Modeling Flashback Propensity using LES and Experiments

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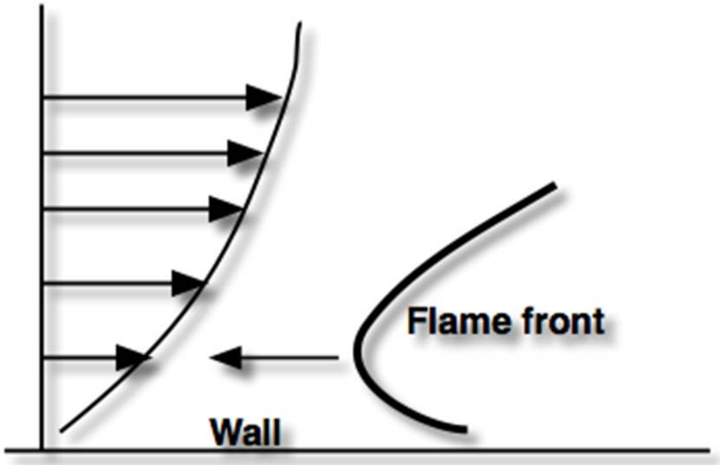
Boundary Layer Flashback

- Many different flashback modes possible
- Hydrogen-based combustion dominated by boundary layer flashback
- Flow near wall is slower than flame speed
  - ➡ Flame propagates upstream
  - ➡ Only wall quenching arrests flame
- Unique physics affects modeling
  - ➡ Turbulent boundary layer affecting flame physics



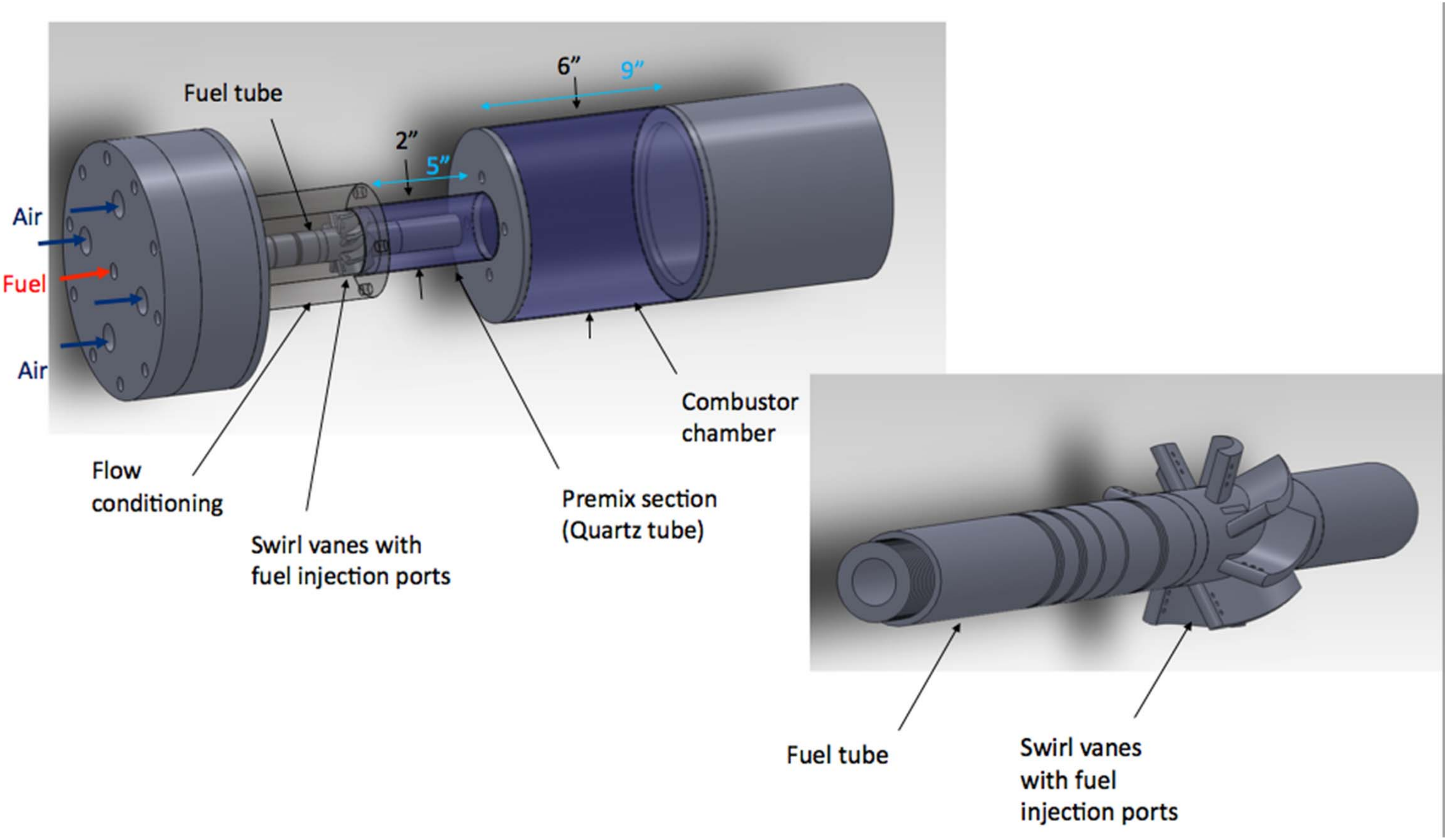
Understanding Flashback Fundamentals

- Previous project
  - ➡ Flashback in swirling flow
  - ➡ Looked at macrsoscopic effects and flow physics
  - ➡ LES modeling based on existing technology
- Current project
  - ➡ Oct. 2013-2016
  - ➡ High pressure effects on flame propagation
  - ➡ Fundamental aspects of LES modeling
    - Flame-wall interactions
  - ➡ Predicting probabilities instead of average flashback

Experimental Program

UT Swirl Burner

- UT high-pressure swirl combustor



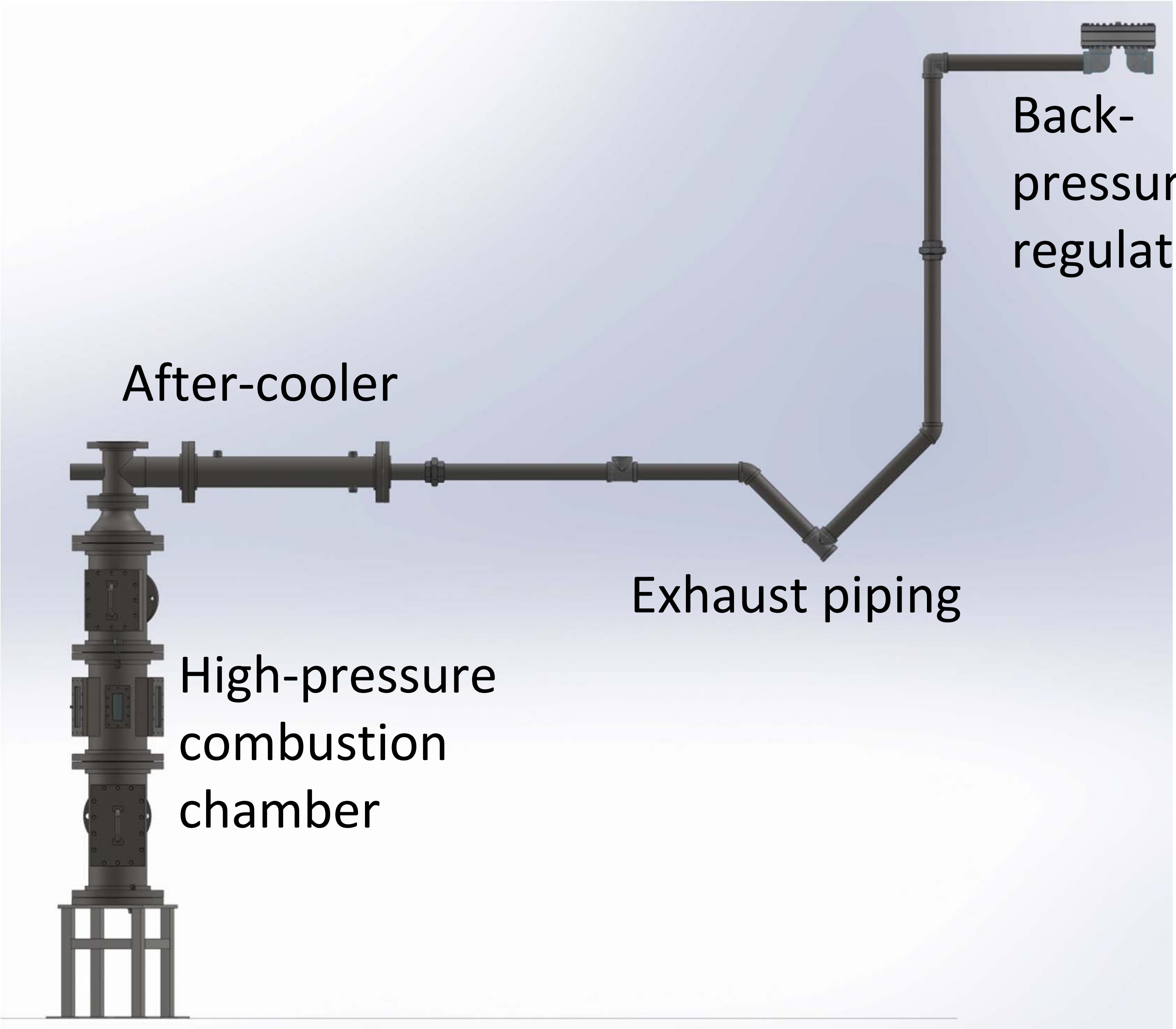
Flashback and Mitigation Strategies

- Flashback at higher pressure
  - Effect of Reynolds number
- Stratification for flashback reduction
  - Fuel profiling
    - Different flow rates through different nozzle inlets
    - Less fuel near walls
      - Push inner boundary layer outside flammability limits
  - Prevent flame anchoring
    - Even with flashback, prevent flame from reaching inlet vanes

Experimental Program

- Two main accomplishments
  - ➡ Complete the High-Pressure Combustion Facility
  - ➡ Develop Radially-Stratified Burner for use at 1 atm and in high-pressure combustor
- High Pressure Combustion Facility
  - ➡ Modular Structure
  - ➡ Stainless Steel
  - ➡ Designed for pressures up to 15 atm
  - ➡ Allows mounting of various combustors
    - Flashback
    - Stratified flames

