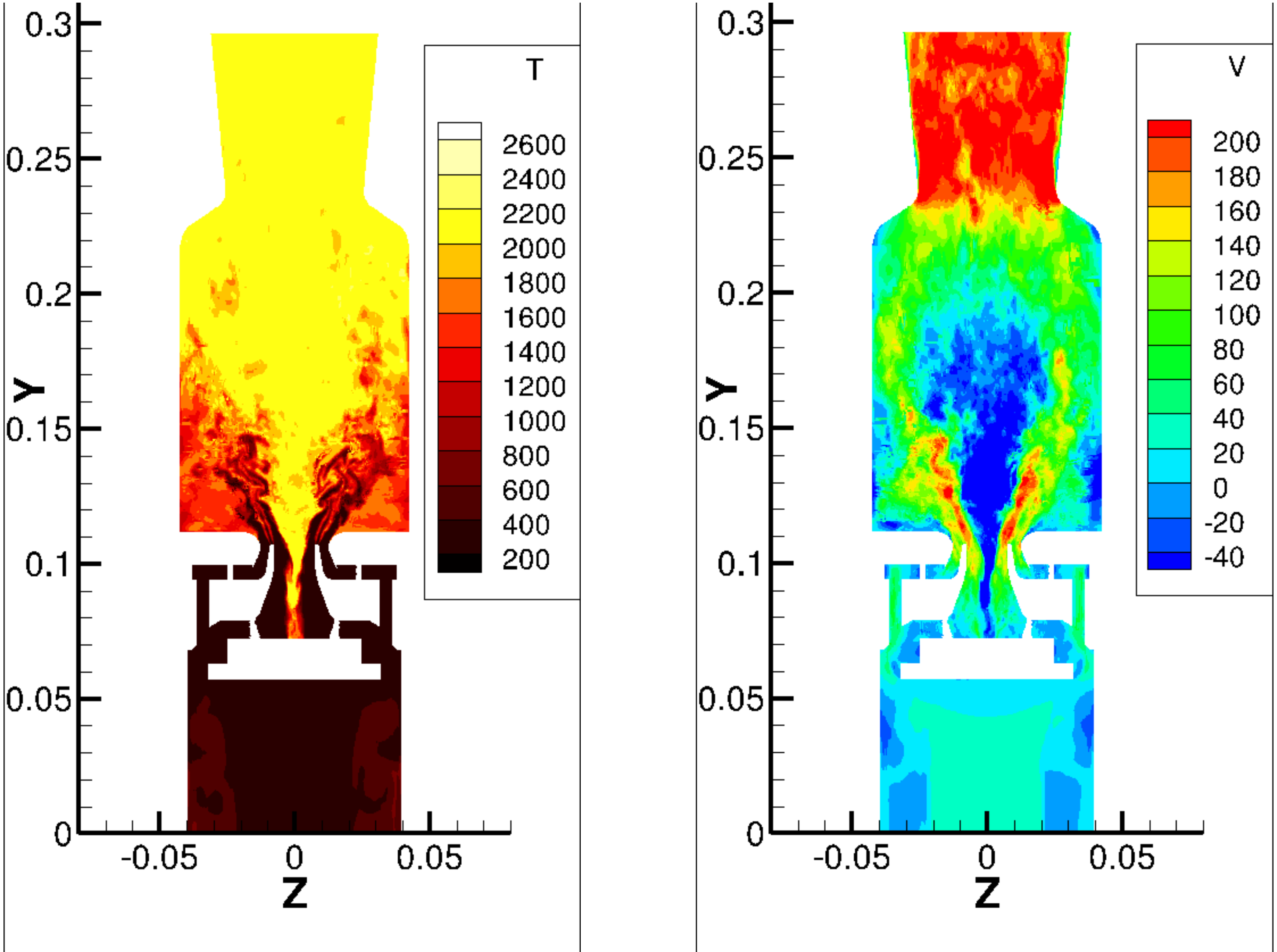
Models	Flamelet Progress Variable (FPV)[1]	FPV with Progress Variable (FPV-Cvar)[2]	Filtered Tabulated Chemistry for LES (F-TACLES)[3]
Flamelet regime	Non-premixed	Non-premixed	Premixed
Tab. variables	$\widetilde{Z}, \widetilde{Z''^2}, \widetilde{C}$	$\widetilde{Z}, \widetilde{Z''^2}, \widetilde{C}, \widetilde{C''^2}$	$\widetilde{Z}, \widetilde{Z''^2}, \widetilde{C}$
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)

Unstable Combustion Processes
Flow Field Results



Unstable Combustion Processes
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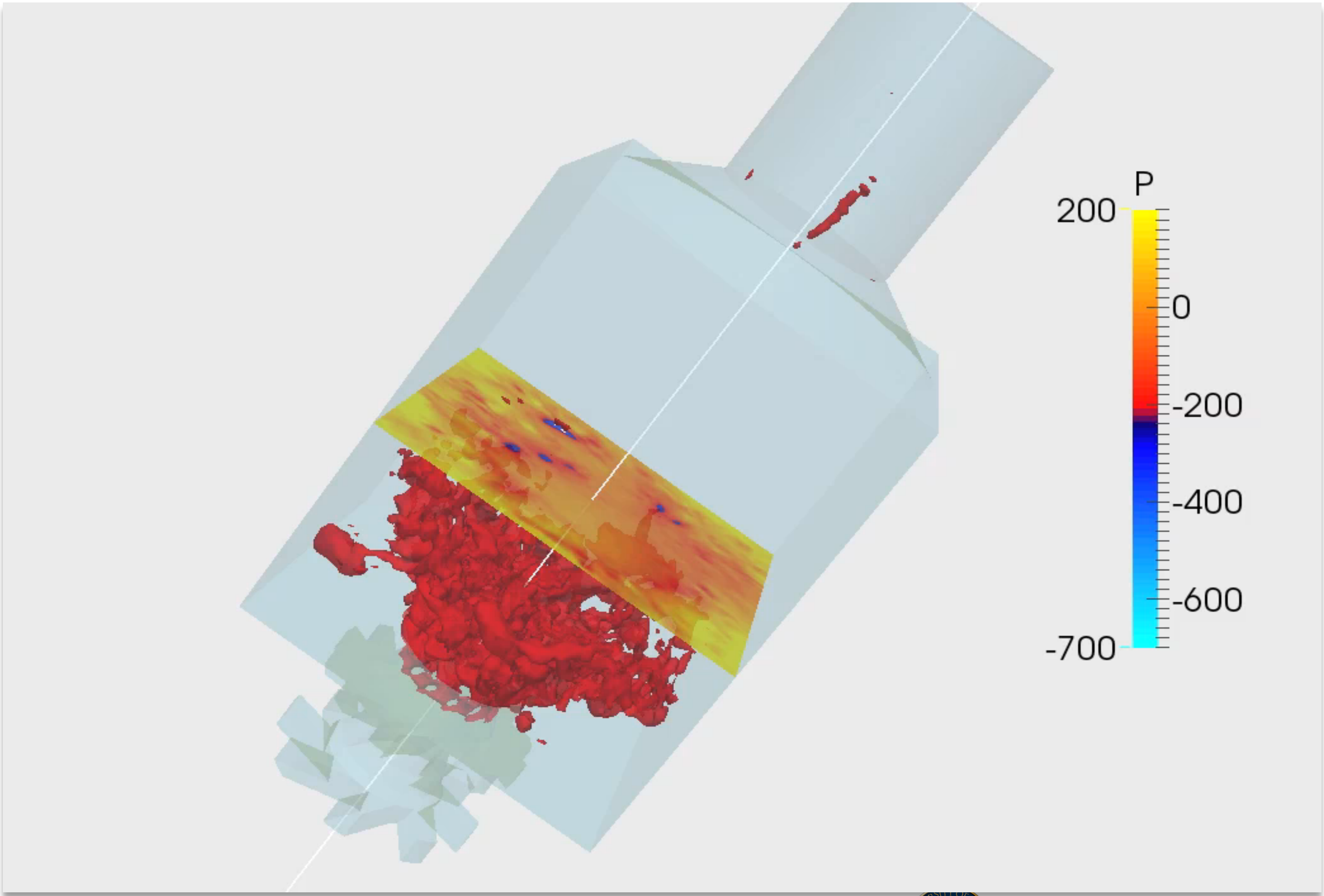
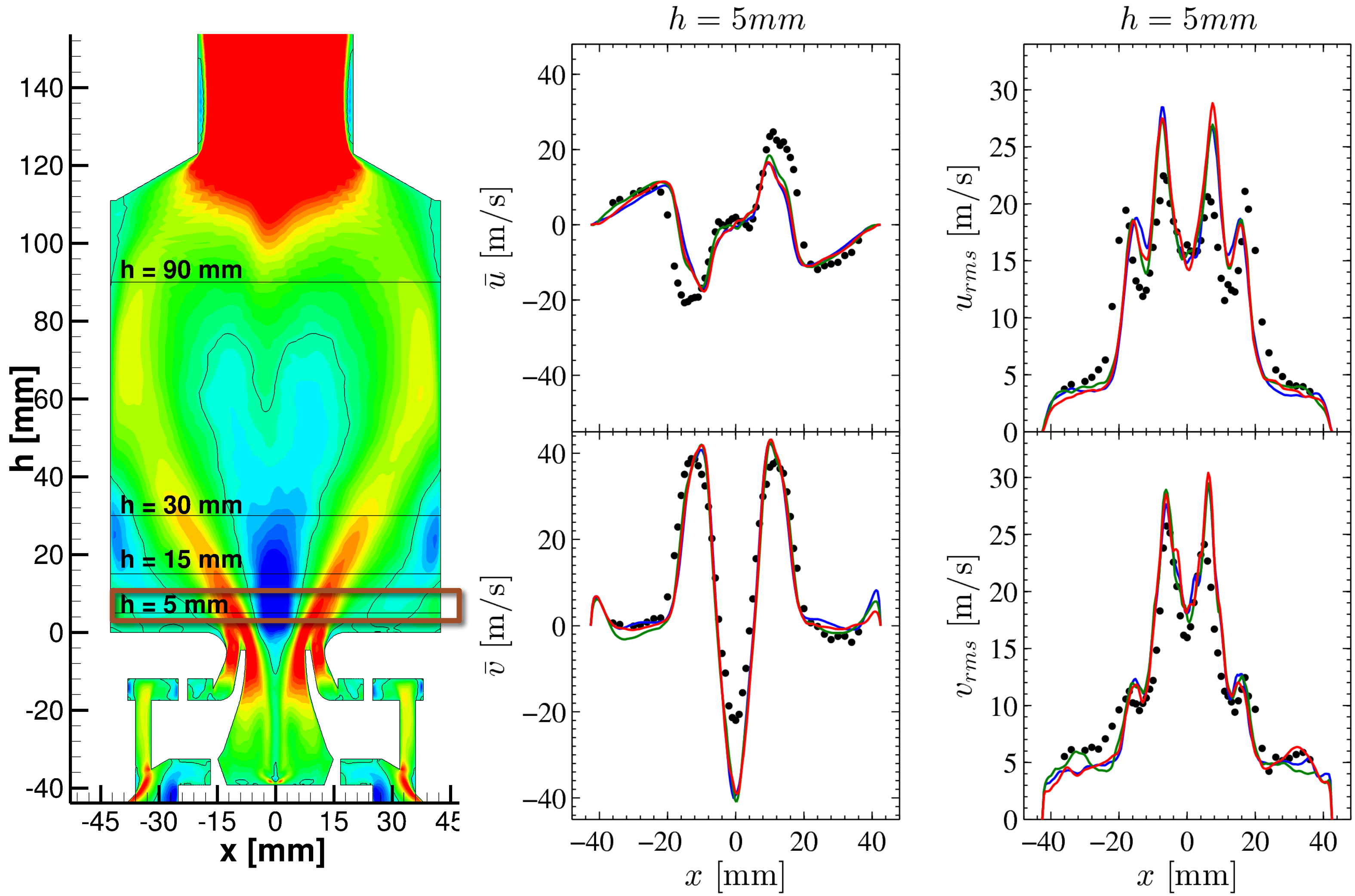
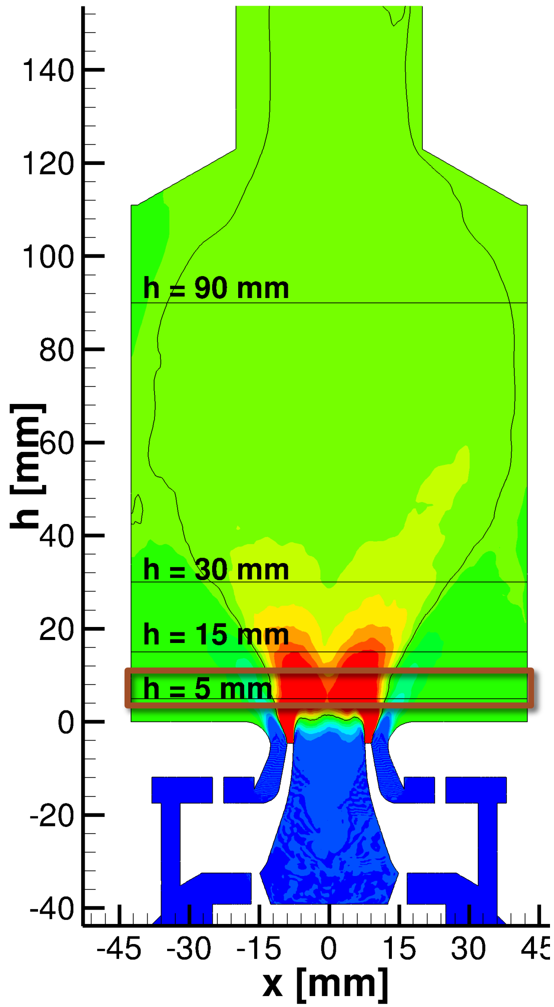


