Joint Computational/Experimental Study of Flashback in Hydrogen-rich Gas Turbines

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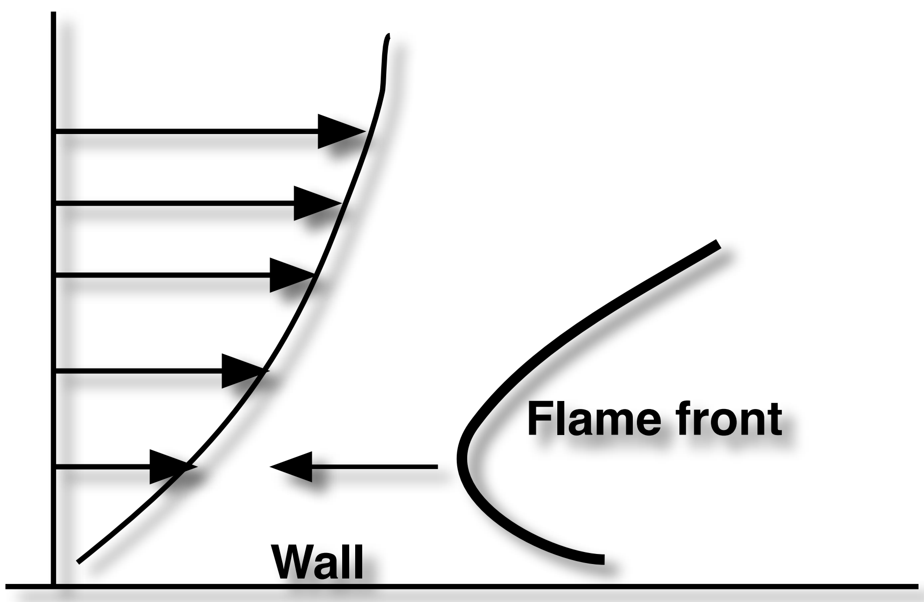
Challenges in Flashback Simulation

- **Unique physics**
  - ➡ Flame propagation in a turbulent boundary layer
  - ➡ Non-uniform equivalence ratio
- **Coupled to upstream processes**
  - ➡ Fuel-injection and mixing affects fuel stratification
- **Input uncertainties**
  - ➡ Chemistry mechanism and boundary condition uncertainties could affect flashback speed + initiation

