Development and Experimental Validation of Large-Eddy Simulation Techniques for the Prediction of Combustion-Dynamic Processes in Syngas Combustion

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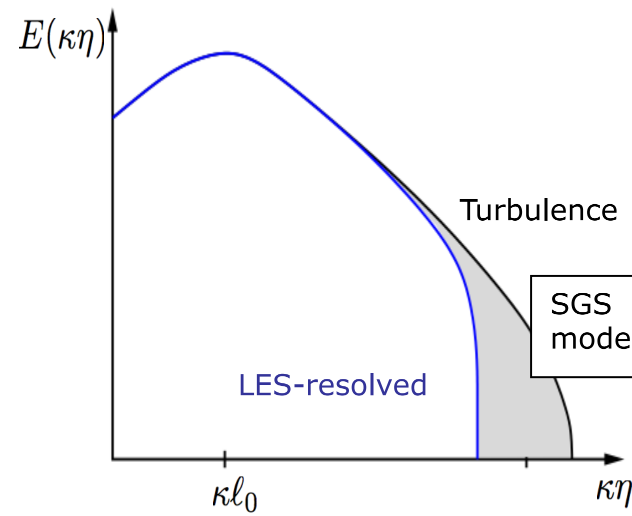
Motivation

- Large-eddy simulation for prediction of turbulent reacting flows
  - Resolves energy-containing scales in turbulent flow
    - Scalar mixing
    - Flame/vortex interaction, swirling and separated flows
    - Flame stabilization
  - Modeling of unresolved scales

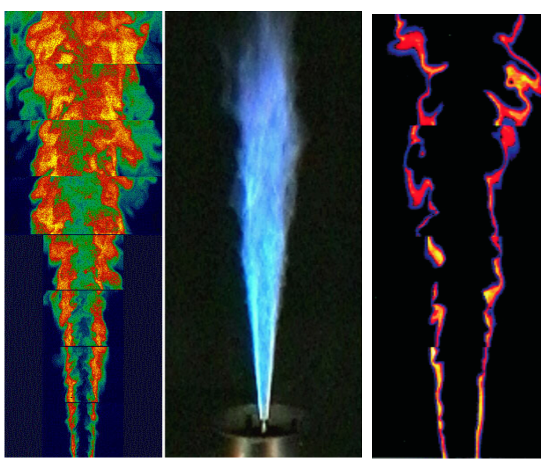


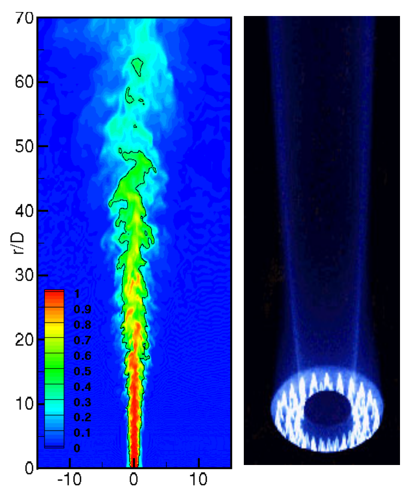
- LES combustion models
  - Structure-free models
    - Transported F/PDF-model, (Direct) Quadrature-methods, MMC
  - Structure-based models
    - Flamelet-formulation, Conditional moment closure

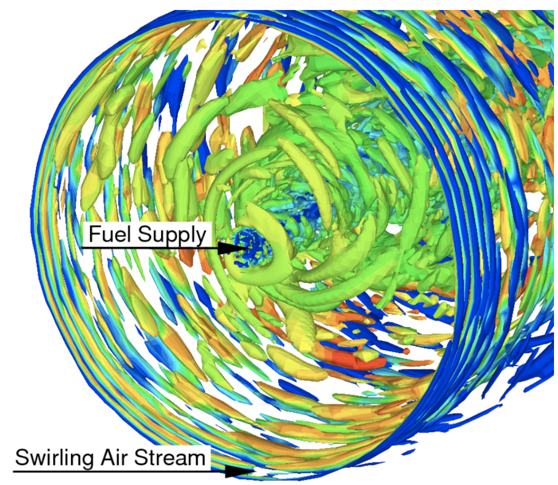
Motivation

- Development and validation of LES-combustion models
  - Using canonical flame configuration under ambient atmospheric conditions
  - Stationary (steady or limit-cycle saturation) conditions

  → Comprehensive experimental databases (space/time resolved, 2D planar imaging)







Motivation

- Gas turbine combustor systems are controlled by
  - (Partially) premixed and stratified mixture composition
  - Flame-dynamic processes: Lift-off, blow-out, and flashback
  - Swirling and recirculating flow regimes
  - High-pressure conditions

- LES combustion models are currently not developed/validated for GT-relevant operating conditions and syngas-fuels, due to
  - Absence of comprehensive and quantitative measurements
  - Limited data for high-pressure environments
  - Realistic fuel mixtures
  - Uncertainties in syngas combustion kinetics

Research Objectives

Joint experimental and computational research program to develop validated simulation techniques for the prediction of autoignition and unstable combustion processes, relevant to oxidation of syngas and HHC-fuels at GT-relevant operating conditions

Research Objectives

Experimental Effort (Driscoll)

- Perform detailed measurements in dual-swirl partially-premixed GT-combustor
- Realistic high-pressure (up to 10 bar) conditions
- Primary fuels: hydrogen, syngas
- Characterization of flame-stabilization mechanisms
  - Flash-back and lift-off
- Establish experimental database for LES-model validation

Computational Effort (Ihme)

- Develop LES-combustion model for prediction of unstable combustion regimes
  - Autoignition
  - Flash-back
  - Flame lift-off
- Evaluation of critical modeling assumptions using DNS-data of Jet-in-Cross-Flow (JICF)
- Model-validation in swirl-stabilized GT-combustor configuration

Overview

- Motivation
- Research Objectives
- LES combustion modeling and turbulence/chemistry interaction
  - Related work: Modeling of autoignition and NO-emissions
  - Research plan
- Experimental investigation of gas-turbine combustor
  - Related work: High-pressure combustor facility
  - Research plan

Objectives

Experimental Effort (Driscoll)

- Conduction detailed measurements in dual-swirl partially-premixed GT-combustor
- Realistic high-pressure (up to 10 bar) conditions
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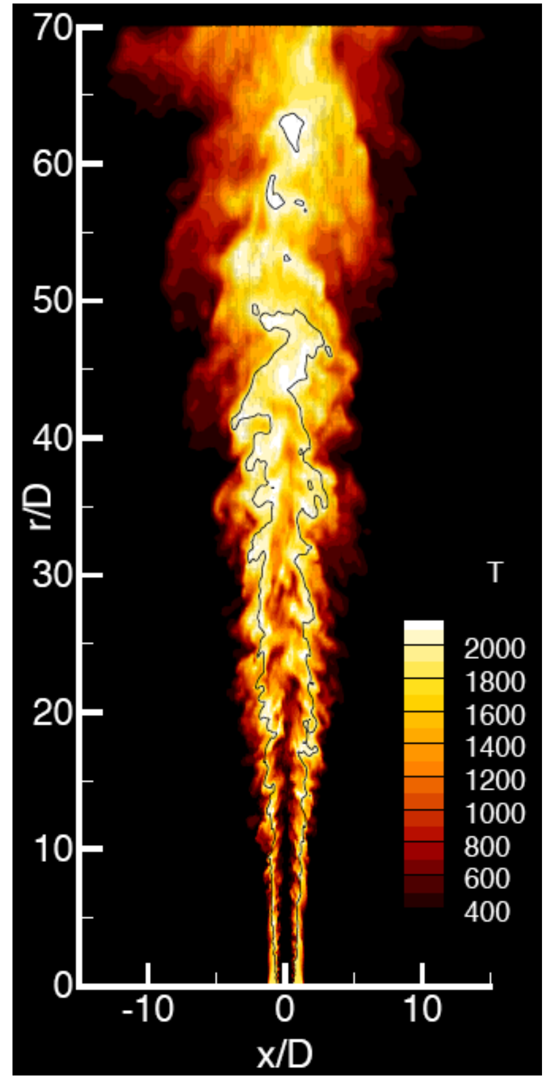
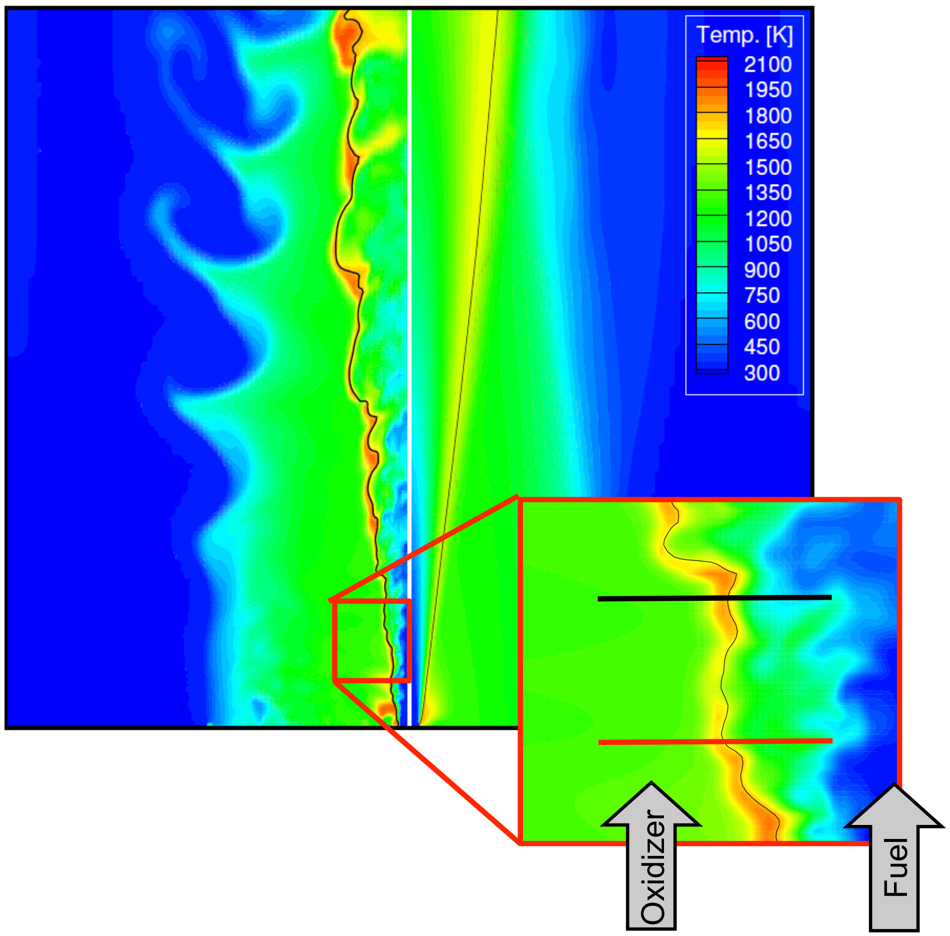
LES Combustion Modeling

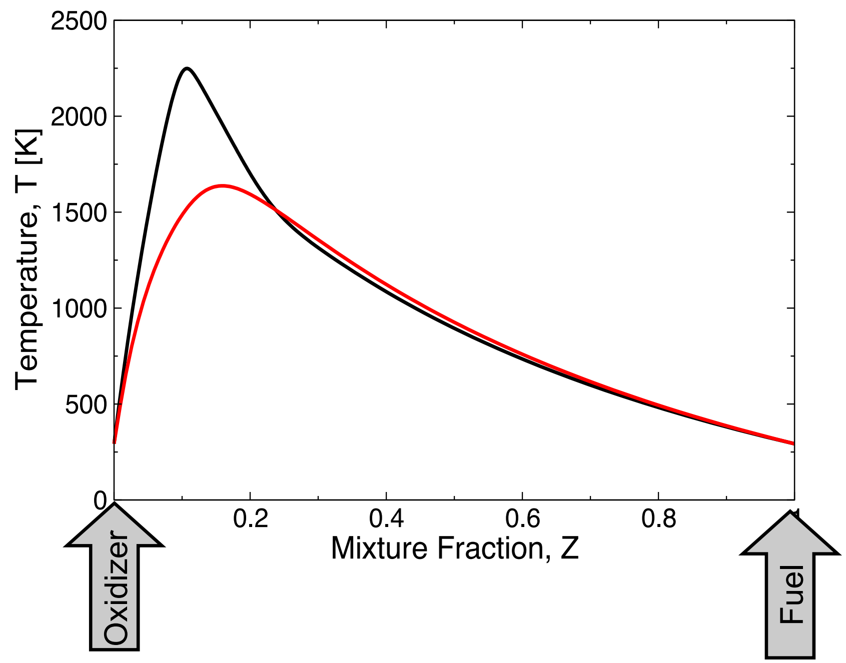
- Flamelet-formulation
  - Representation of turbulent flame as unsteady reaction-diffusion layer that is embedded in turbulent flame
  - Interaction of flame structure with turbulent environment leads to stretching, deformation, and extinction of flame
- Advantage of flamelet formulation
  - Parameterization of combustion process in terms of reduces set of scalars
    - Mixture fraction
    - Scalar dissipation rate
    - Reaction progress parameter
  - Tabulation of reaction chemistry



LES Combustion Modeling

- LES flamelet-based combustion model





LES Combustion Modeling

- Flamelet formulation is obtained by transforming governing equations for species and temperature conservation into mixture fraction space

$$\partial_t \rho \boldsymbol{\psi} + \nabla \cdot (\rho \boldsymbol{u} \boldsymbol{\psi}) = \nabla \cdot (\rho \alpha \nabla \boldsymbol{\psi}) + \rho \dot{\boldsymbol{\omega}}$$

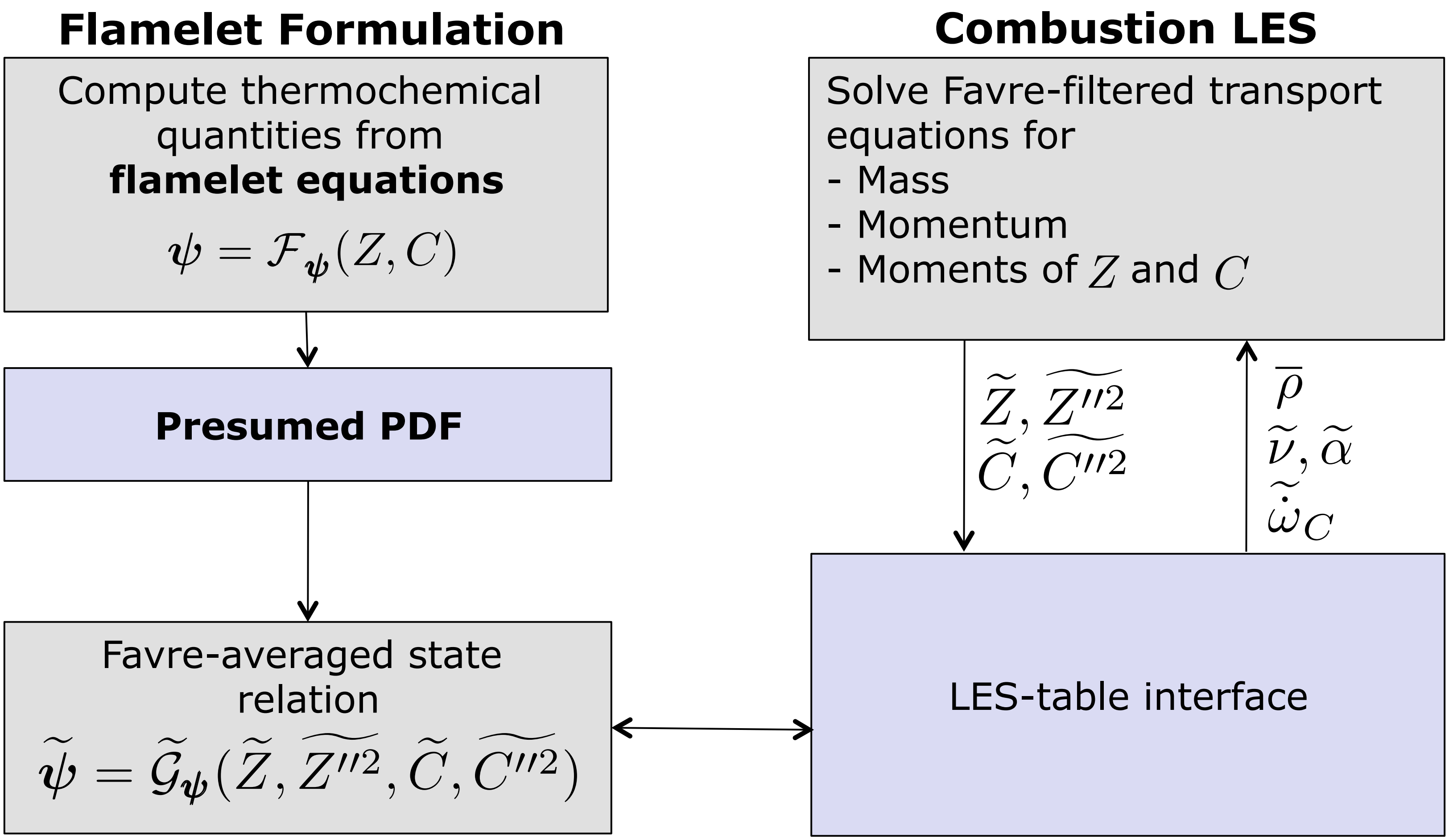
Transformation: $(t, \boldsymbol{x}) \rightarrow (t, Z(t, \boldsymbol{x}), \xi_1, \xi_2)$

$$\frac{\partial \boldsymbol{\psi}}{\partial t} - \frac{\chi_Z}{2} \frac{\partial^2 \boldsymbol{\psi}}{\partial Z^2} = \dot{\boldsymbol{\omega}}$$