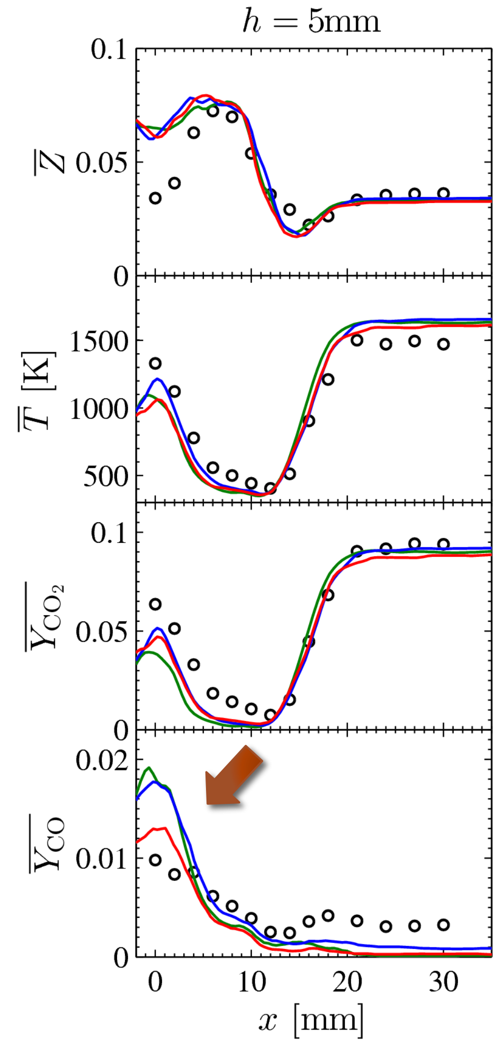
Simulation Results: Mean and RMS Velocities (h=5mm)



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

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





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

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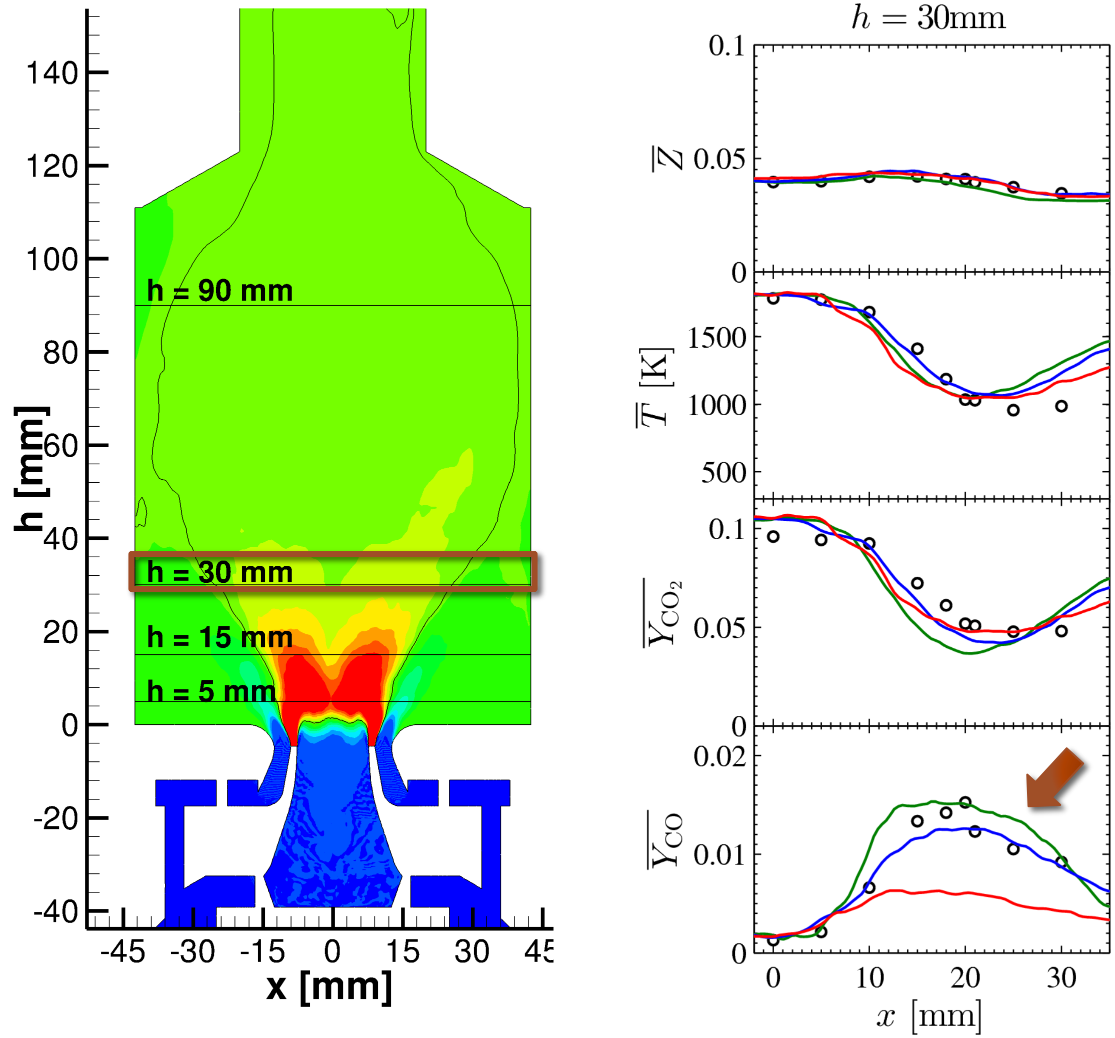
Simulation Results: Temperature and Species (h=30mm)



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

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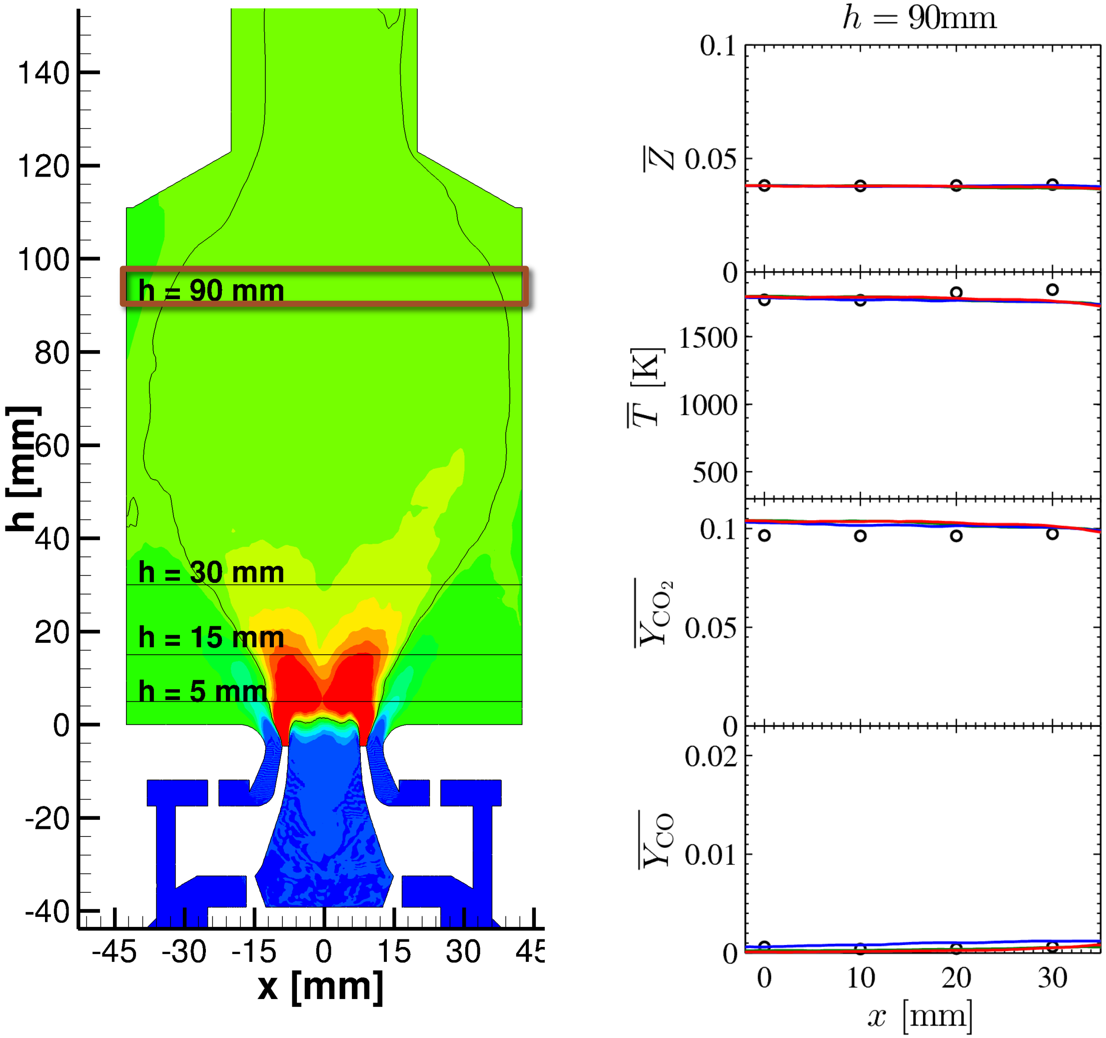
Simulation Results: Temperature and Species (h=90mm)