High-Pressure Combustion Facility



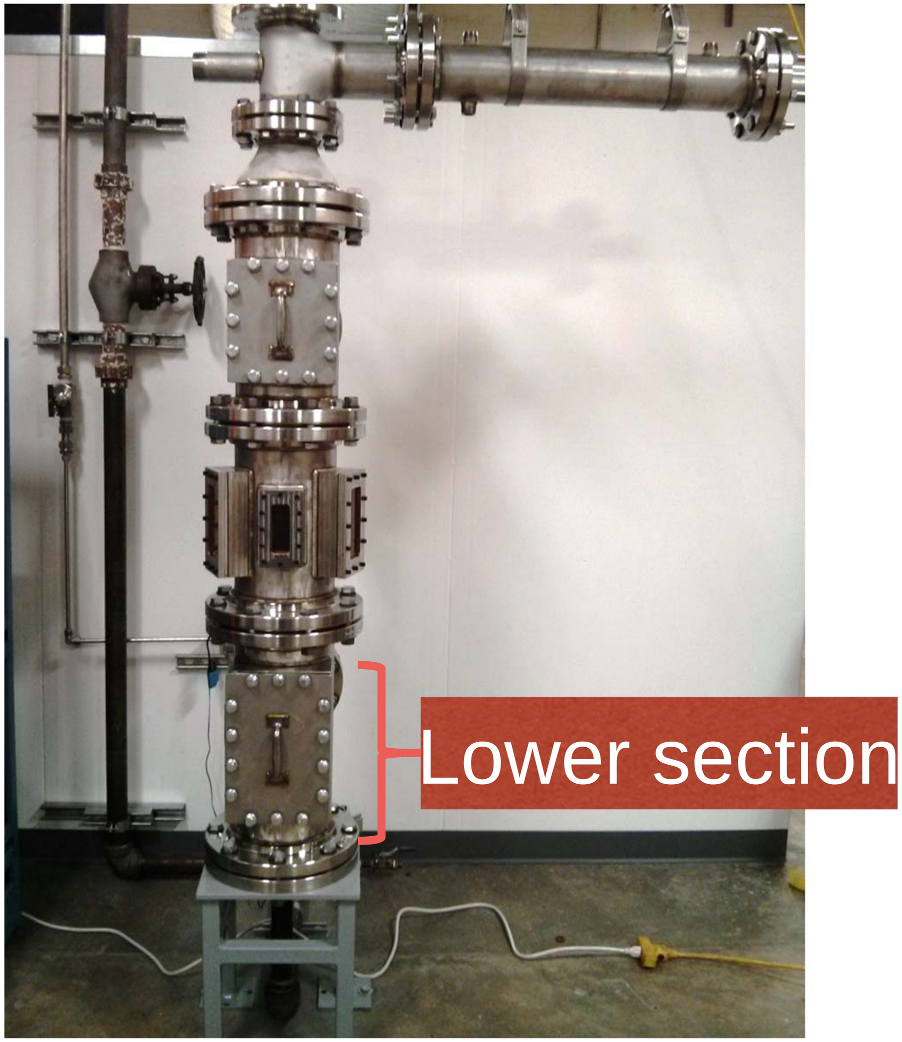
Back-pressure regulator

After-cooler

Exhaust piping

High-pressure combustion chamber

High-Pressure Combustion Facility

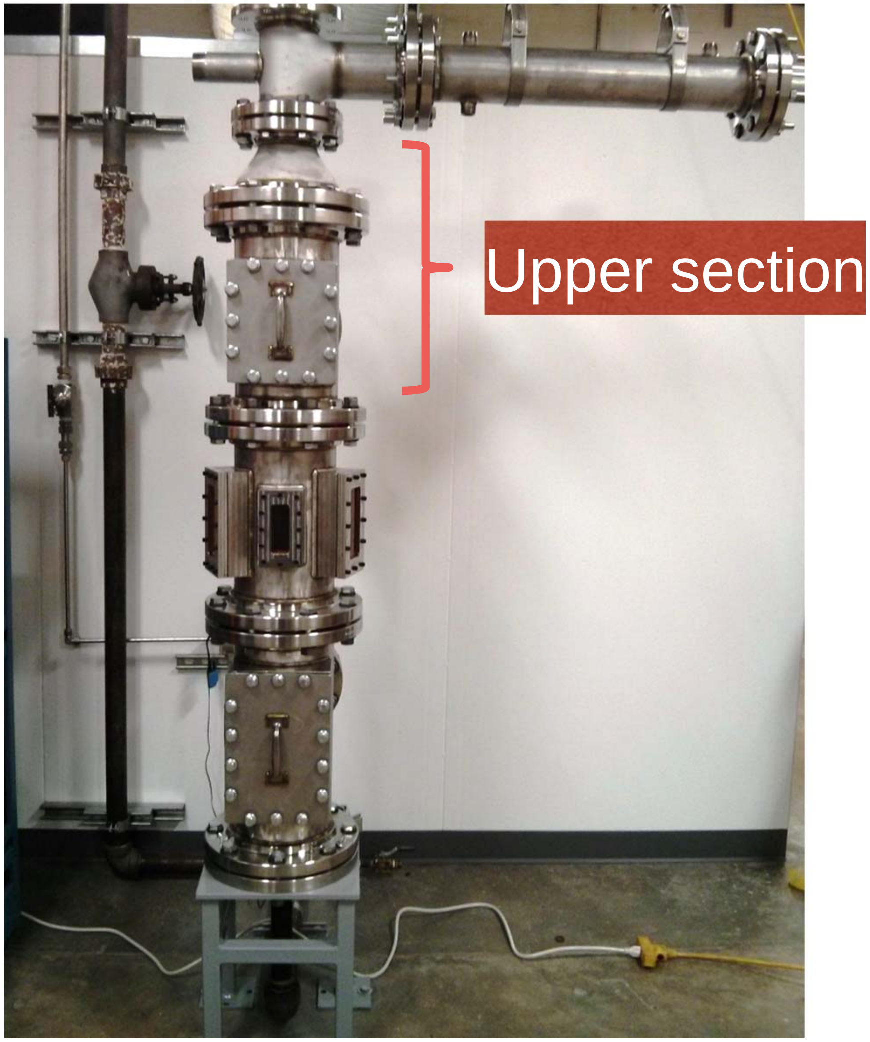


- Lower section
    - ➡ Access port for installation
    - ➡ Gas supply ports to the internal burner assembly

High-Pressure Combustion Facility

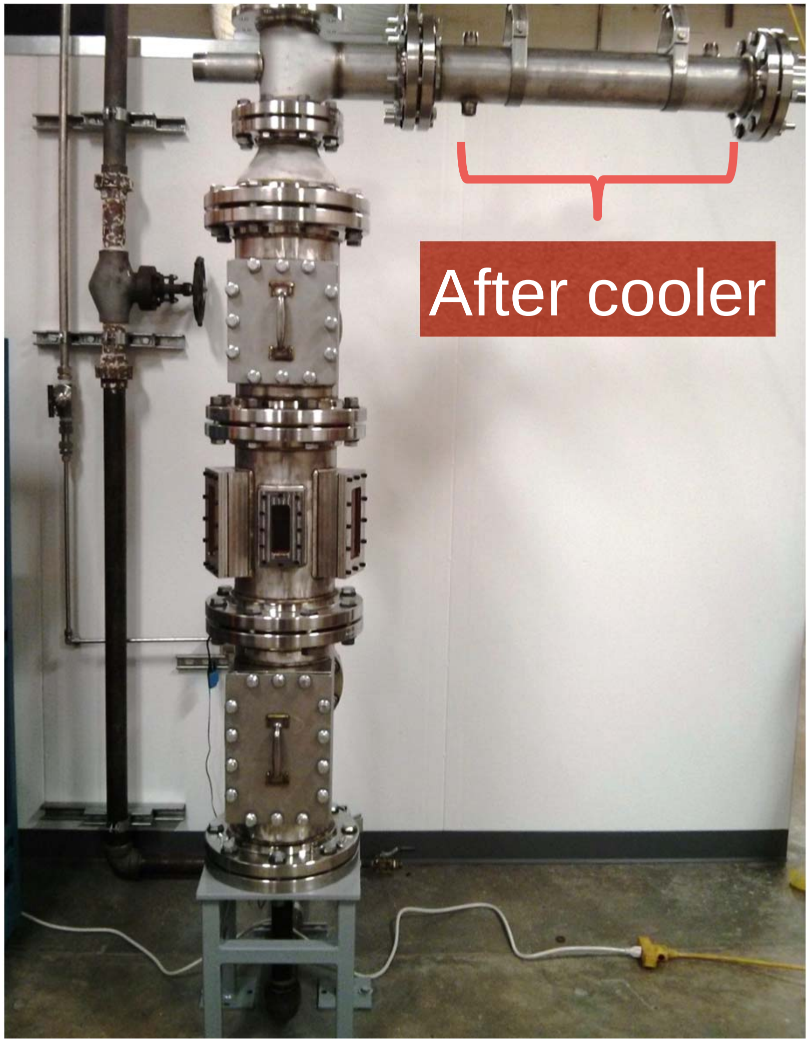
- Combustion Chamber
  - ➡ Contains three windows for laser diagnostics
  - ➡ High-speed stereo PIV
  - ➡ Chemi-luminescence
  - ➡ PLIF
- Uses shroud air-flow for cooling windows