$\boldsymbol{\psi}$ . . . Vector of thermochemical quantities
$\boldsymbol{\omega}$ . . . Source term
Z . . . Mixture fraction
χ_Z . . . Scalar dissipation rate

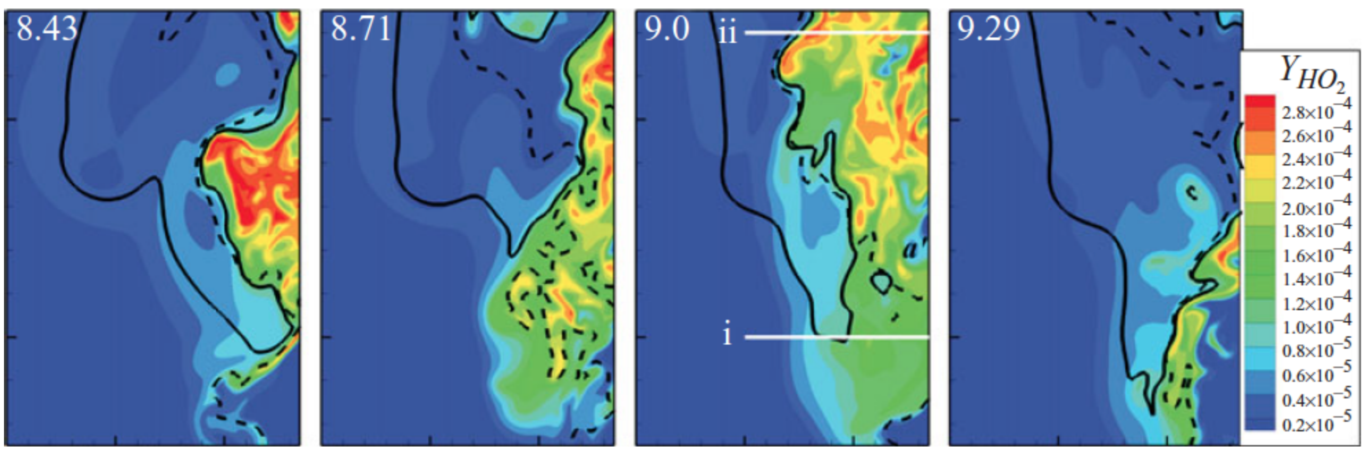
LES Combustion Modeling

- Model formulation and implementation



LES Combustion Modeling

- Modeling challenges
  - Kinetics-controlled combustion regime
  - Turbulence/chemistry interaction
  - Accurate description of temporal flame-evolution
    - Chemistry not in steady-state (reduced Damkoehler number)
    - Transient ignition and extinction processes
    - Scalar mixing

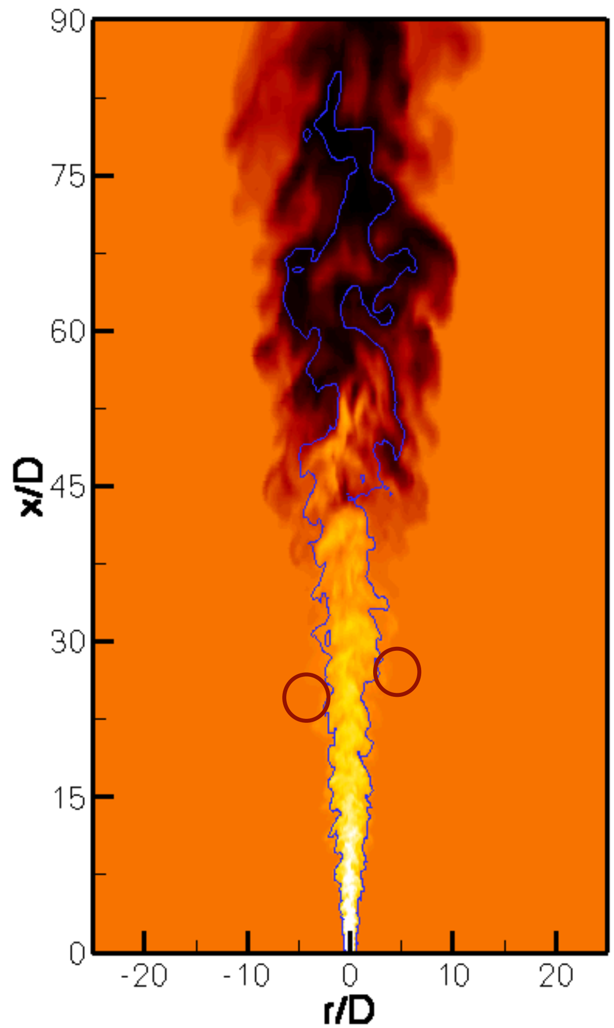


Yoo et al., JFM, 640 (2009)

LES Combustion Modeling
- Flame Autoignition -

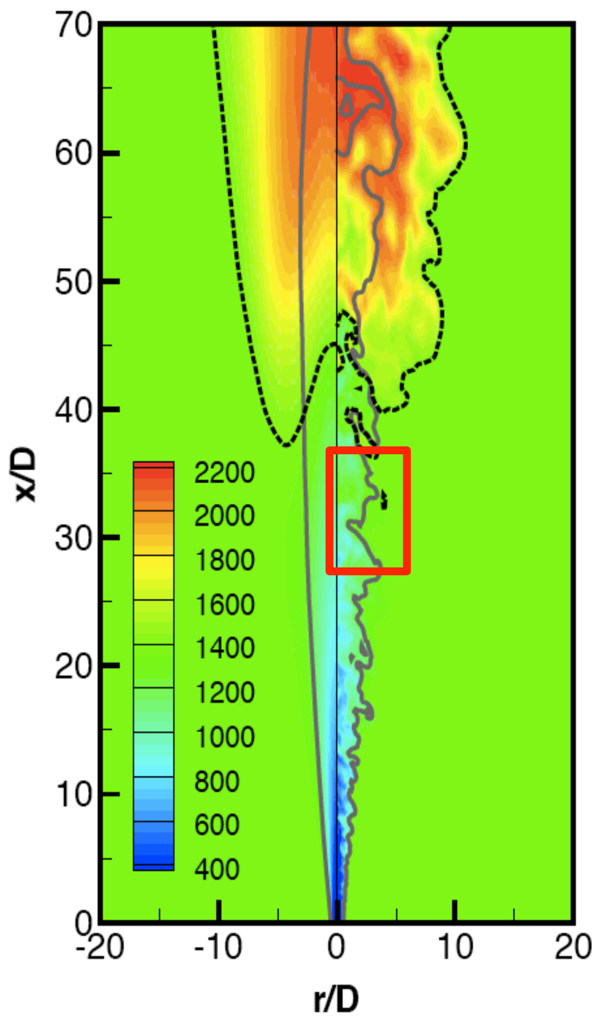
Application: LES-Modeling of Autoignition

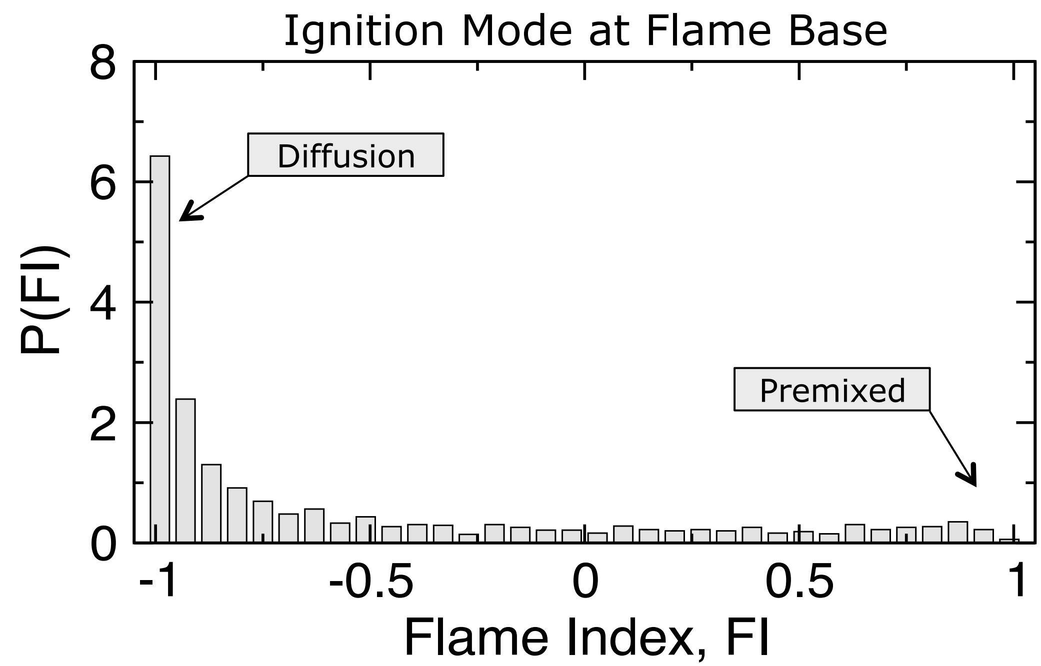
- Experimental configuration
  - Lifted flame in vitiated co-flow
  - Fuel: methane/air 1:2
  - Co-flow temperature: 1350 K
  - Co-flow composition from premixed H_2-Air reaction product
- Computational setup
  - Grid: 2.5 Mio grid points
  - Reaction Chem.: GRI-Mech. 2.11



[1] Cabra, Chen, Dibble, Karpetis, Barlow, CF, 143, 2005

Application: LES-Modeling of Autoignition

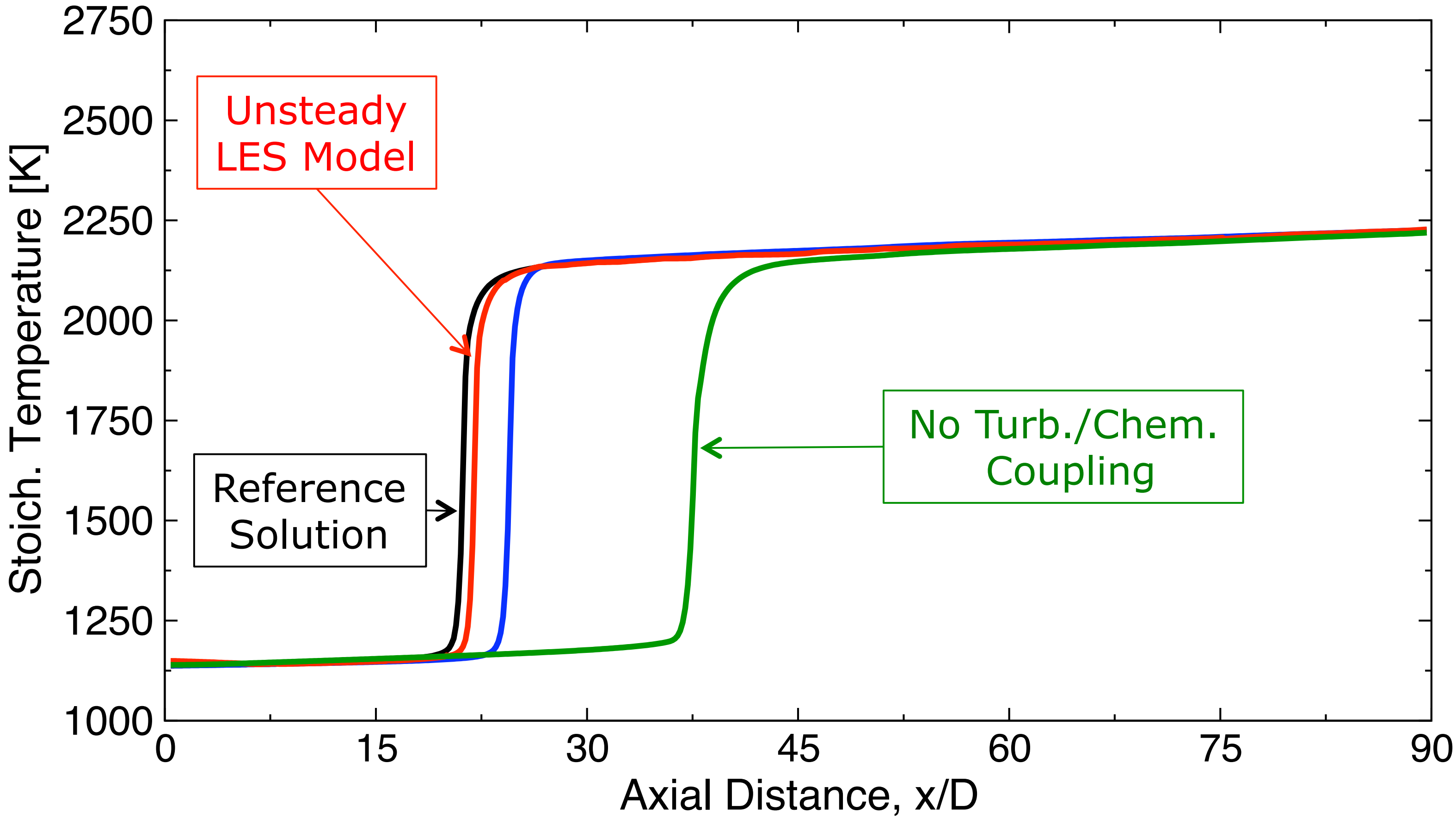




- Ignition conditions: low-strain region at most-reactive mixture composition
- Ignition occurs primarily in diffusion regime
- Location of flame-base controlled by HO_2-radical pool that is formed upstream of flame

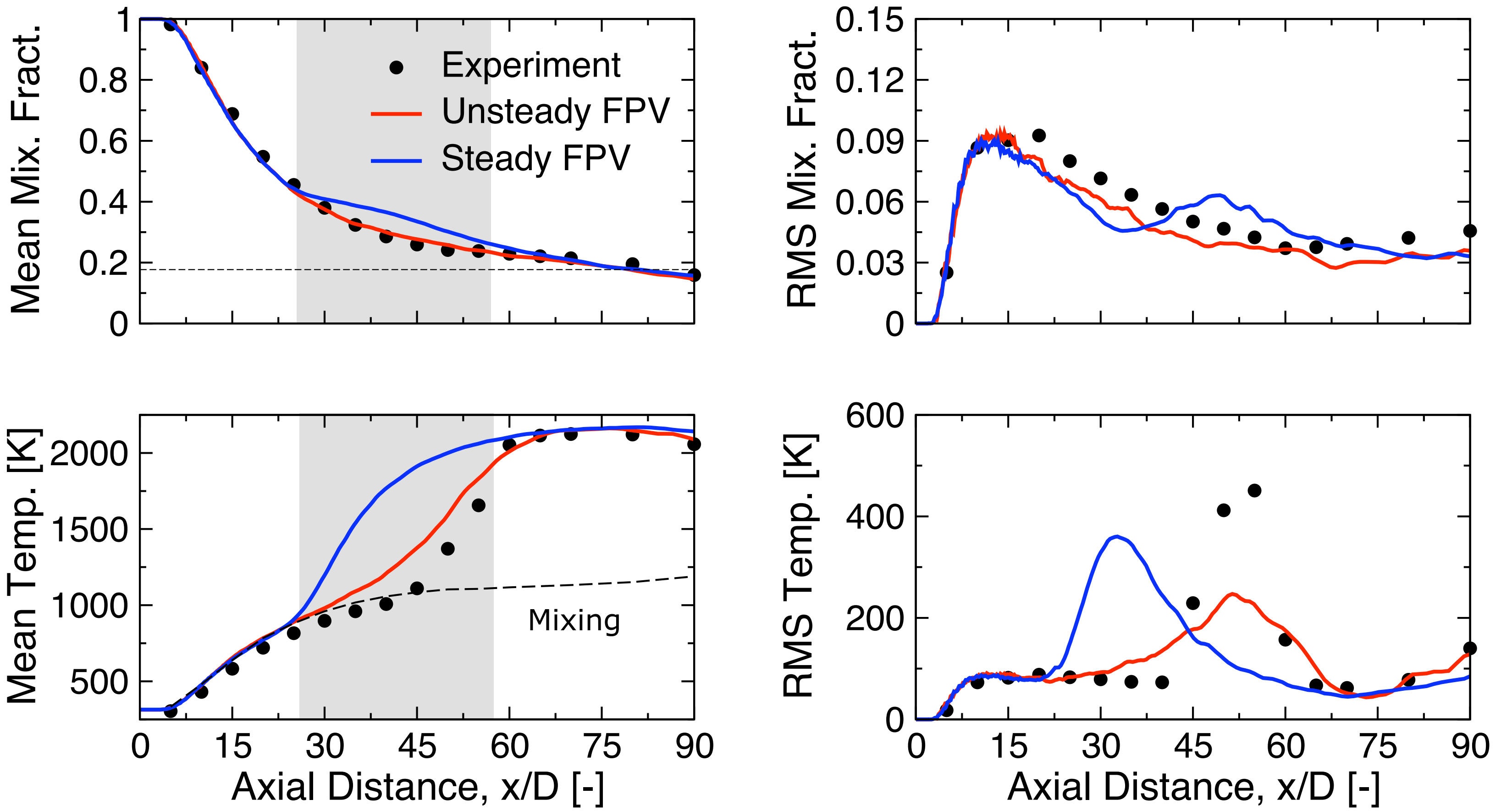
Application: LES-Modeling of Autoignition