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

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LES Model Evaluation

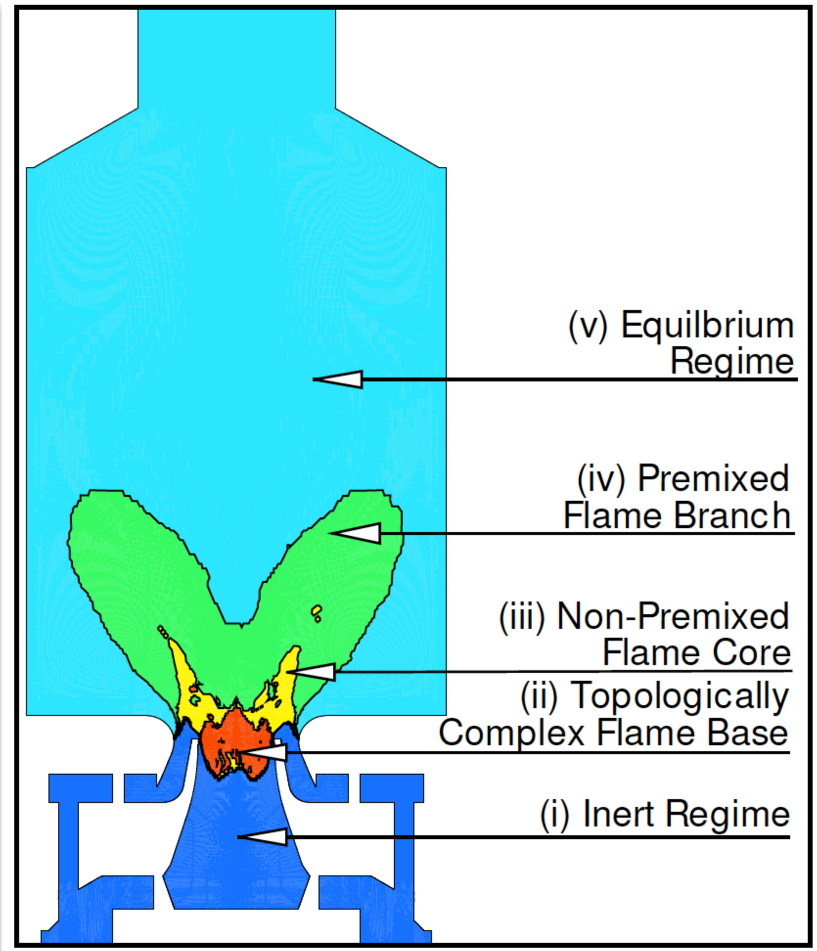
Main observation

- Prediction of velocity field insensitive to LES-combustion model selection
- Temperature and major species equally well predicted by all models
- Depending on flame region, minor species (CO, NO) exhibit substantial model sensitivities

Combustion modes

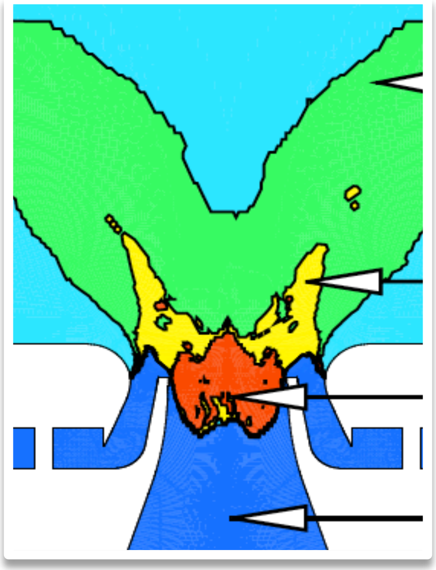
- Different combustion modes simultaneously present
- Selection of monolithic model often unsuccessful for predicting combustor performance

➔ Need for adaptive modeling combustion models



When is a model "good" enough

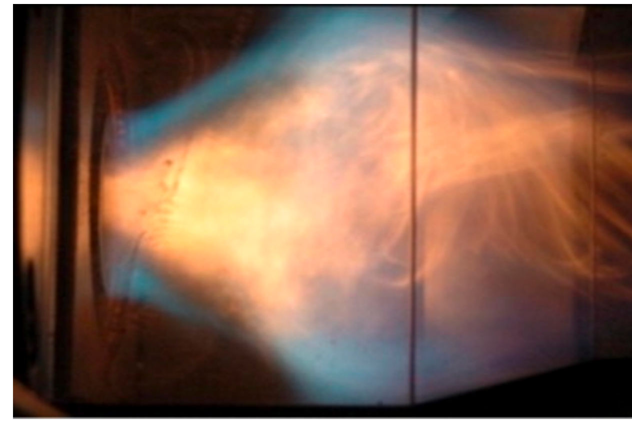
FIDELITY-ADAPTIVE COMBUSTION MODEL



Performance of Combustion Models

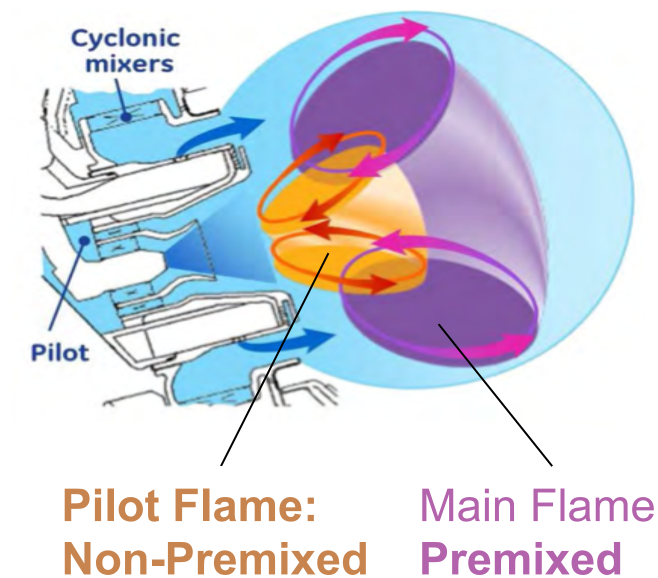
Model error depends on

- Quantities of interest (T, CO2, CO, NO)
- Combustion-physical processes (autoignition, local extinction/re-ignition)
- Combustion regimes: premixed, non-premixed, multiphase



Model selection

- Single-mode combustion model
- Global control of error
- Balance between computational efficiency and accuracy
- Dependence of model accuracy on quantities of interest



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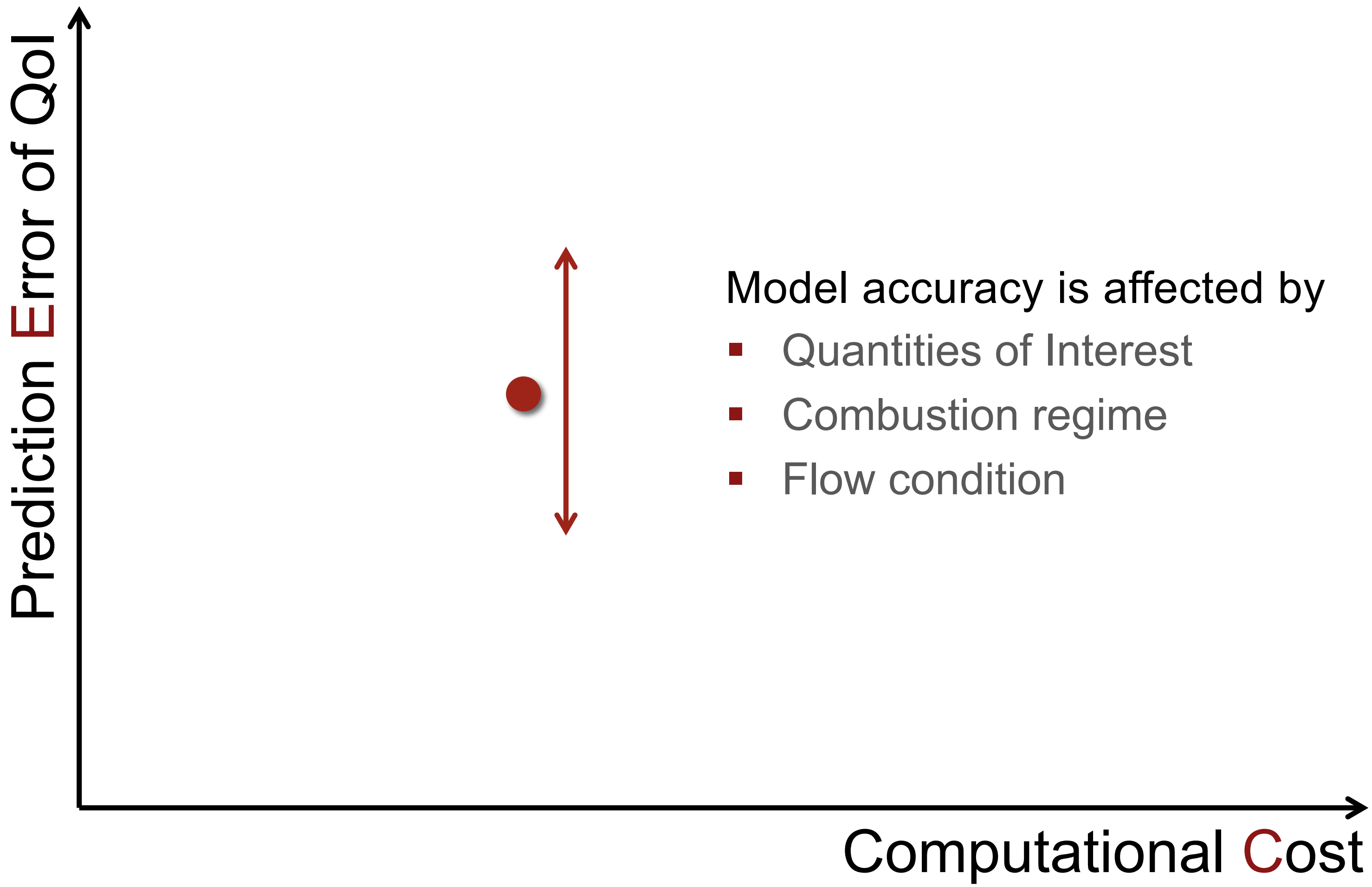
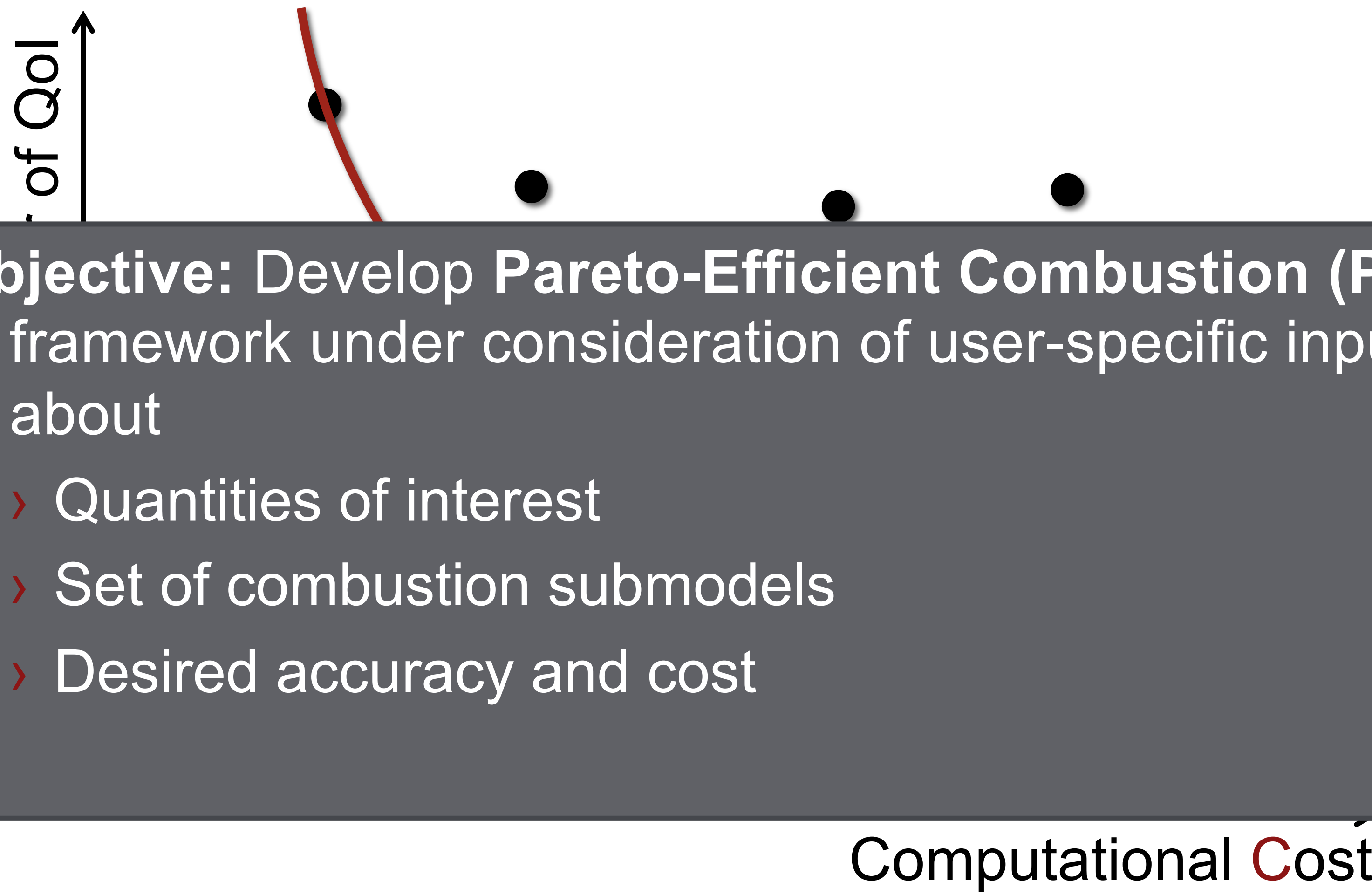
Performance of Combustion Models