High-Pressure Combustion Facility



- Upper Section
  - ➡ Access ports for installation and calibration

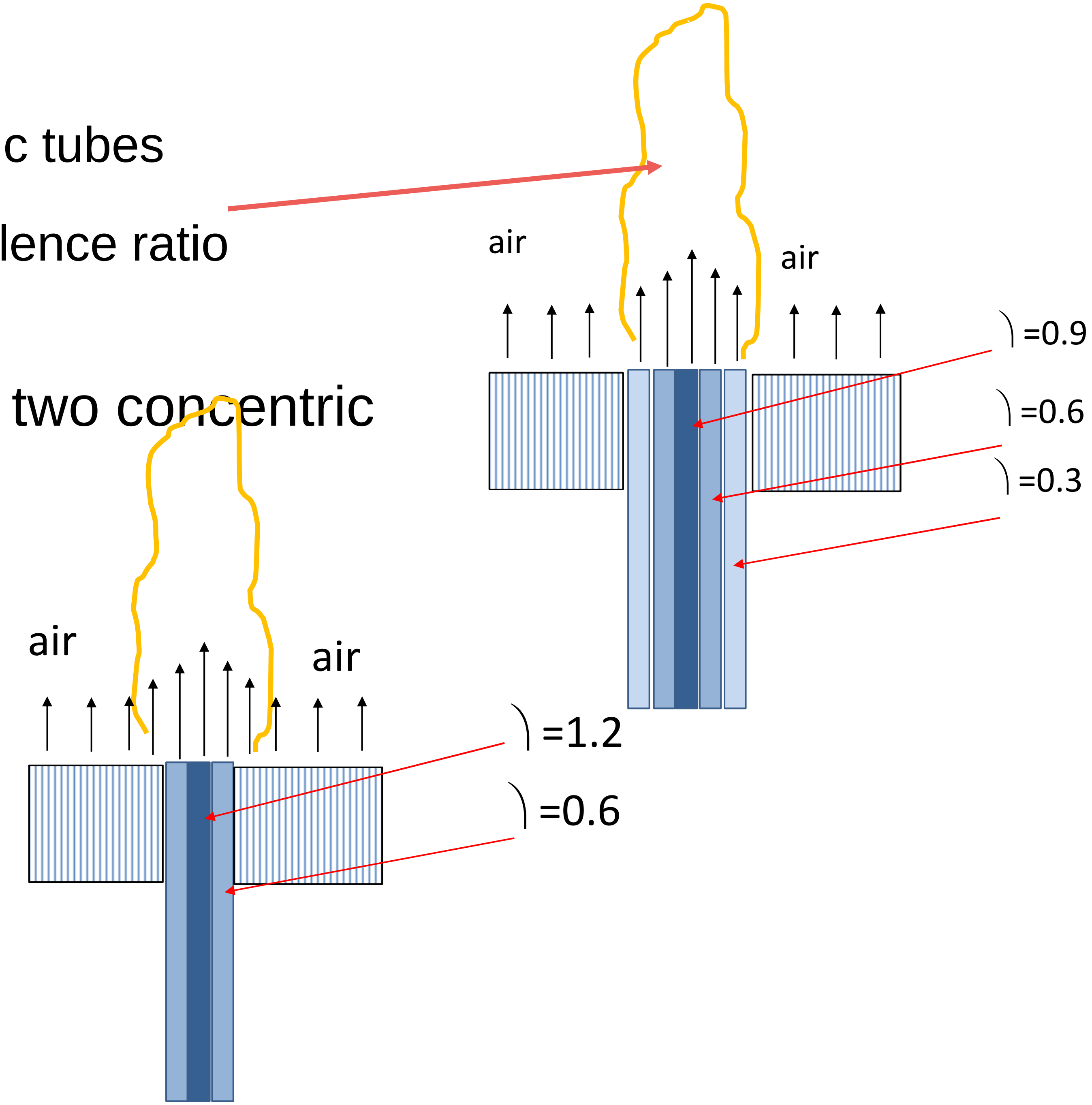
High-Pressure Combustion Facility



- After cooler
  - ➡ Shell and tube heat exchanger made using copper coils

Radially-stratified Flame Burner

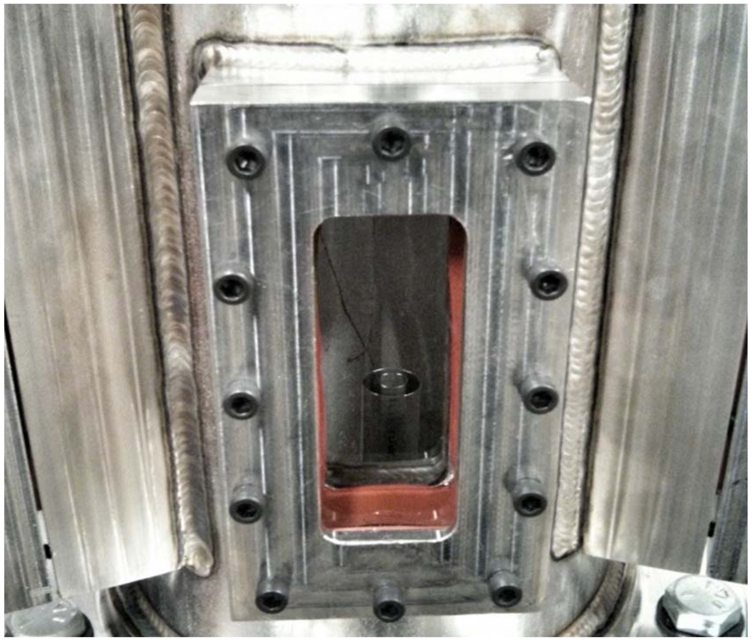
- Burner design
  - ➡ Multiple concentric tubes
    - Different equivalence ratio mixtures
- Initial design with two concentric tubes



Radially-stratified flame burner

- Two concentric nozzles of dia. 0.5” and 1”
- Long nozzles ensure fully developed flow
- Concentric tubes will be surrounded by a co-flow section (under construction)

Stratified burner



Stratified burner mounted in chamber

Stratified Burner

- Stratified burner currently undergoing testing for flame stability with CH4-air
- Rich mixtures in both nozzles is stable at high Reynolds numbers
- Lean outer flow and rich inner flow is lifted flame for Reynolds number > 3000
- Hydrogen addition should give wider stability limits

Methane-air stratified

Methane-air stratified flames at 1 atm

Inner nozzle only
Ø = 2.72, Re = 4776

Outer nozzle only
Ø = 2.12, Re = 3915

Both nozzles
Inner Ø = 4.08
Outer Ø = 1.9

Planned work

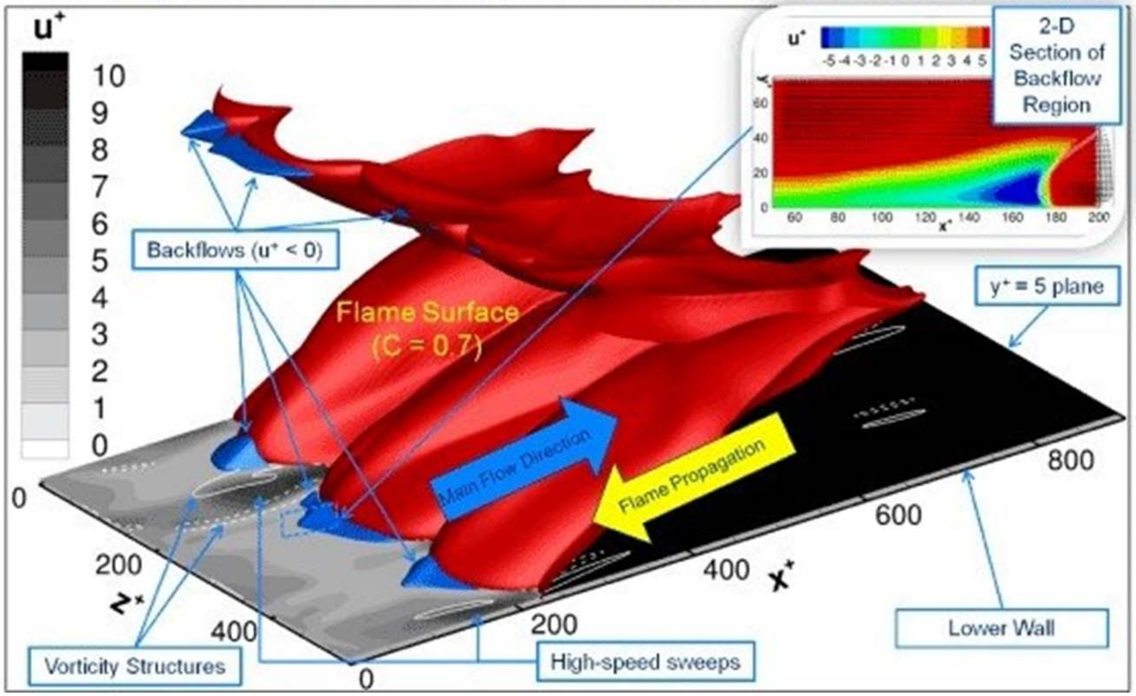
- Use $H_2/CH_4/N_2$/air pre-mixtures to widen stability limits
- Make extensive measurements at 1 atm
  - ➡ PIV
  - ➡ Temperature imaging (Rayleigh scattering using DLR fuel – $H_2/CH_4/N_2$)
  - ➡ OH/CH PLIF
- Make measurements at elevated-pressure conditions

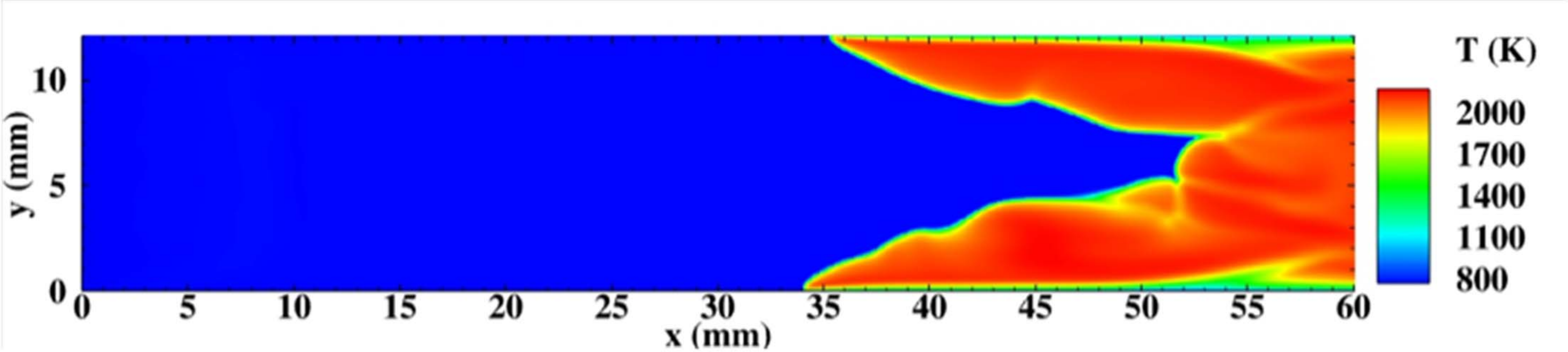
Methane-air stratified

LES Modeling of Flashback

LES Modeling of Flame Flashback

- Experimental data is not refined enough to test model hypotheses
  - ➡ Use of DNS data
  - ➡ Sandia National Lab.
    - Chen and co-workers


