Turbulent Flames and the Role of Chemistry

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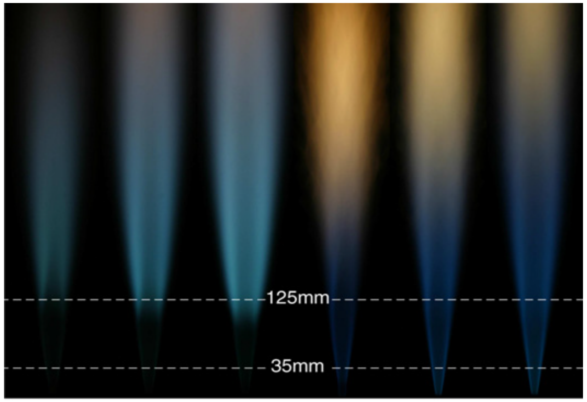
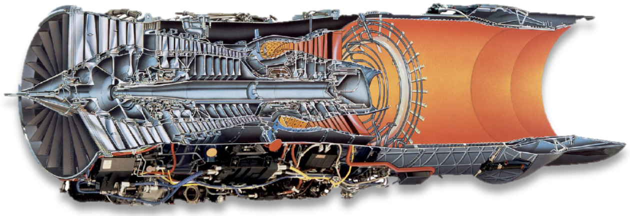
Sponsor: ONR, AFOSR, DoE

Motivation

- Advanced combustion strategies rely on
  - Low/moderate temperature combustion
  - High-pressure operating conditions
  - (Ultra)Lean and stratified combustion
  - Emerging and alternative fuel combustion
- Challenges
  - Shift from mixing-controlled to kinetics-controlled combustion regime
    - Increasing relevance of ignition-kinetics and low-temperature chain-branching reactions
    - Increasing significance of turbulence and turbulence/chemistry interaction
    - Finite-rate chemistry effects
  - Operation near stability limit





Motivation

- Objective
  - Development of high-fidelity combustion for prediction of turbulent reacting flows under consideration of
    - Finite-rate chemistry
    - Turbulence/chemistry coupling
    - Transient combustion-dynamical processes
- Relevance
  - Identify and isolate combustion-physical processes
  - Combustor-design, control, and optimization
  - Guide experimental instrumentation

Overview

- Motivation
- LES-combustion modeling
  - Flamelet-based formulation
- ***Part 1:*** Modeling and simulation of combustion-physical processes: LES of lifted vitiated flames
- ***Part 2:*** Guide experimental instrumentation: Turbulent inhomogeneities and facility-effects?
- Summary and conclusions

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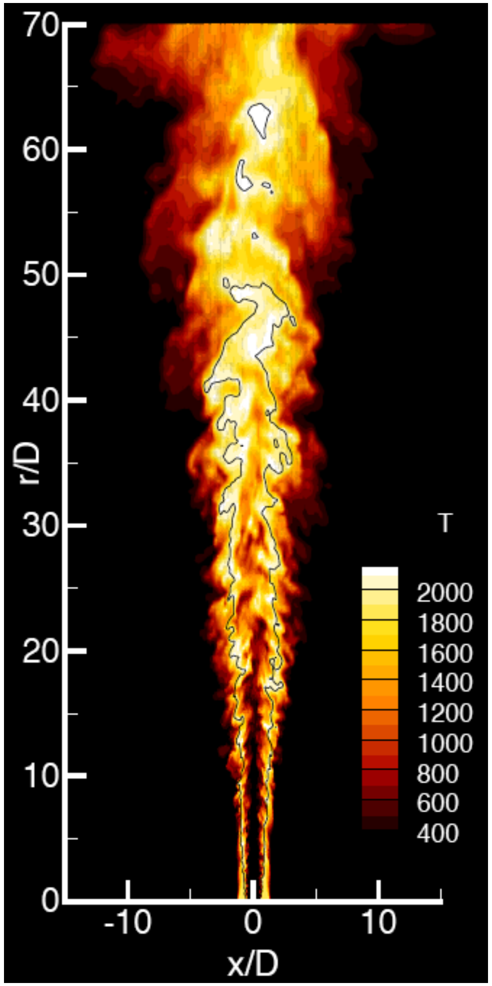
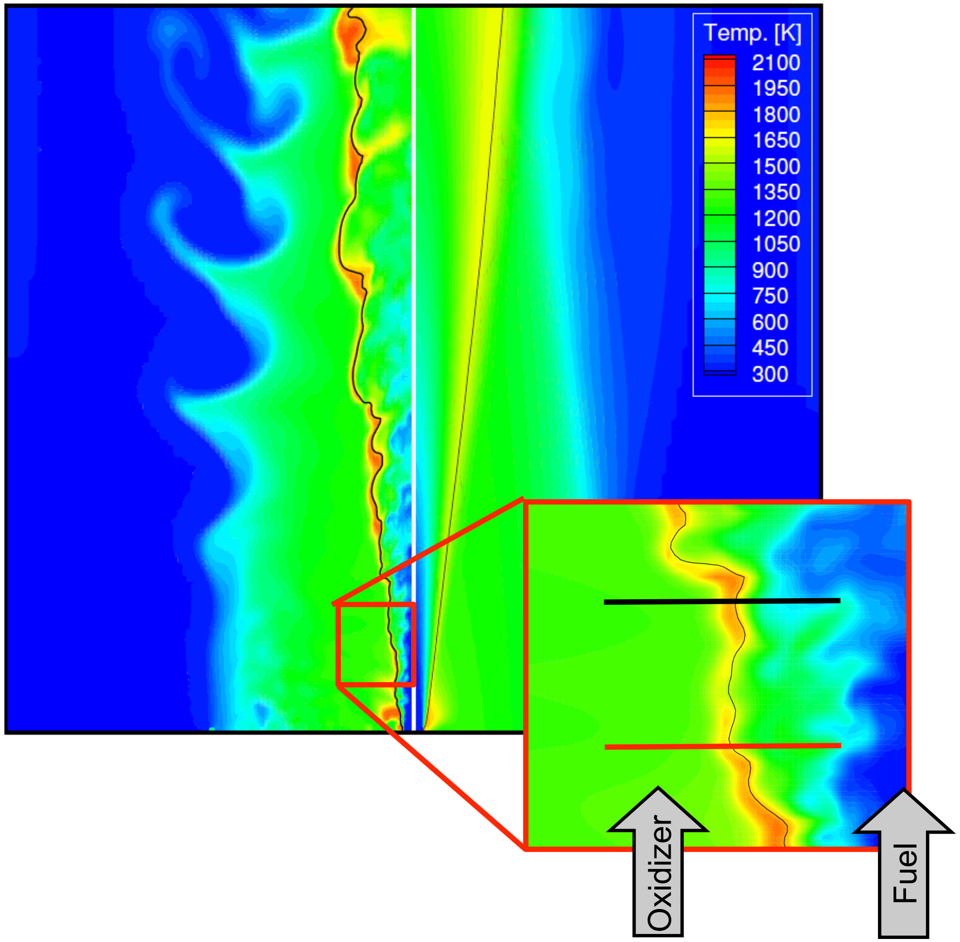
LES Combustion Modeling

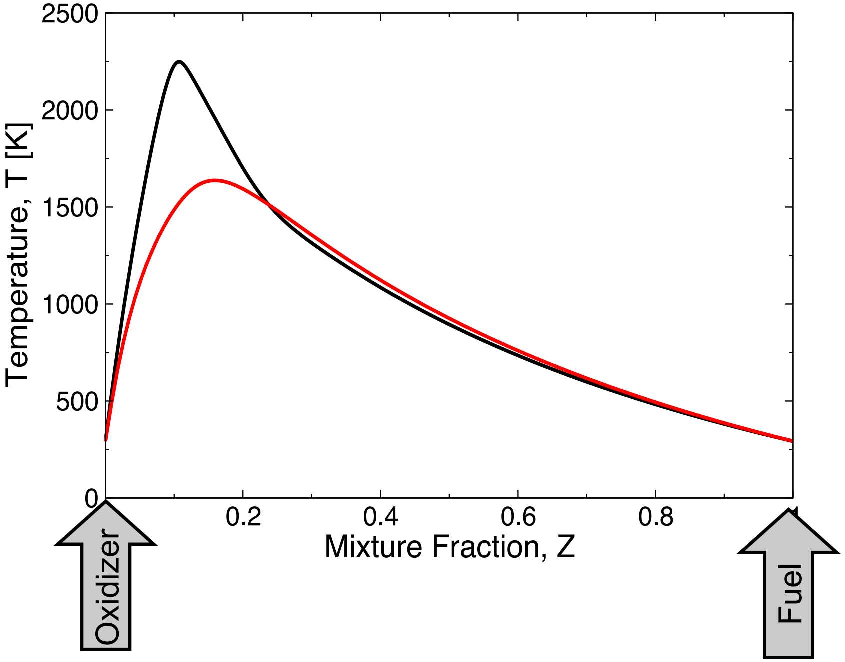
- LES Flamelet-based combustion models
  - Representation of turbulent flame as unsteady reaction-diffusion layer that is embedded in turbulent flame
  - Interaction of flame structure with turbulent environment leads to stretching, deformation, and extinction of flame