- Prediction of ignition location and role of turb./ chemistry coupling

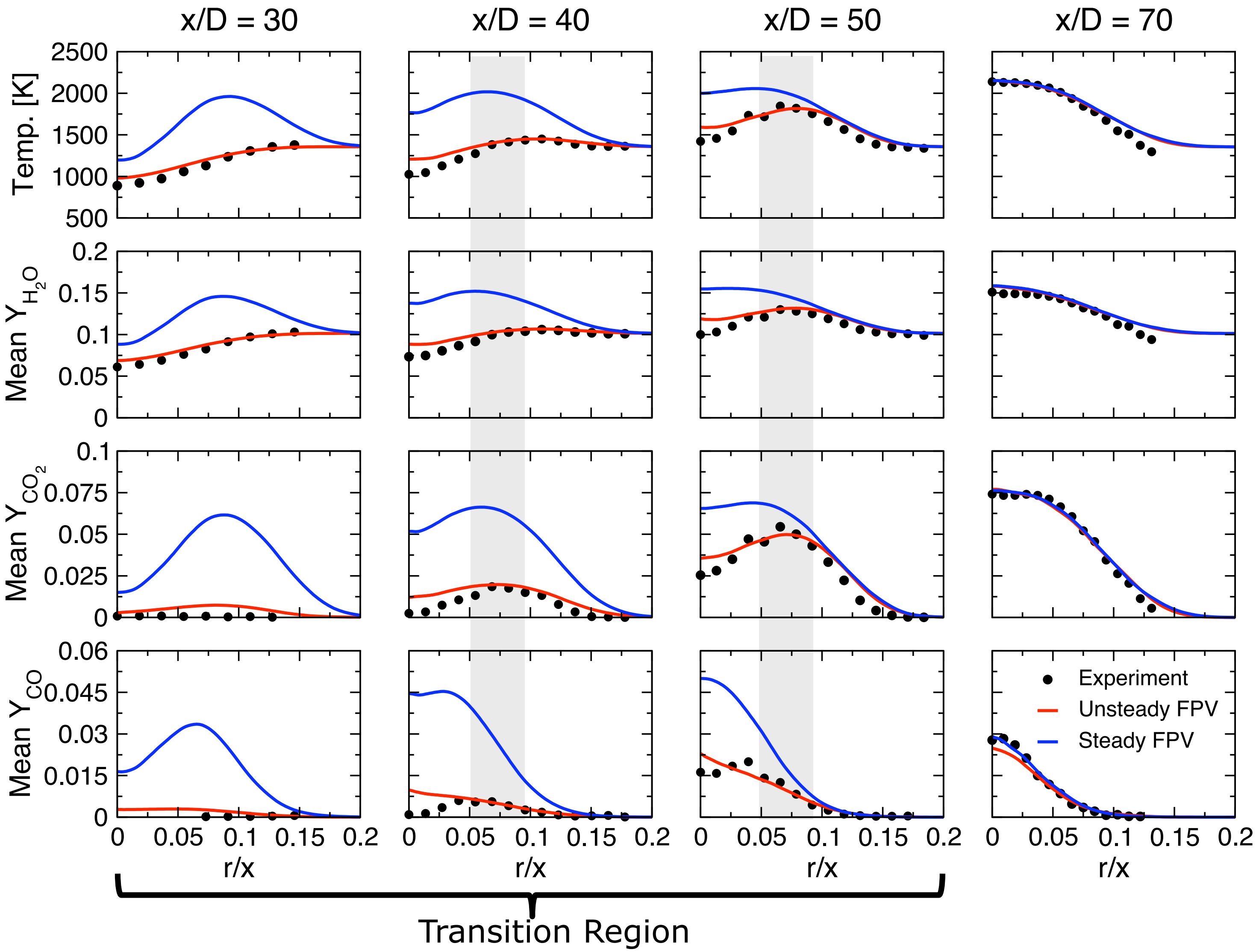


Application: LES-Modeling of Autoignition

- Centerline profiles



Application: LES-Modeling of Autoignition



LES Combustion Modeling
- NO Pollutant Emissions -

LES-Modeling of NO-Emissions

- NO-formation evolves on time-scales that are slow compared to major species conversion
  - Employ flamelet/progress variable model
  - Solve additional transport equation for NO mass fraction

$$\partial_t(\rho Y_{\mathrm{NO}}) + \nabla \cdot (\rho \boldsymbol{u} Y_{\mathrm{NO}}) = \nabla \cdot (\rho \alpha \nabla Y_{\mathrm{NO}}) + \rho \dot{\omega}_{\mathrm{NO}}$$

  - Model of chemical reaction rate

$$\dot{\omega}_{\mathrm{NO}} + \dot{\omega}_{\mathrm{NO}}^{+} + \dot{\omega}_{\mathrm{NO}}^{-}$$

Formation rate ($\dot{\omega}_{\mathrm{NO}}^{+}$)

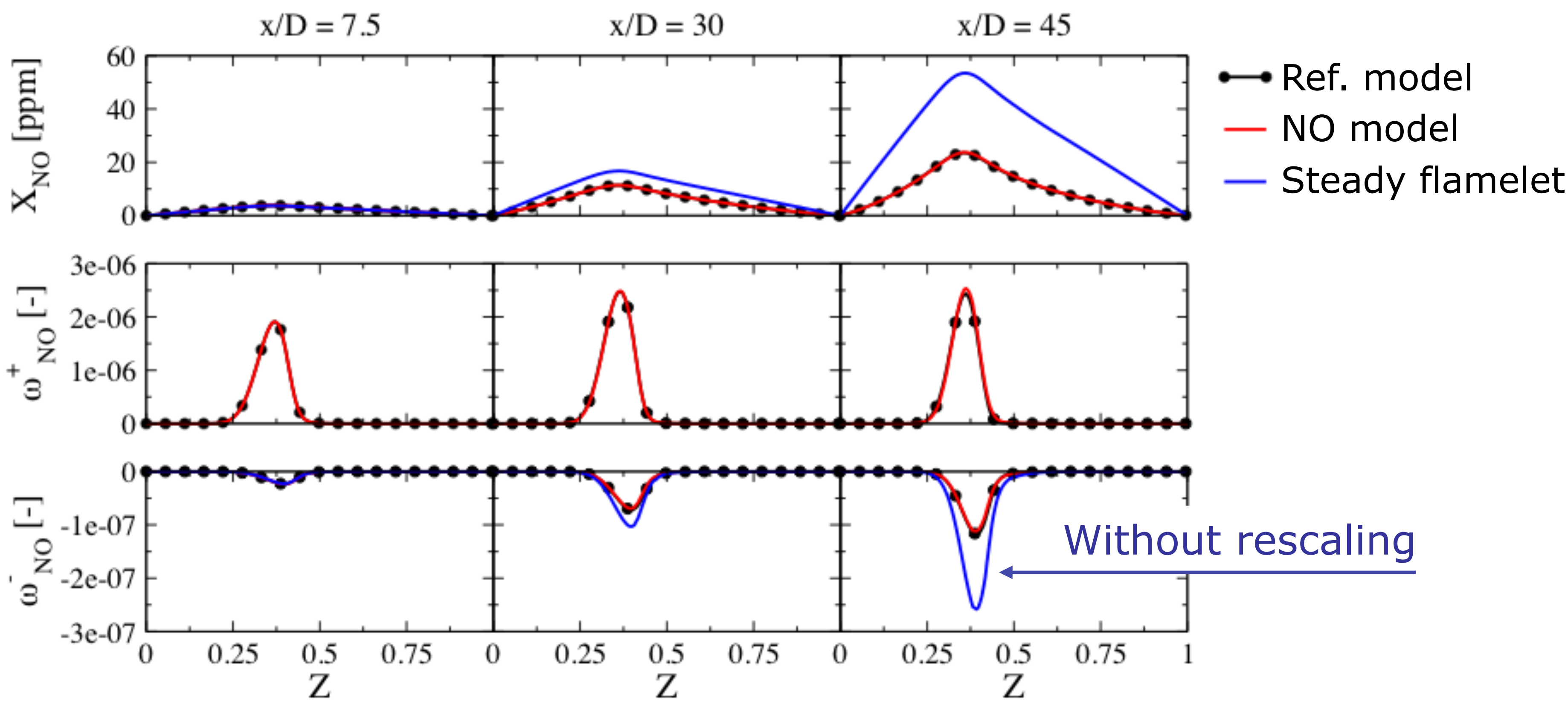
Consumption rate ($\dot{\omega}_{\mathrm{NO}}^{-}$) requires modeling

  - Rescale consumption-rate with steady-state NO-mass fract.

$$\dot{\omega}_{\mathrm{NO}} = \dot{\omega}_{\mathrm{NO}}^{+} + Y_{\mathrm{NO}} \frac{\dot{\omega}_{\mathrm{NO}}^{-}}{Y_{\mathrm{NO}}^{\mathrm{SS}}}$$

LES-Modeling of NO-Emissions

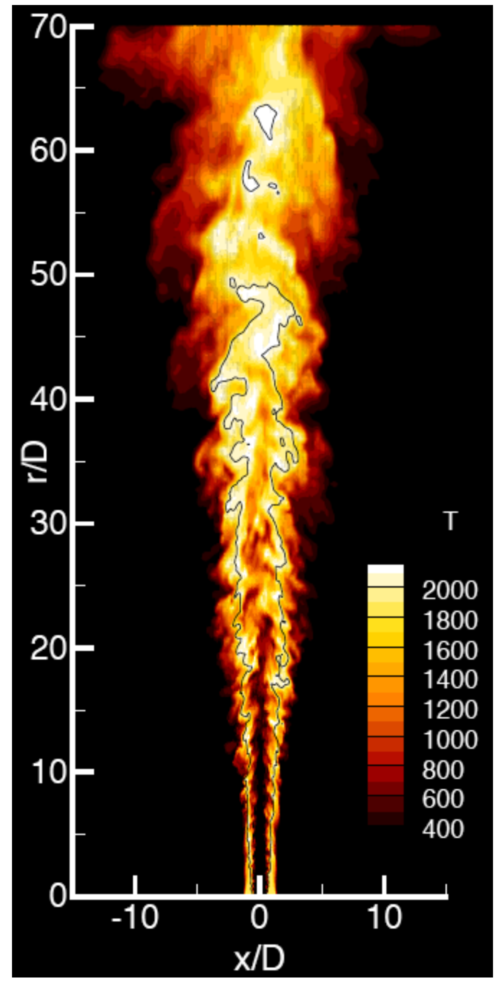
- Zeldovich mechanism



Flame Extinction and Reignition

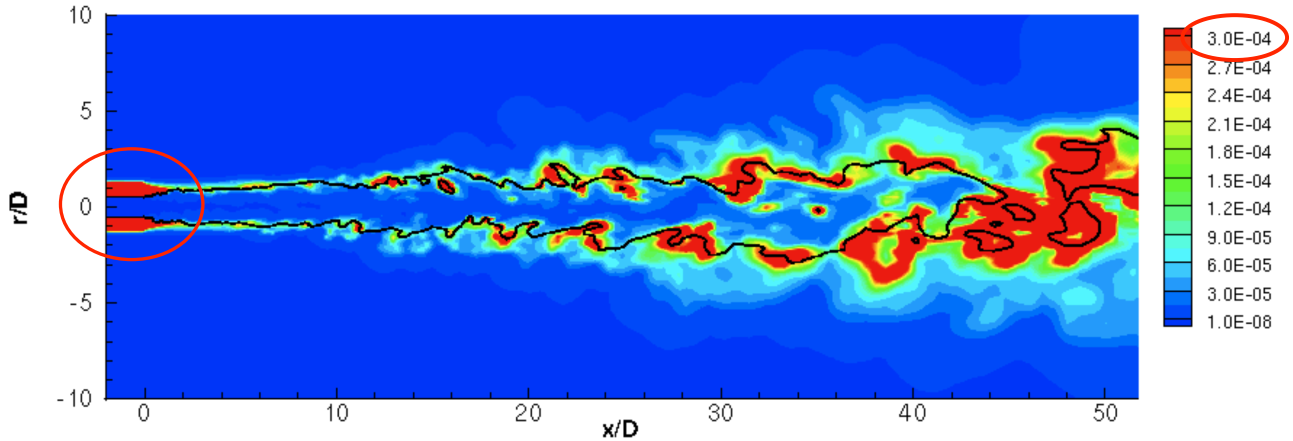
- Experimental setup
  - Sandia D configuration
  - Partially premixed jet flame
  - Fuel stream
    - $X_{CH4}/X_{Air} = 1/3$
    - Jet diameter: D = 7.2 mm
    - Reynolds-number: 22,400
  - Pilot-stabilized flame

- NO-Mechanisms
  - GRI-Mech. 2.11
  - Zeldovich mechanism
  - Prompt NO-mechanism
  - Nitrous oxide mechanism

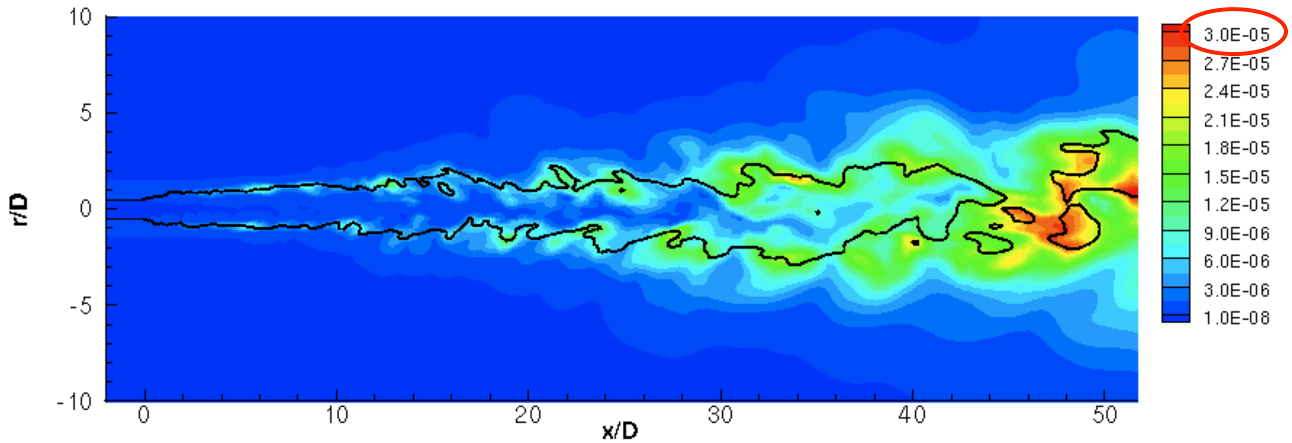


LES-Modeling of NO-Emissions

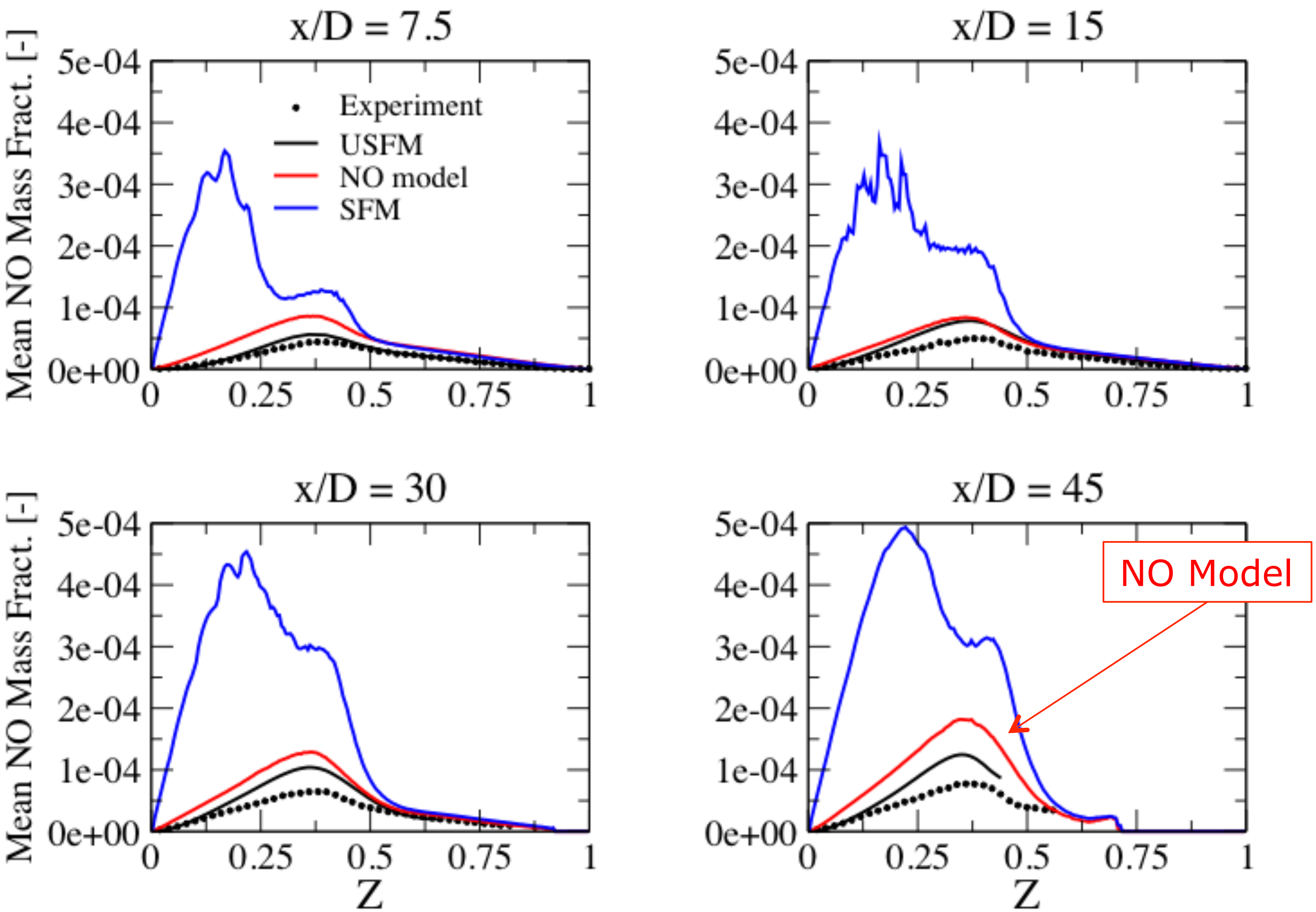
NO from steady model



NO from extended model formulation



LES-Modeling of NO-Emissions



Research Objectives

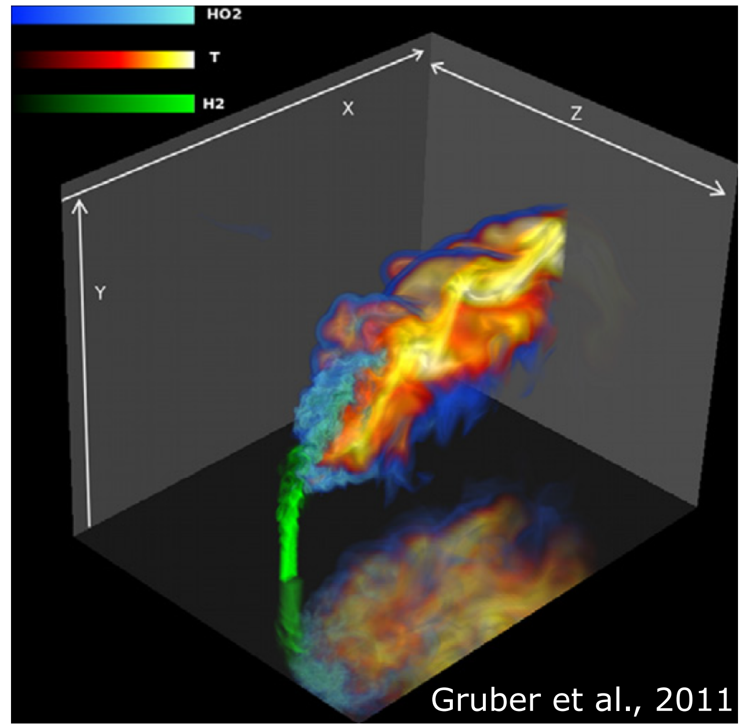
Research Plan

- Research Objectives
  - Develop LES-combustion model for prediction of unstable combustion regimes under GT-relevant operating conditions