DNS of premixed H2-air flame flashback in turbulent channel

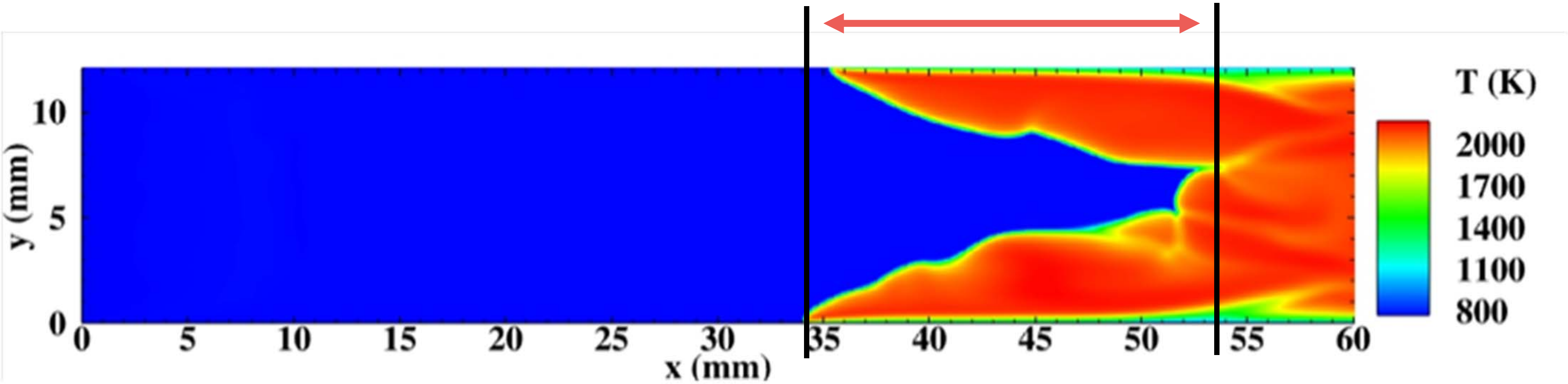


Modeling Approach

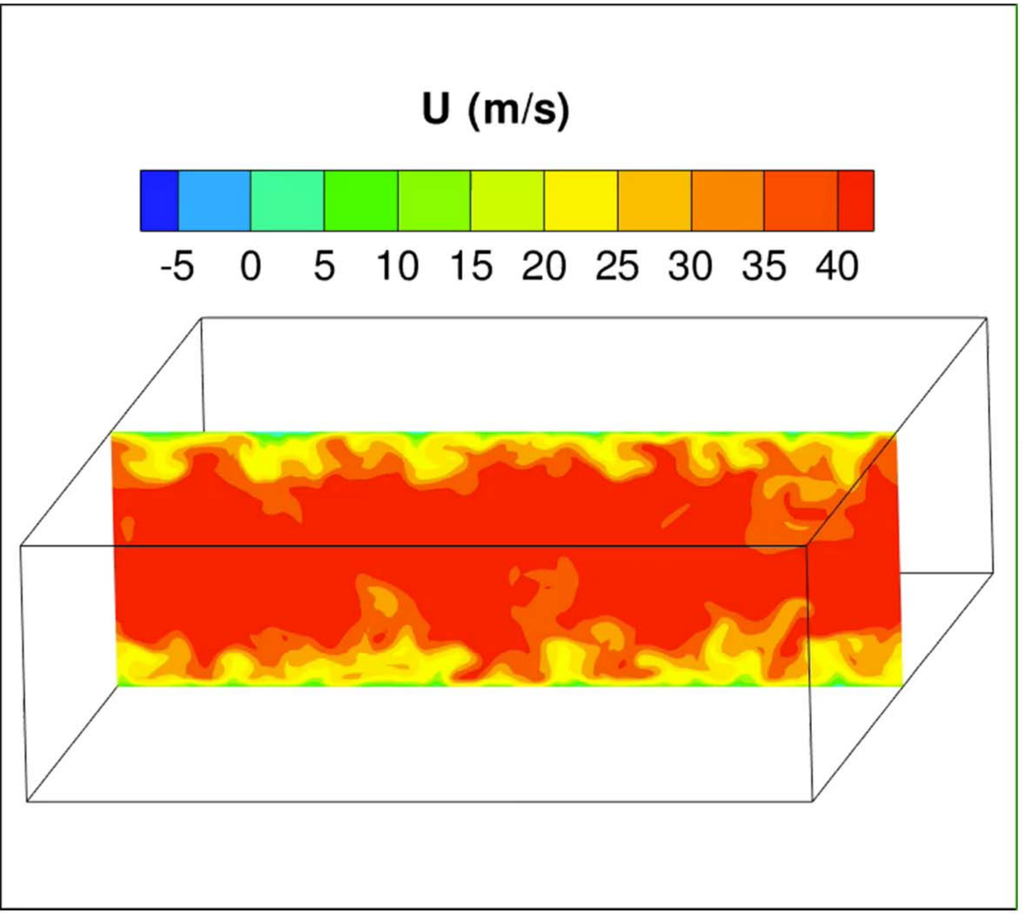
- Flame-front described using progress variable
  - ➡ Flame structure through flamelet model
    - This is strictly not necessary
  - ➡ Progress variable source term determined to predict the correct laminar flame speed
- Modeling issues
  - ➡ Near-wall heat loss effects
  - ➡ Small-scale flame wrinkling
  - ➡ Numerical solution of the progress variable equation

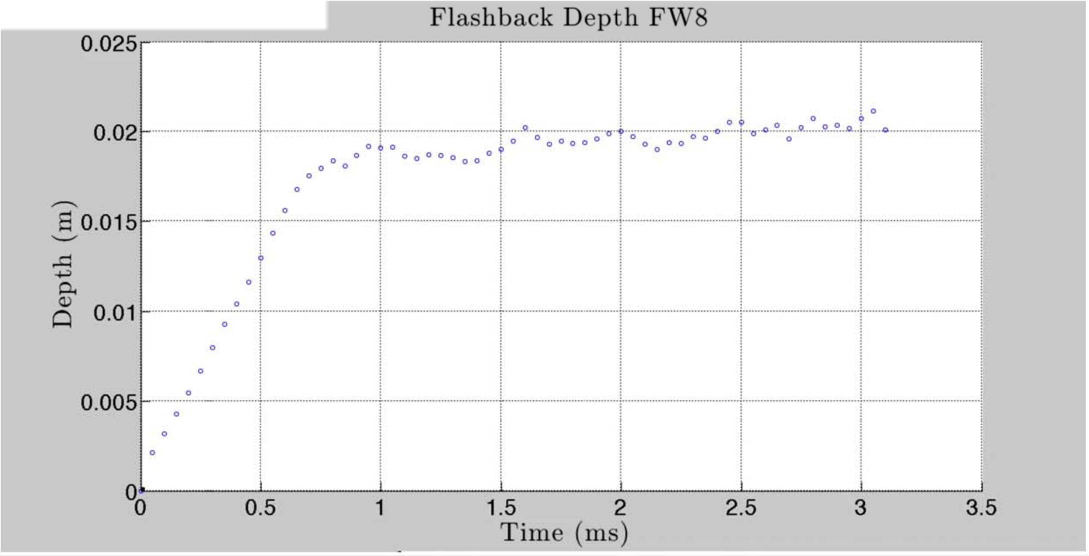
DNS Statistics

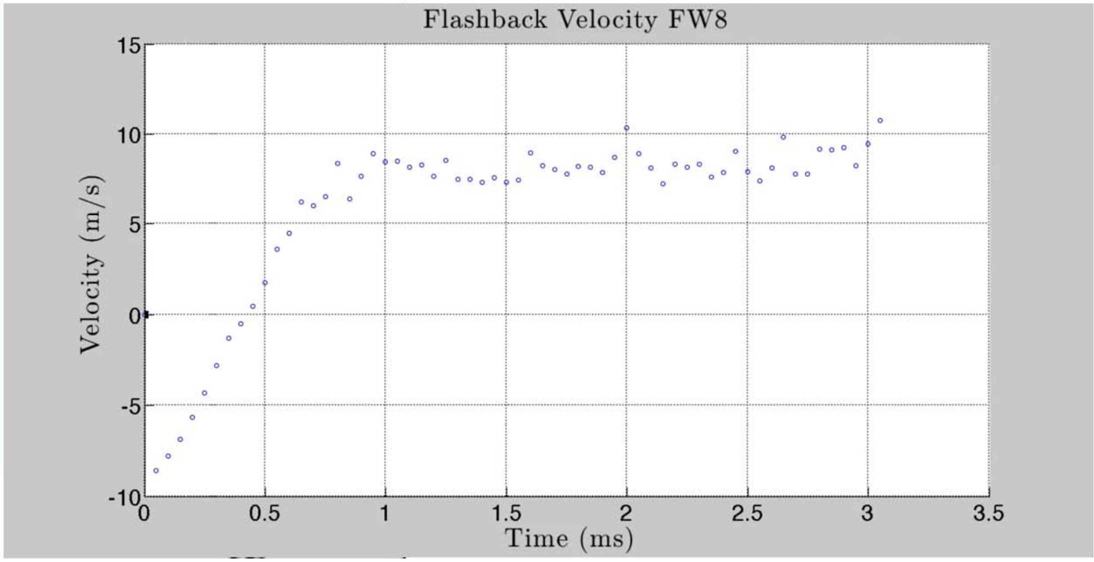
- DNS represents a single realization of flashback
  - ➡ No statistical information
- Derived statistical quantities
  - ➡ Flame depth
  - ➡ Spanwise averaged flame propagation velocity
    - Computed at leading edge



LES Statistics

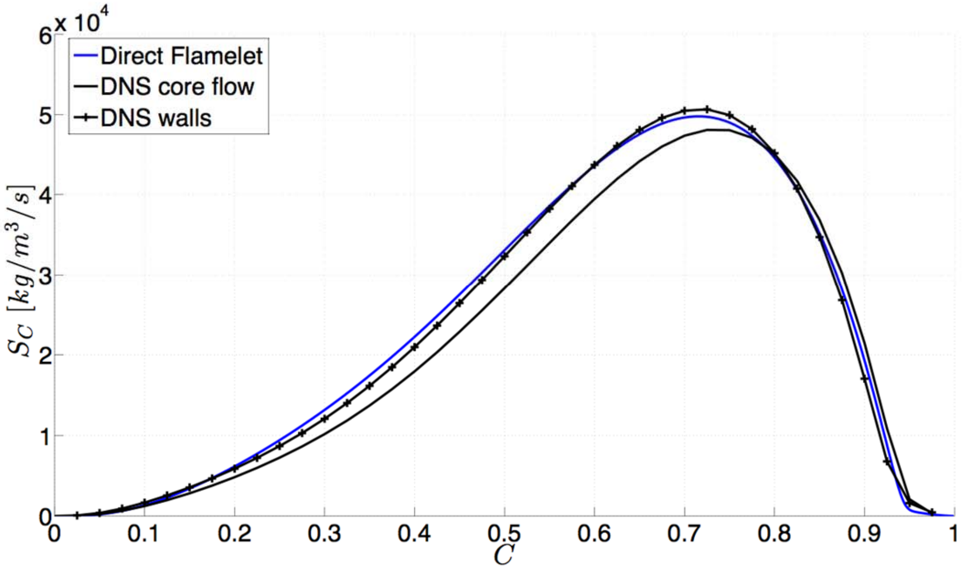


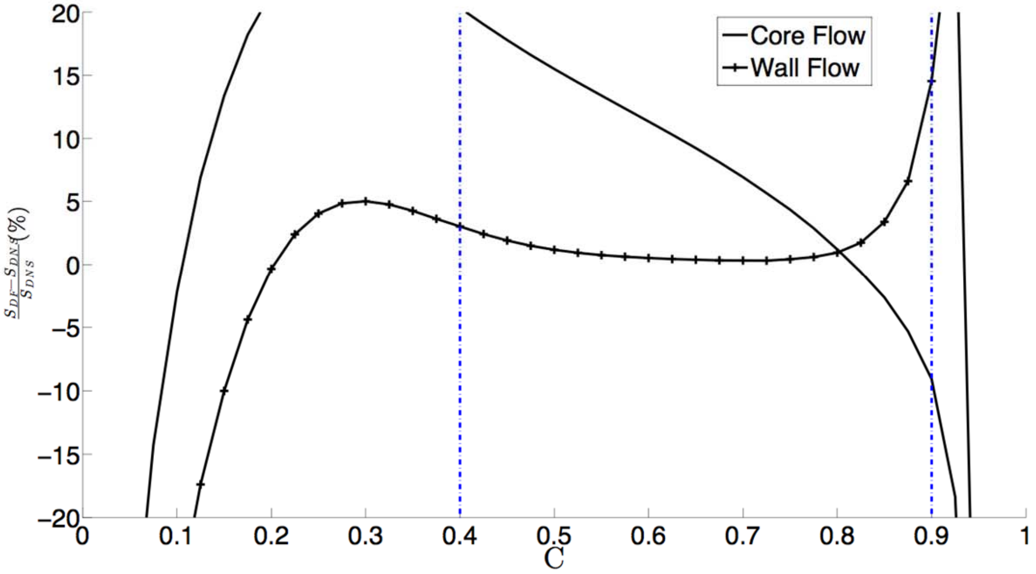




Flamelet Model Errors

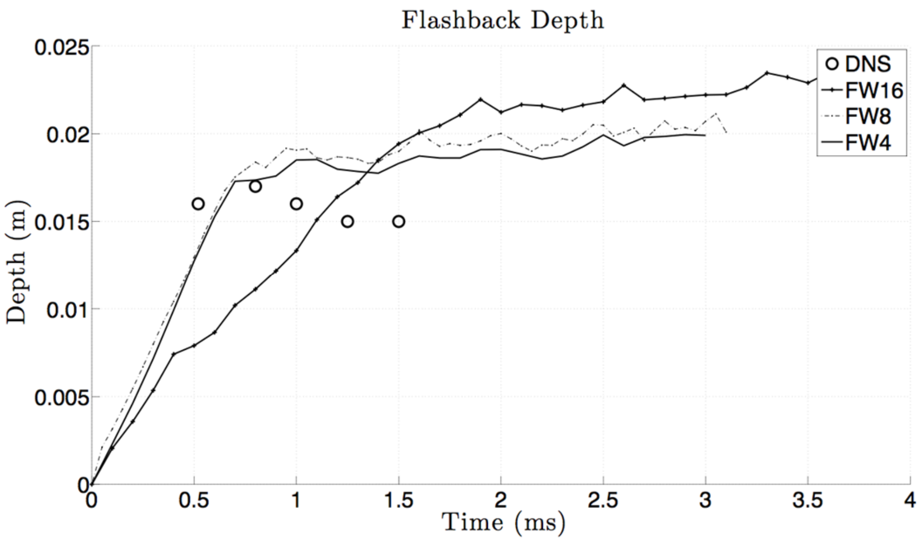
- Flamelet assumption used to obtain progress variable source term
  - ➡ Evaluated also from DNS data