Performance of Combustion Models

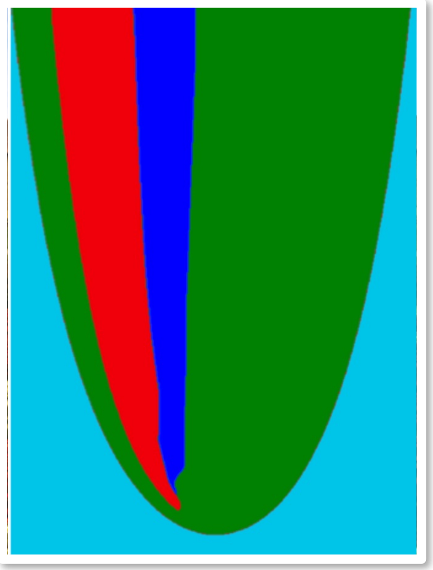


Objective: Develop **Pareto-Efficient Combustion (PEC)** framework under consideration of user-specific input about

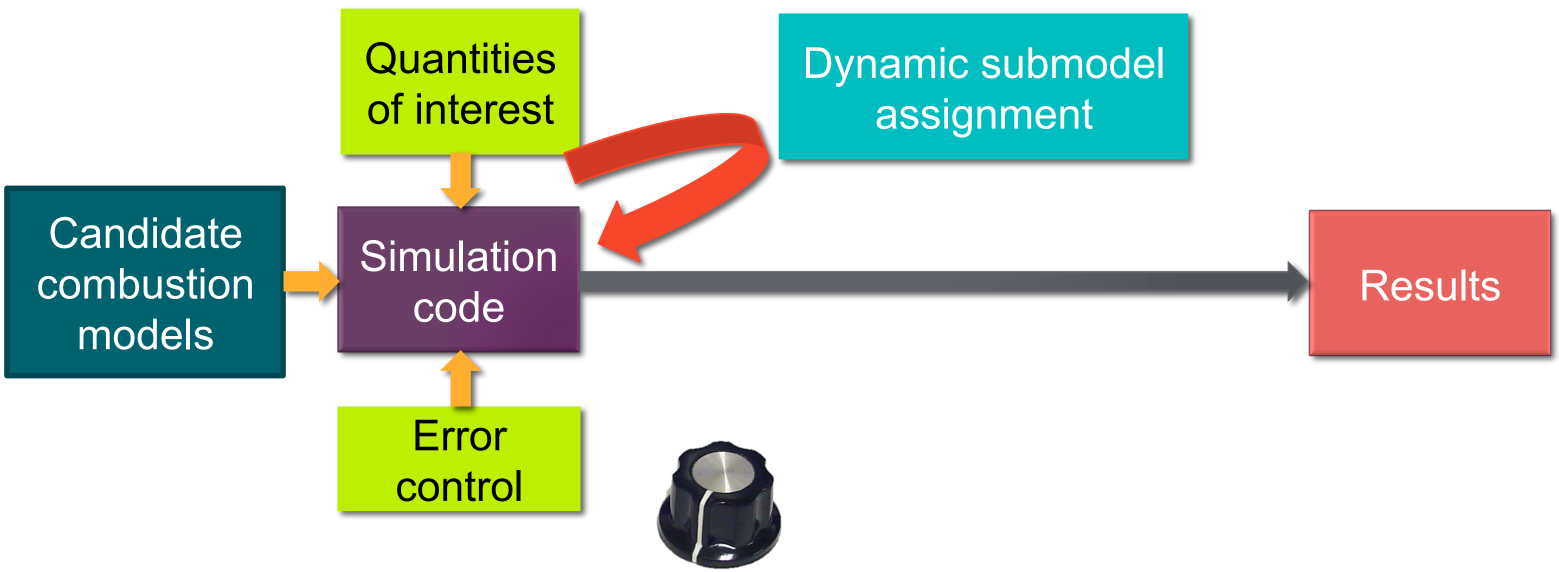
- Quantities of interest
- Set of combustion submodels
- Desired accuracy and cost

PEC-Modeling Framework

PARETO-EFFICIENT COMBUSTION MODEL



PEC Modeling Framework



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PEC Modeling Framework

User input

- Set of quantities of interest: $Q = \{Y_{CO2}, Y_{CO}, Y_{H2O}, Y_{NO}, \ldots\}$
- Set of candidate combustion models: *M*
  - Reaction-transport manifolds: FPV, FPI, FGM, Inert Mixing, …
  - Chemistry manifold: detailed chemistry, skeletal, reduced, …
- Penalty term λ for cost/accuracy trade-off

PEC algorithmic components

- Model selection
- Error assessment
- Coupling between subzones and different models
- Computational considerations

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PEC algorithmic components

- **Model selection**
- Error assessment
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PEC Modeling Framework
Model Selection

- Model assignment $\mathcal{M} : \Omega \to M$

Physical domain (Ω)

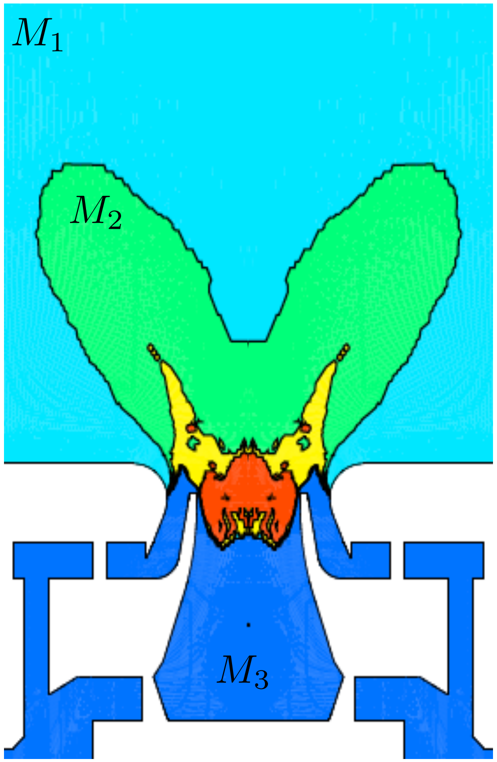
Set of candidate models (M)
{FPV, FPI, Detailed Chemistry, …}

- Solve optimization problem

$$\min_{\mathcal{M}:\Omega\to M} \mathcal{E}(\mathcal{M}) + \lambda \mathcal{C}(\mathcal{M})\,,$$

with

- Model error: $\mathcal{E}(\mathcal{M}) = \int_\Omega \left| e^{\mathcal{M}}(\mathbf{x}) \right| d\mathbf{x}\,,$
- Cost: $\mathcal{C}(\mathcal{M}) = \int_\Omega \left| c^{\mathcal{M}}(\mathbf{x}) \right| d\mathbf{x}\,.$