- Approach
  - Model developments: Extension of unsteady flamelet/ progress variable approach to stratified flame-regimes
  - A priori model analysis: Systematic evaluation of critical model assumptions in flamelet-formulation using DNS-data of JICF configuration
  - A posteriori analysis: LES-model validation in dual-swirl gas turbine combustion

Research Plan: A priori Analysis

- Configuration
  - A priori analysis utilizes DNS of JIHC, performed at Sandia Nat'l Lab (J.H. Chen)
- Mixture composition
  - Fuel: N_2/H_2 (350 K, 50 m/s)
  - Oxidizer: Air (750 K, 255 m/s)
- Thermoviscous transport
  - Mixture-averaged transport properties
- Parametric variations
  - Momentum ratio
  - Injector angles and flame stability regimes

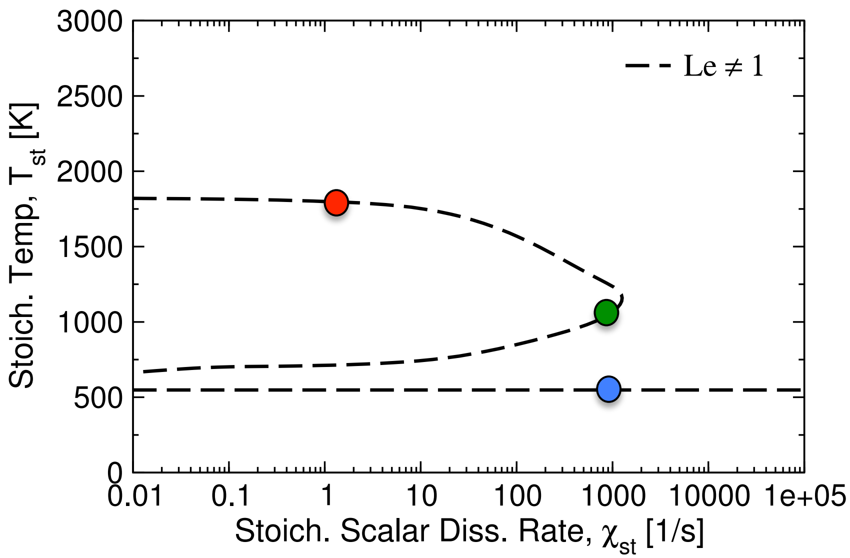


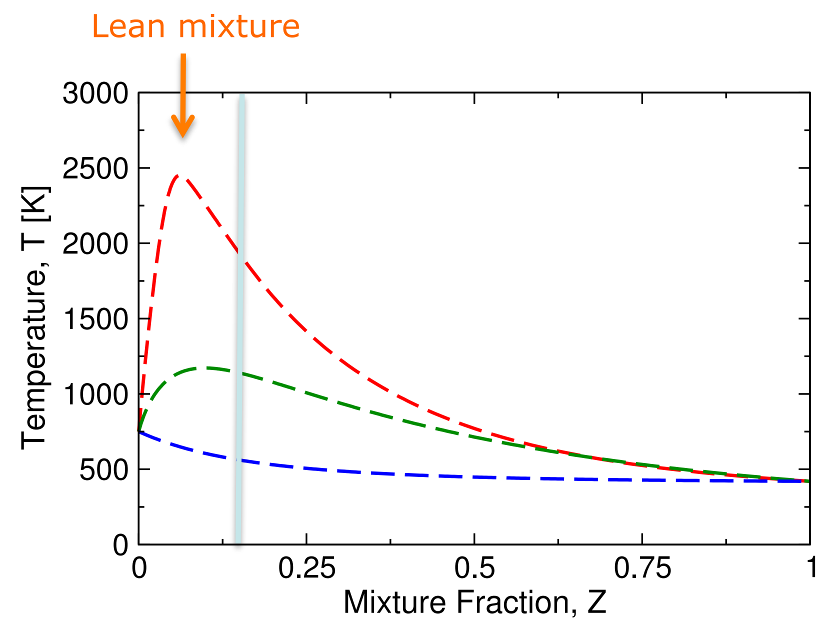
Gruber et al., 2011

Research Plan: A priori Analysis

- Lewis number effects
  - Preferential diffusion shifts flame location and heat-release to lean mixture

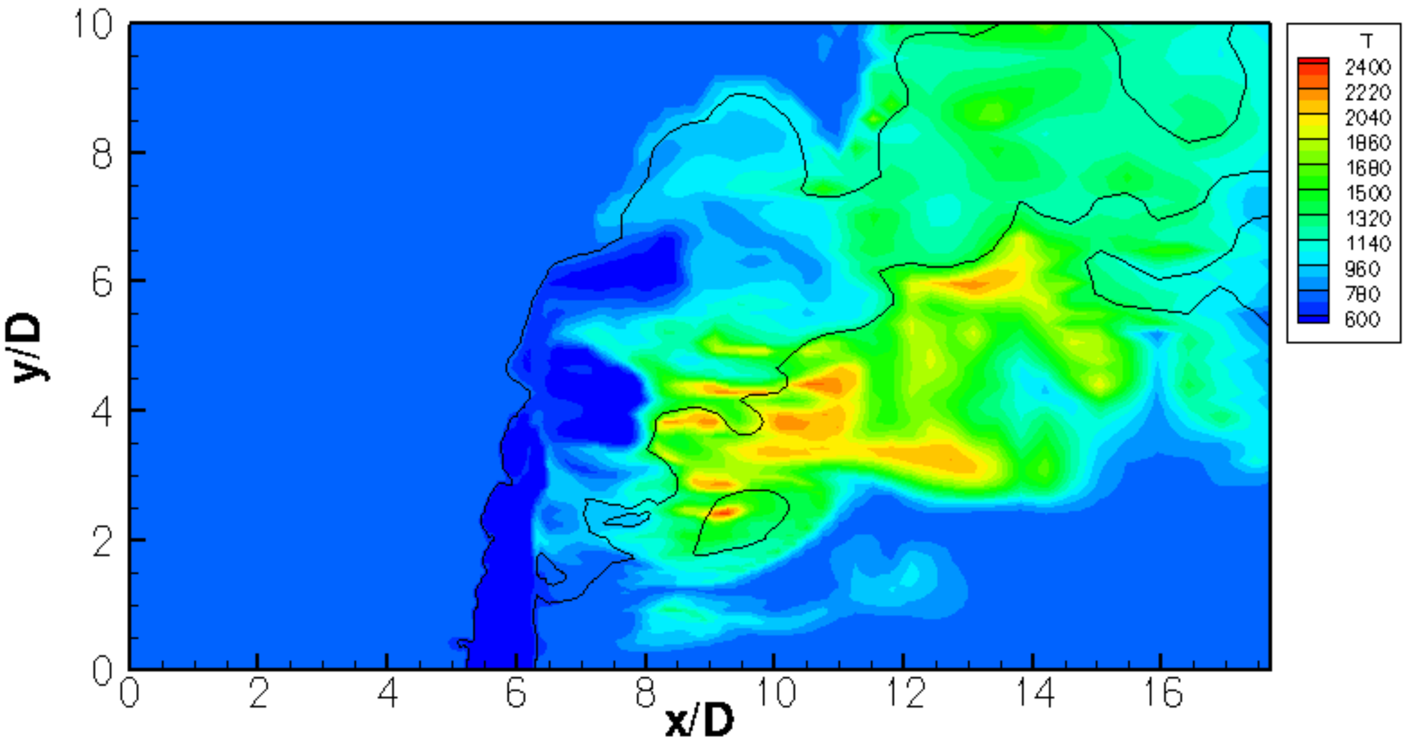
    → Flame-destabilization





Research Plan: A priori Analysis

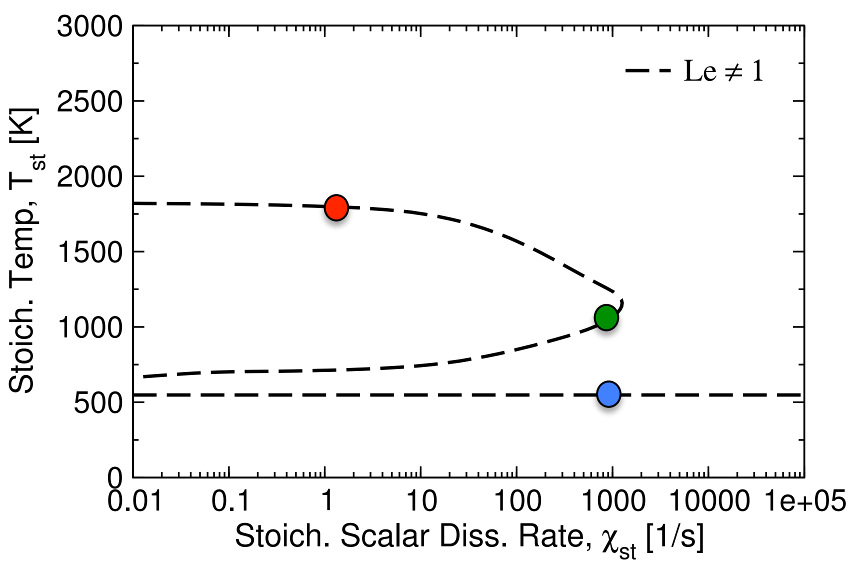
- Lewis number effects: Non-unity Lewis-number
  - Flame blow-off due to shift of flame location to lean mixture

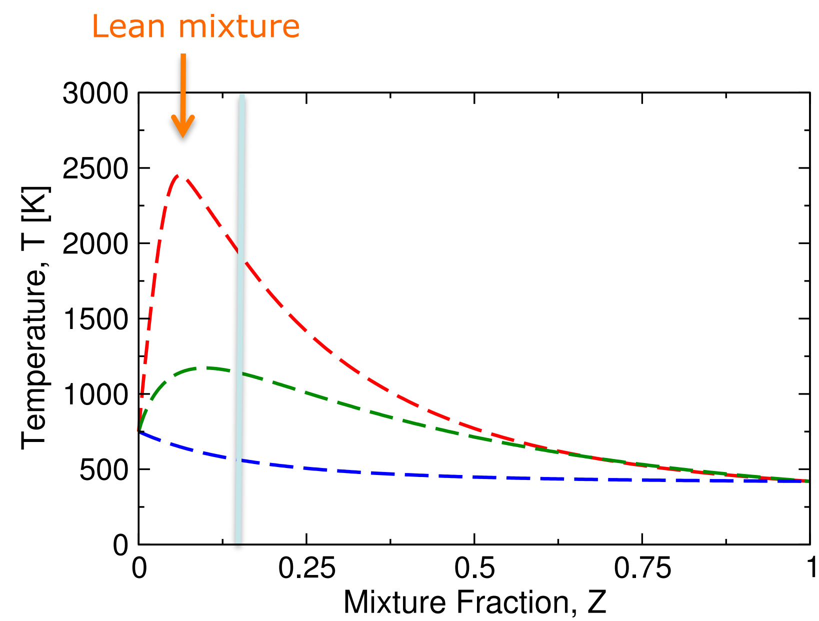


Research Plan: A priori Analysis

- Lewis number effects
  - Preferential diffusion shifts flame and heat-release to lean mixture

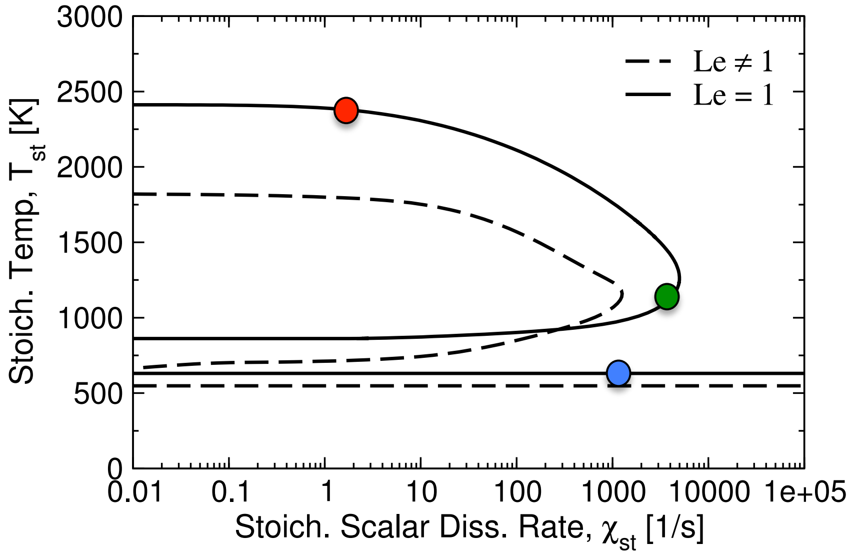
    → Flame-destabilization

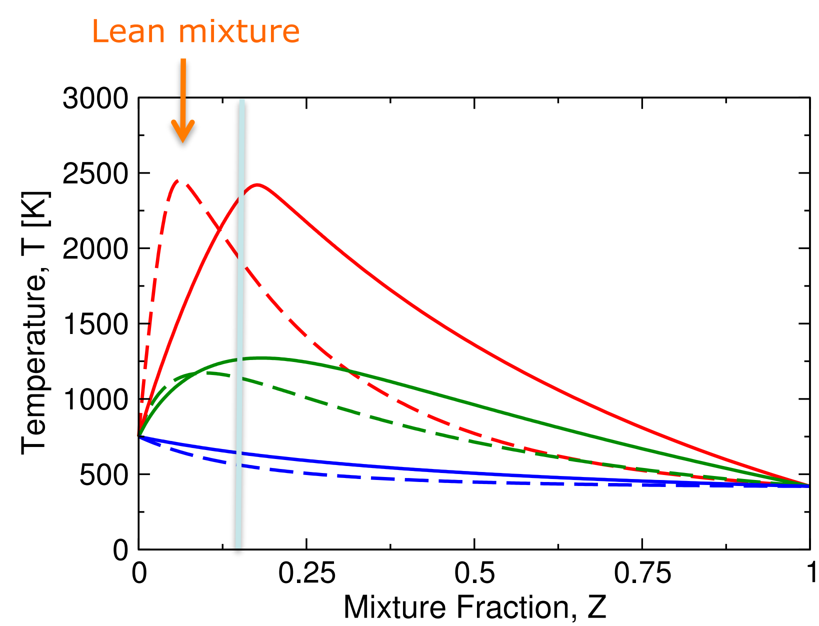




Research Plan: A priori Analysis

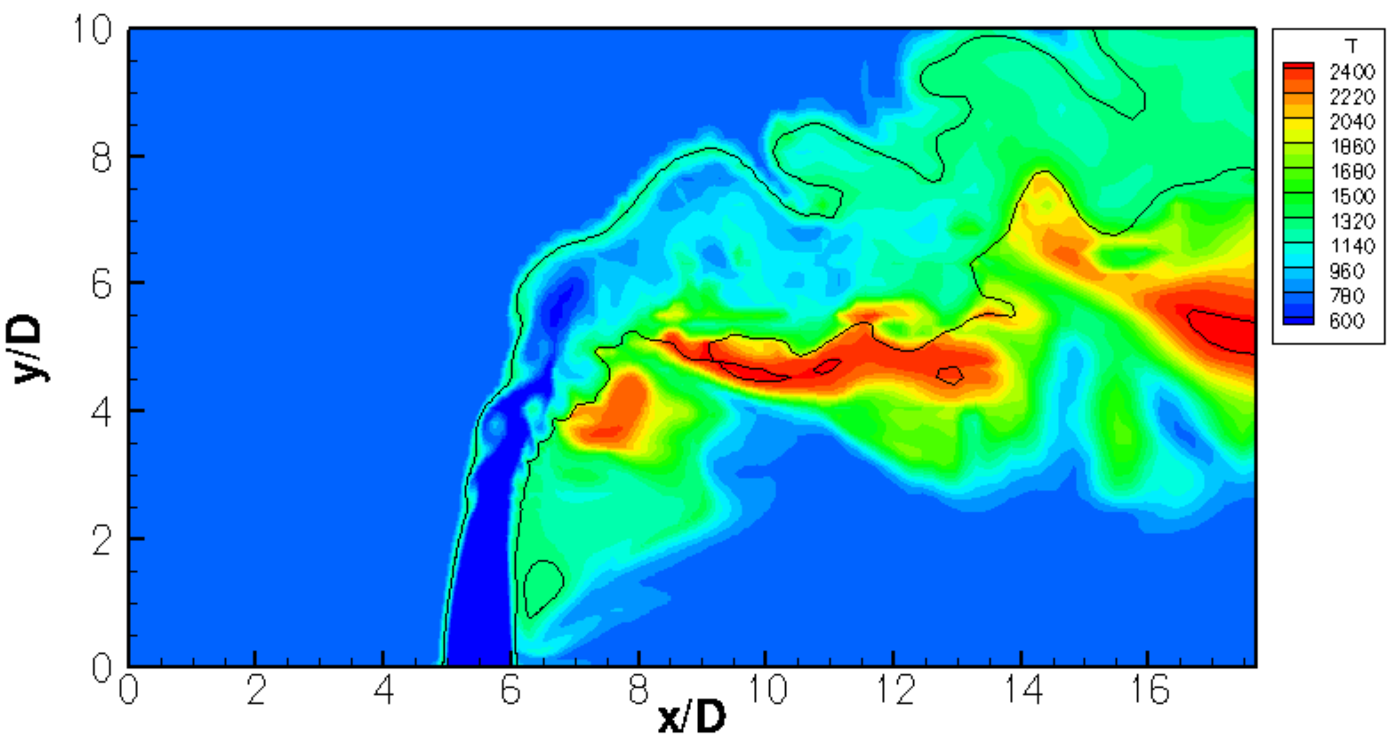
- Lewis number effects
  - Turbulent mixing leads to enhanced thermo-diffusive transport and shift of flame-structure to stoichiometric condition