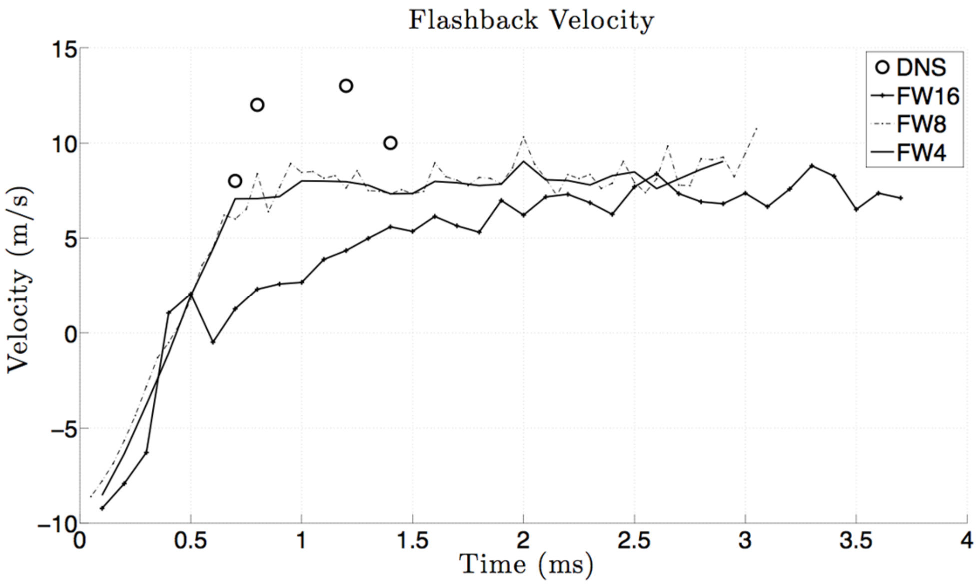




LES Results - Filter Width Effect

- LES conducted for different grid sizes
- Filtered flame model used
  - ➡ FTACLES approach of Fiorina and co-workers

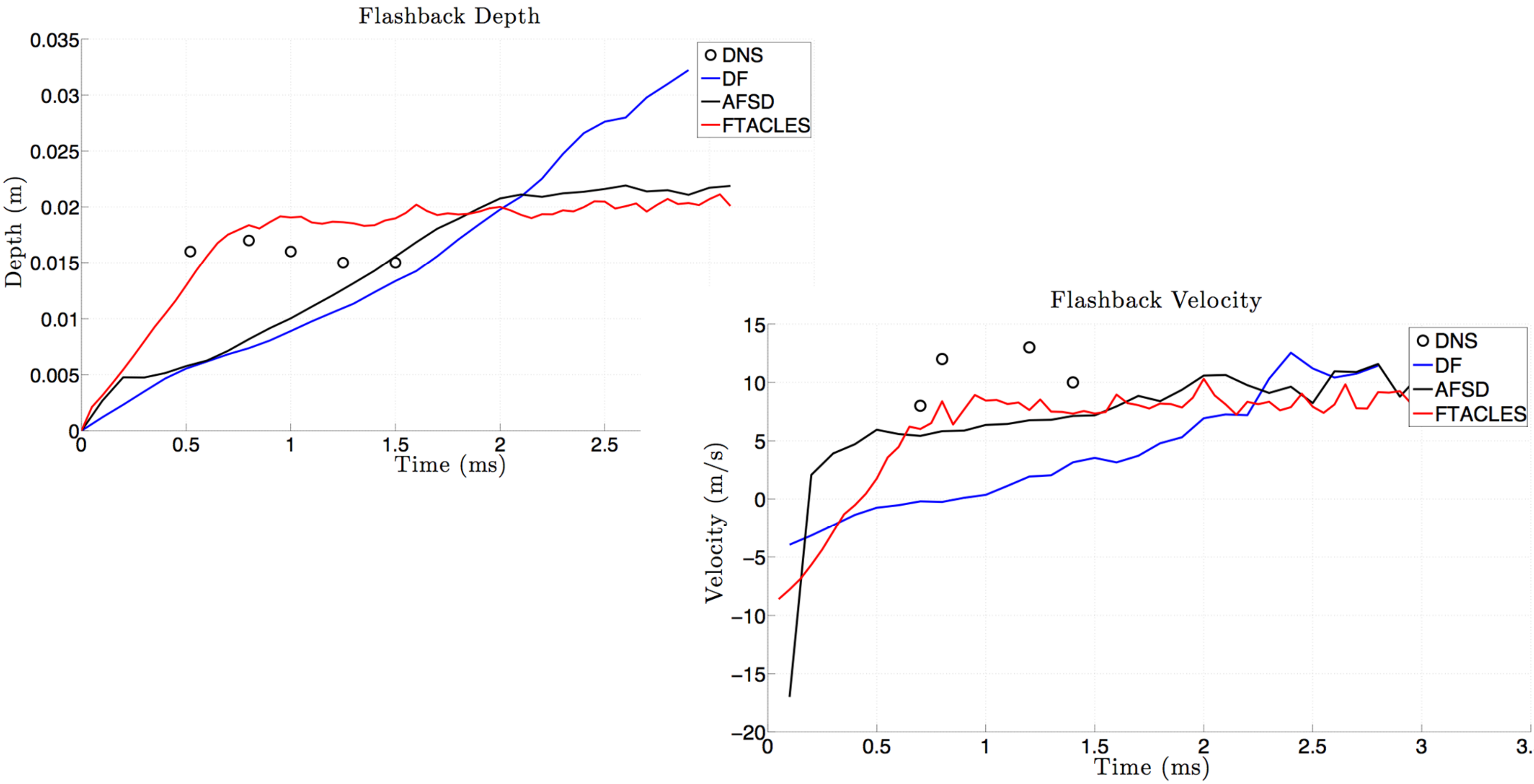




FW = Filter Width, indicates ratio of LES to DNS grid size

LES Results - Model Performance

- Different source term approximations for progress variable tested
- FTACLES approach determined to be most suitable



Moving Beyond Averages

Computational Modeling

- Computational modeling a.k.a CFD targets statistical stationarity
  - ➡ Flow does not change with time
  - ➡ Flow is turbulent but the mean is constant
  - ➡ Why?
    - Allows for ``Equilibrium Assumptions''
- What can CFD do?
  - ➡ Predict mean evolution of quantities
    - Average NOx at outlet
    - Mean and fluctuations of temperature
  - ➡ Cannot be trusted for transient problems

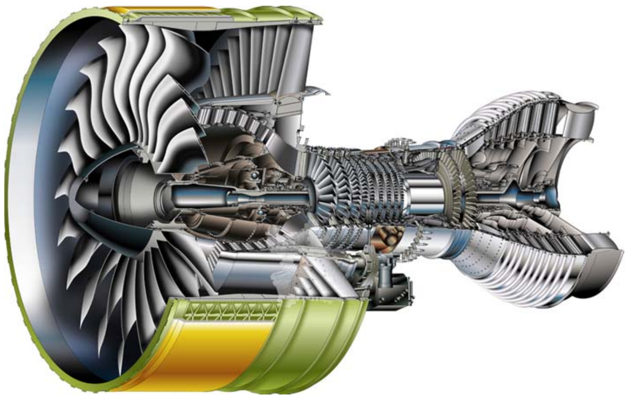
Fundamentals of CFD Modeling

- At core of all CFD models lies Equilibrium Assumption (EA)
  - ➡ Not a single assumption but spans a suite of assumptions
- Examples of EA
  - ➡ At many different scales
    - Molecular thermodynamics (thermal equilibrium)
    - Spectral equilibrium (turbulence and scalar spectrum are similar)
    - Turbulence equilibrium (established spectrum)
- Why EA?
  - ➡ Makes modeling simpler (which is the goal of modeling)
  - ➡ Valid in many situations

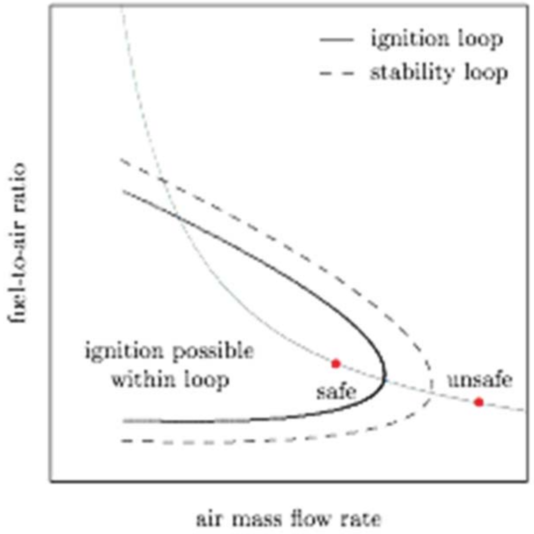
EA with Averaging

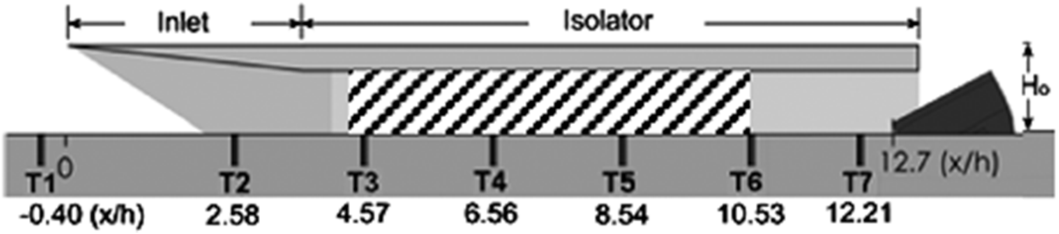
- All turbulence simulations use some form of averaging
  - RANS uses ensemble averaging
  - LES uses spatial averaging followed by ensemble averaging
    - The second part is not normally discussed
      - Important for transient flow problems
- Averaging further limits the utility
  - Turbulent flow is chaotic
  - Predicting average events is useful, but not critical
  - More importantly, experiments are ideally suited for this purpose
    - Simulations may not ``predict'' new information not already obtainable
      - Granted, experiments are expensive!

Rethinking CFD: Motivating Physics

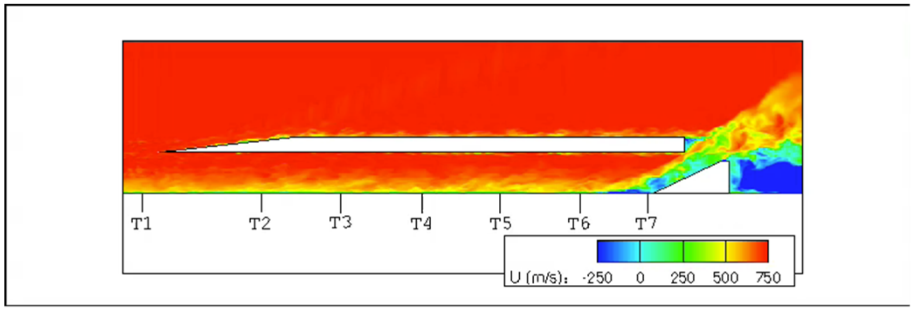


High Altitude Relight





Supersonic Isolator Unstart



Flame Flashback in Confined Geometries

Changing the Simulation Target

- Simulations are designed to predict this:
  - ➡ What is the average speed of flashback?
- Simulations should predict this:
  - ➡ What is the probability that the flashback speed > some value?