PEC Modeling Framework

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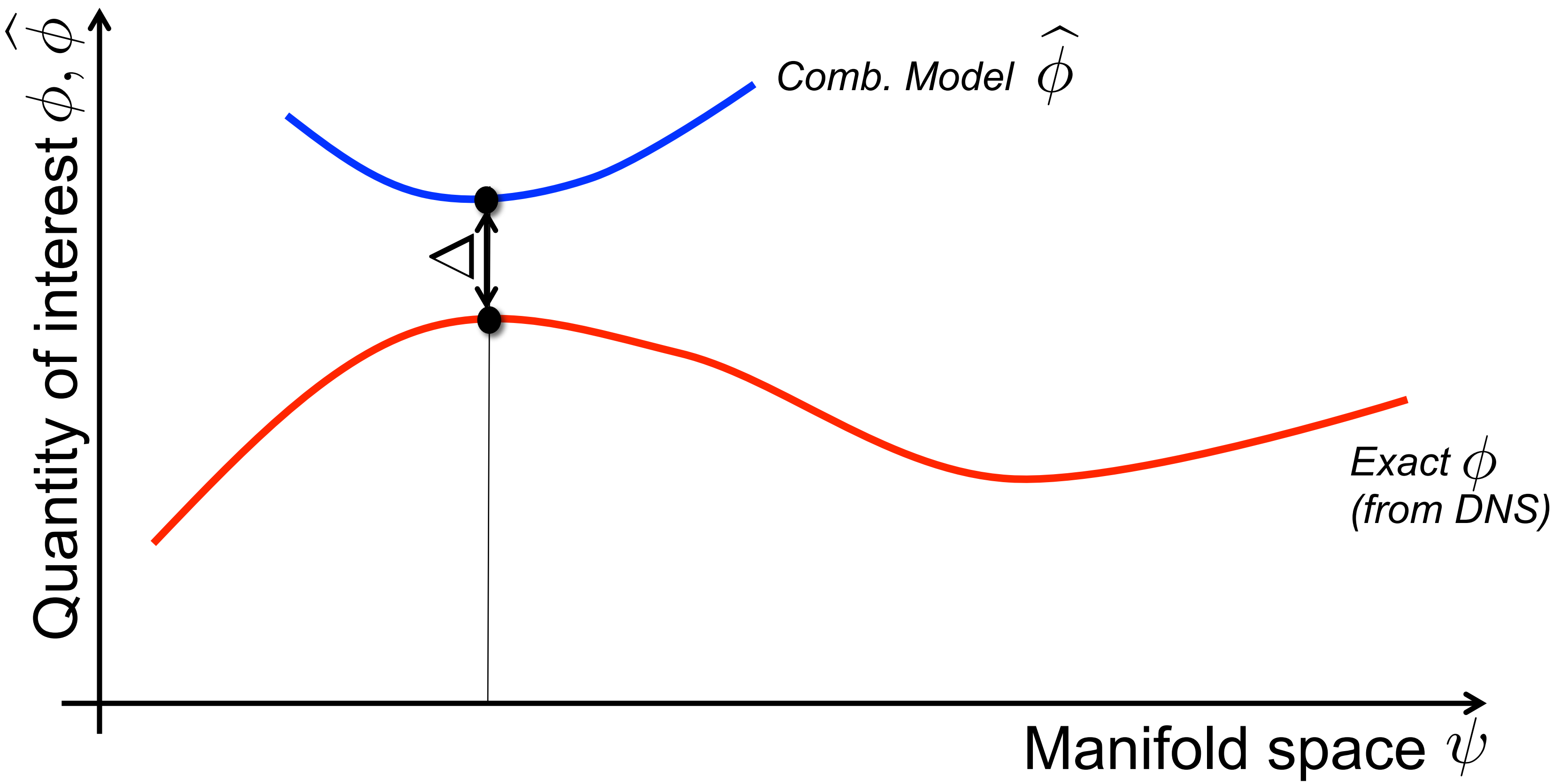
PEC algorithmic components

- Model selection
- **Error assessment**
- Coupling between subzones and different models
- Computational considerations

PEC Modeling Framework
Error Assessment – Key idea

- Evaluate model error $\Delta = \widehat{\phi} - \phi$

✖ ✔



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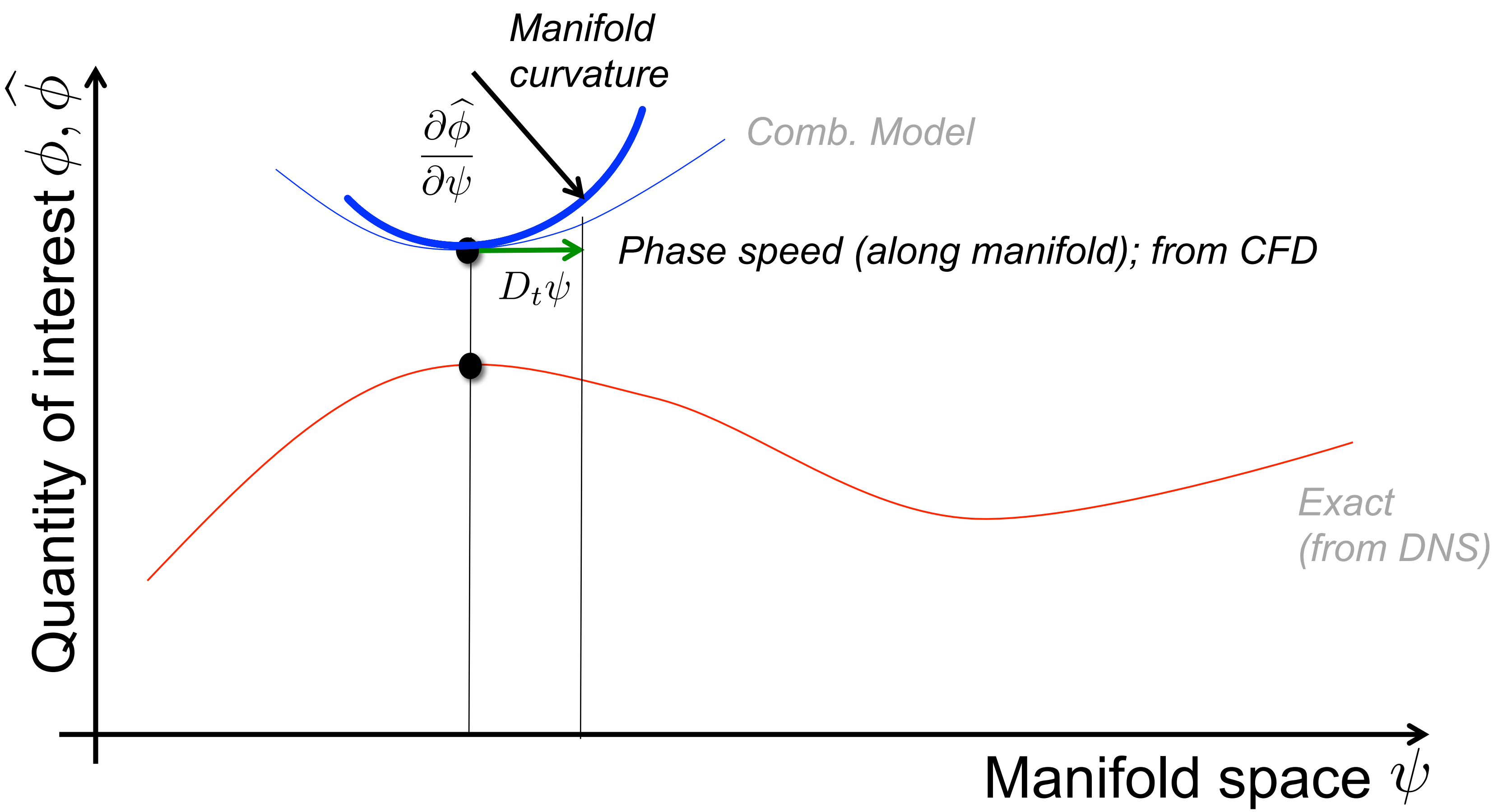
PEC Modeling Framework
Error Assessment – Key idea

- Evaluate model error $\Delta = \widehat{\phi} - \phi$
- Instead, evaluate compatibility of combustion model and CFD-solution



PEC Modeling Framework
Error Assessment

- Evaluate compatibility by expanding error: $\Delta = \widehat{\phi} - \phi$

- Drift from manifold[1] for each QoI and candidate model

$$\mathcal{D} = D_t \Delta\big|_{\Delta=0}$$

Manifold curvature

$$= D_t \phi\big|_{\phi=\widehat{\phi}} - \frac{\partial \widehat{\phi}}{\partial \psi} \cdot D_t \psi$$

Phase speed

- Relate model error to manifold drift (for QoI's)

$$e^{\mathcal{M}} = \frac{1}{|Q|} \sum_{\alpha \in Q} w_\alpha \mathcal{D}_\alpha^{\mathcal{M}}$$

1 Pope, S. B. "Small scales, many species and the manifold challenges of turbulent combustion, Proc. Combust. Inst. 34, 2013

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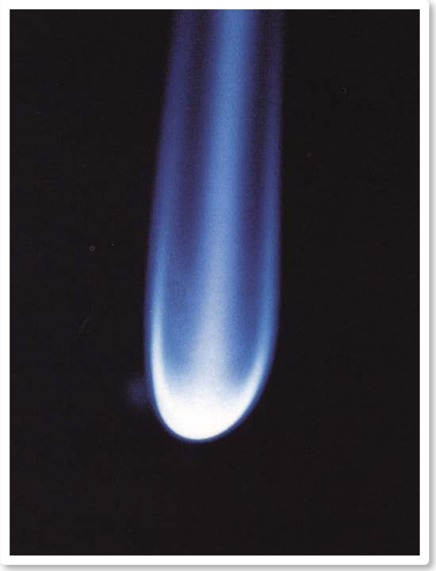
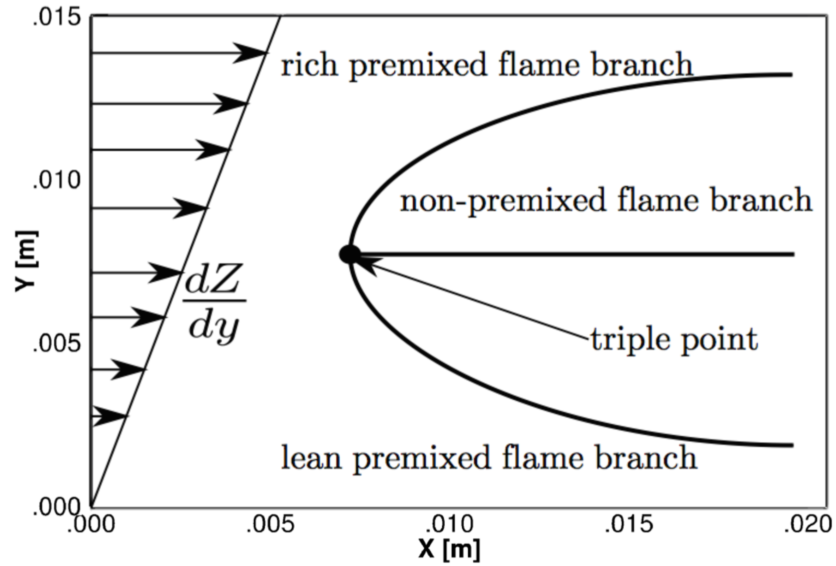
Results