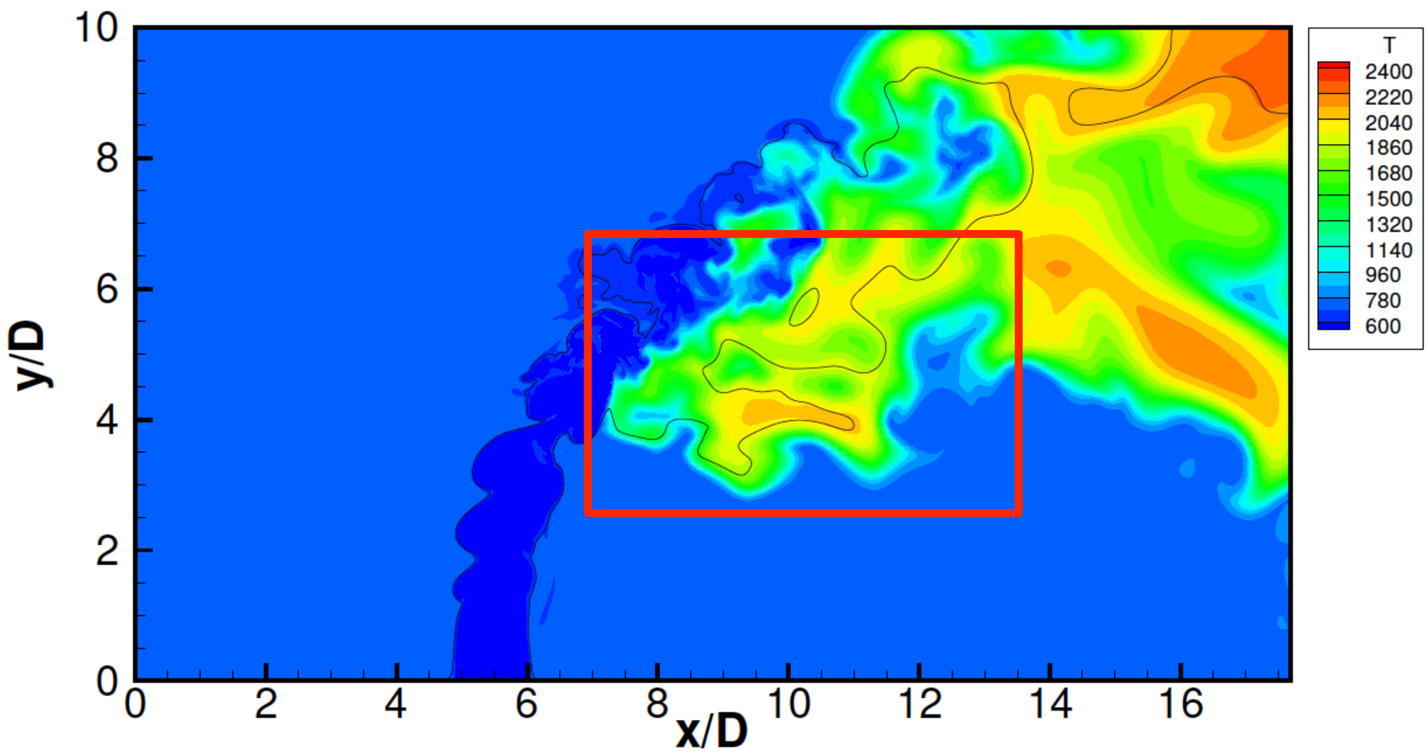
Research Plan: A priori Analysis

- Lewis number effects: Unity Lewis-number
  - Turbulent mixing lead to enhanced thermo-diffusive transport → flame-stabilization



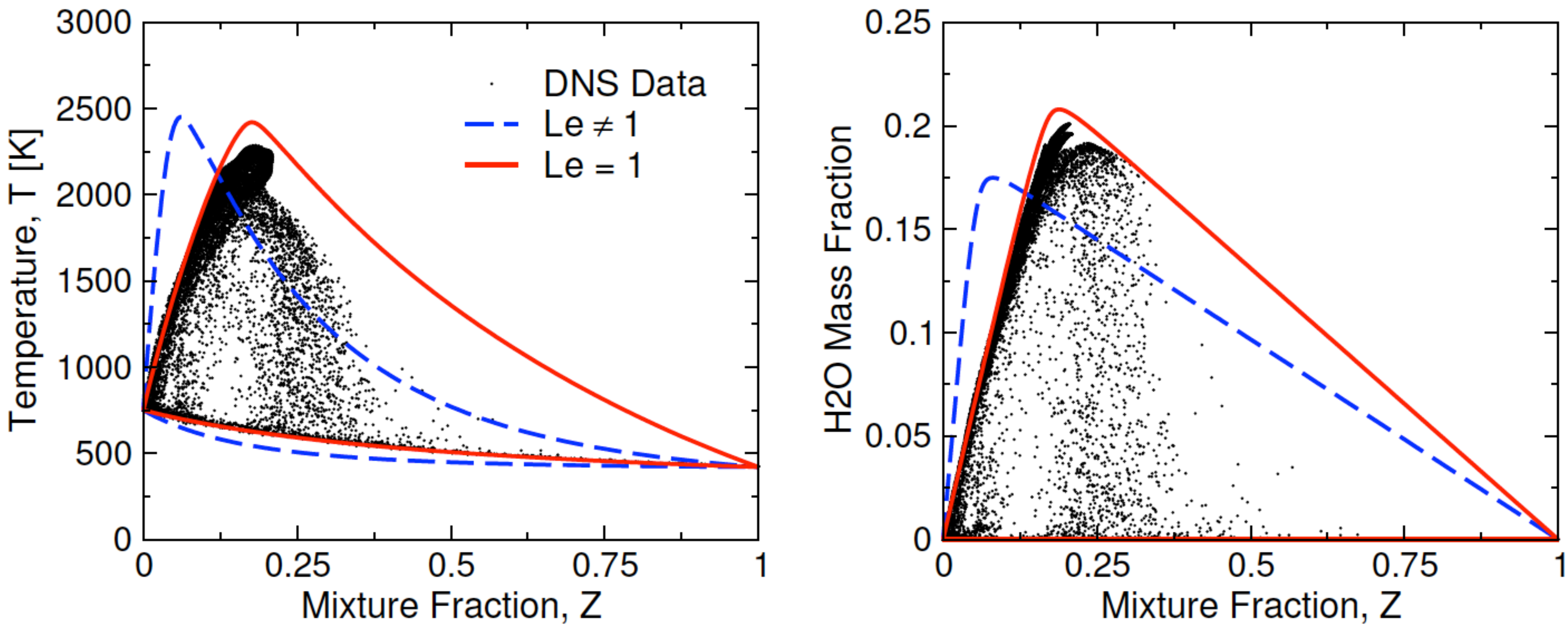
Research Plan: A priori Analysis

- Lewis number effects
  - Instantaneous temperature field from DNS-data



Research Plan: A priori Analysis

- Lewis number effects
  - Comparison against DNS-database



→ Turbulent unity Lewis-number representation is accurate even for low-Reynolds-number HHC-flows

Research Plan

(1) Perform large-eddy simulations with steady and unsteady flamelet model

(2) Assess flamelet-modeling assumptions

- Closure models for turbulence/chemistry interaction
- SGS-scalar mixing and dissipation rate models
- Ignition and flame-stabilization processes

(3) A posteriori LES-model validation using dual-swirl-stabilized partially premixed GT-combustor

Objectives

Experimental Effort (Driscoll)

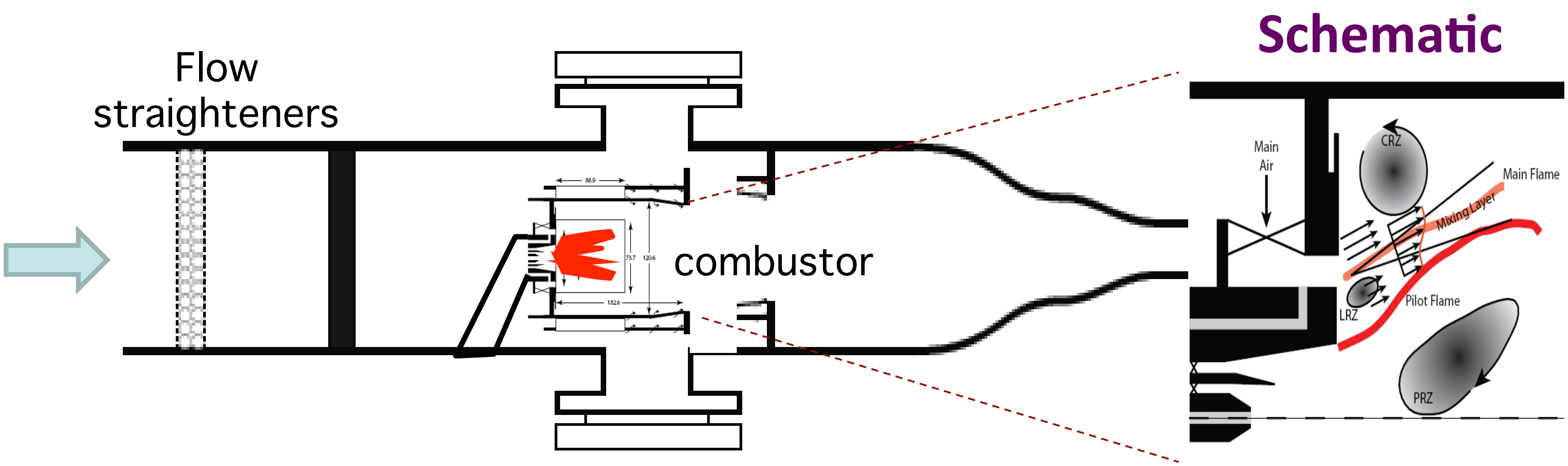
- Perform detailed measurements in dual-swirl partially-premixed GT-combustor
- Realistic high-pressure (up to 10 bar) conditions
- Primary fuels: hydrogen, syngas
- Characterization of flame-stabilization mechanisms
  - Flash-back and lift-off
- Establish experimental database for LES-model validation

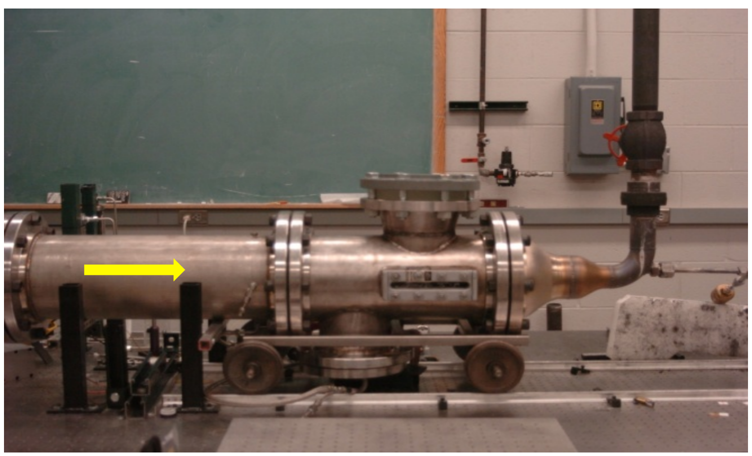
Computational Effort (Ihme)

- Development of LES-combustion model for prediction of unstable combustion regimes
  - Autoignition, flash-back, and blow-out
- Evaluation of critical modeling assumptions using DNS-data of vitiated H_2/air Jet-in-Cross-Flow (JICF) configuration
- Model-validation using swirl-stabilized GT-combustor configuration

High-Pressure Gas Turbine Combustion

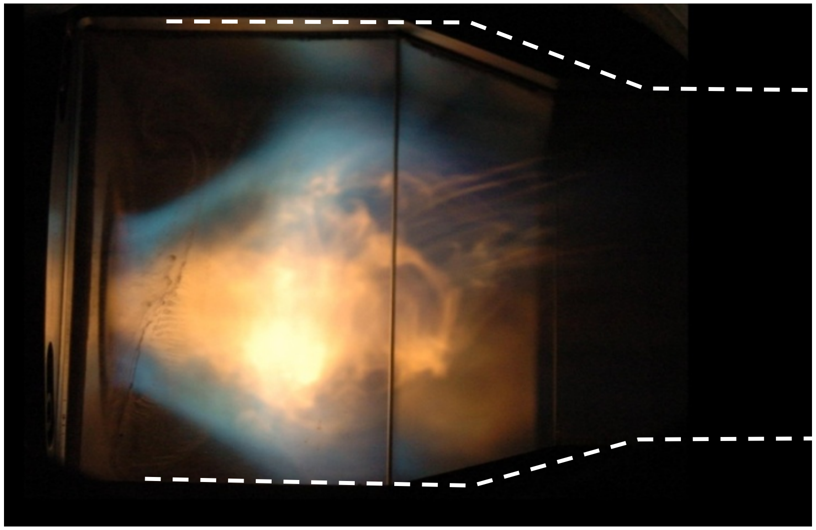
- Michigan High Pressure Gas Turbine Combustor Facility

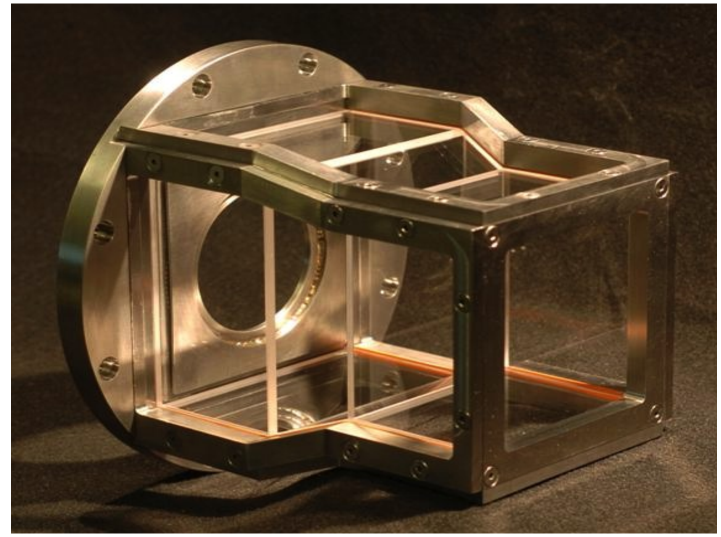




- Flame-tube: 5” diameter
- Rig Capabilities: 10 atm and 940 K
- Mass flow-rate: 0.5kg/s
- Diagnostics: PIV, LDV, PLIF (Flame)