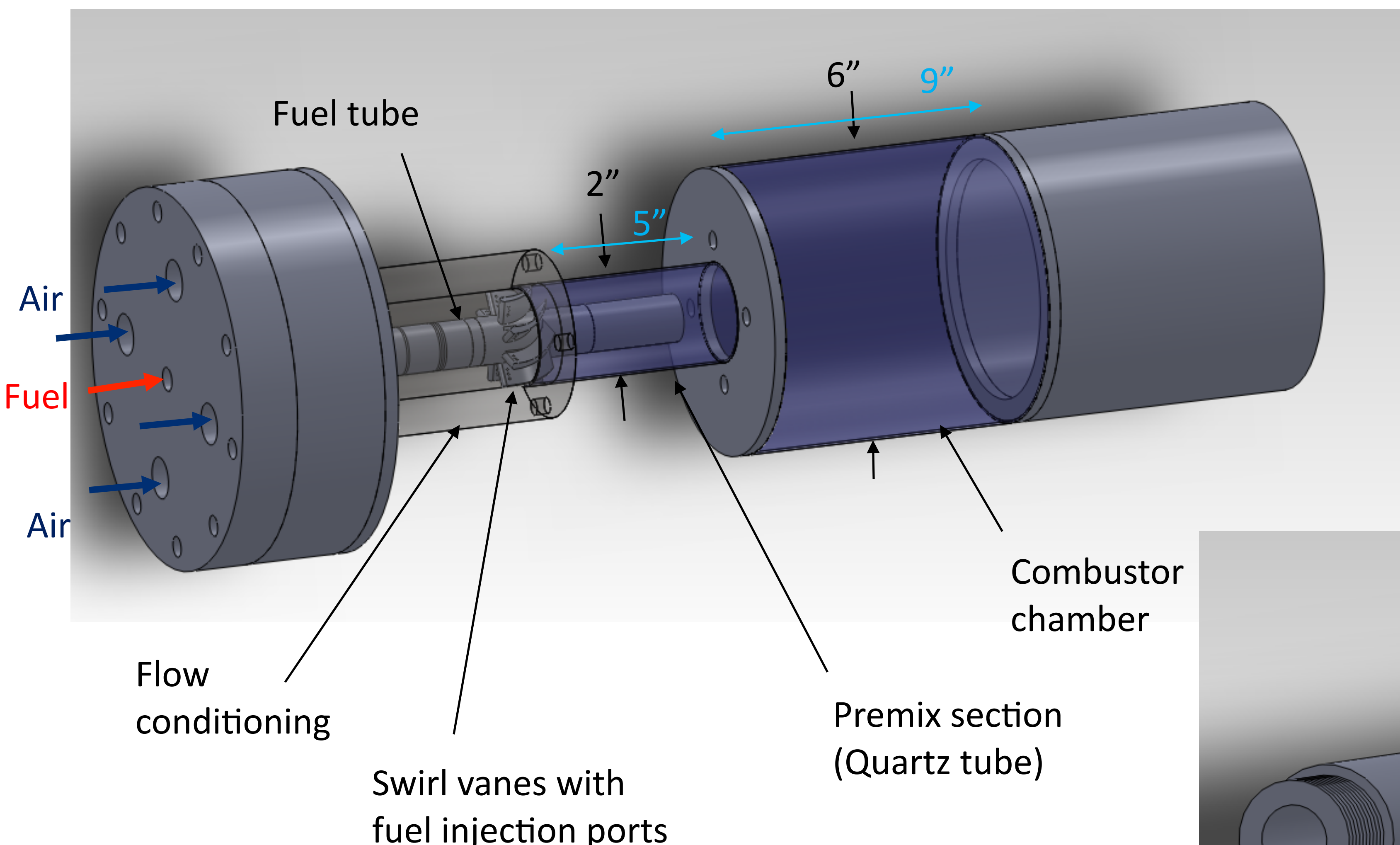


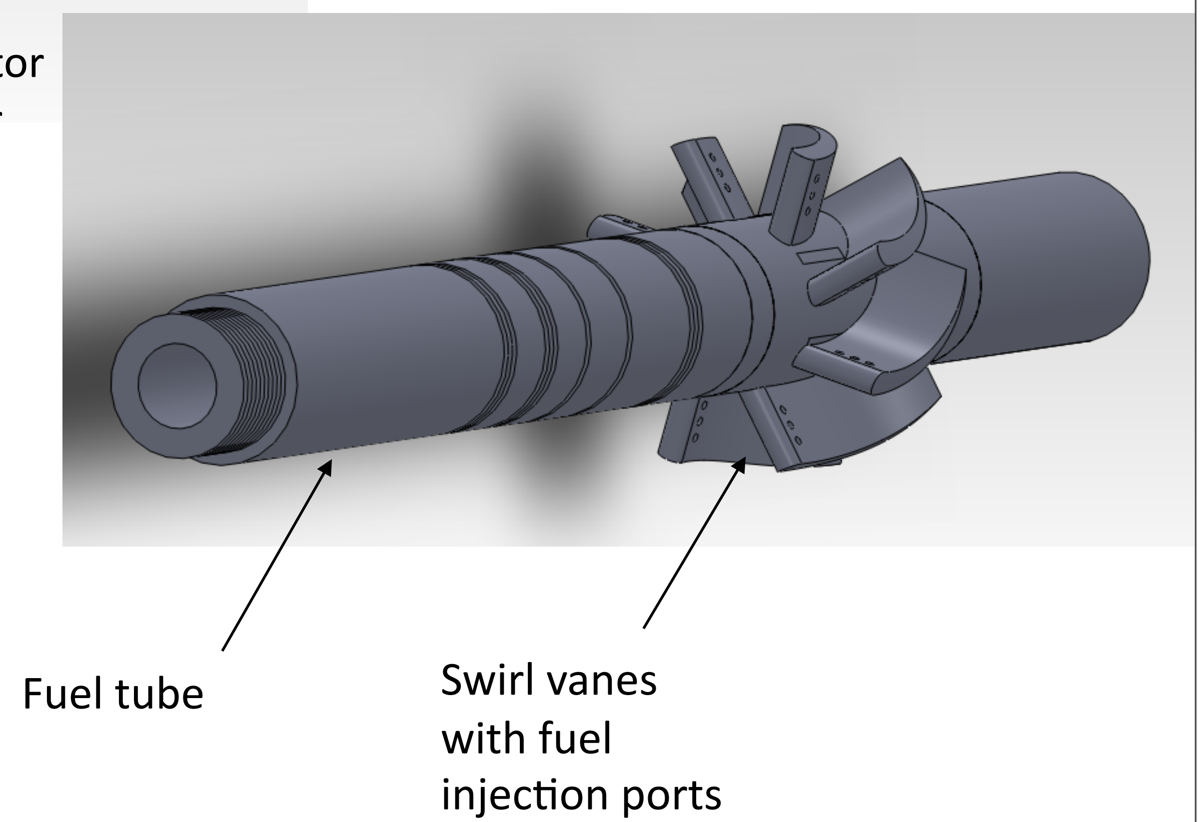
Operating Hypotheses

- **Both Large eddy simulation (LES) and Reynolds-averaged Navier-Stokes (RANS) approaches necessary**
- **Models developed should be applicable in complex geometries**
  - ➡ Restricts model formulation
- **Rigorous validation procedures necessary**
  - ➡ Individual processes (flame-wall interaction, jet mixing etc.) need to be validated
  - ➡ Interaction of processes also need to be tested
- **It is not sufficient to produce predictions, but also uncertainty in the predictions**
  - ➡ A statistical framework for uncertainty evaluation needed