LES Combustion Modeling

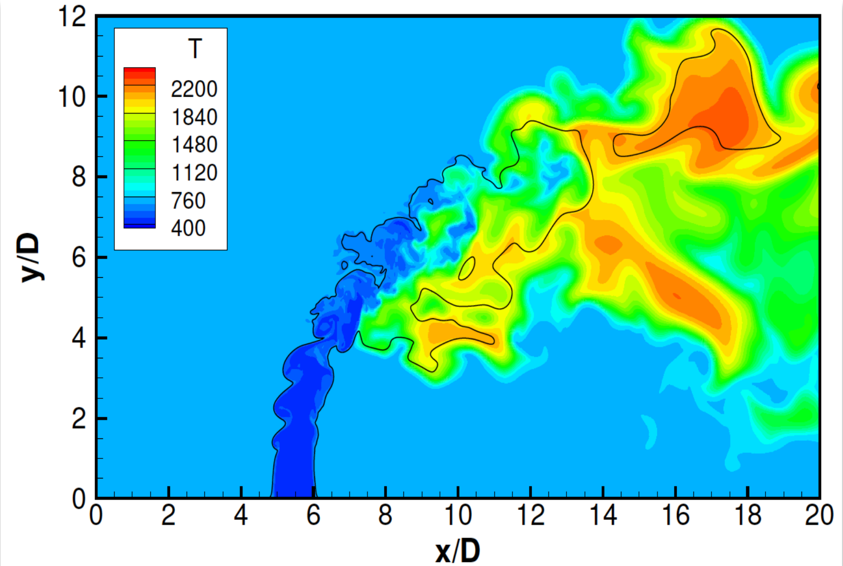
- LES flamelet-based combustion model

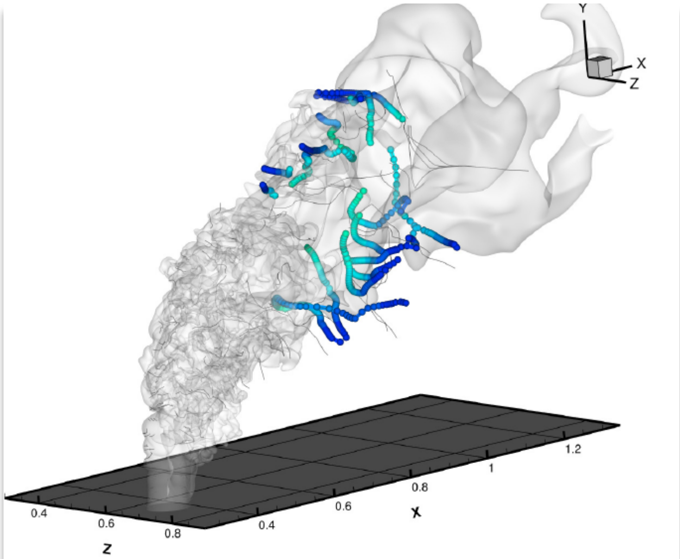




LES Combustion Modeling

- Flamelet-structure in turbulent reacting flows
  - Analysis Tools: DNS-database[1] of reacting jet-in-cross-flow
    - Fuel: N2-diluted H2-jet, 350 K
    - Oxidizer: Air, 750 K
- Extract instantaneous local flamelet structure from DNS-database





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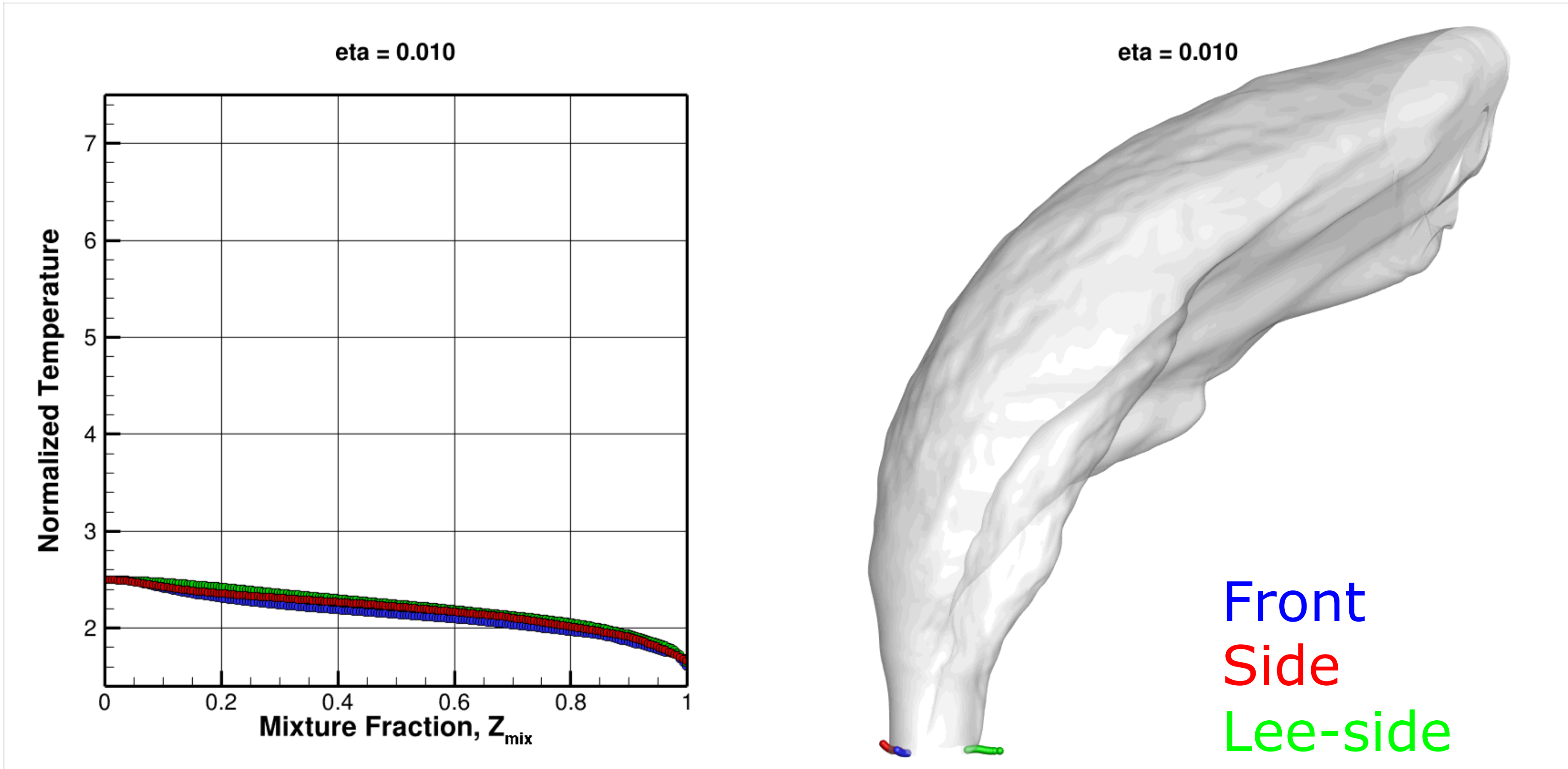
[1] Grout et al. Proc. Combust. Inst. 2011; Kolla et al. US Nat. Meeting 2011

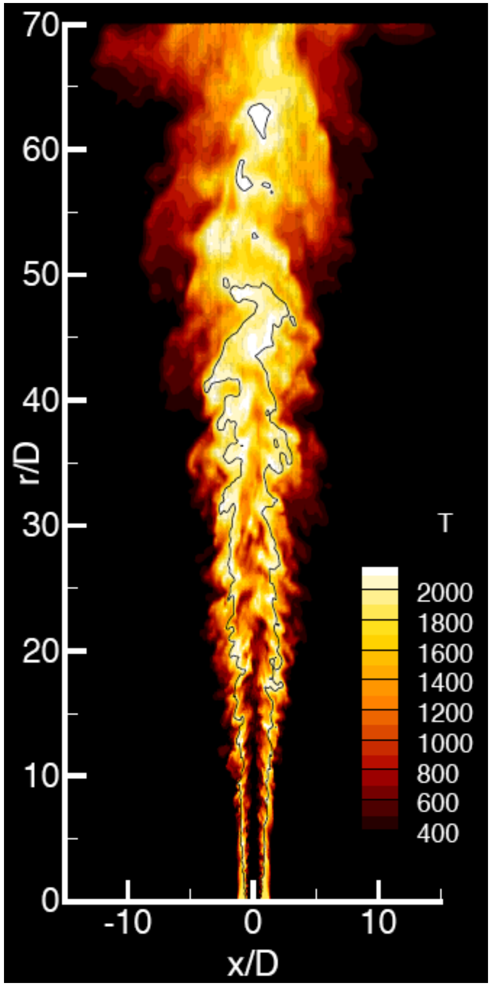
LES Combustion Modeling

- Evolution of 1D-flamelet-elements in JICF



LES Combustion Modeling

- LES Flamelet-based combustion models
  - Parameterization of combustion process in terms of reduces set of scalars
  - Account for detailed chemistry
  - Tabulation of reaction chemistry
  - Consideration of turbulence chemistry coupling



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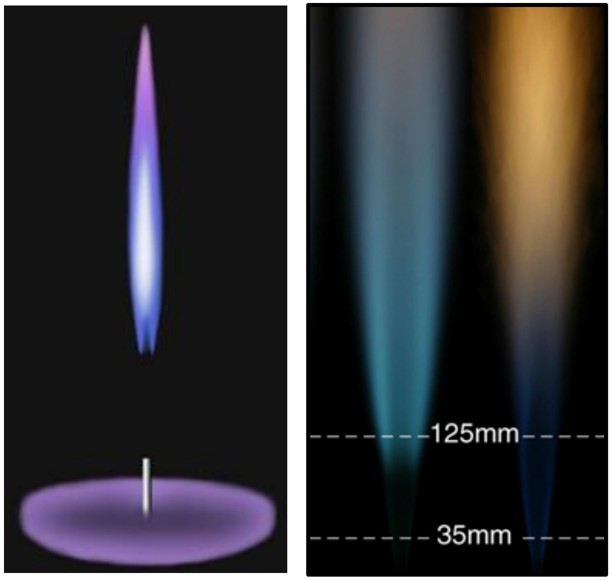
Autoignition in Turbulent Flames

- Modeling challenges in predicting autoignition in turbulent flames
  - Autoignition is transient process; requires accurate description of temporal flame-evolution
  - Flame stability and ignition dynamics strongly dependent on scalar mixing and flame/turbulence interaction



- Modeling approach[1]
  - Autoignition requires consideration of transient species formation,
    described by unsteady flamelet equations
  - Turbulence/chemistry interaction: Presumed PDF-closure to consider effects of subgrid-mixing and unresolved flame structure