High-Pressure Gas Turbine Combustion



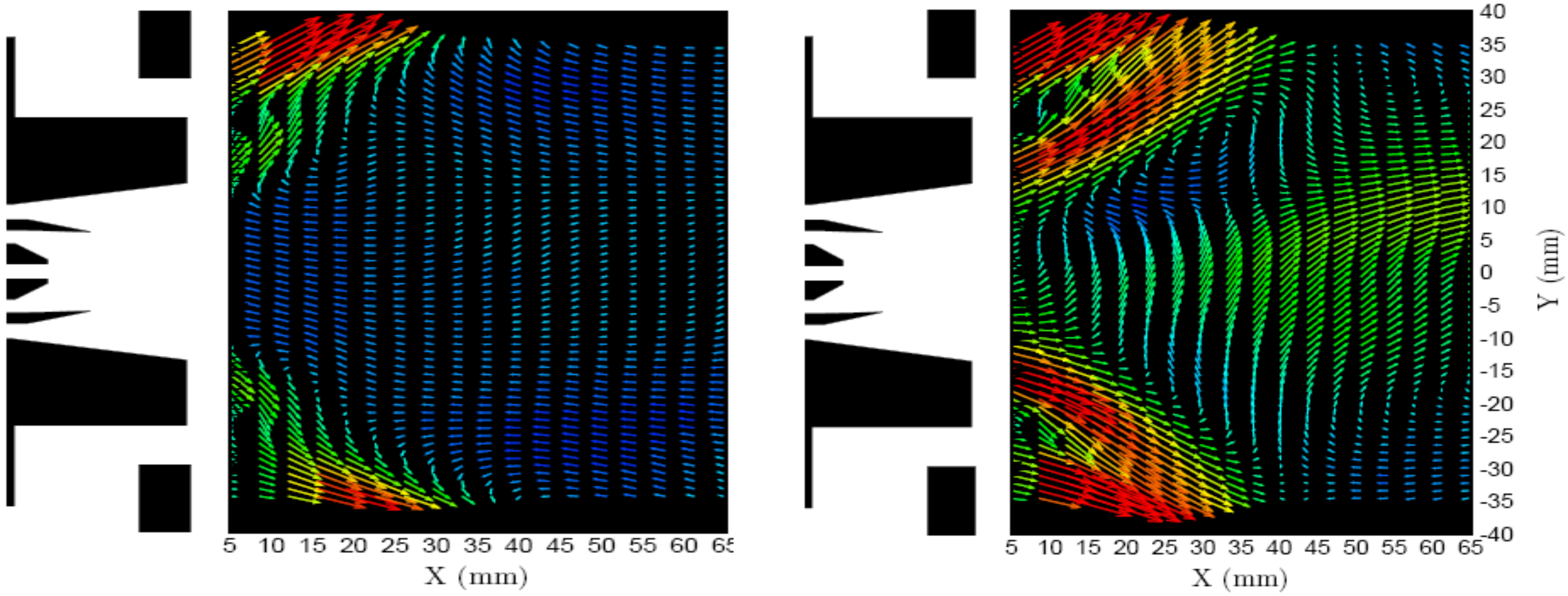


Case	Temperature [R/K]	Pressure [psia/atm]	Mass flow rate [lbm/s]	Comment
1	**760/678**	**36/2.4**	**0.47**	**achieved**
2	801/700	45/3.1	0.58	achieved
3	**907/760**	**66/4.5**	**0.85**	**achieved**
4	907/760	29.4/2	Main & Pilot	achieved
5	907/760	14.7/1	Main & Pilot	achieved
7	1200/922	150/10	0.95	achievable

High-Pressure Gas Turbine Combustion

- Effect of heat release on flow field structure

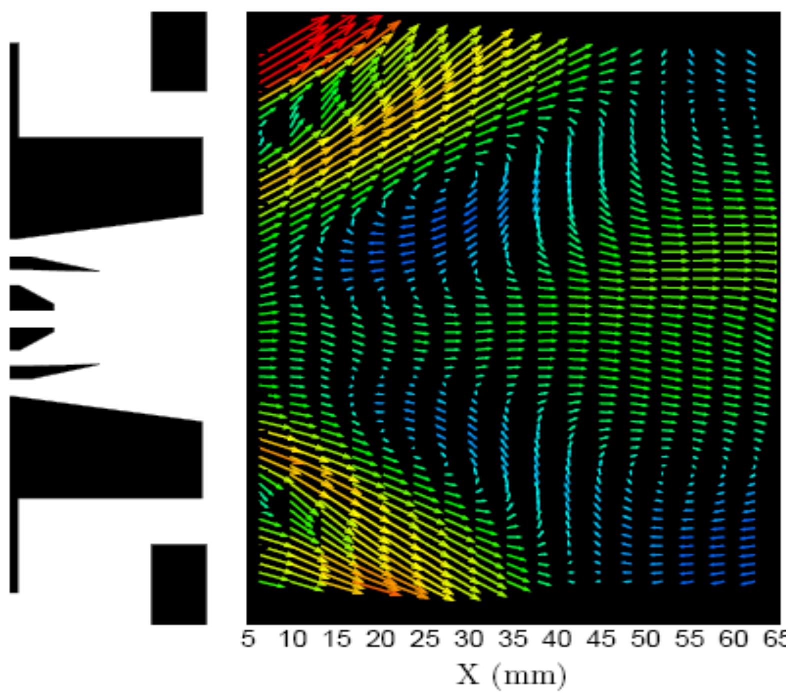
Case 3: Nonreacting, 4.5 atm **Case 3: Reacting, 4.5 atm**



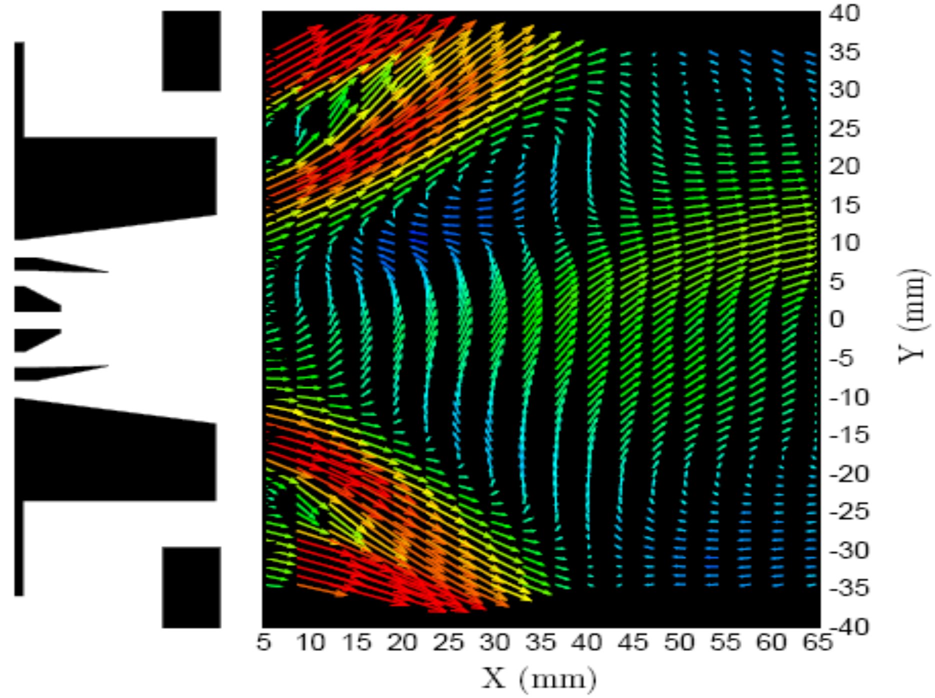
High-Pressure Gas Turbine Combustion

- Mean Flow Field

Case 1 Reacting, 2.4 atm

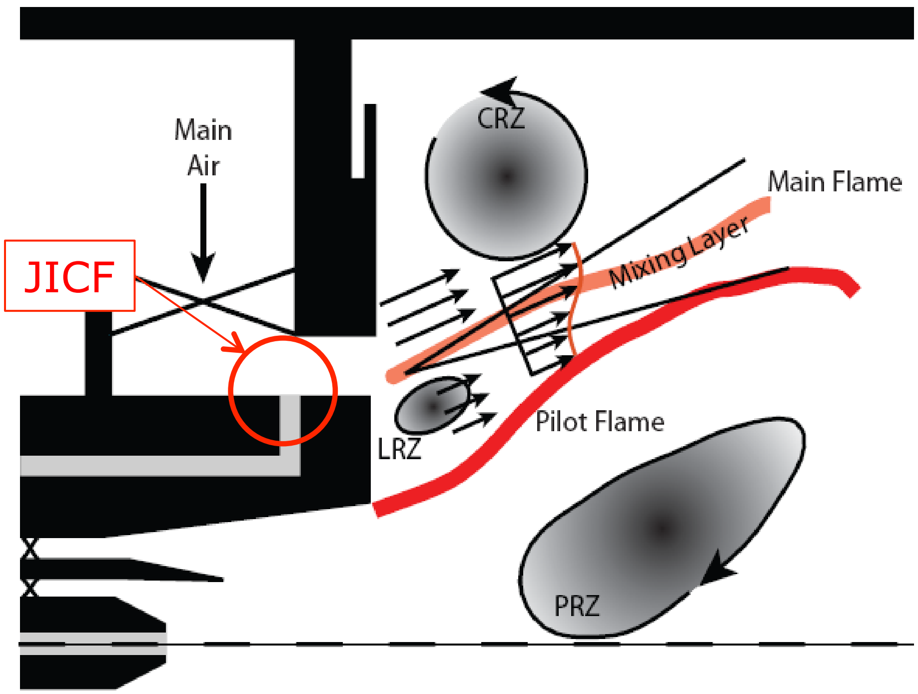


Case 3 Reacting, 4.5 atm

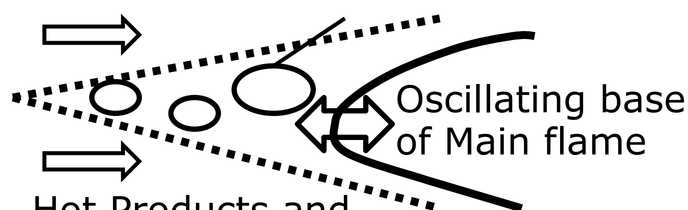


High-Pressure Gas Turbine Combustion

- Sources of Unsteadiness



- Anchor point of Main flame (liftoff, flashback)
- Shed vortices in shear layer
- Oscillating recirculation zones
- Spray combustion time delay
- Flame area oscillates

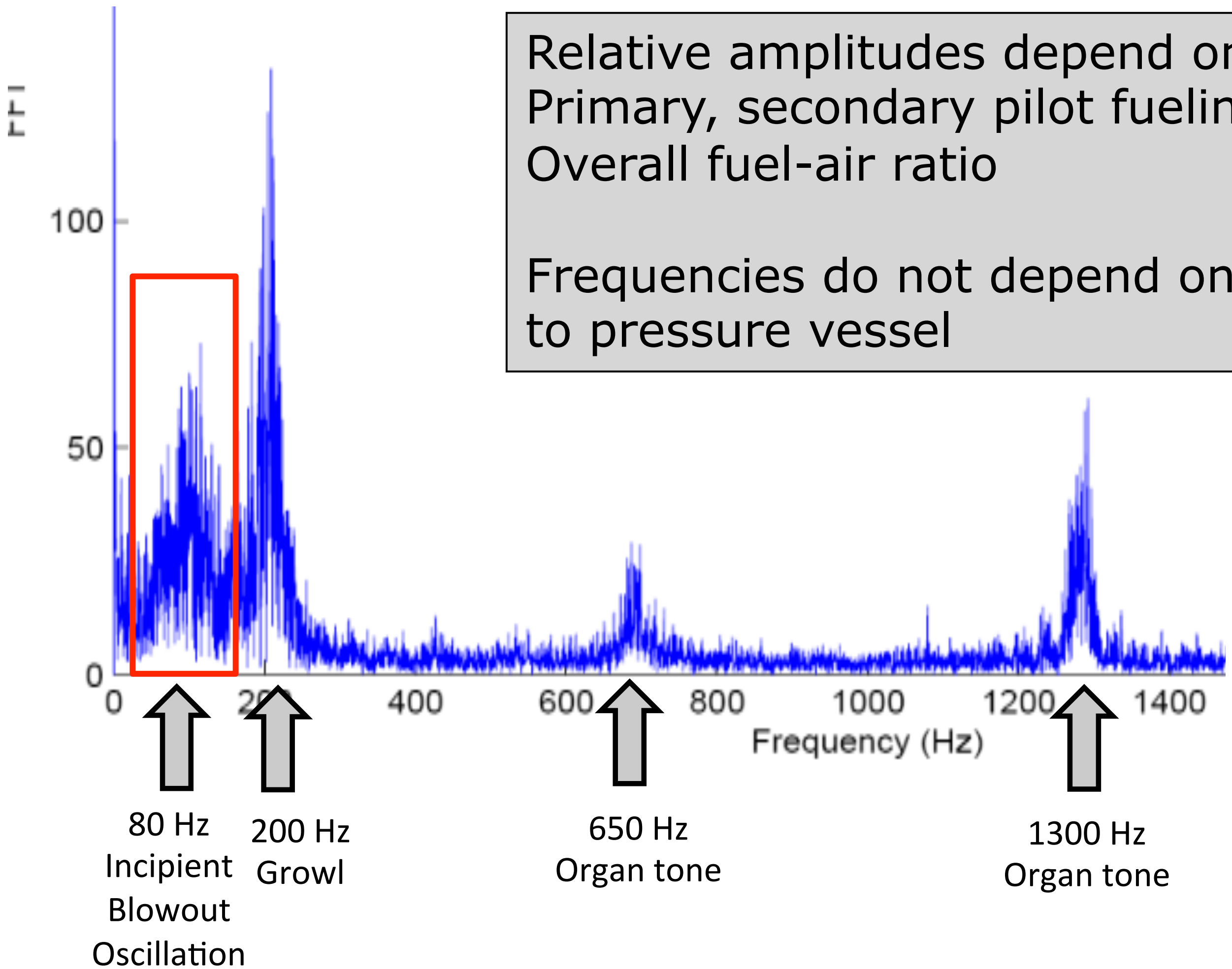


High-Pressure Gas Turbine Combustion

- Pressure spectra in TAPS combustor

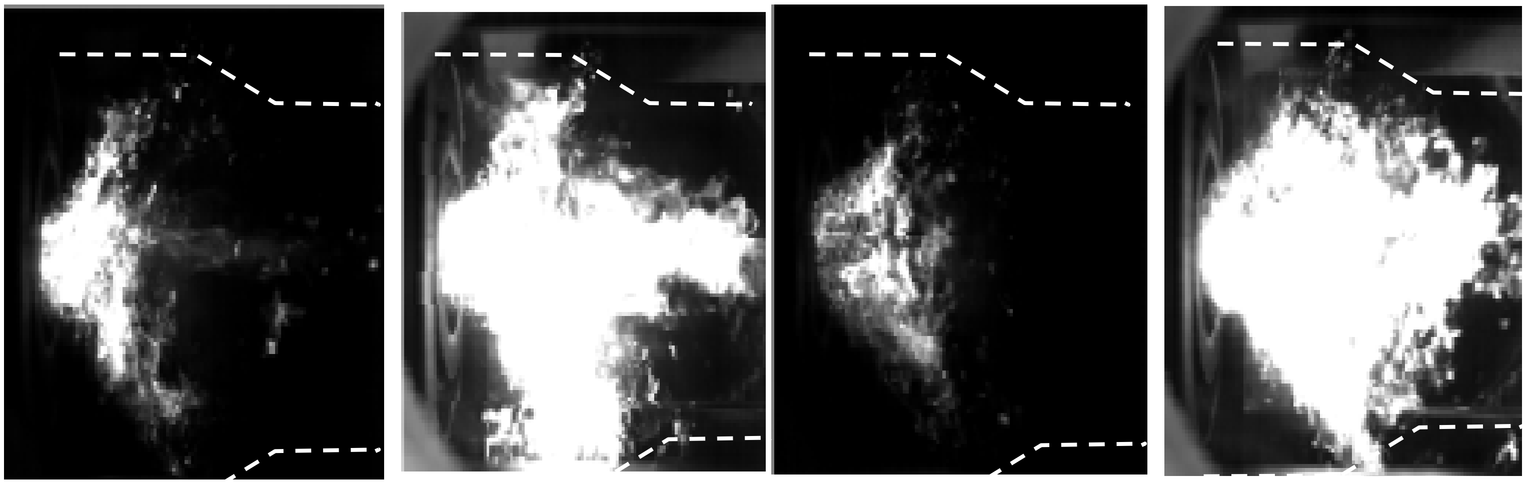
Relative amplitudes depend on:
Primary, secondary pilot fueling
Overall fuel-air ratio

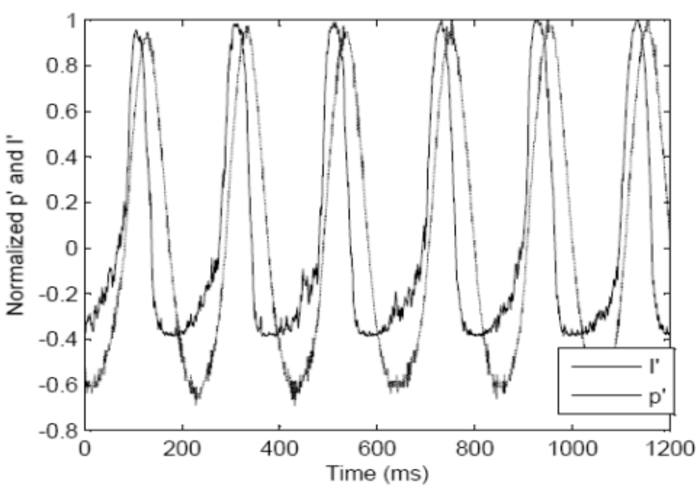
Frequencies do not depend on changes to pressure vessel