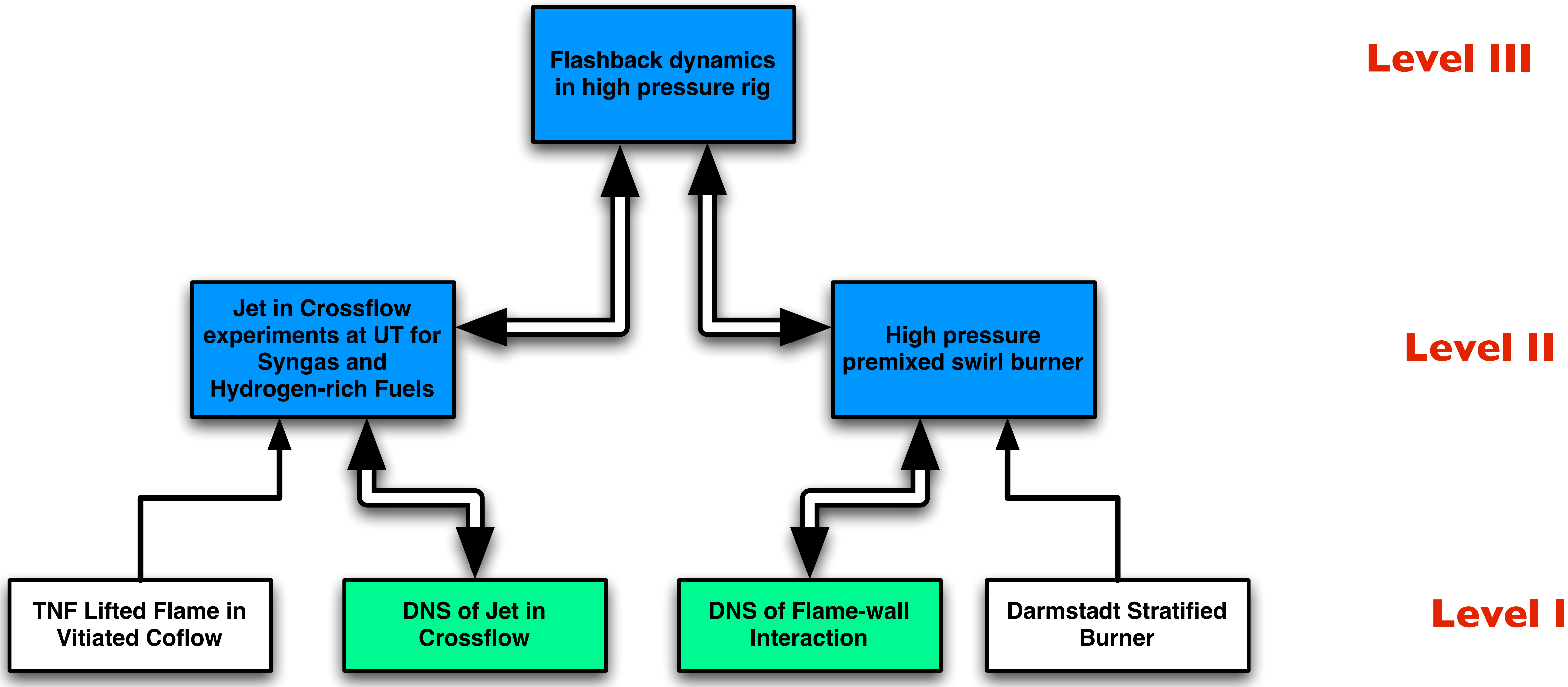
Target-based Flashback Modeling

- **UT high-pressure swirl combustor**





Hierarchical Validation Pyramid



- Level 1 - Fundamental data from legacy expts. and direct numerical simulations (DNS)
- Level 2 - UT re-configurable experiments designed for validation
- Level 3 - UT target system experiments

Topics of Discussion

- **Quadrature approach (DQMOM) for modeling combustion of jets-in-crossflow**
  - ➡ Formulation of DQMOM approach
  - ➡ Implementation in OpenFOAM general purpose CFD solver
- **Analysis of flame-wall interaction using direct numerical simulation (DNS) data**
- **Bayesian approach for uncertainty quantification**
  - ➡ Formulation and UQ of syngas chemistry mechanisms
- **Preliminary studies of UT swirl burner**
  - ➡ Experimental and LES studies

Direct Quadrature Method of Moments (DQMOM) Approach for LES/RANS of Turbulent Combustion

DQMOM Basics

- **Probability density function (PDF) approach**
  - ➡ Solve a high-dimensional transport equation for joint-PDF of gas phase scalars
- **In LES calculations, the filtered moments of the composition vector are required**

$$\widetilde{\phi} = \int \mathcal{G}(\zeta) P_\xi(\zeta; \mathbf{x}, t) d\zeta$$

- **PDF transport equation**

Chemical Source

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j}\left[P\widetilde{u_j|\zeta}\right] = -\frac{\partial}{\partial \zeta_\alpha}\left[P\widetilde{\mathcal{M}_\alpha|\zeta}\right] - \frac{\partial}{\partial \zeta_\alpha}\left[P S_\alpha\right]$$

Conditional Diffusion

  - ➡ Condition diffusion requires a model for scalar dissipation rate

Modeling PDF Transport Equation

- **PDF transport equation**

Chemical Source

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j}\left[P\widetilde{u_j|\zeta}\right] = -\frac{\partial}{\partial \zeta_\alpha}\left[P\widetilde{\mathcal{M}_\alpha|\zeta}\right] - \frac{\partial}{\partial \zeta_\alpha}\left[P S_\alpha\right]$$

Conditional Diffusion

- **PDF equation is high-dimensional**
  - ➡ If N species present in chemistry, N+5 dimensions
- **Lagrangian Monte-Carlo approach typically used**
  - ➡ Stochastic in nature
  - ➡ Numerical stability is highly flow dependent
  - ➡ Difficult to maintain numerical accuracy in complex geometries
  - ➡ Highly expensive for realistic flow configurations