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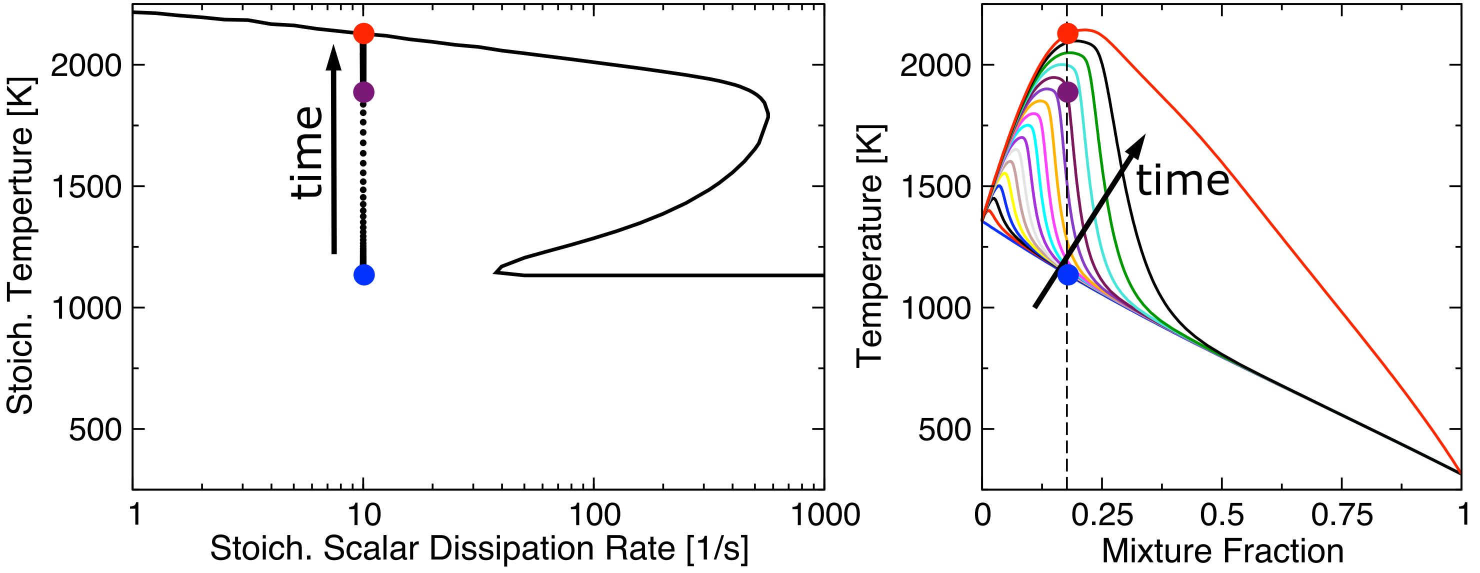
[1] Ihme & See, Combustion & Flame, 157, 2010

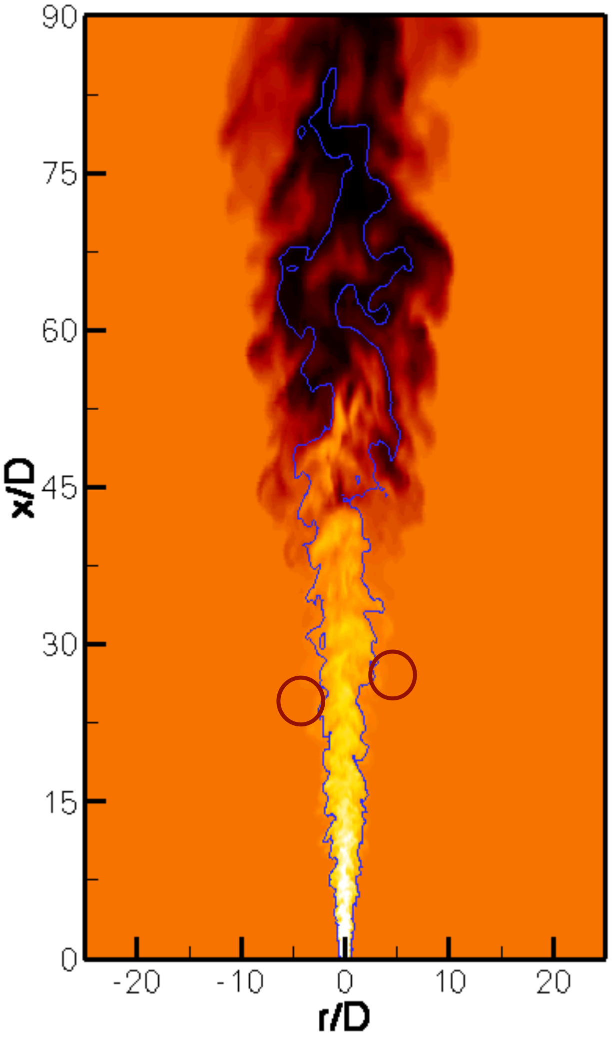
Autoignition in Turbulent Flames

- Conditions for flame-ignition in diffusion flames
  - Autoignition is transient process
  - Sufficiently low scalar dissipation rate
  - Flame ignition occurs under conditions corresponding to “most-reactive mixture”
  - Build-up of radical pool through chain-branching reaction



Autoignition in Turbulent Flames

- 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 2.11, (also used GRI 3.0, USC-mech II)
  - 5-dimensional chemistry table with grid-refinement



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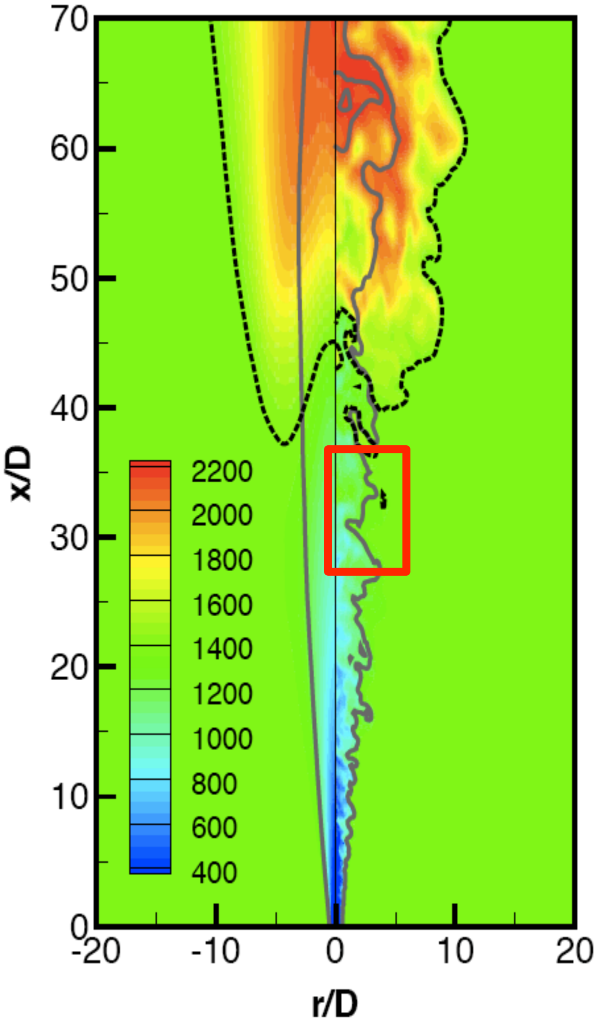
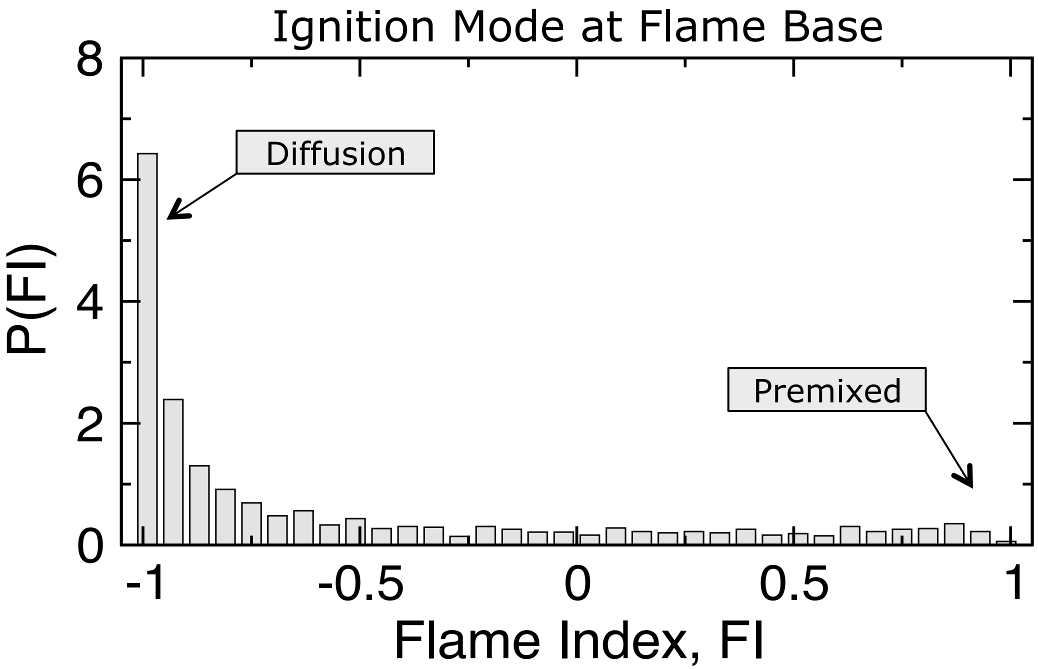
[1] Cabra, Chen, Dibble, Karpetis, Barlow, CF, 143, 2005