TRIBRACHIAL
FLAME



Model Problem: Tribrachial Flame

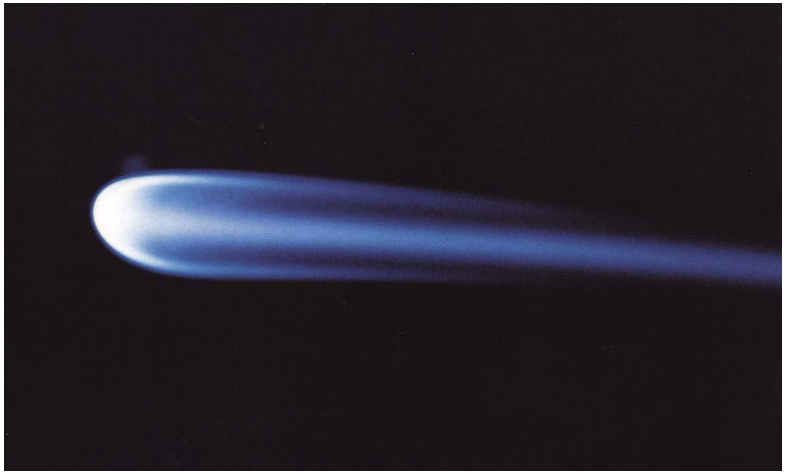


Configuration

- CH4-Air laminar flame
- Stratification of reactants

Combustion submodels

- Reaction-transport manifold
  - Flamelet Progress Variable (FPV)
  - Flame Prolongation of ILDM (FPI)
  - Inert Mixing (IM)
- Chemistry Manifold
  - Detailed chemistry (DC): GRI 3.0
  - Skeletal mechanism (SC): DRM-19



Kioni, et al. CnF (1993)
Dold CnF (1989)
See, Ihme PCI (2014)
Pierce & Moin (2001)
Fiorina et al. CnF (2010)

Results
Stationary Flame

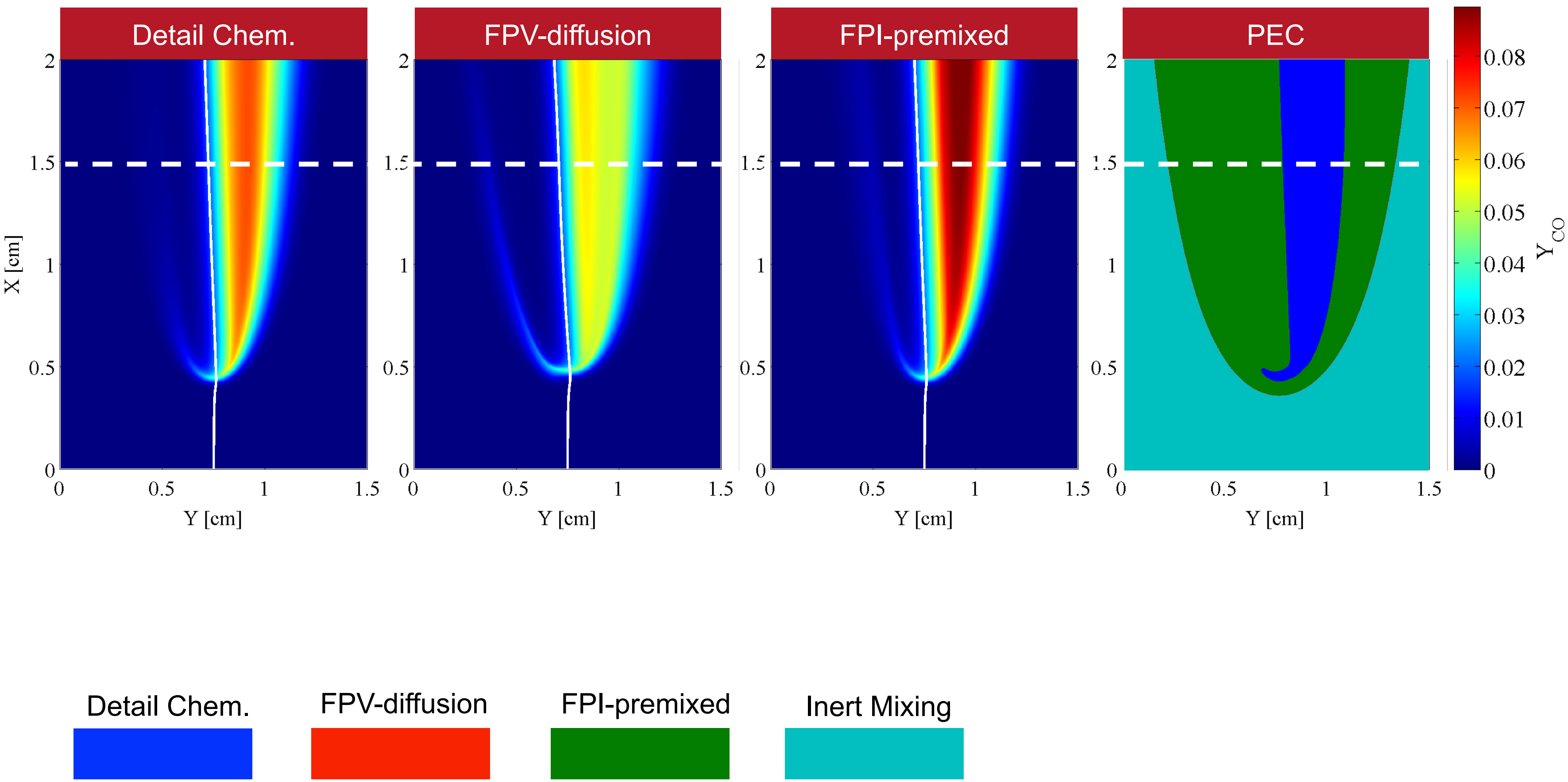
Baseline Case

Candidate Models	Quantities of Interest	Penalty
1) DC: Detailed chemistry 2) SC: Skeletal chemistry 3) FPI: premixed flamelet model 4) FPV: diffusion flamelet model 5) Inert mixing model	$\{CO, CO_2, H_2, H_2O, NO\}$	0.2

Results
Stationary Flame

PEC-setup: *M = {DC, FPV, FPV, IM}, Q={CO2, CO, H2O, H2, NO}, λ = 0.2*

Results: mass fraction of CO



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Stationary Flame

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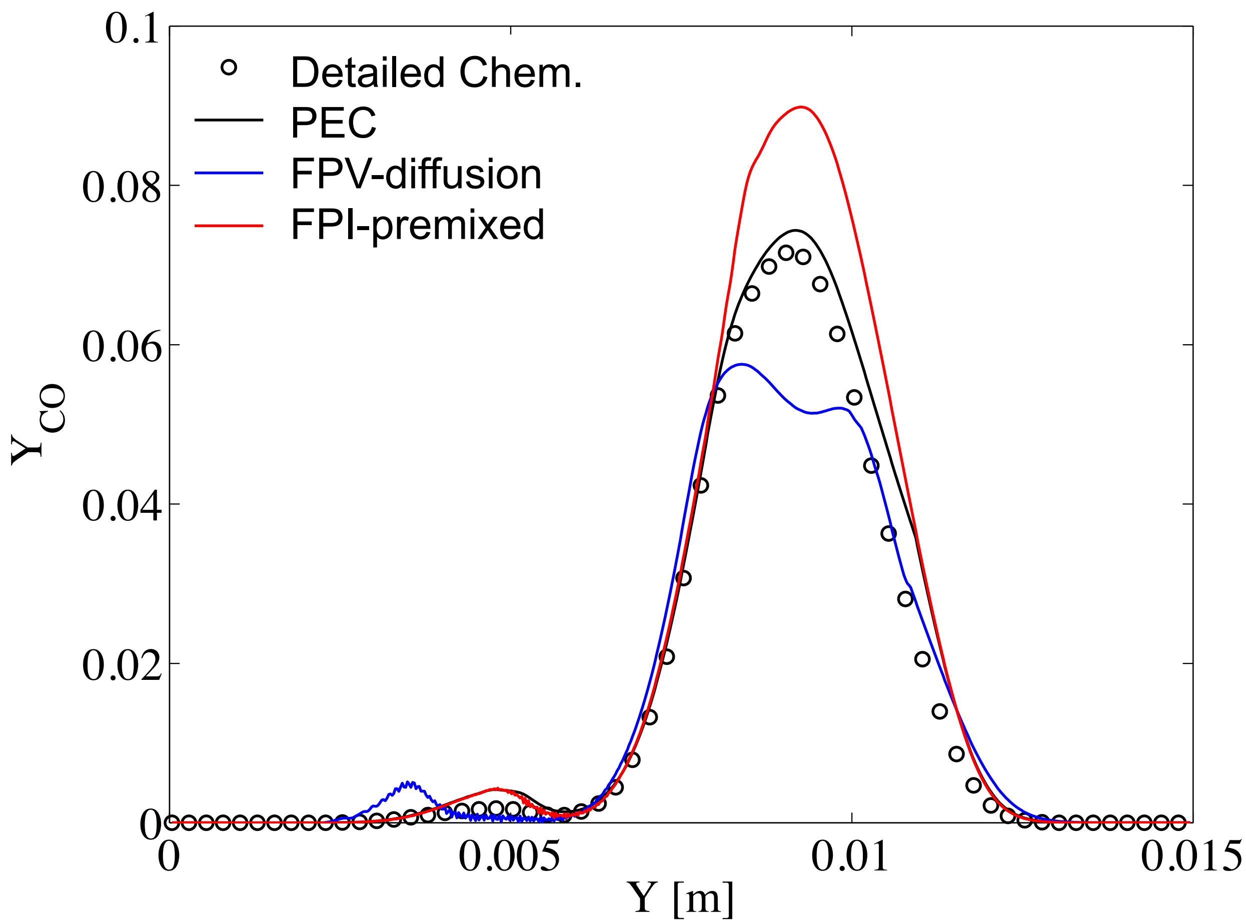