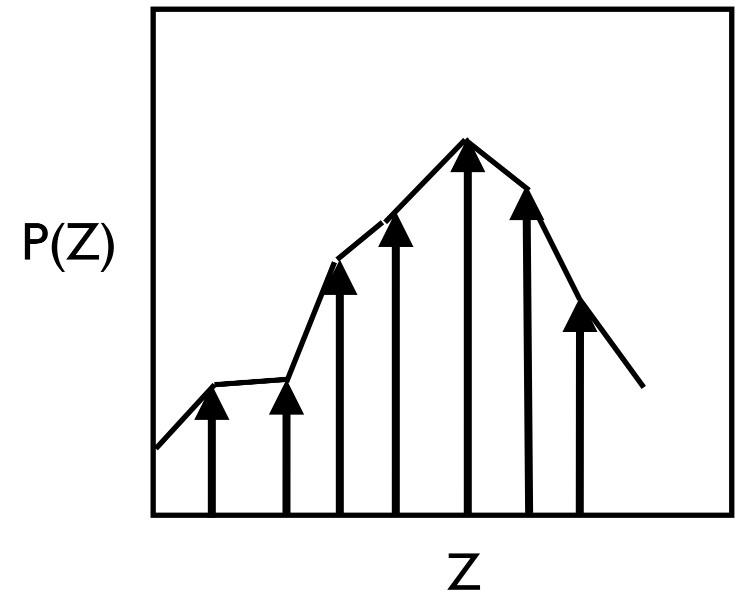
Eulerian DQMOM Approach

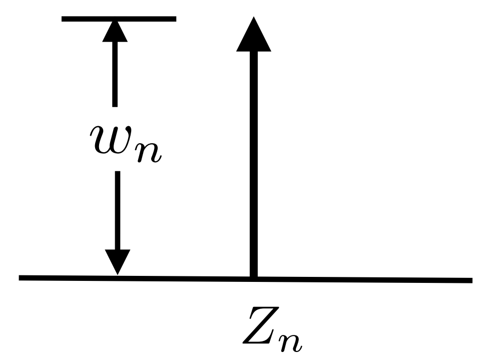
- **DQMOM uses dirac-delta functions to discretize the PDF**

- **Each delta-function characterized by a weight and abscissa**
  - ➡ Transport equations for these two variables can be formulated

- **Similar in structure to scalar transport equations**

$$\frac{\partial w_n}{\partial t} + \overline{U_i}\frac{\partial w_n}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\Gamma \frac{\partial w_n}{\partial x_i}\right) + a_n$$





Implementation in OpenFOAM

- **Eulerian PDF approach**
  - ➡ Easy transition to commercial and open source codes
- **OpenFOAM open source platform**
  - ➡ C++ libraries for solving partial differential equations
  - ➡ Arbitrary geometries handled using unstructured grids
  - ➡ MPI-based parallelization

Abscissas

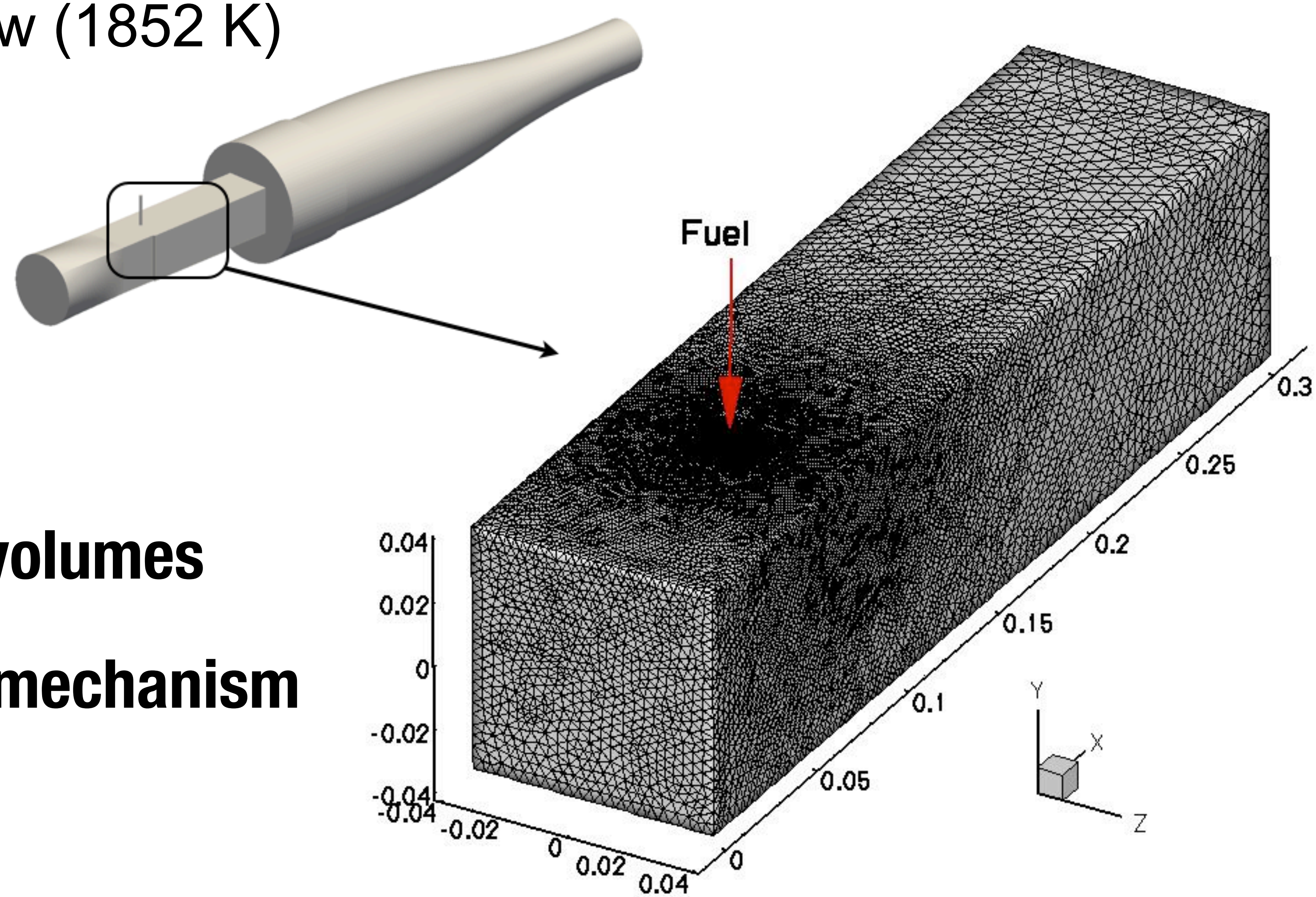
```
solve
(
    fvm::ddt(rho, G1[i])
  + mvConvection->fvmDiv(phi, G1[i])
  - fvm::laplacian(turbulence->muEff(), G1[i])
 ==
    rho*mixingSource[i]
  + chemistry1.RR(i)
);
```