Autoignition in Turbulent Flames

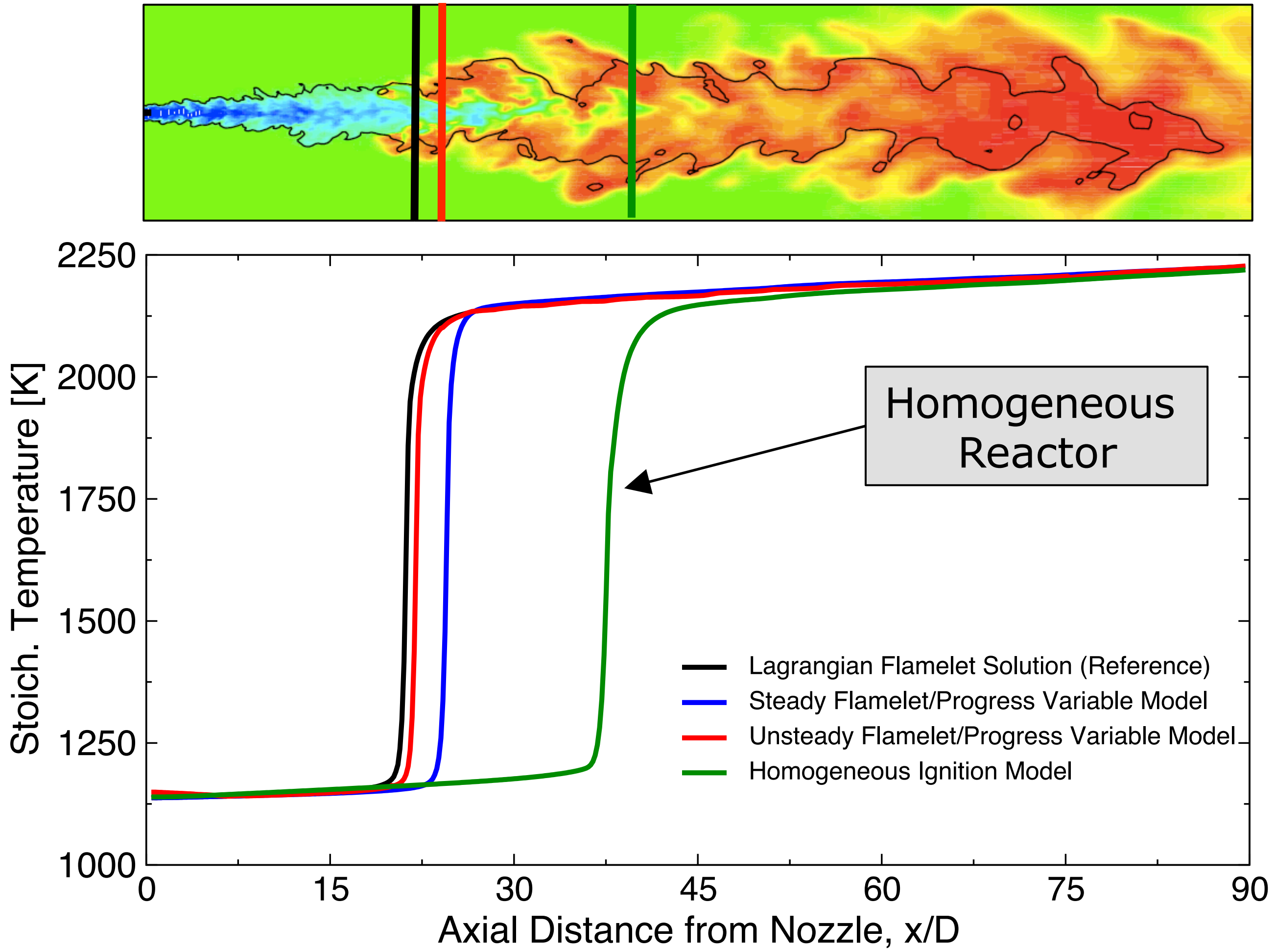




- Ignition conditions: low-strain region at most-reactive mixture composition
- Ignition occurs primarily in diffusion regime
- Location of flame-base controlled by HO_2-radical pool that is formed upstream of flame