High-Pressure Gas Turbine Combustion

- Insipient blowout dynamics in TAPS combustor

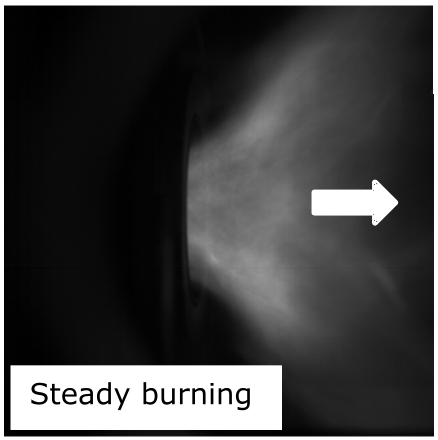


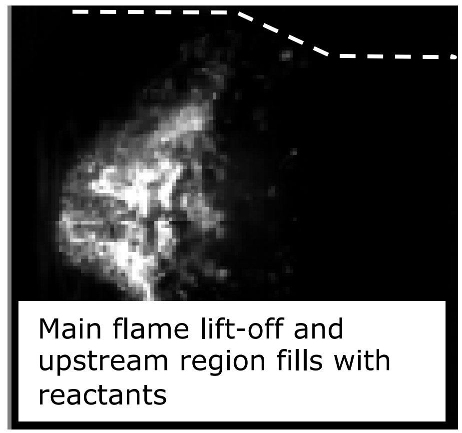


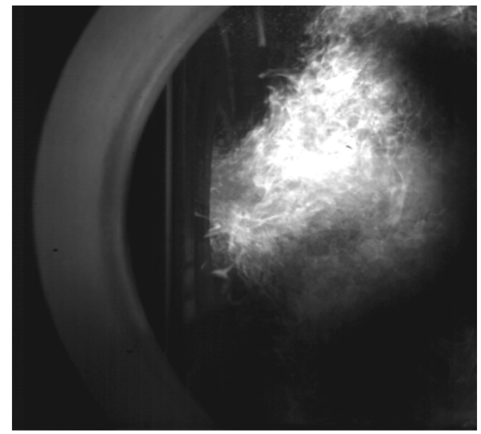
Pressure and flame luminosity are highly correlated and periodic but low frequency

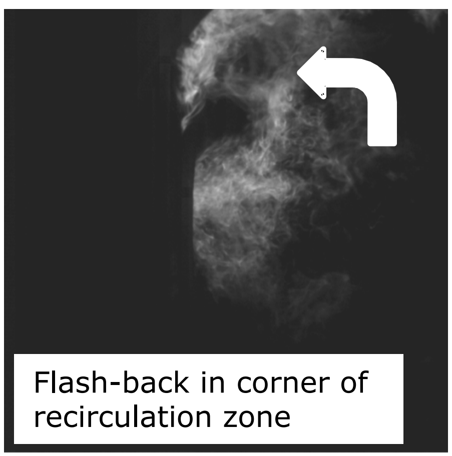
High-Pressure Gas Turbine Combustion

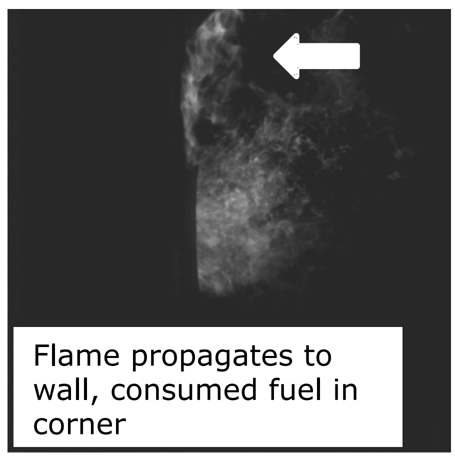
- Flame Anchoring











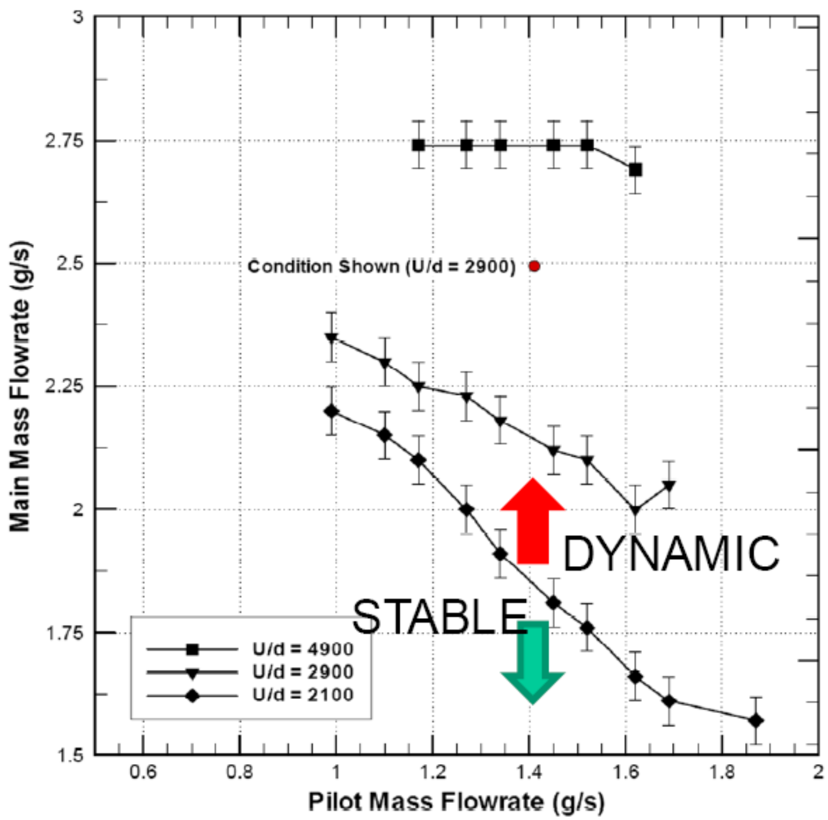
Off-design condition (low pilot fiuel flow)

4.5 atm/760 K

High sped movies at 1000 fps

High-Pressure Gas Turbine Combustion

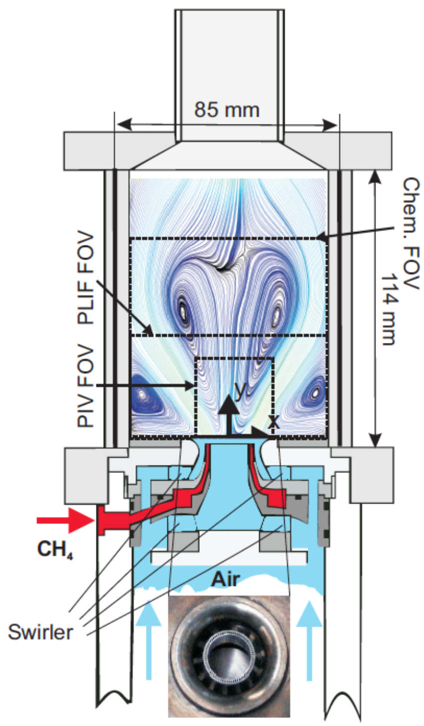
- Boundary of dynamics in TAPS combustor for 20 Hz incipient blowout instability

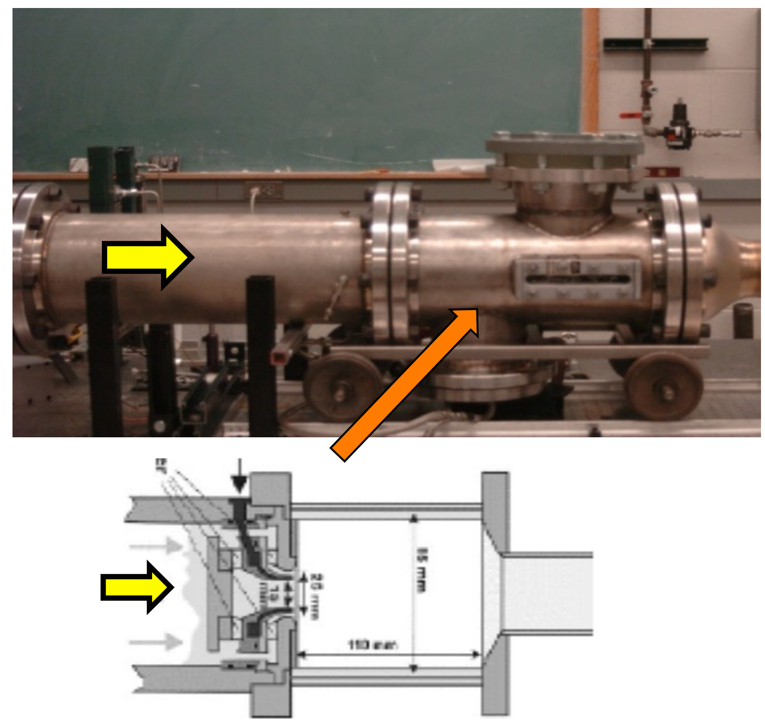


Research Efforts

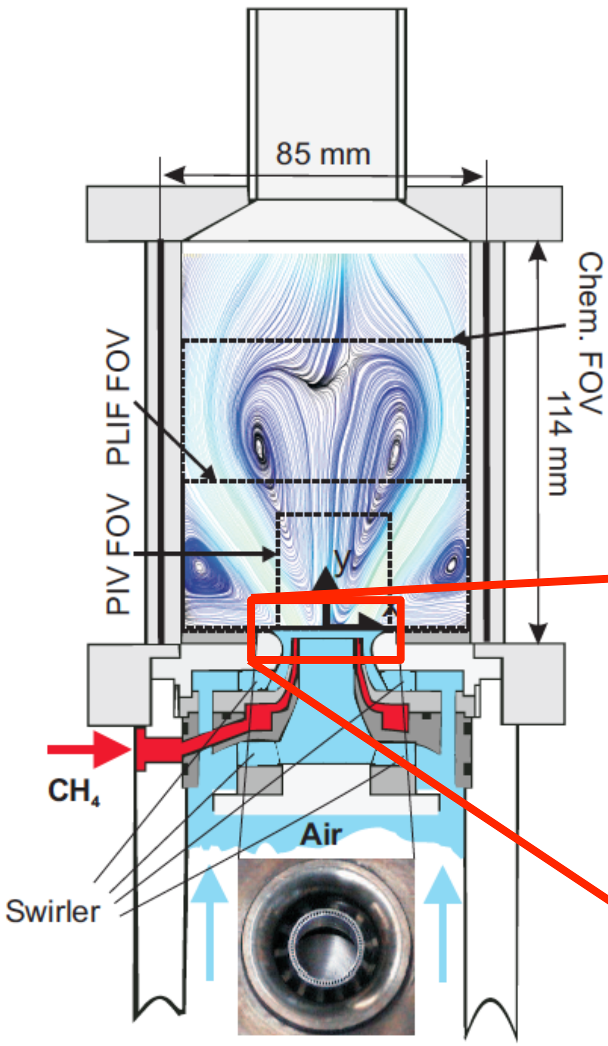
Dual-swirl Gas Turbine Combustor

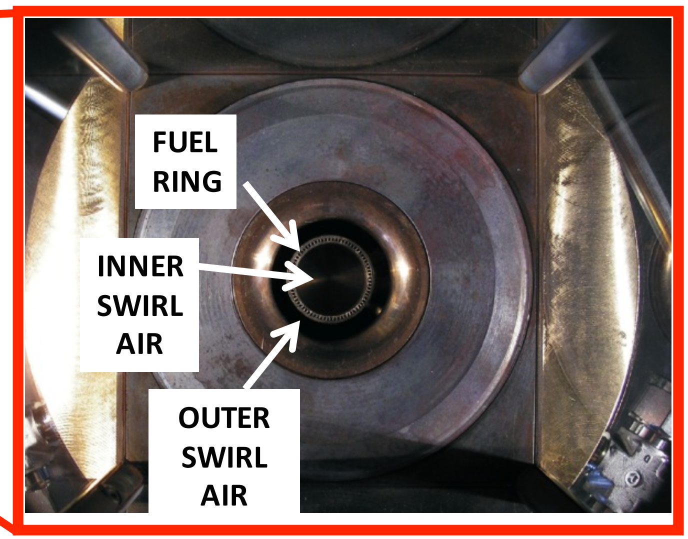
- Research efforts
  - Integrate DLR dual-swirl gas turbine combustor in the UM-high pressure gas turbine facility
  - Instrumentation with high-speed diagnostics, PIV, and PLIF





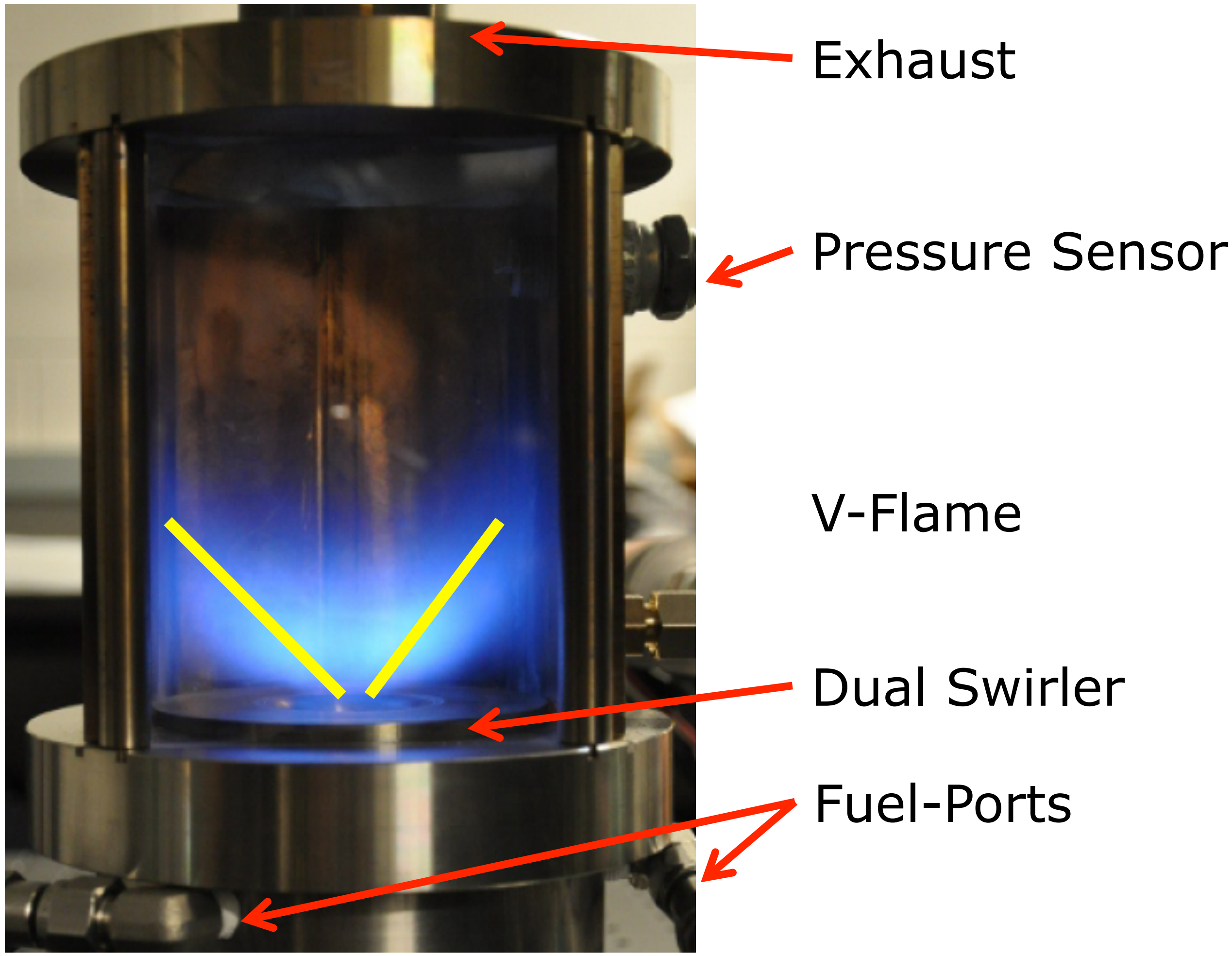
Dual-swirl Gas Turbine Combustor





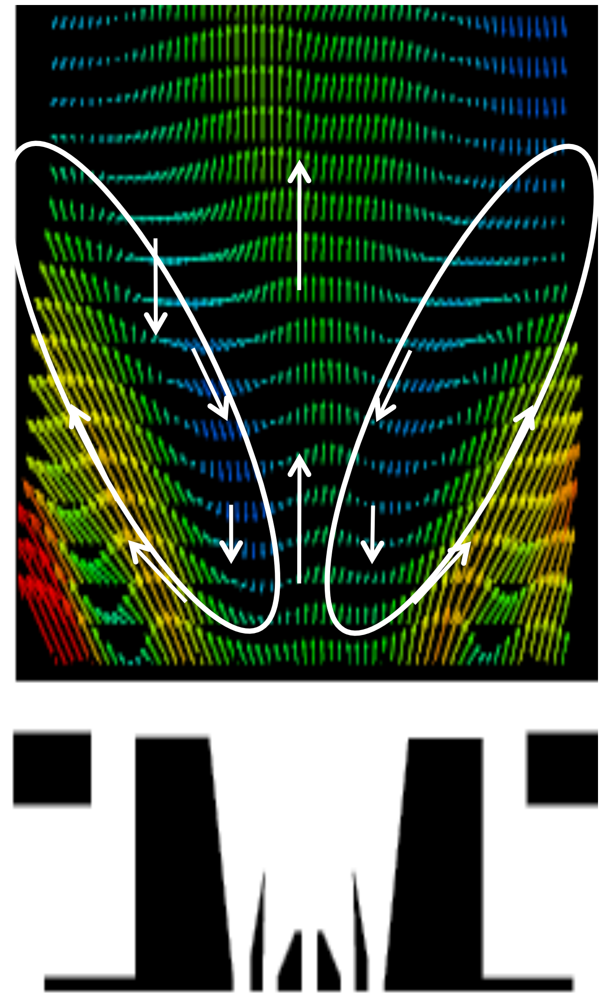
Dual-swirl Gas Turbine Combustor

- Burner setup



Dual-swirl Gas Turbine Combustor

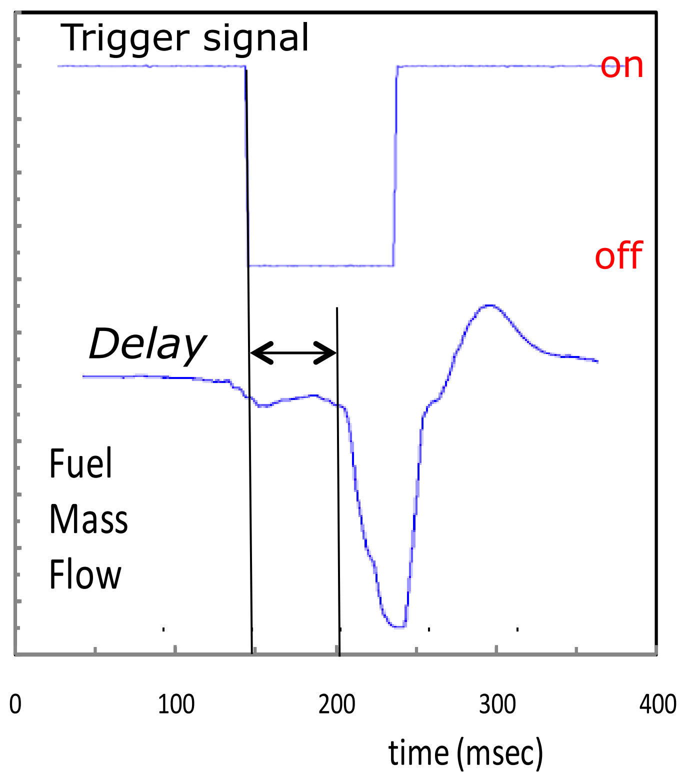
- Experimental instrumentation
  - Particle Image Velocimetry (PIV)
    - Instrumentation has been setup; Calibration experiments are currently conducted
    - Identify relevant operating conditions for PIV-analysis
  - High-speed chemiluminescence for dynamic flame imaging and flame-shape analysis
  - Pressure sensors
  - Thermocouples