Weights

```
solve
(
    fvm::ddt(rho,w1)
  + mvConvection->fvmDiv(phi,w1)
  - fvm::laplacian(turbulence->muEff(),w1)
);
```

Simulation of Jet-in-Crossflow Configuration

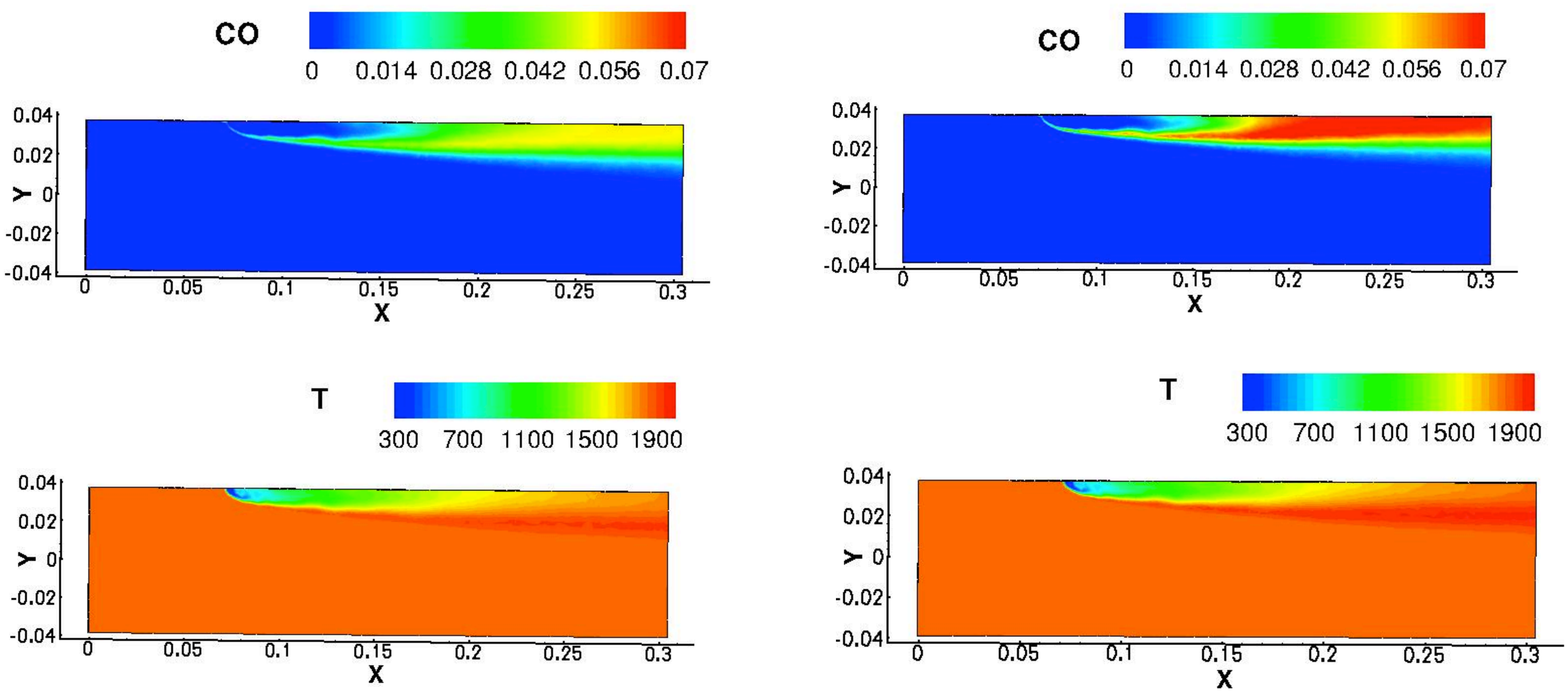
- **Experiment from Lieuwen's group (GaTech Univ.)**
  - ➡ Methane/hydrogen mixture (300K)
  - ➡ Vitiated air crossflow (1852 K)



- **Simulation details**
  - **1.7 million control volumes**
  - **7-species Linstedt mechanism**