Autoignition in Turbulent Flames

- Effects of turbulence and scalar mixing

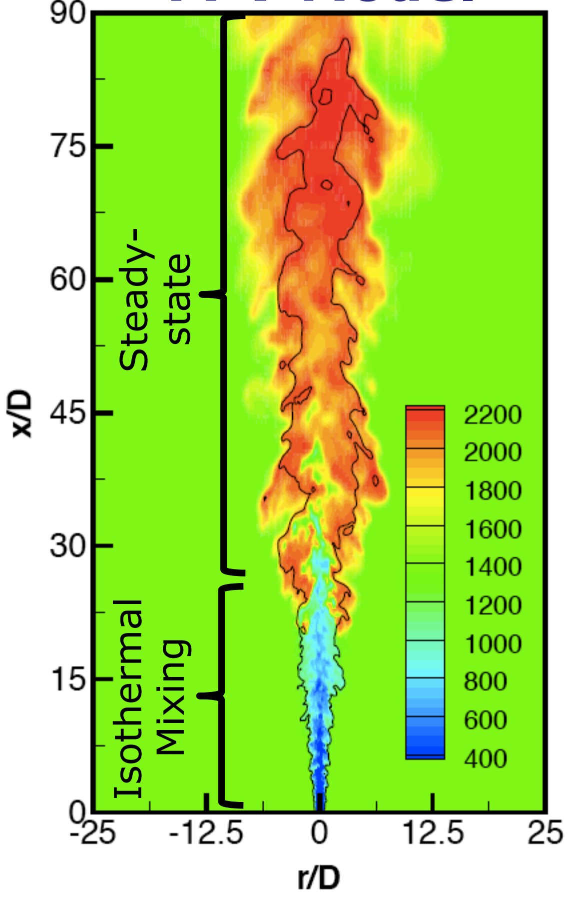


Homogeneous Reactor

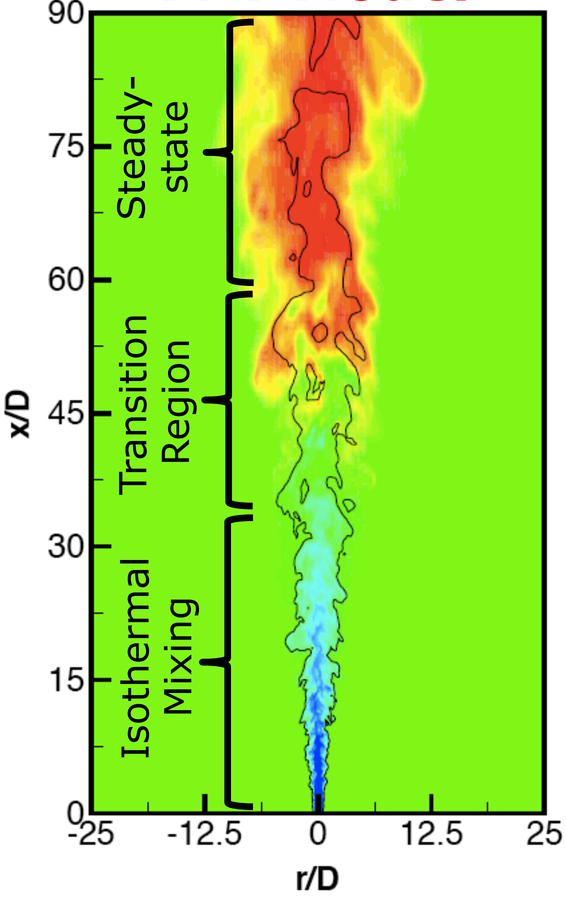
Autoignition in Turbulent Flames

- Instantaneous temperature field

Steady FPV Model

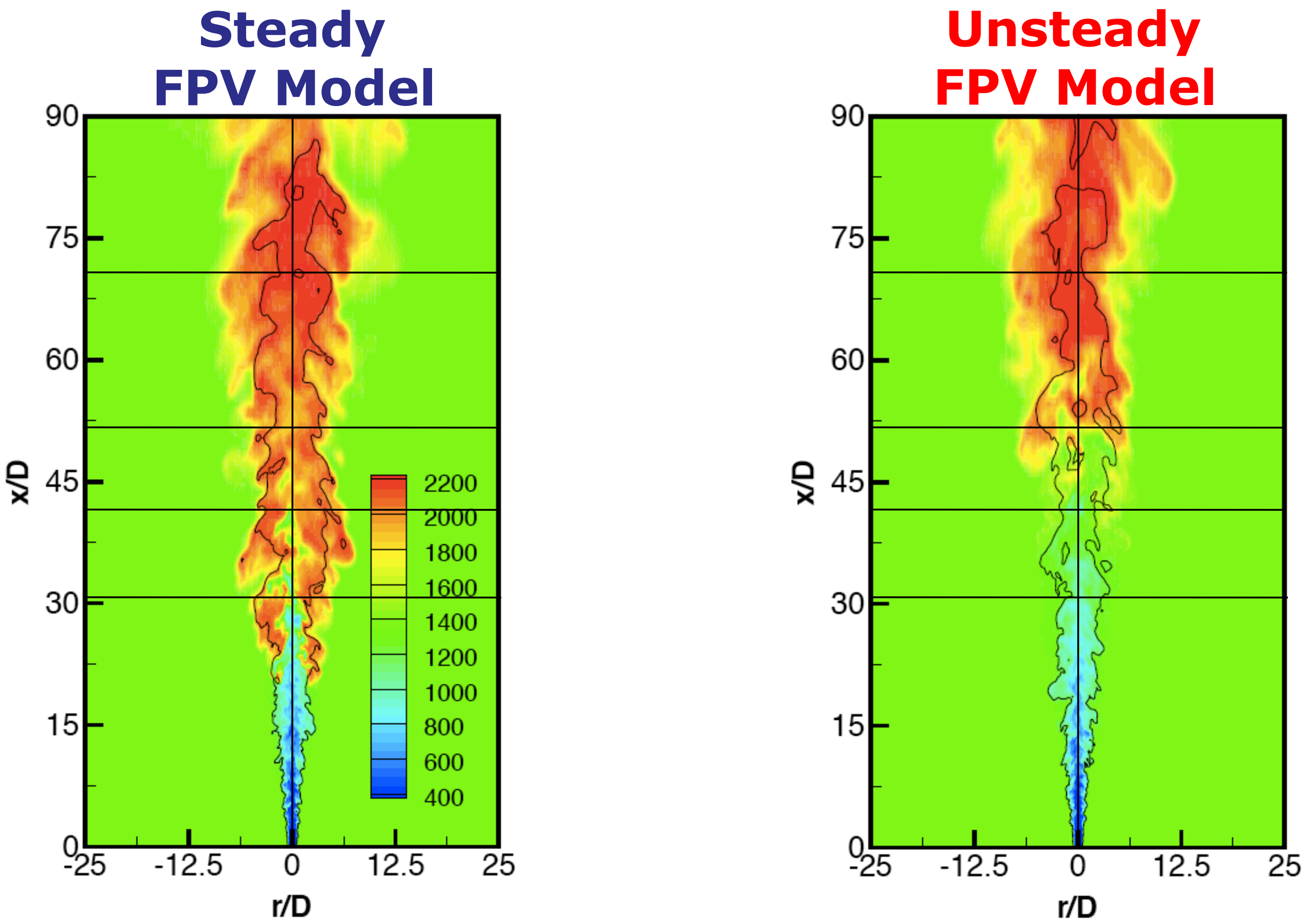


Unsteady FPV Model



Autoignition in Turbulent Flames

- Instantaneous temperature field

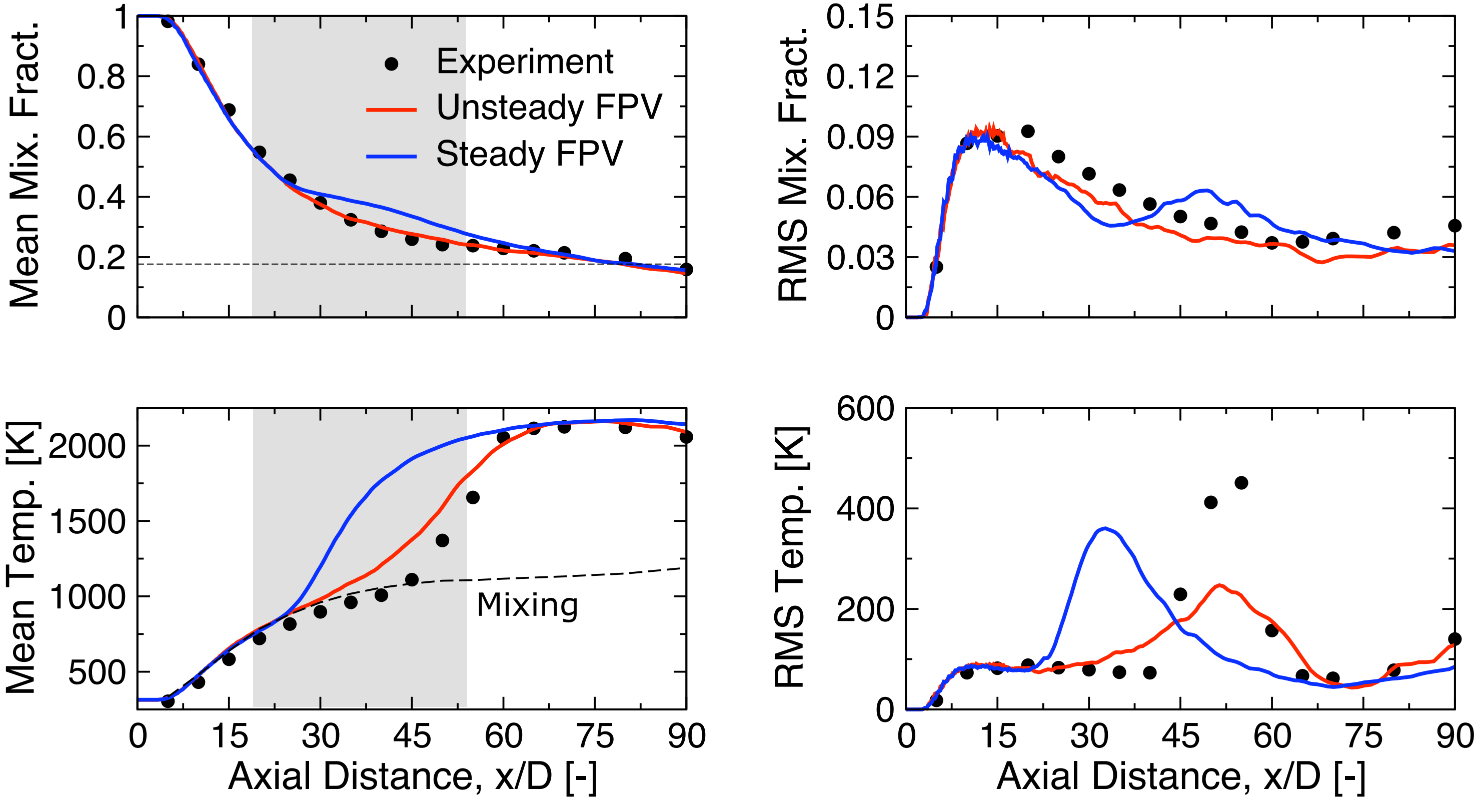


Steady FPV Model

Unsteady FPV Model

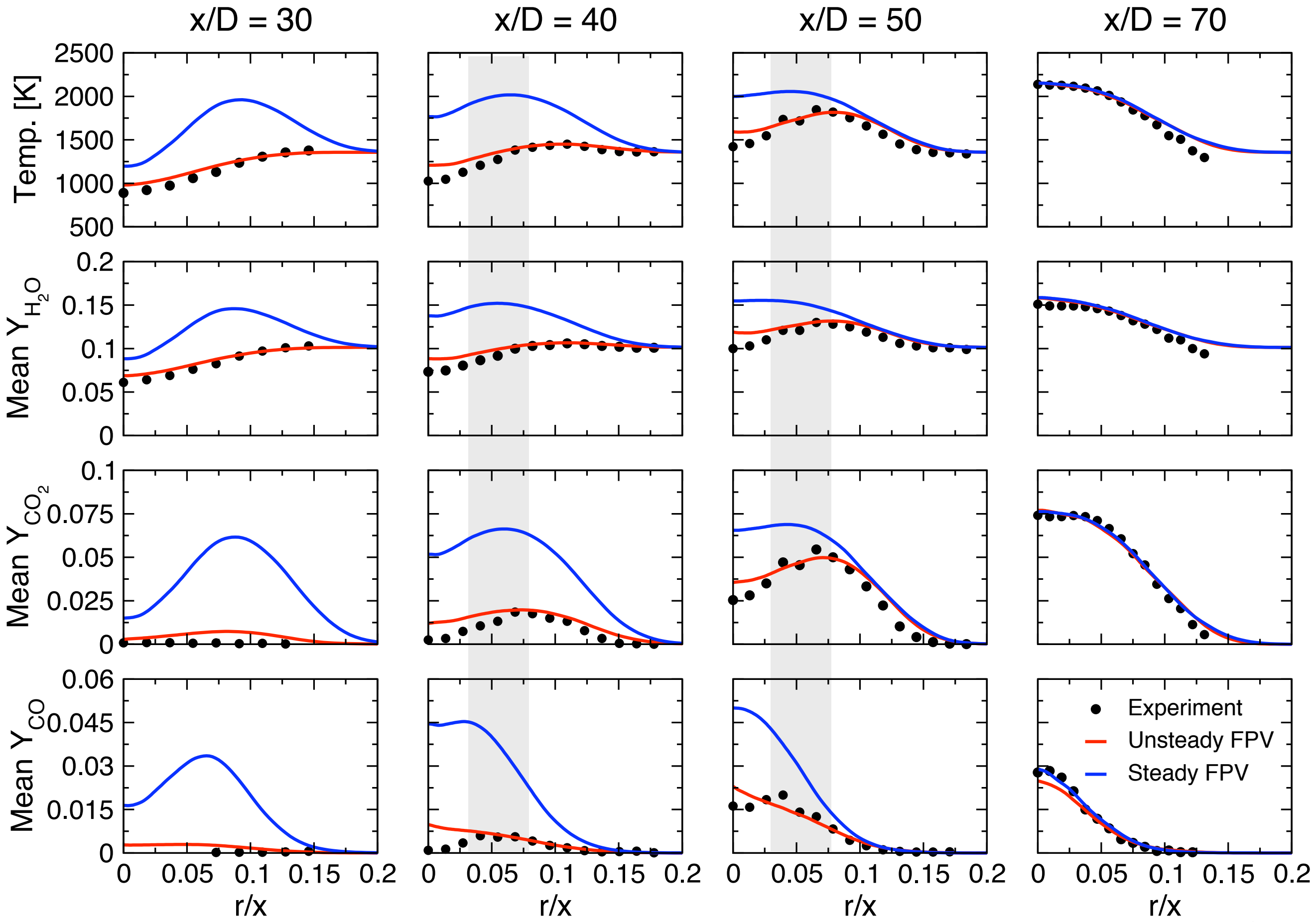
Autoignition in Turbulent Flames

- Centerline profiles



Autoignition in Turbulent Flames

- Radial profiles



Nozzle down-stream direction

Summary and Conclusions

- LES-modeling of lifted vitiated flames

- Key modeling components
  - Transient flame evolution
  - Accurate description of turbulent mixing and scalar dissipation rate

- Combustion-physical insights
  - Transient flame evolution
  - Identified significance of flame/turbulence interaction

→ Homogeneous reactor-model under-predicts ignition onset

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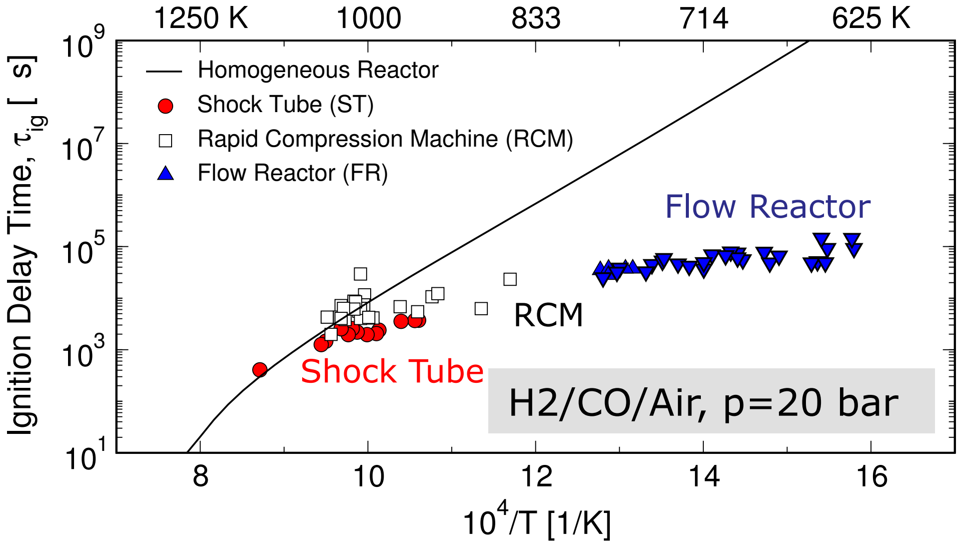
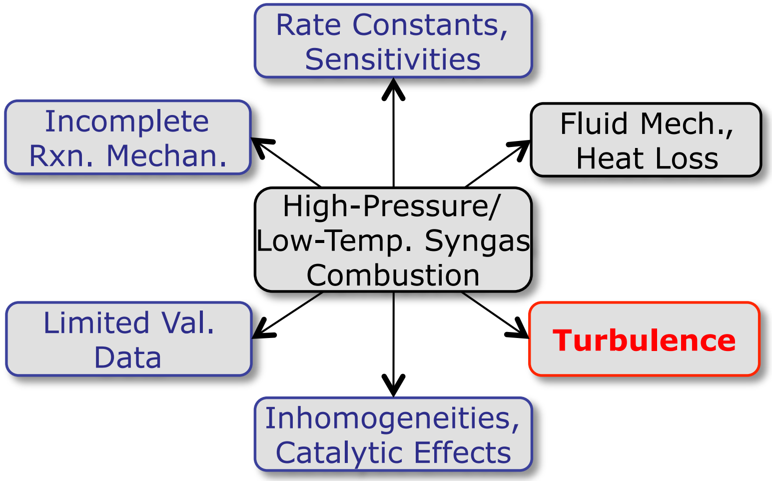
Turbulent Inhomogeneities and Facility Effects

- Question: Can we apply “lessons-learned” from LES simulations to characterize experimental facilities?
  - Shock-tubes
  - Flow-reactors
  - Rapid compression machines

- Source of non-idealities in experimental facilities[1,2,3]





High-Pressure/ Low-Temp. Syngas Combustion

Rate Constants, Sensitivities

Incomplete Rxn. Mechan.