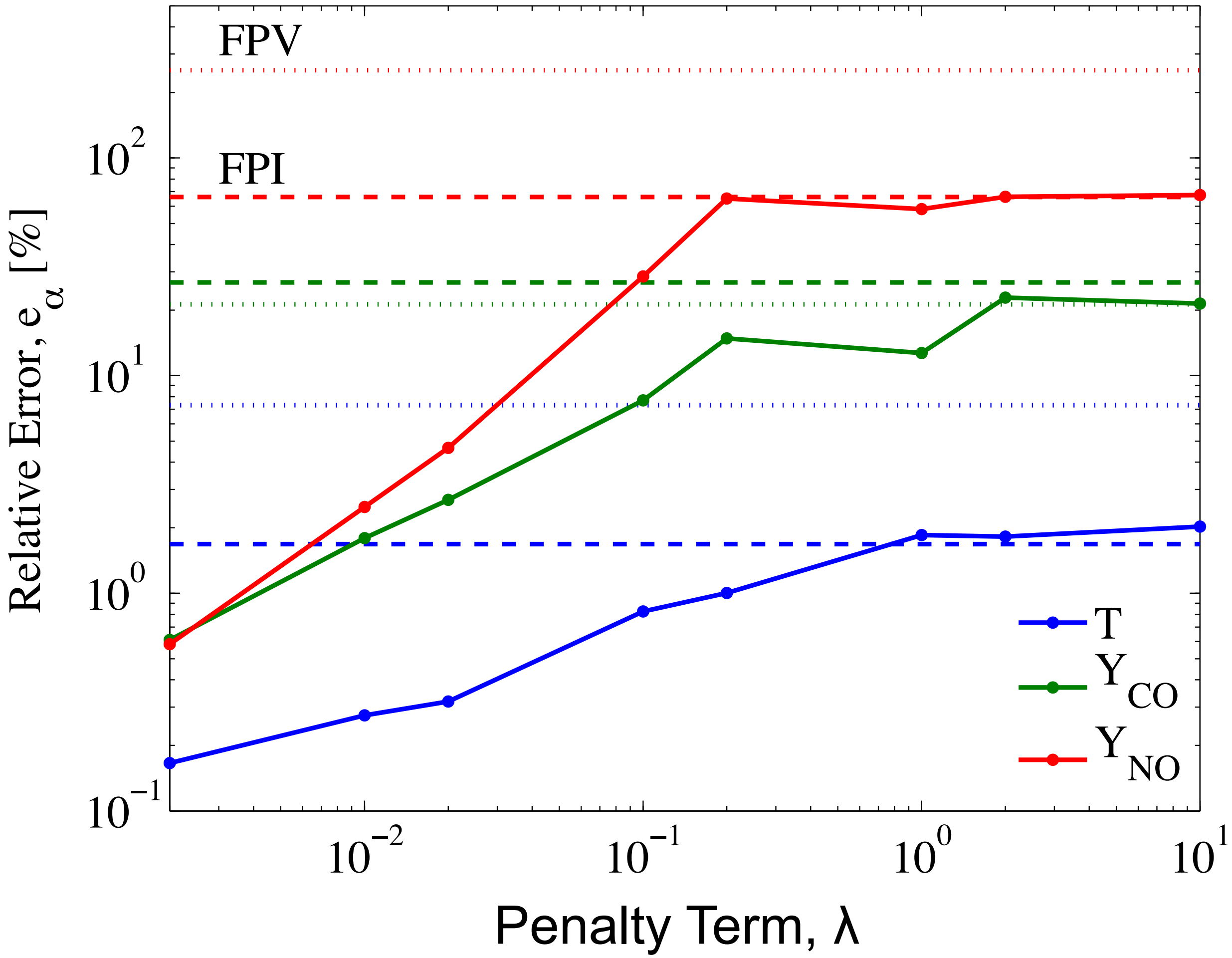
Results
Stationary Flame

Cost/accuracy trade-off

Candidate Models	Quantities of Interest	Penalty
1) DC: Detailed chemistry 2) SC: Skeletal chemistry 3) FPI: premixed flamelet model 4) FPV: diffusion flamelet model 5) Inert mixing model	$\{CO, CO_2, H_2, H_2O, NO\}$	2×10^{-3} ⋮ 10

Results
Stationary Flame

PEC-setup: *M = {DC, SC, FPV, FPV, IM}*, *Q={CO2, CO, H2O, H2, NO}*



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Results
Stationary Flame

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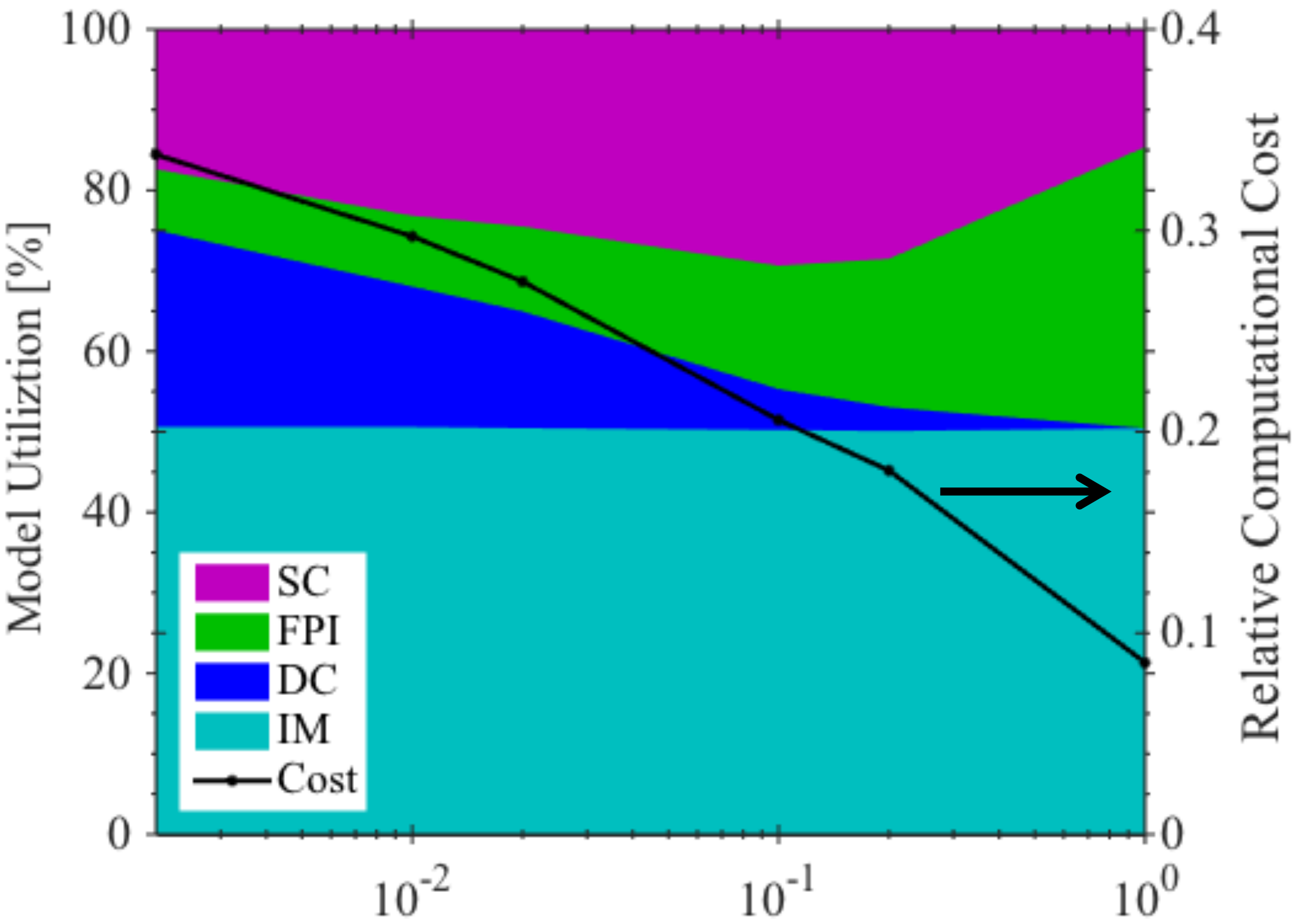
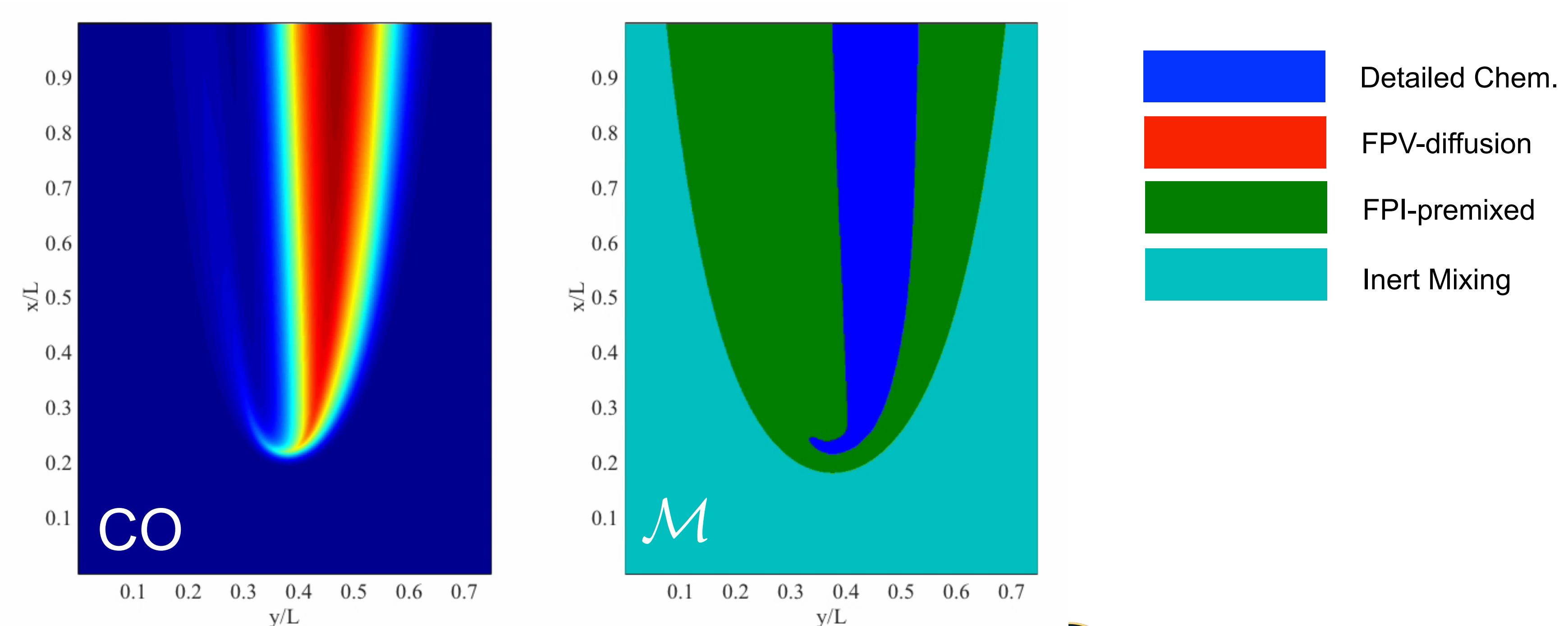