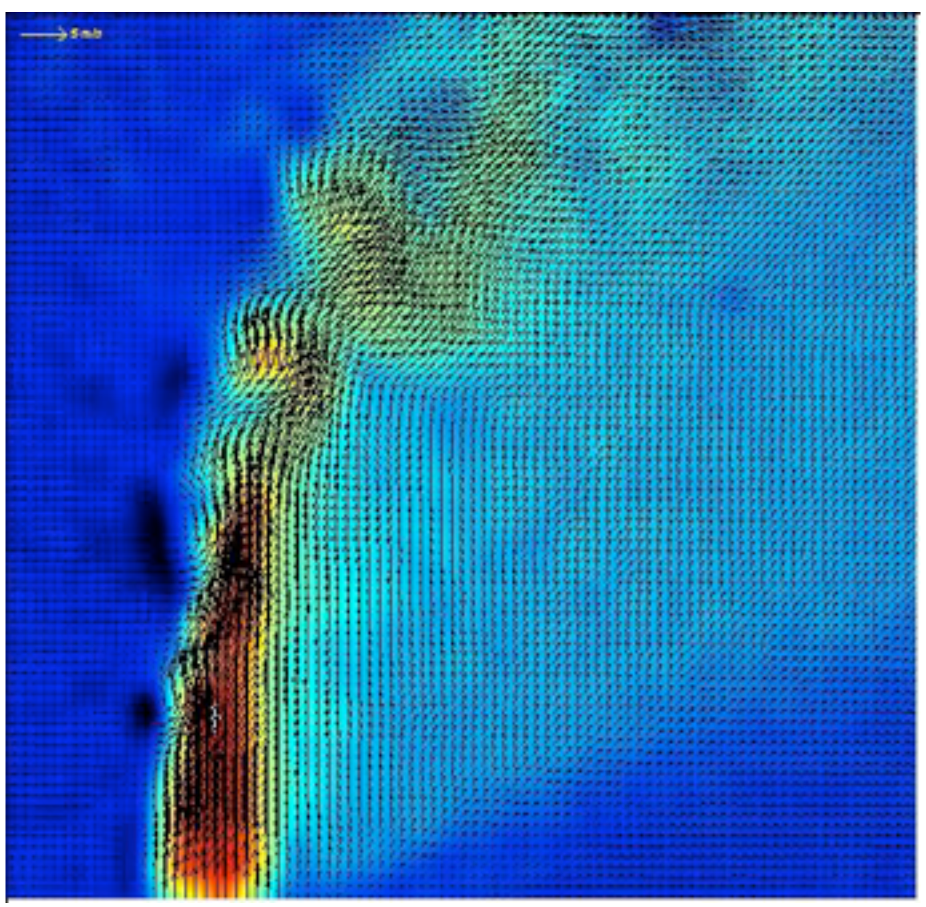
Species Distribution

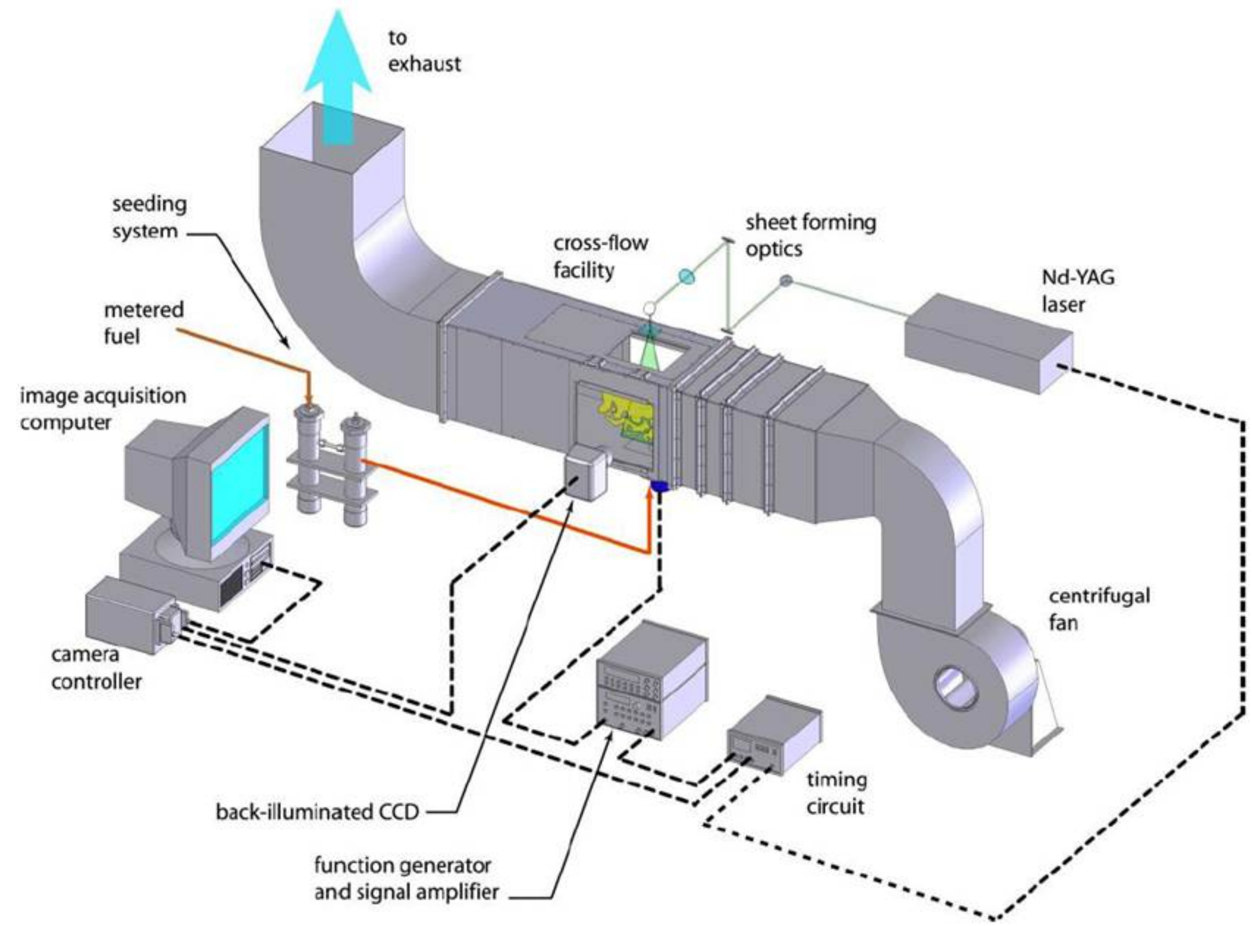
- **DQMOM results compared with no-combustion model simulation**
  - ➡ DQMOM predicts lower combustion rates
  - ➡ Finite-rate mixing slows reactions