Fluid Mech., Heat Loss

Limited Val. Data

Turbulence

Inhomogeneities, Catalytic Effects

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1 Petersen et al., Comb. & Flame, 149, 244 (2007); 2 Chaos & Dryer, Combust. Sci. and Tech., 180, 1053 (2008); 3 Burke, Chaos, Dryer, & Ju, Comb. & Flame, 157, 618 (2010)

Turbulent Inhomogeneities and Facility Effects

- Research Objectives
  - Use high-fidelity simulation and non-equilibrium formulation to isolate parametric contributions of non-idealities in experimental facilities

  - Research emphasis
    - Identify parametric sensitivities
    - Reconcile observed differences between experiments and detailed model-formulations

  - Facilities
    - Shock-tube
    - Flow-reactor
    - Rapid compression machine

Turbulent Inhomogeneities and Facility Effects

Shock-Tube

- Non-ideal processes in shock-tubes

1. Non-ideal rapture of diaphragm[#]

  - Finite opening time of diaphragm
  - Contribution to shock attenuation: 30%

2. Boundary layer growth[$]

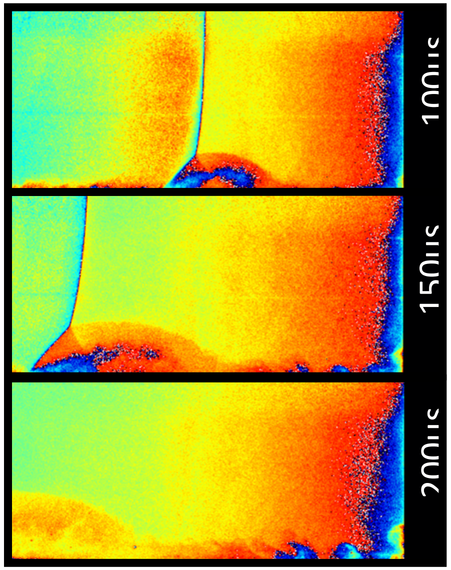
  - Formation of viscous boundary layer behind initial shock

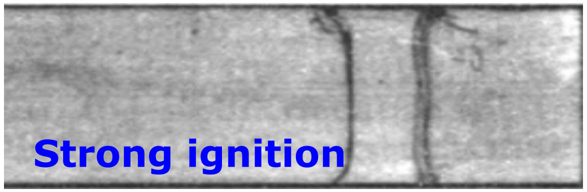
3. Shock reflection and bifurcation[%]

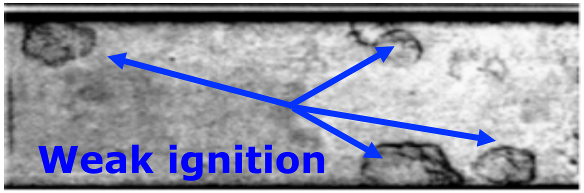
  - Lift-off of boundary layer resulting in formation of separation region

4. Inhomogeneous ignition and weak-to-strong ignition transition[$]

  - Ignition proceeds as multi-dimensional heterogeneous process







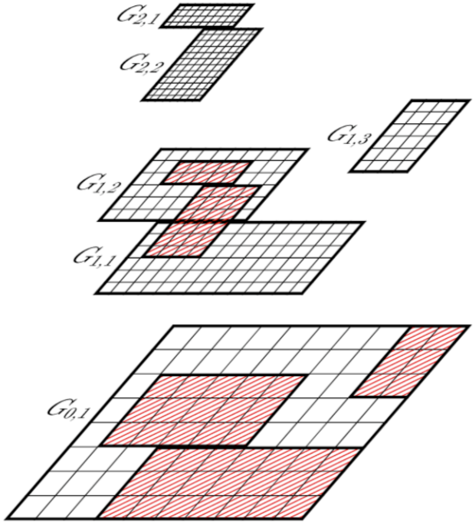
Petersen, E. L. & Hanson, R., Shock Waves, 10 (2001); $ Mirels, H., NACA-TN 3278 (1956); Mirels, H., NACA-TN 3401 (1955); %Yoo, Mitchell, Davidson, Hanson, Shock Waves, 21, 2011

Turbulent Inhomogeneities and Facility Effects

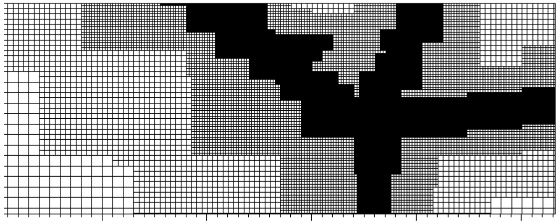
Shock-Tube

- Modeling challenges in simulating shock-tubes
  - Disparity of spatial and temporal scales

$$\underbrace{\frac{1}{150\,\mathrm{Re}_\tau^{2/7}}}_{\boxed{\text{Geometric shock-tube domain}}} L \sim \frac{1}{\mathrm{Re}_\tau}\delta \sim \delta_v \sim \underbrace{\frac{\mathrm{Re}_\tau\,\mathrm{M}}{\mathrm{M_t}}}_{\boxed{\text{Shock Thickness}}}\xi$$



- Solution method: Adaptive mesh refinement
  - AMR exploits multiscale nature of hydro-dynamic problem by locally adjusting computational effort to maintain uniform level of accuracy$^{\#,\$}$



\# Deiterding, R., Computers & Structures, 87, 769, 2009; \$ Berger, M. & Colella, P., JPC, 1982 (1988); % C. Pantano, et al. JCP, 221 (1) (2006) 63–87.

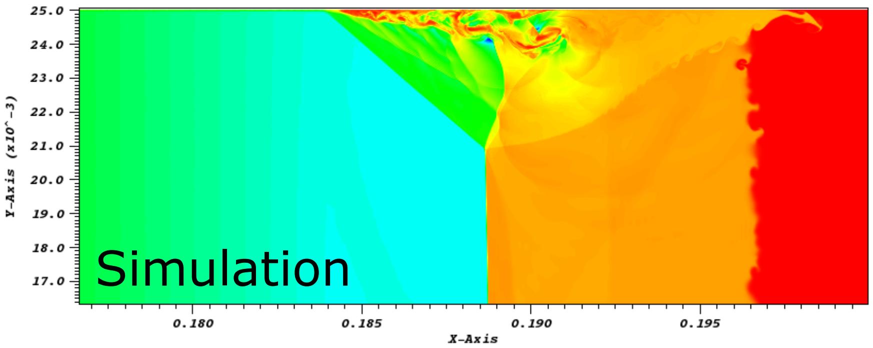
Turbulent Inhomogeneities and Facility Effects

Shock-Tube

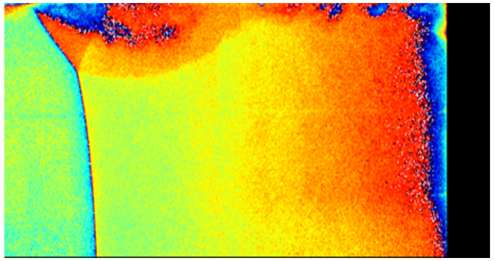
- Shock-bifurcation
  - Simulation of Ar-diluted H_2/O_2 mixture at 5 and 10 bar pressure

    →Relevant condition for weak and strong ignition regime

    →Adiabatic and isothermal wall conditions
  - Shock tube setup
    - Length: 1m
    - Diameter: 5 cm
    - Helium in driver section
  - Target condition:
    - T_5=1100 K, p_5=10 bar
  - Chemical mechanism:
    - Burke et al.[1] (2011)



Experiment[2]



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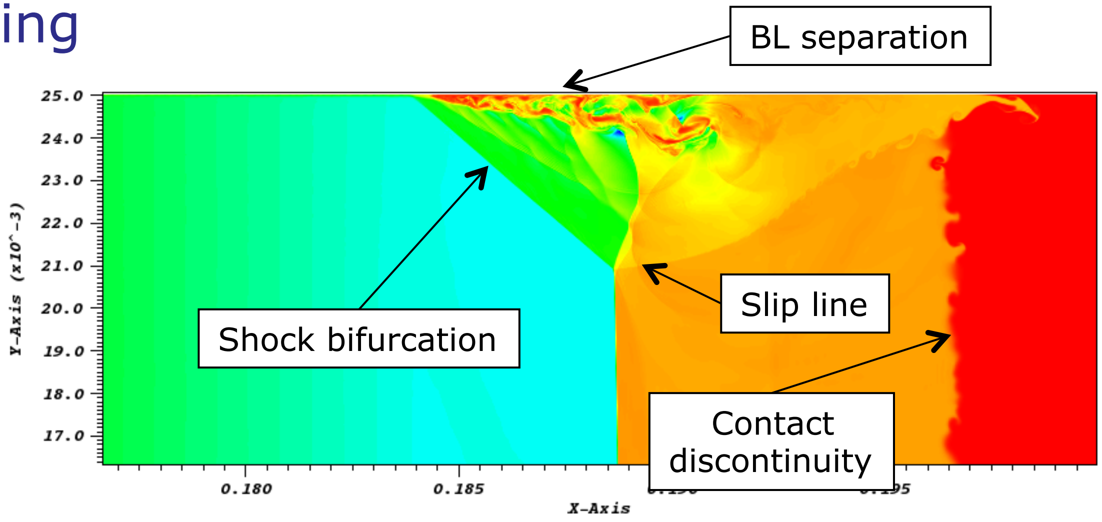
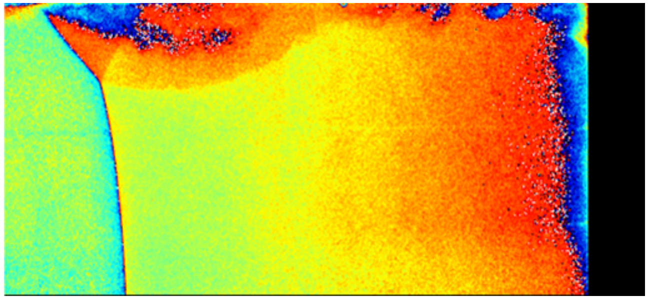
1 Burke, Chaos, Ju, Dryer, Klippenstein, IJCK, 44, 2011