    Or

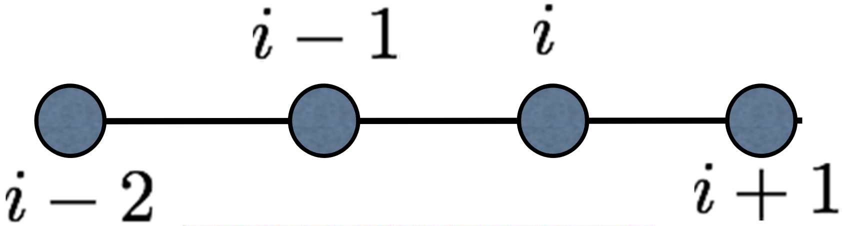
  - ➡ What is the fastest propagation speed?

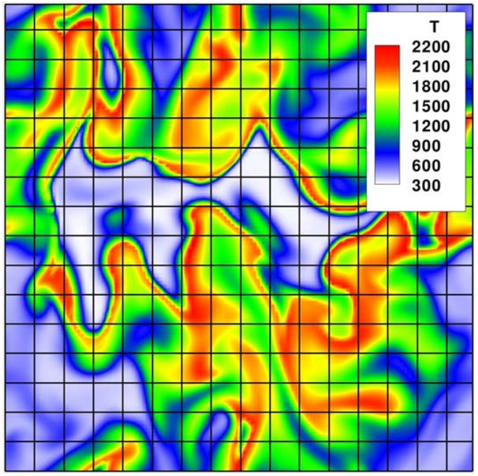
Three Approaches to Understanding LES

- Adrian (1977) provided one of the first studies on the implied meaning of filtering
  - ➡ Discussed this in terms of two different simulations approaches
  - ➡ Termed here as coarse DNS and filtered LES approaches
- Moser’s ideal LES approach (1998)
  - ➡ Similar to Adrian’s second approach
- Pope’s self-conditional LES approach (2010)
  - ➡ Seeks to restate the CFD modeling problem
  - ➡ Unique model terms arise

Statistical Definition of LES

- Consider a continuous velocity field $\mathbf{u}(\mathbf{x},t)$

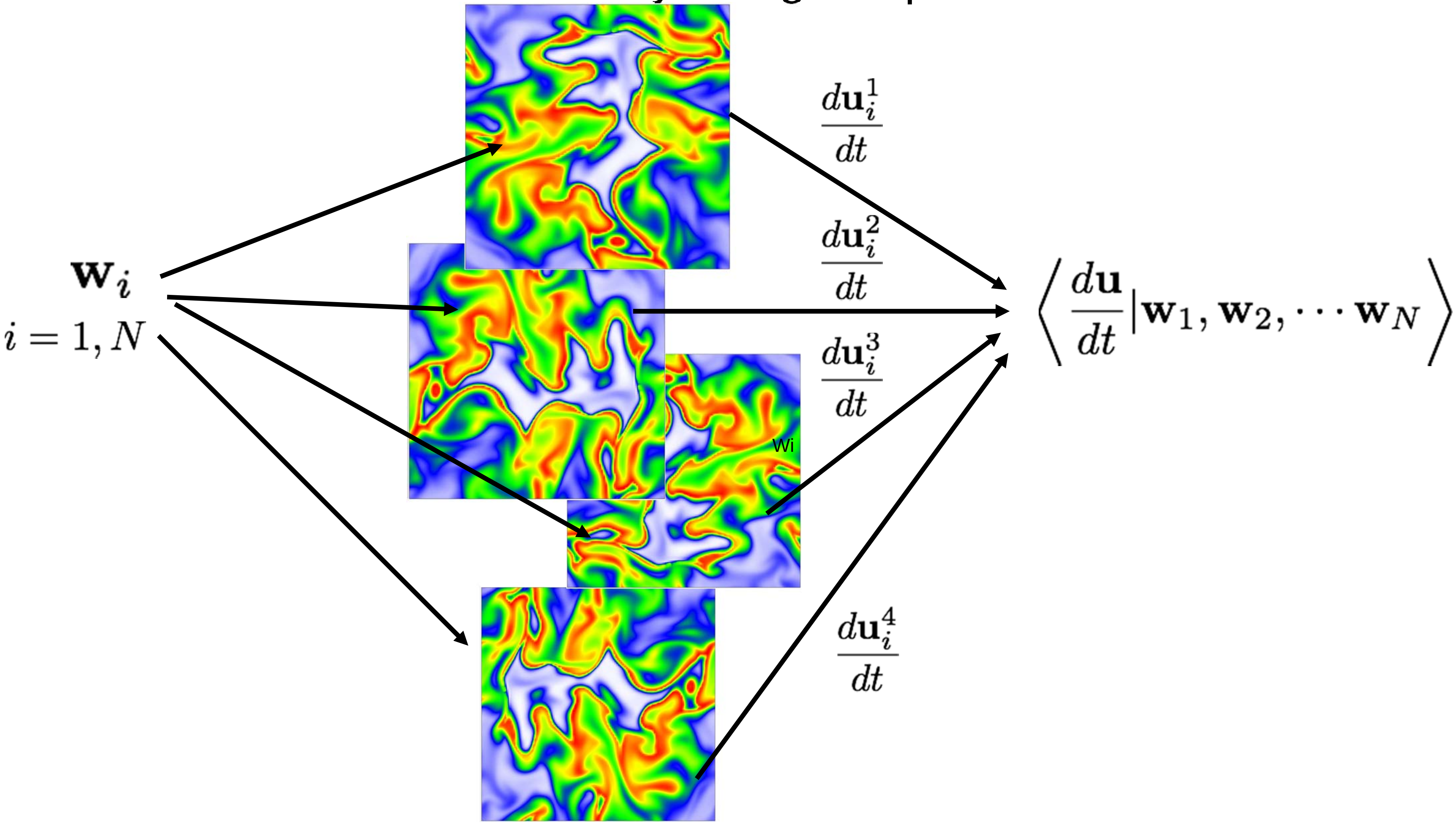




- Consider a computational grid of discrete points
  - ➡ Mesh points are spaced larger than the smallest flow scales
  - ➡ Velocity denoted by $\mathbf{w}_i$
- Knowledge of $\mathbf{w}_i$ alone does not determine the evolution of $\mathbf{u}(\mathbf{x},t)$
  - ➡ For a given $\mathbf{w}_i$ there are multiple possible transitions from $\mathbf{u}(\mathbf{x},t)$ to $\mathbf{u}(\mathbf{x},t+\Delta t)$
  - ➡ Transition should be described probabilistically
- How do we evolve $\mathbf{w}_i$?

Understanding Filtered Evolution

- Consider representation of velocity on a mesh
  - ➡ W_i is the vector of velocity at a given point



$$\mathbf{w}_i$$

$$i = 1, N$$

$$\frac{d\mathbf{u}_i^1}{dt}$$

$$\frac{d\mathbf{u}_i^2}{dt}$$

$$\frac{d\mathbf{u}_i^3}{dt}$$

$$\frac{d\mathbf{u}_i^4}{dt}$$

$$\left\langle \frac{d\mathbf{u}}{dt} \middle| \mathbf{w}_1, \mathbf{w}_2, \cdots \mathbf{w}_N \right\rangle$$

Multi-point Probability Density Function

- Consider the following event

$$\mathbf{E}_n = \{\mathbf{v}_1 < \mathbf{u}(\mathbf{x},t) < \mathbf{v}_1 + d\mathbf{v}_1, \mathbf{v}_2 < \mathbf{u}(\mathbf{x},t) < \mathbf{v}_2 + d\mathbf{v}_2, \cdots, \mathbf{v}_n < \mathbf{u}(\mathbf{x},t) < \mathbf{v}_n + d\mathbf{v}_n\}$$

➡ n refers to the number of grid points in the computational grid

➡ The event refers to multi-point velocity information

- The joint-PDF evolves according to

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial \mathbf{v}_n}\left(\left\langle \frac{d\mathbf{u}}{dt} | \mathbf{E}_n \right\rangle P\right) = 0.$$

- The best solution from the LES reproduces the multi-point PDF accurately

Conditional Evolution Equations

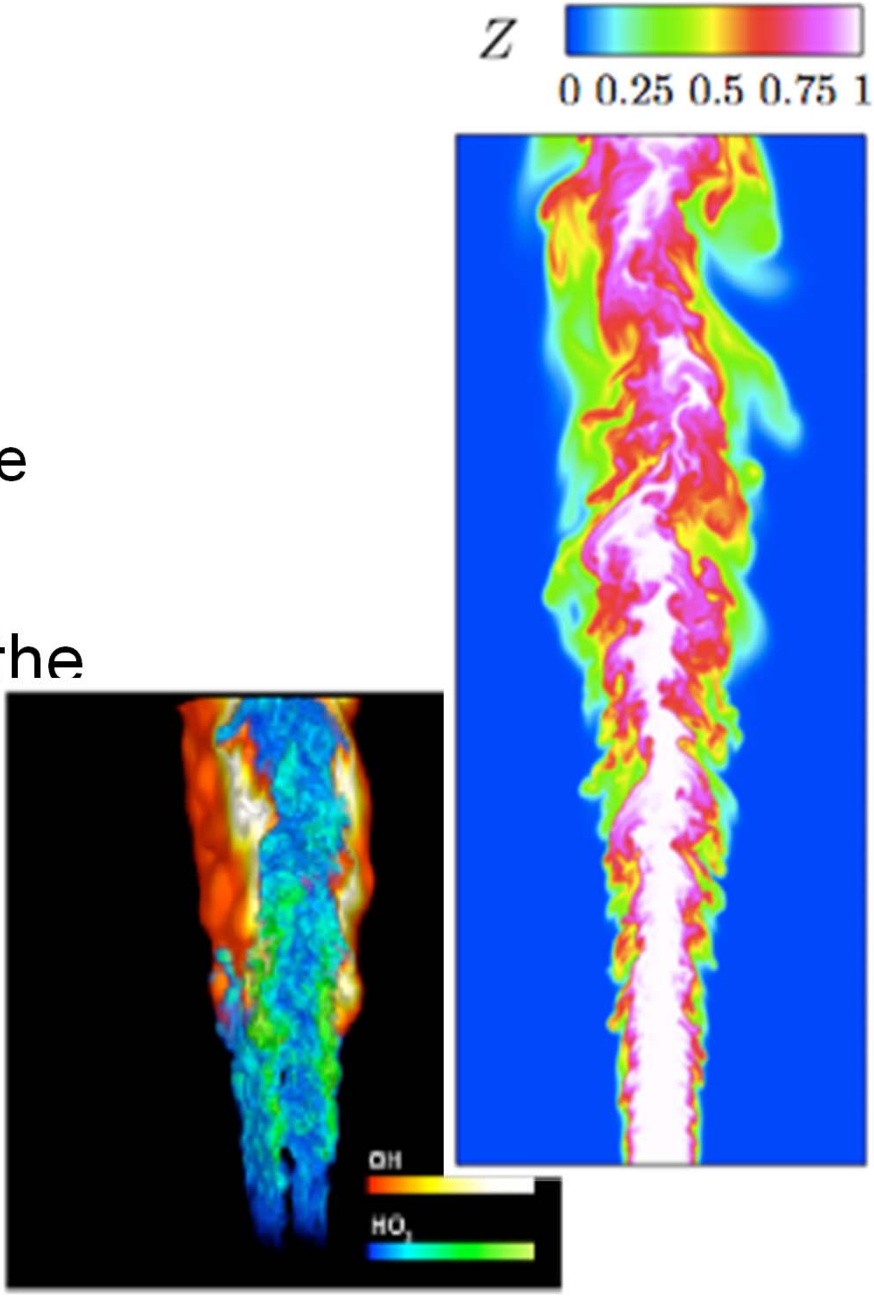
- How do we evolve $\mathbf{w}_i$?
  - ➡ The solution should capture the multi-point PDF correctly

$$\mathbf{w}_\alpha(t+\Delta t) = \mathbf{w}_\alpha(t) + \left\langle \frac{d\mathbf{u}}{dt} | \mathbf{E}_n = \{\mathbf{w}_1, \mathbf{w}_2, \cdots, \mathbf{w}_n\} \right\rangle \Delta t$$