UT JICF Configurations

- **Objective is to develop joint velocity/scalar statistics for methane/hydrogen fuel mixtures**
- **3-component PIV measurements completed**

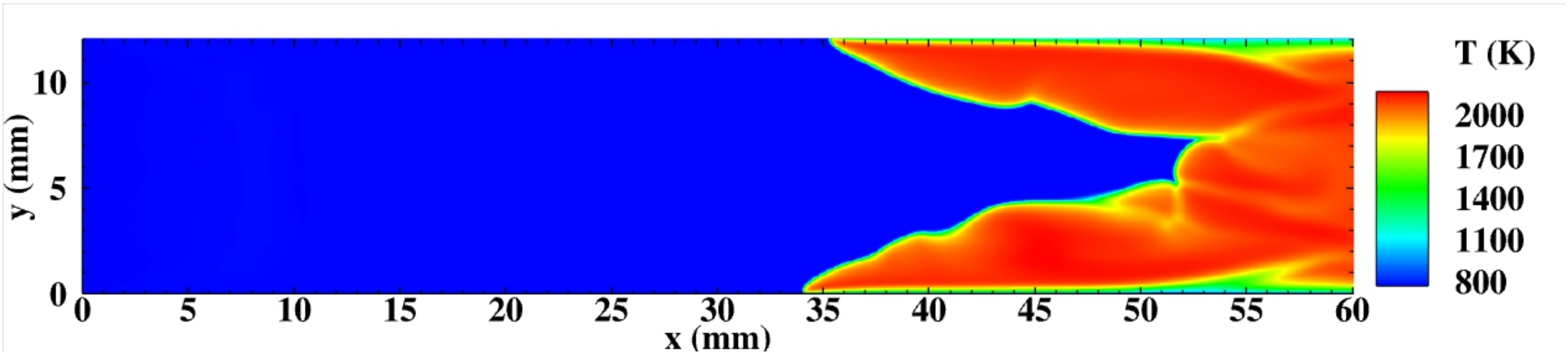




DNS-based Analysis of Flame Propagation Through Turbulent Boundary Layers

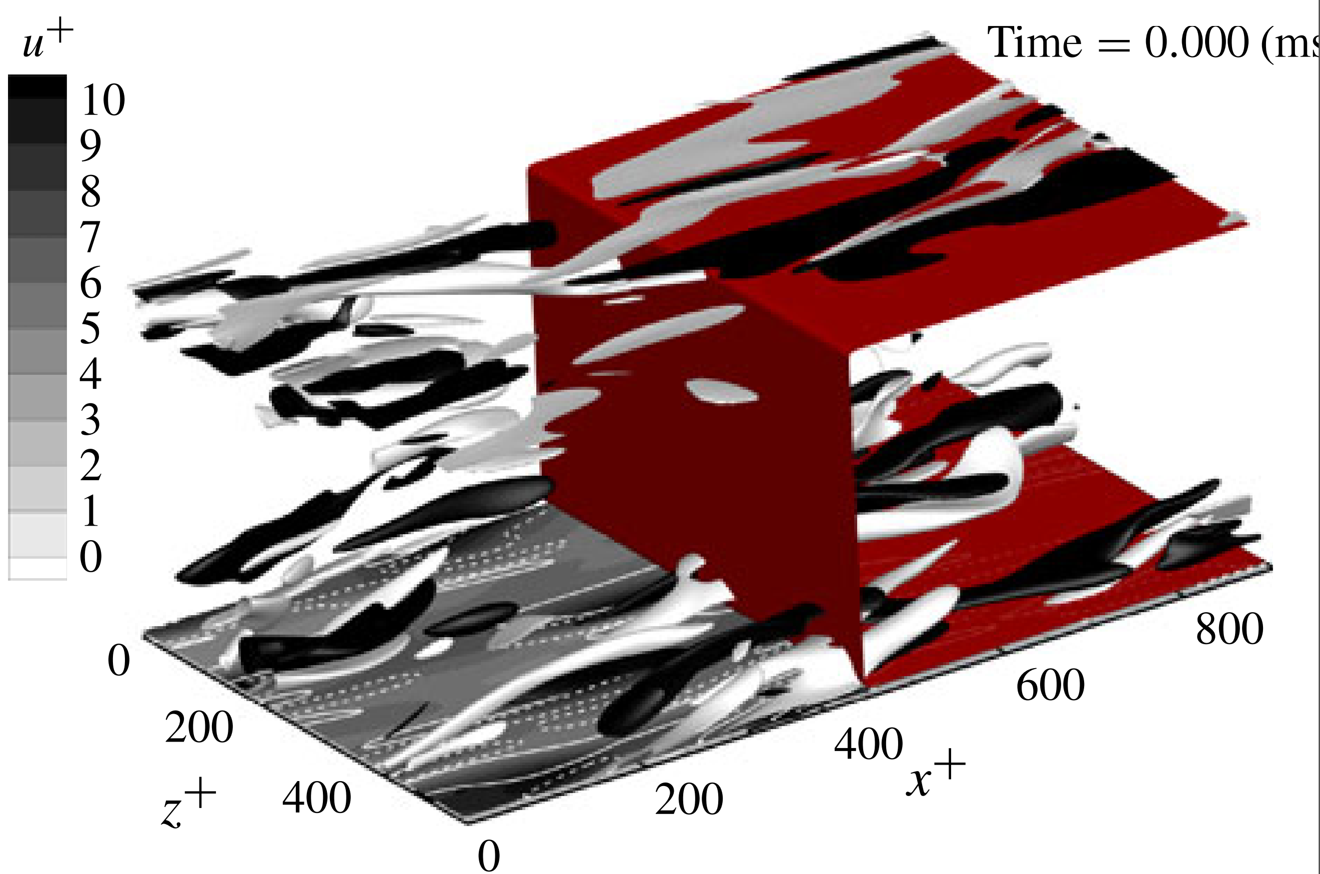