2 Yoo, Mitchell, Davidson, Hanson, Shock Waves, 21, 2011

Results: Shock Bifurcation

- Shock-bifurcation
  - Instantaneous temperature evolution shows rich flow-field structure: Boundary layer separation, Shock-bifurcation, Boundary heating





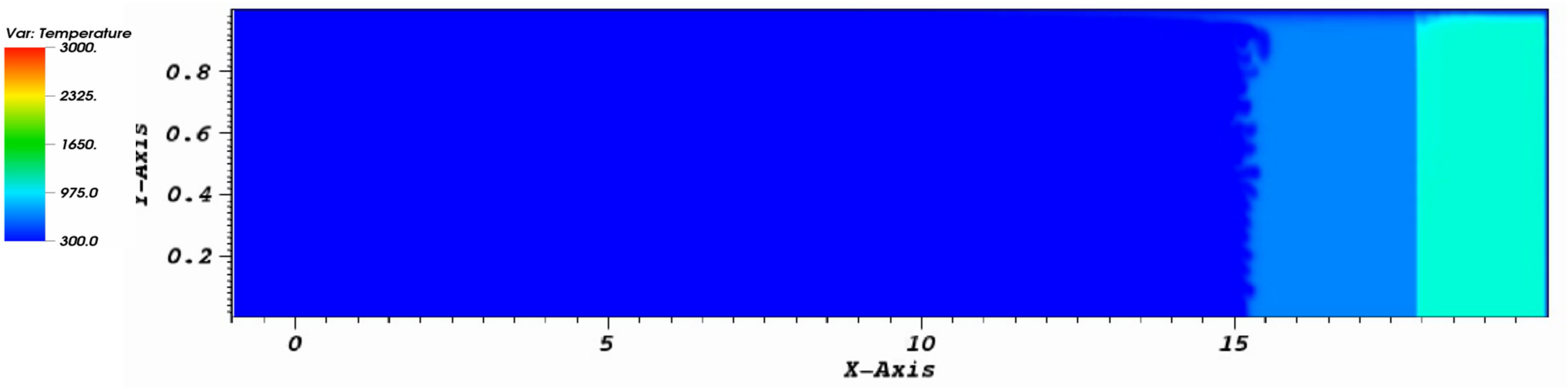
Toluene PLIF Measurements#

Yoo, Mitchell, Davidson, Hanson, Shock Waves, 21, 2011

Turbulent Inhomogeneities and Facility Effects

Shock-Tube

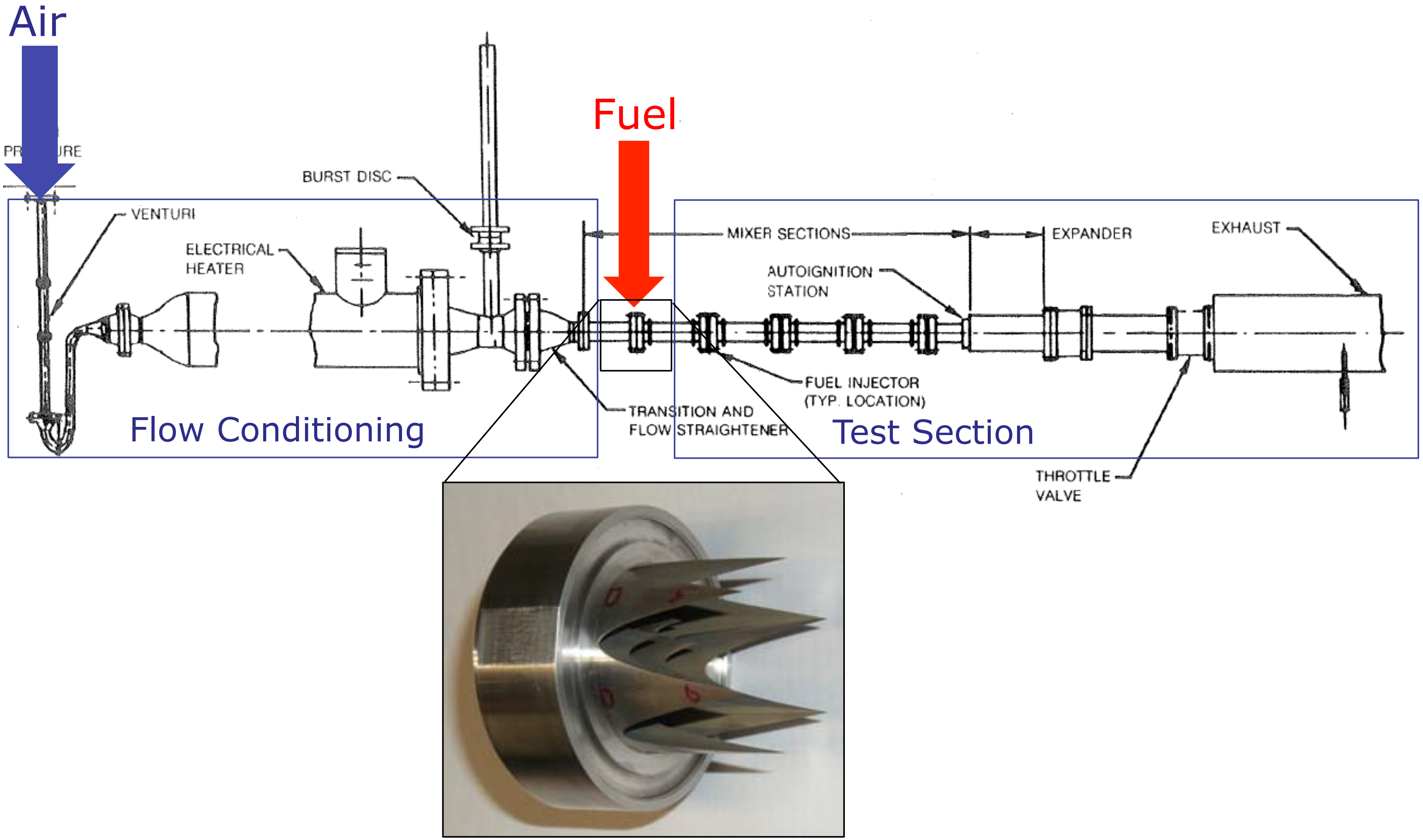
- Ignition
  - Isothermal wall



  - Observations:
    - Ignition is initiated at end-wall
    - Flame propagation towards unburned mixture (region of favorable pressure gradient)
→ non-homogeneous ignition

Turbulent Inhomogeneities and Facility Effects

Flow-Reactors



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

Turbulent Inhomogeneities and Facility Effects

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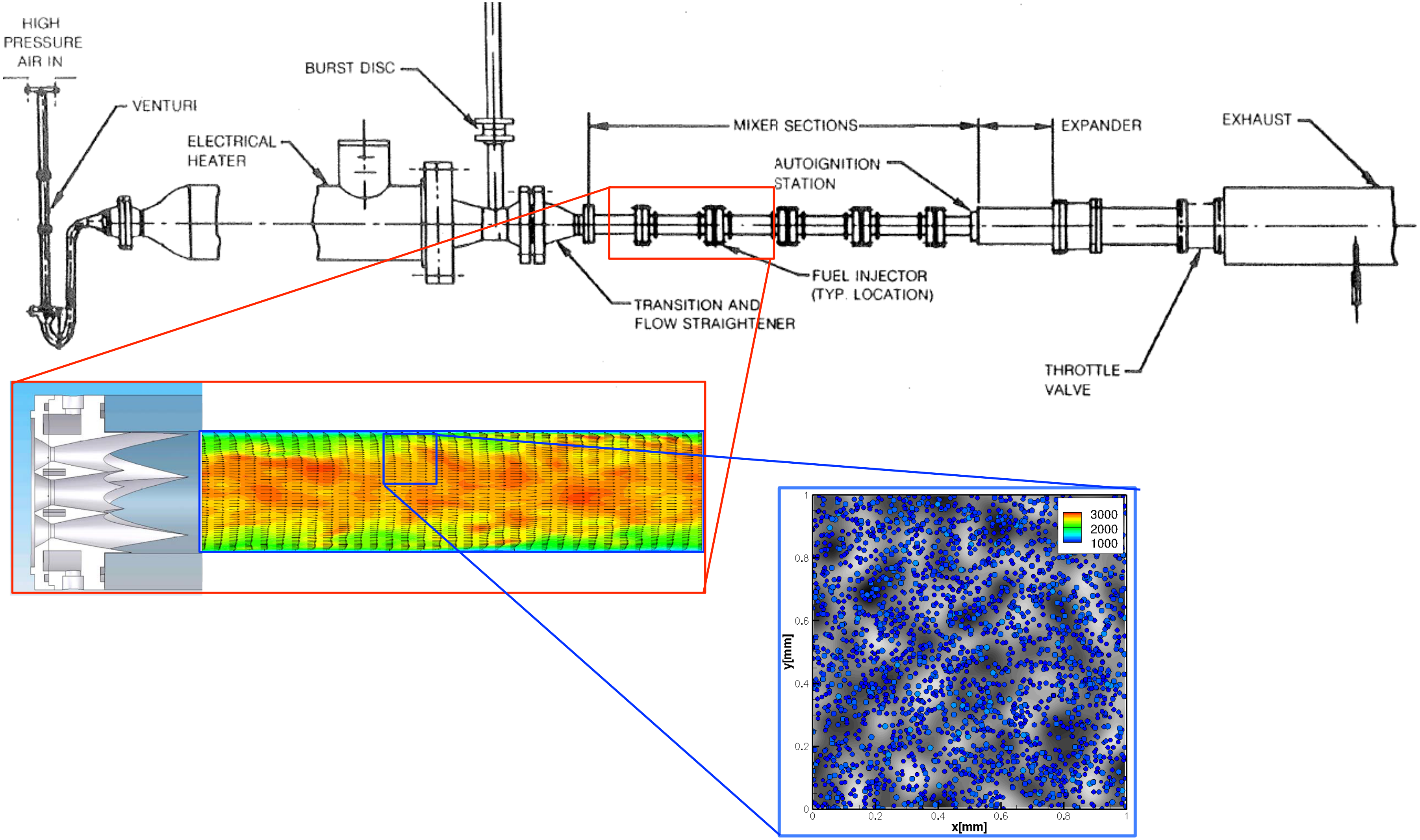