PIV-measurements in TAPS-combustor

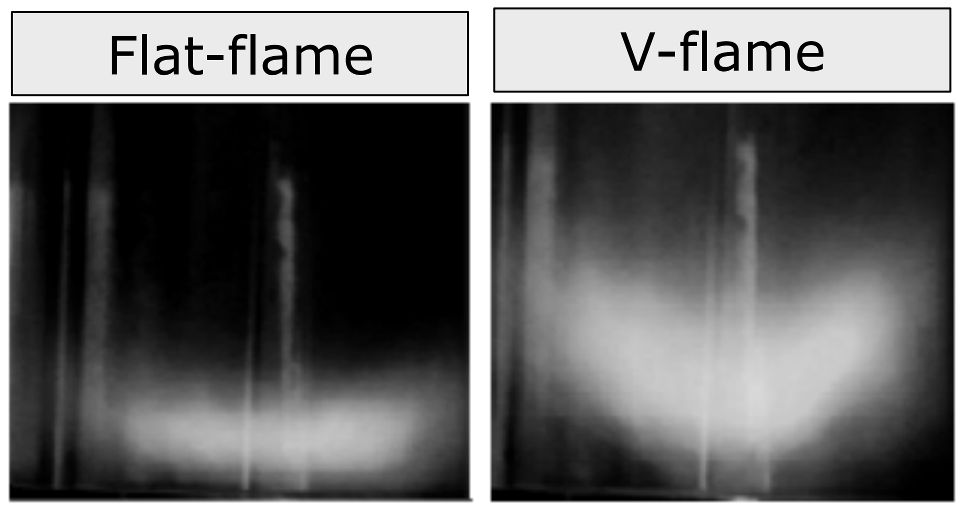
Dual-swirl Gas Turbine Combustor

- Manufactured and installed combustor, instrumentation with externally-controlled fuel valves
- Fuel modulation



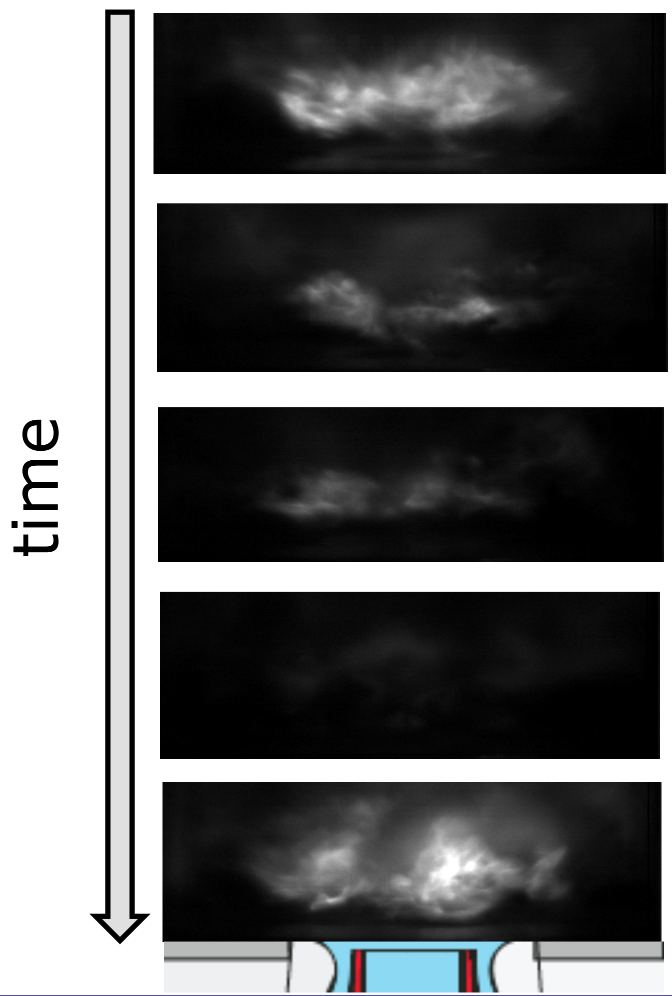
Dual-swirl Gas Turbine Combustor

- Operating condition:
  - Rapid increase in fuel flow rate results in modulation of flame shape



Dual-swirl Gas Turbine Combustor

- Flame modulation sequence



Flame initially above lean limit

Rapid decreased of fuel supply

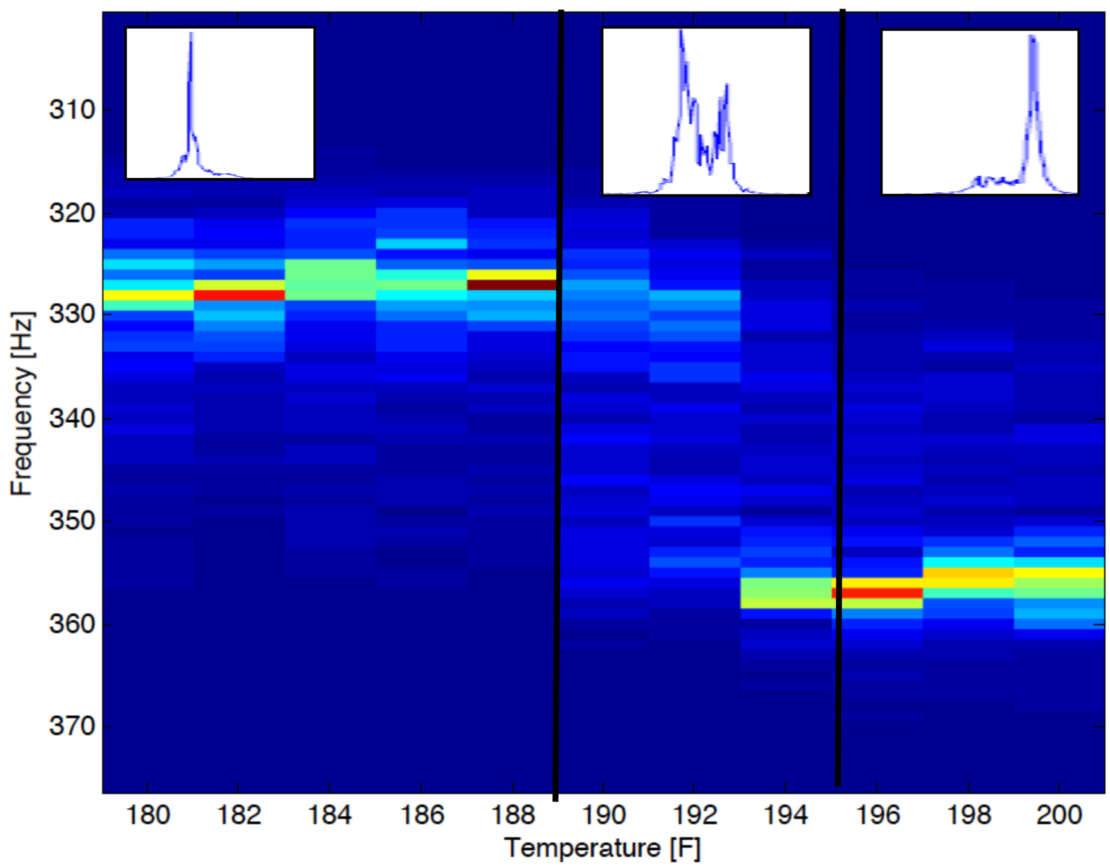
Reduction of flame luminosity

Flame temporarily extinguished

Flame reignites with fuel-injection

Dual-swirl Gas Turbine Combustor

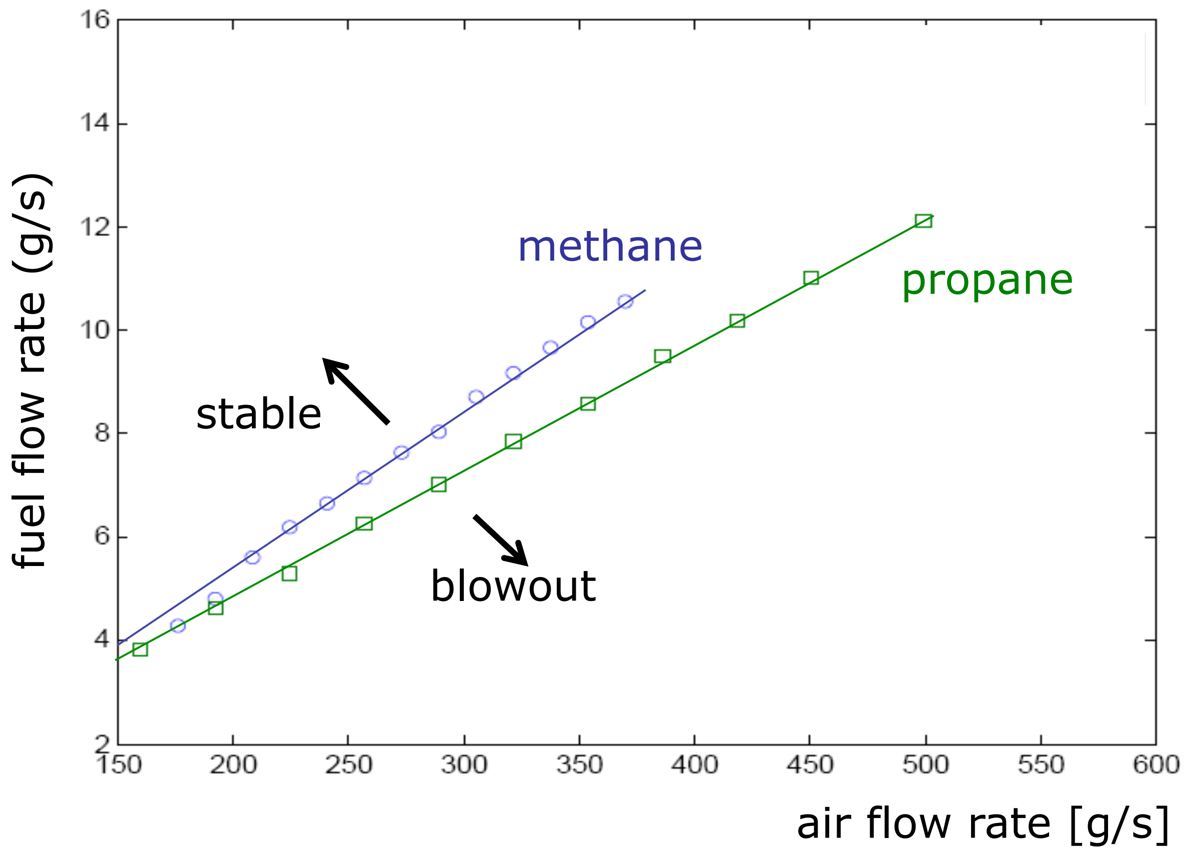
- Drift in acoustic frequency due to variations in air temperature (by heat-transfer to burner and nozzle)



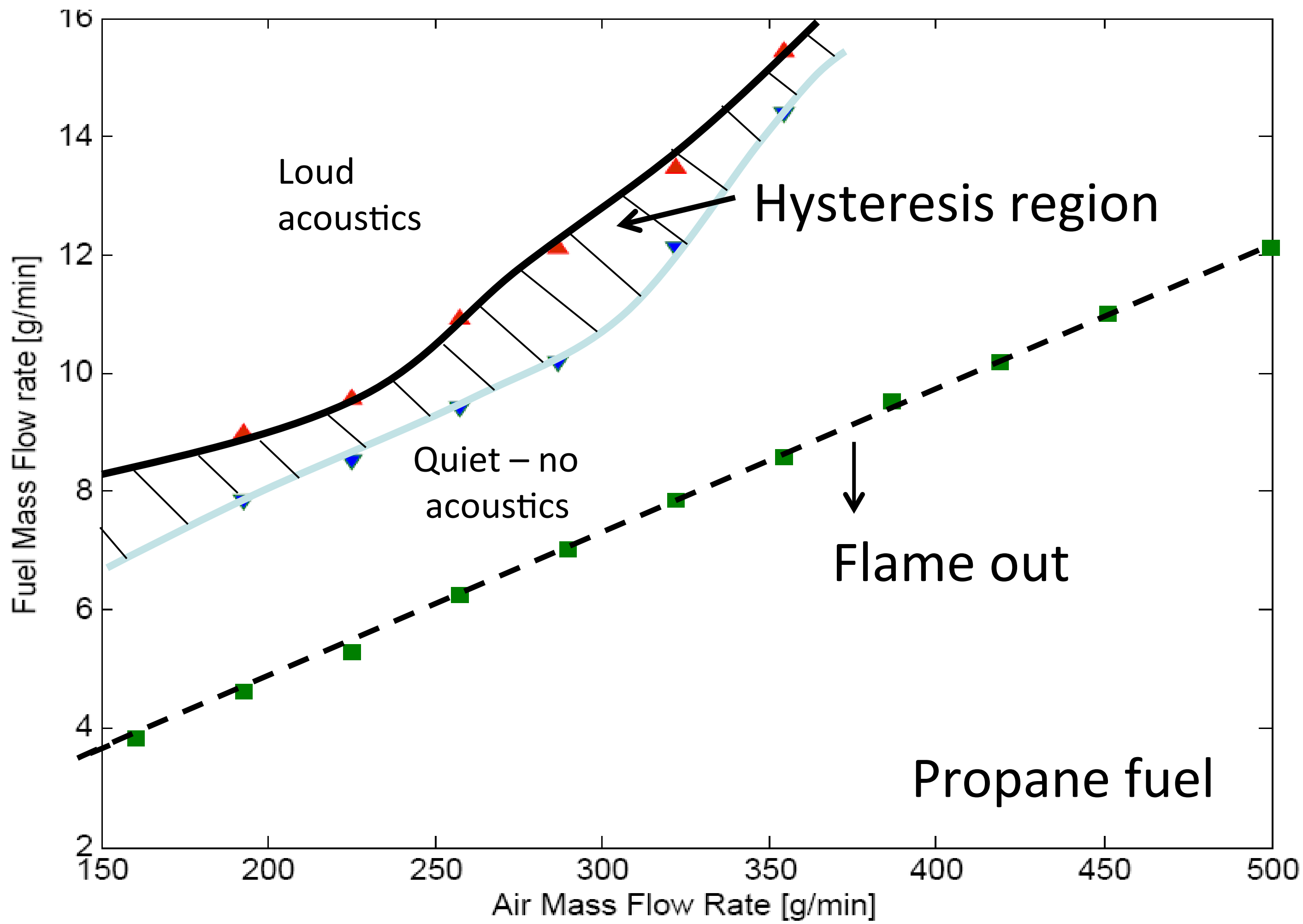
two distinct combustion frequencies are present dependent on air-temperature

Dual-swirl Gas Turbine Combustor

- Measured dynamics associated with lean blowout limits for methane and propane fuels



Dual-swirl Gas Turbine Combustor: Hysteresis



Research Plan

1) Characterize and measure stable GT-operating regime for lean syngas fuel mixtures

2) Complete setup of PIV/PLIF systems

3) Conduct phase-locked experiments to analyze combustion instability regimes

4) Develop metric to characterize unstable combustion mechanism and transition btw. flame lift-off, flashback and propagating combustion regimes

5) Measurements for different HHC-fuel compositions and equivalence ratios

Research Objectives

Experimental Effort (Driscoll)

- Perform detailed measurements in dual-swirl partially-premixed GT-combustor
- Realistic high-pressure (up to 10 bar) conditions
- Primary fuels: hydrogen, syngas
- Characterization of flame-stabilization mechanisms
  - Flash-back and lift-off
- Establish experimental database for LES-model validation

Computational Effort (Ihme)

- Develop LES-combustion model for prediction of unstable combustion regimes
  - Autoignition
  - Flash-back
  - Flame lift-off
- Evaluation of critical modeling assumptions using DNS-data of Jet-in-Cross-Flow (JICF)
- Model-validation in swirl-stabilized GT-combustor configuration