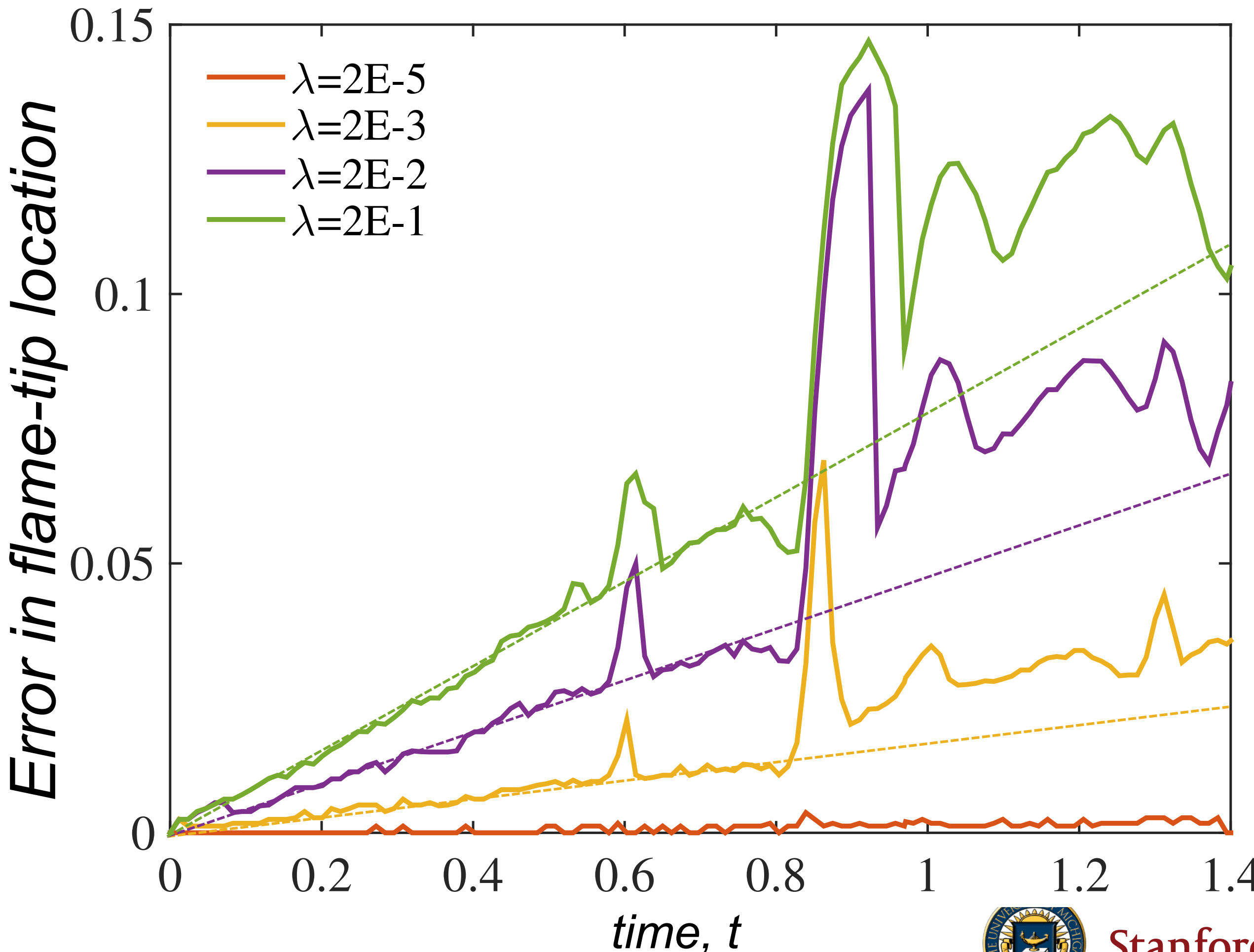
Results
Transient Flame

- Transient flame simulation by seeding inflow with turbulent velocity profile
- PEC-parameters
  - QoI: $Q = \{Y_{\mathrm{CO_2}}, Y_{\mathrm{H_2O}}, Y_{\mathrm{H_2}}, Y_{\mathrm{CO}}, Y_{\mathrm{NO}}\}$
  - Candidate combustion models: FPI, FPV, IM, DC
  - Penalty term: λ = 0.2

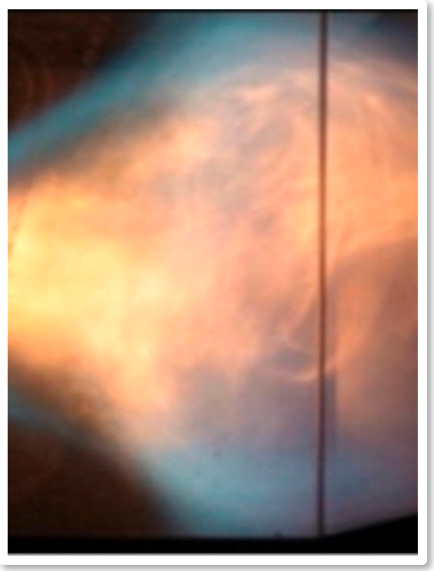


Results
Transient Flame

- Prediction of flame-tip location (relative to DNS ($\lambda=0$) results)



Application to LES



Extension of PEC to LES

Extension of drift term to filtered LES quantities

$$\mathcal{D}^{\mathcal{M}} = \widetilde{D}_t \langle \Delta \rangle |_{\widetilde{\Delta}=0}$$

$$= \widetilde{D}_t \langle \phi \rangle |_{\langle \phi \rangle = \widehat{\langle \phi \rangle}} - \frac{\partial \widehat{\langle \phi \rangle}}{\partial \langle \psi \rangle_\alpha} \widetilde{D}_t \langle \psi \rangle_\alpha$$

Closure model: For reactive scalar transport equation, $\widetilde{D}_t \langle \Delta \rangle$ appears in unclosed form

$$\widetilde{D}_t = [\widetilde{D}_t] + \left(\widetilde{D}_t - [\widetilde{D}_t] \right)$$

Closure Model

Closure Error

Closure for filtered drift term

$$[\mathcal{D}]^{\mathcal{M}} = \left[\widetilde{D}_t \right] \langle \phi \rangle |_{\langle \phi \rangle = \widehat{\langle \phi \rangle}} - \frac{\partial \widehat{\langle \phi \rangle}}{\partial \langle \psi \rangle_\alpha} \left[\widetilde{D}_t \right] \langle \psi \rangle_\alpha$$

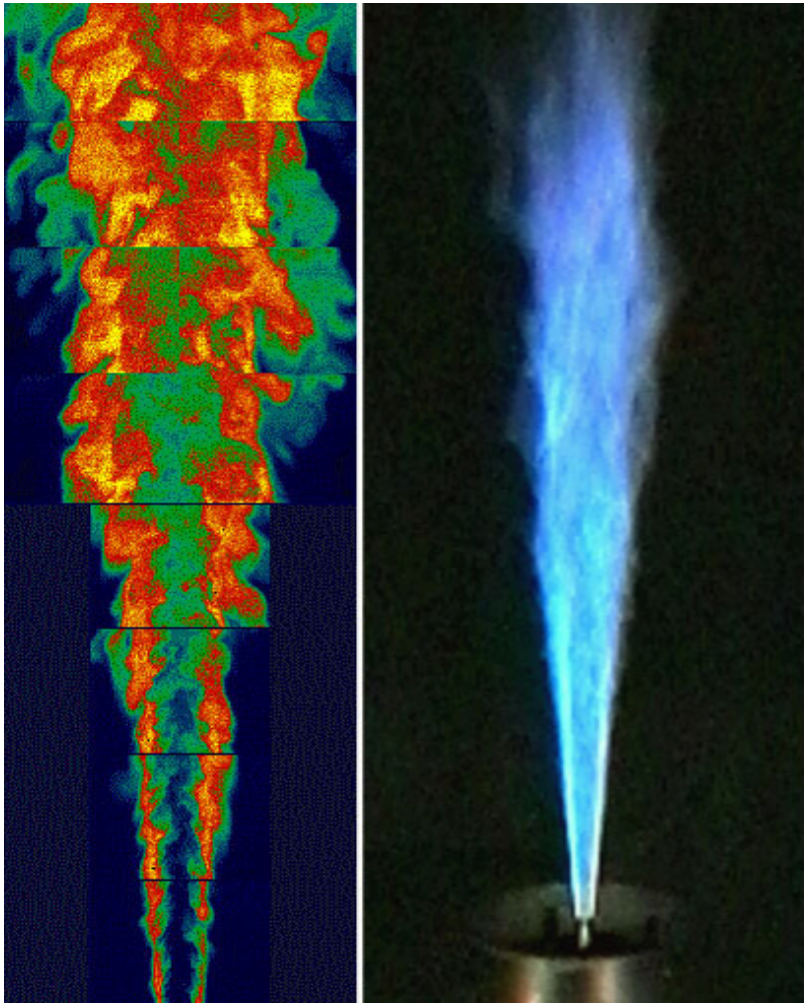
Extension of PEC to LES

Application to DLR flame

- N_2-diluted CH_4/Air-flame
- Re = 15,200 (Ub=42.2 m/s)
- Nozzle diameter: D=8 mm
- Fuel-stream: $CH_4/H_2/N_2$

Model assignment

- Inert mixing
- FPV-diffusion
- Finite rate (GRI 3.0) based on instantaneous drift)



Meier, Barlow, Chen, and Chen, Combust. Flame, 123 (2000)
Schneider, Dreizler, Janicka, and Hassel, Combust. Flame, 135 (2003)

Extension of PEC to LES

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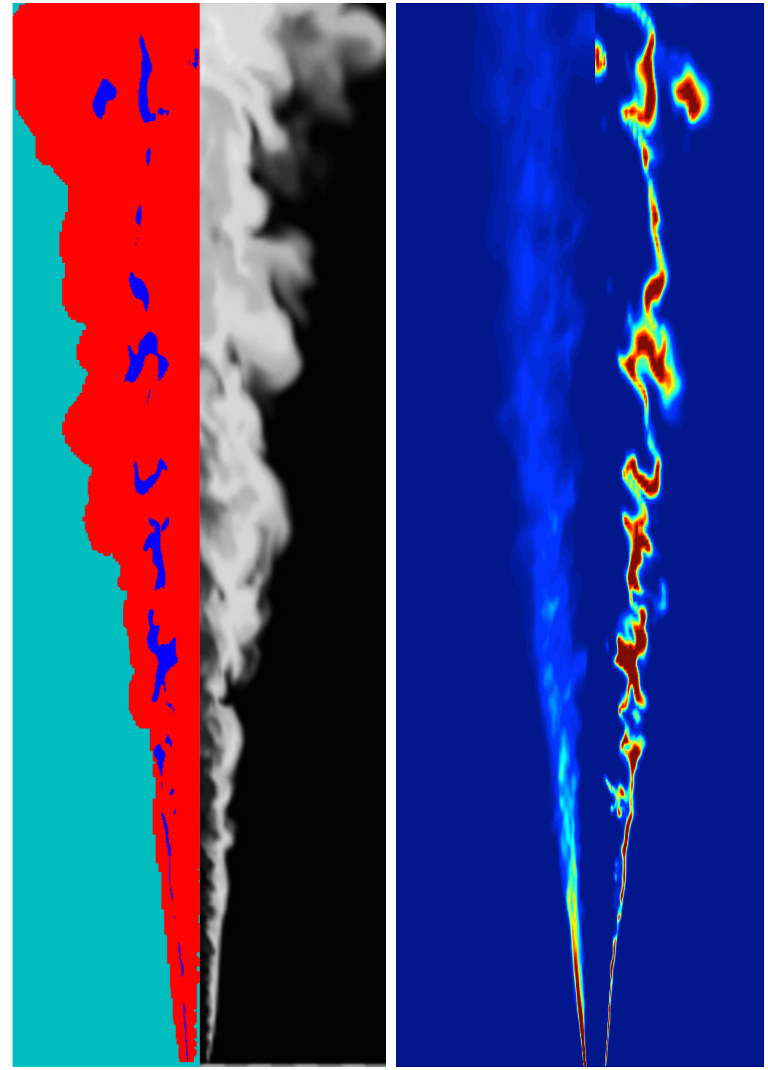

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Summary and Conclusions

- Developed a Pareto-Efficient combustion (PEC) framework for the general description of complex flame configurations
- PEC-input parameters
  - Set of quantities of interest
  - Set of candidate combustion models
  - Penalty term
- Application of PEC to laminar and turbulent flame, demonstrating
  - Adaptation of model assignment
  - Computational cost adjustable by 40X
  - Consistently more accurate than single-regime model

Wu, H., See, Y. C., Wang, Q., and Ihme, M., “A Pareto-efficient combustion framework with submodel assignment for predicting complex flame configurations.” Combustion and Flame, in press.