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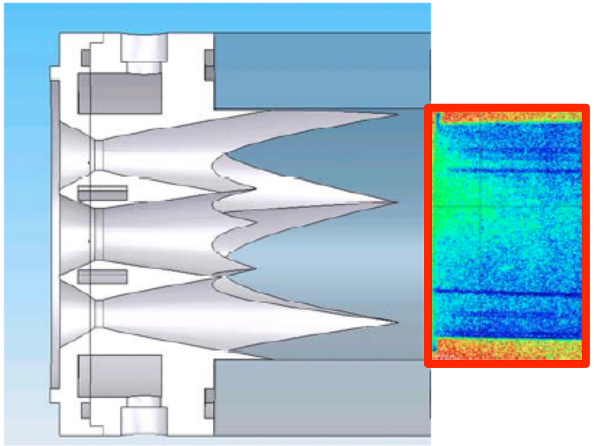
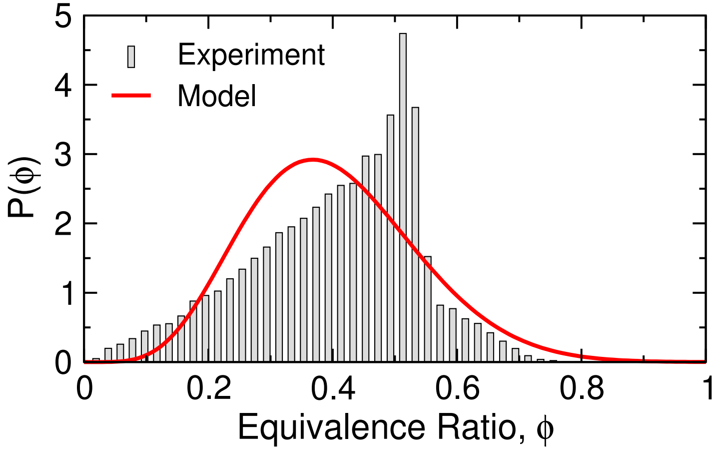
Turbulent Inhomogeneities and Facility Effects

Flow-Reactors

- 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 $Re = 10^4$





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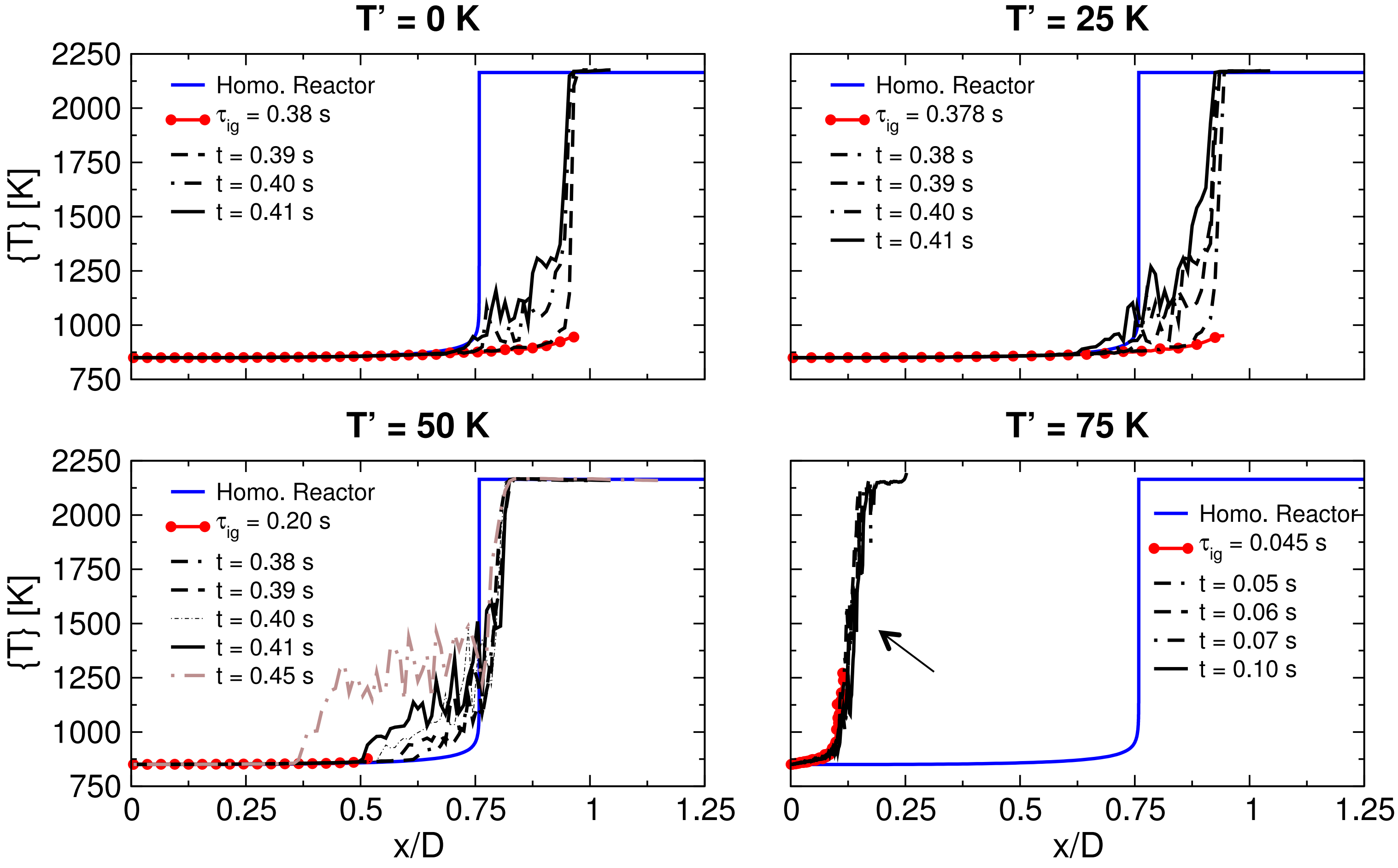
1 Santoro (2009)

2 Samuelsen et al. (2003)

Turbulent Inhomogeneities and Facility Effects

Flow-Reactors

- Mixture variation: ϕ=0.4; ϕ’=0.135
- Temperature variation: T=850 K; T′ = {0, 25, 50, 75} K



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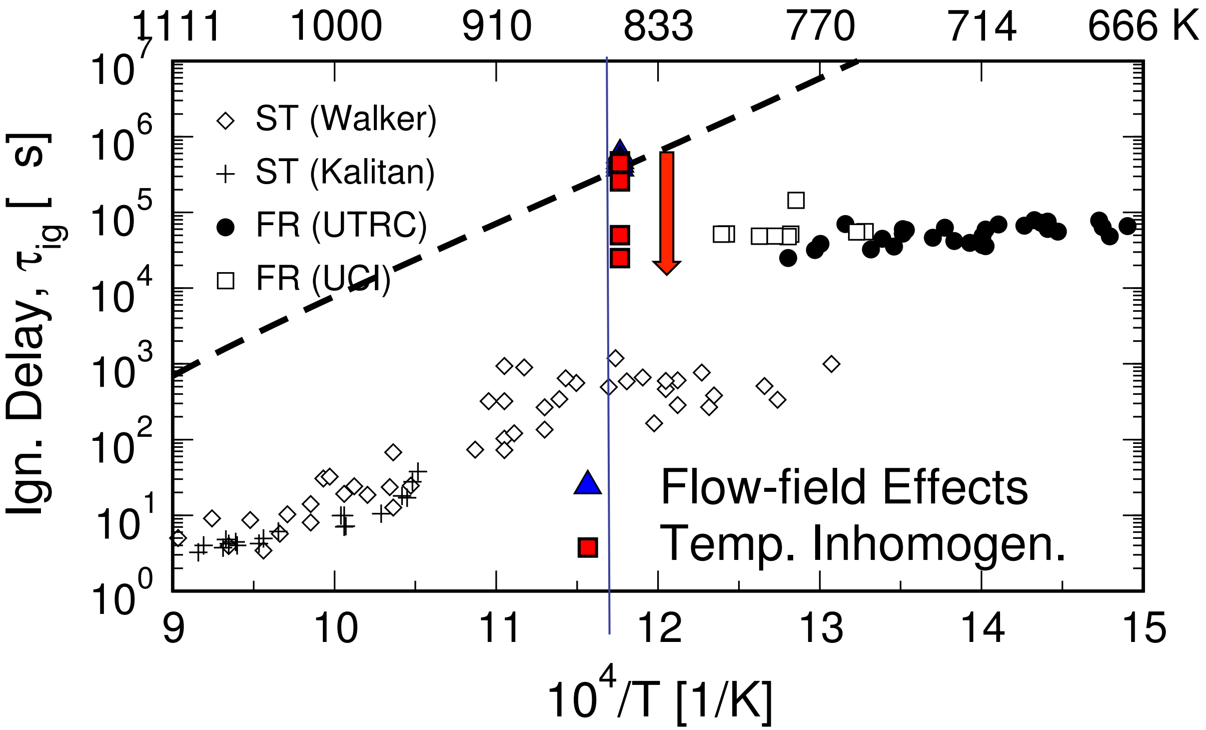

Summary and Conclusions

- Turbulence/chemistry coupling processes
  - Increased relevance for low-Damkoehler/high-Karlovitz combustion processes: oxygen-diluted comb.; autoignition; preheat-comb.
  - Turbulence promotes mixing, exchange of radicals and enthalpy
  - Ignition occurs at preferred sites: “most-reactive” mixture and regions of low strain

- Validated high-fidelity LES combustion models have been developed and are available to accurately capture ignition processes
  - Models rely on experimental data

- Simulations can assist and complement experimental investigations
  - Identify experimental sensitivities
  - Guide potential modifications to mitigate facility effects
  - Reconcile discrepancies btw. experiments and theory
  - Example: Turbulence/chemistry coupling in shock-tubes and flow-reactors