    - The best solution evolves the conditional mean of all possible realizations
  - ➡ Note that the best solution evolves the average path and is a statistically averaged result
    - It is important to think of LES computations also in such average terms

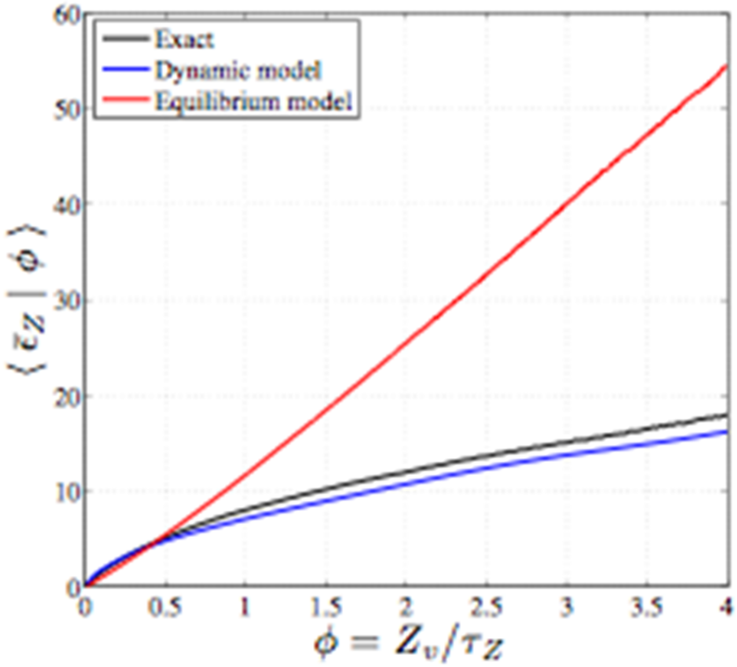
Developing Conditional Models in LES

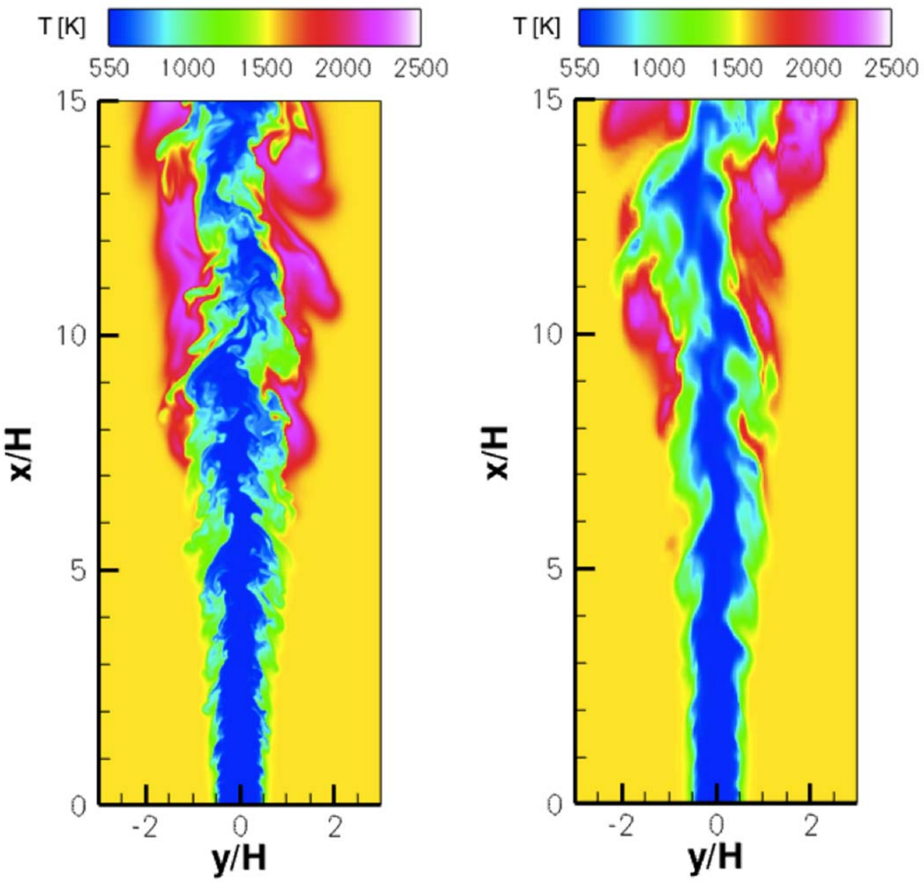
- From conditional evolution equations, a set of model terms could be extracted
    - ➡ Similar to conventional LES
    - ➡ Unresolved stress, subfilter variance etc.
- Models in LES should also obey the conditional average formulation
- Consider scalar dissipation rate
    - ➡ Very important for combustion simulations
- Lifted flame configuration



Conditionally Averaged Combustion Models

- New optimal estimator based model selection
  - ➡ Provides an estimate of the least error that could be made with a given set of input variables
  - ➡ Model form chosen to be close to this error





DNS **LES**

From Kaul et al. (2013), Proc. Comb. Inst.

Multi-time Formulations

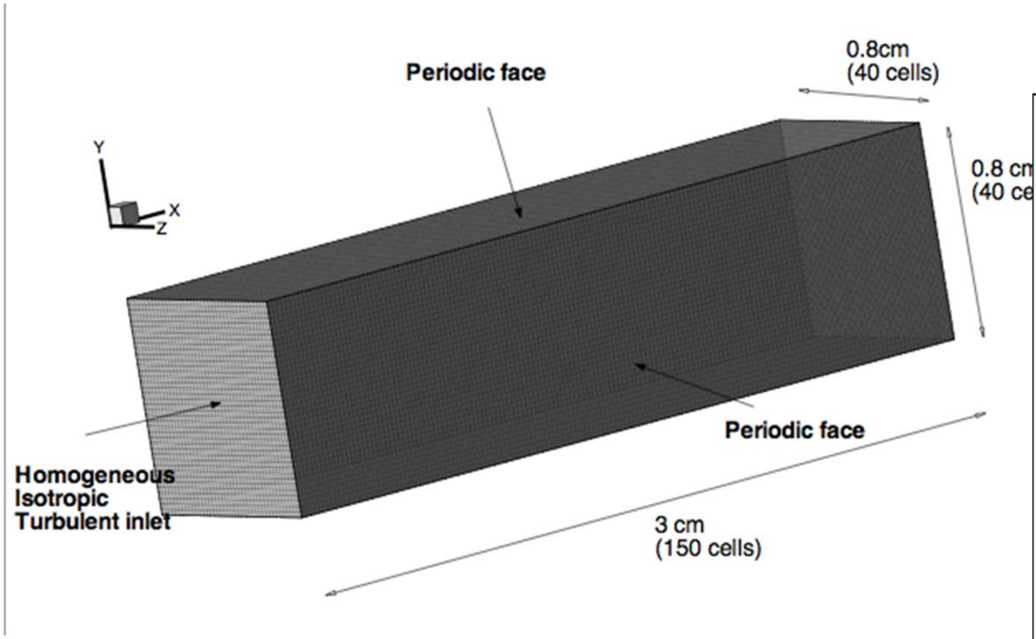
- CFD has to move beyond one-point one-time models
  - ➡ Multi-time models for transient flow behavior

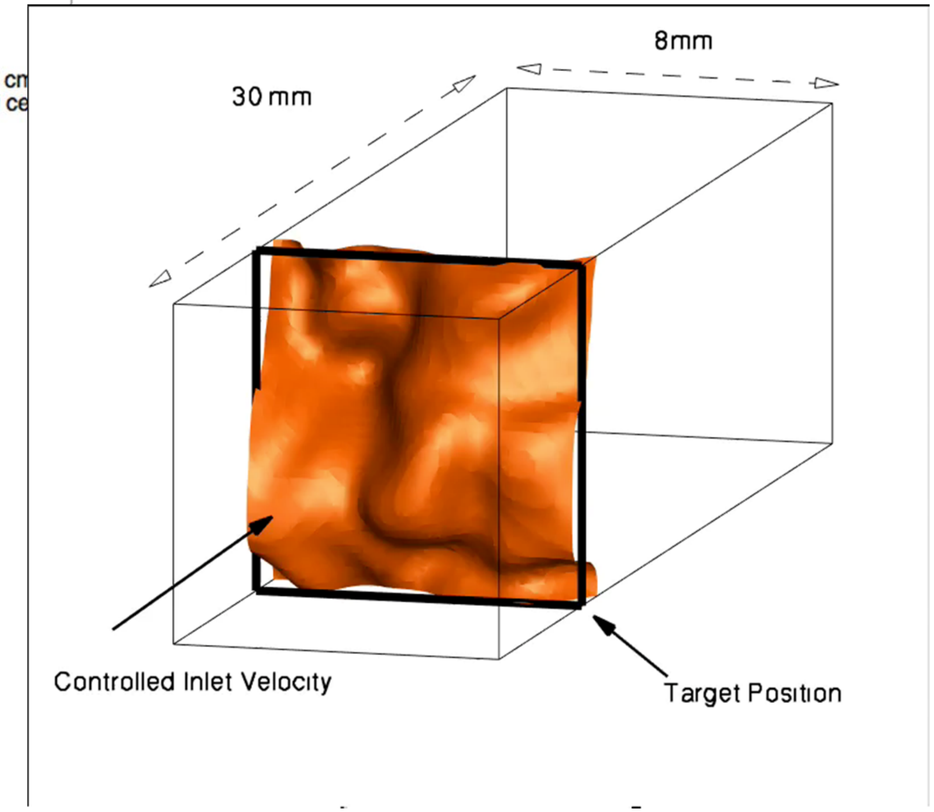
$$\frac{d\mathbf{w}}{dt} = \left\langle \frac{d\mathbf{u}}{dt} | \mathbf{w}(t), \mathbf{w}(t - \Delta t), \cdots \right\rangle$$

- Current project
  - ➡ Understand variability in flashback
  - ➡ Devise modeling methods for predicting ``extreme events”
  - ➡ Map the limitations of LES in predicting such transient flows

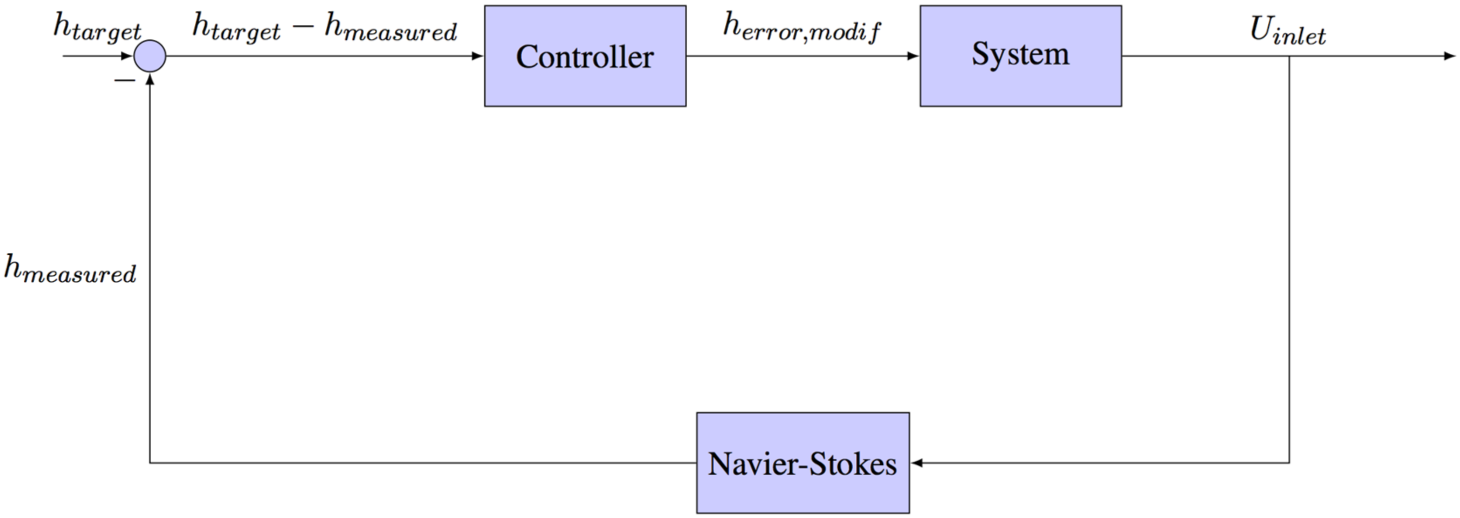
Constrained Premixed Flame

- Flame propagation in homogeneous isotropic turbulence
- Flame location fixed using a control loop



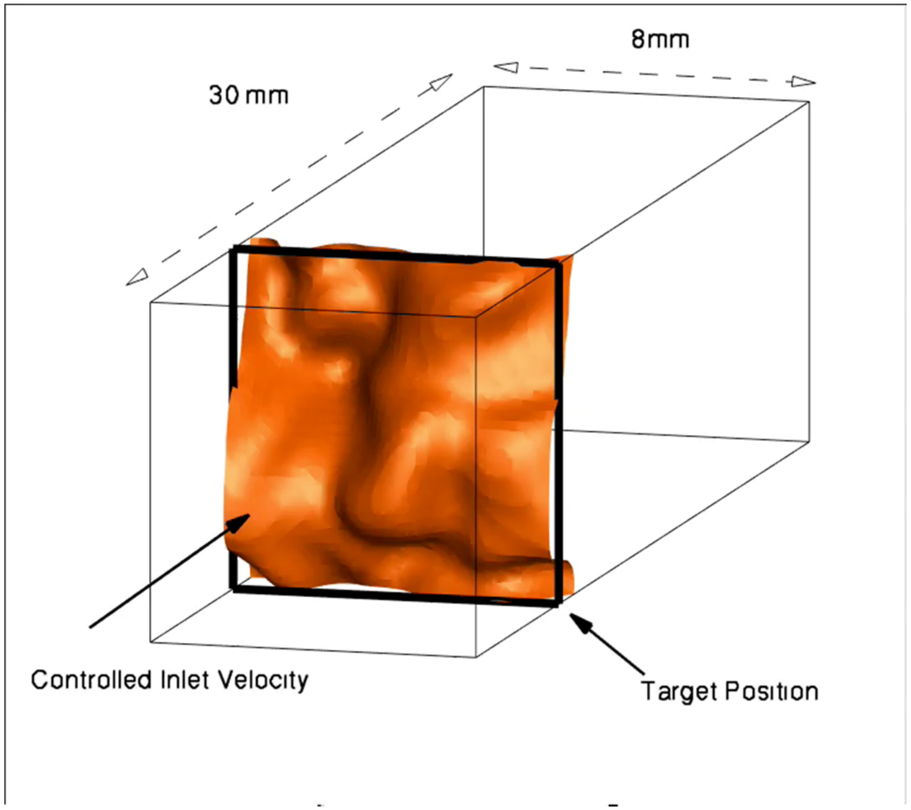


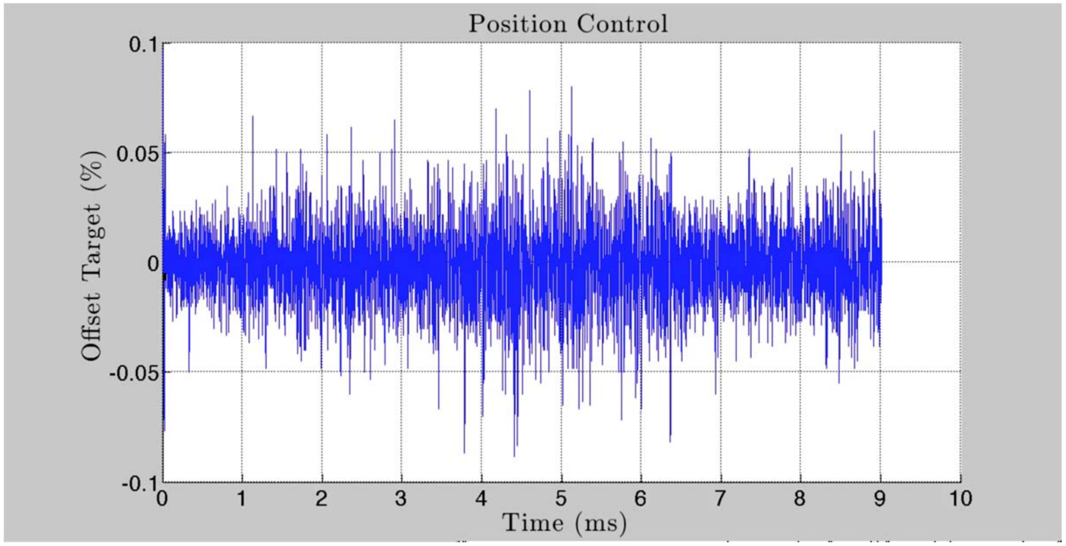
Position Control Algorithm

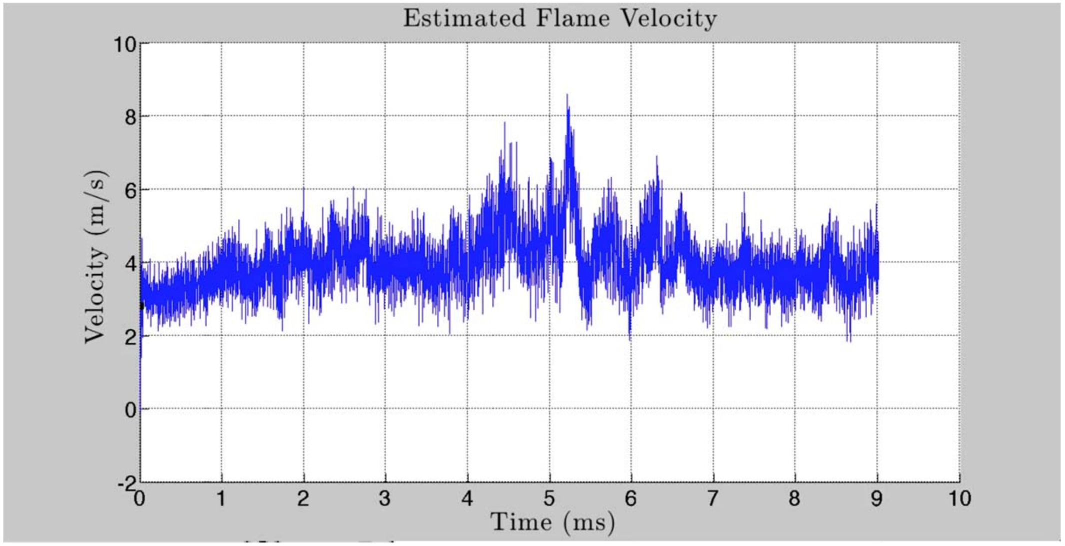


- Flame position adjusted by changing inflow velocity
  - ➡ Response time adjusted to ensure stability
  - ➡ Total adjustment a small fraction of the flame propagation velocity

Flame Evolution

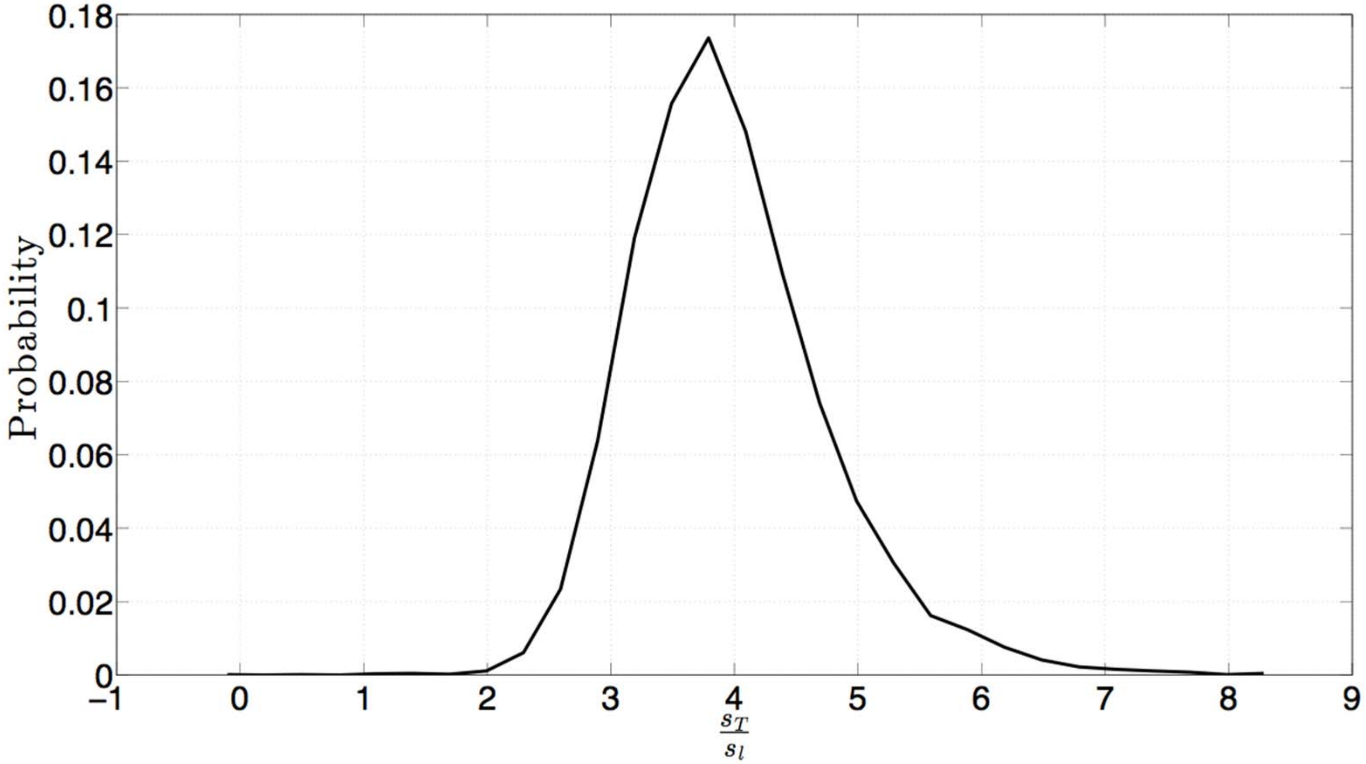



Position Control


Estimated Flame Velocity

PDF of Flame Propagation Velocity

- Strong asymmetry in flame propagation
  - ➡ Faster velocities are more common than slower velocities



Conclusions

- High-pressure setup constructed
  - ➡ Initial stratified flame studies underway
- LES of flashback
  - ➡ Progress variable approach predicts DNS statistics reasonably accurately
  - ➡ Flame wrinkling effects at larger filter widths need to be studied
- New modeling strategy for CFD
  - ➡ Towards probabilistic modeling of transient flows
  - ➡ Homogeneous cases used to understand time correlation of extreme events