Flame Propagation

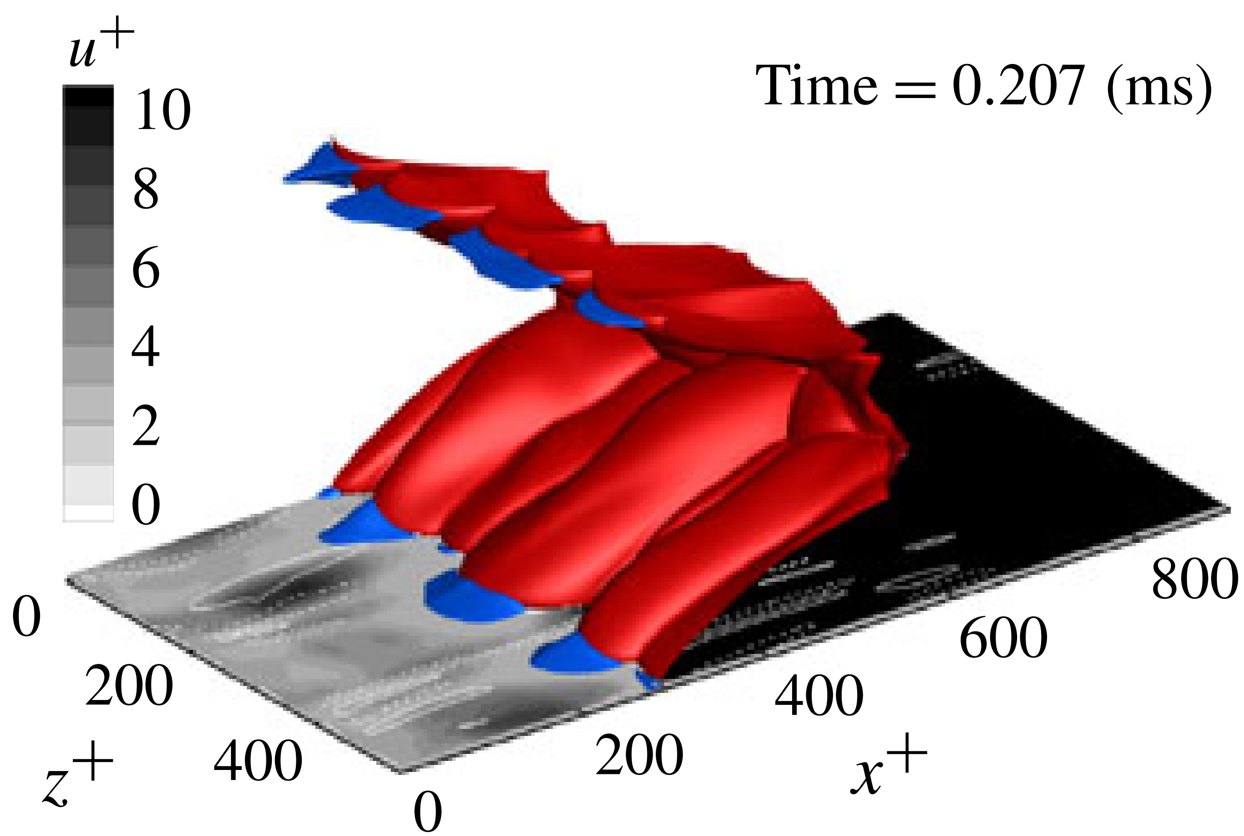
- **Premixed flame propagation generally studied in free-stream or shear layer turbulence**
- **Wall-bounded flows**
  - ➡ Exhibit significant flow anisotropy
  - ➡ Turbulence modified through flame propagation
    - Similar to shock-turbulence interaction



Sandia Flashback DNS

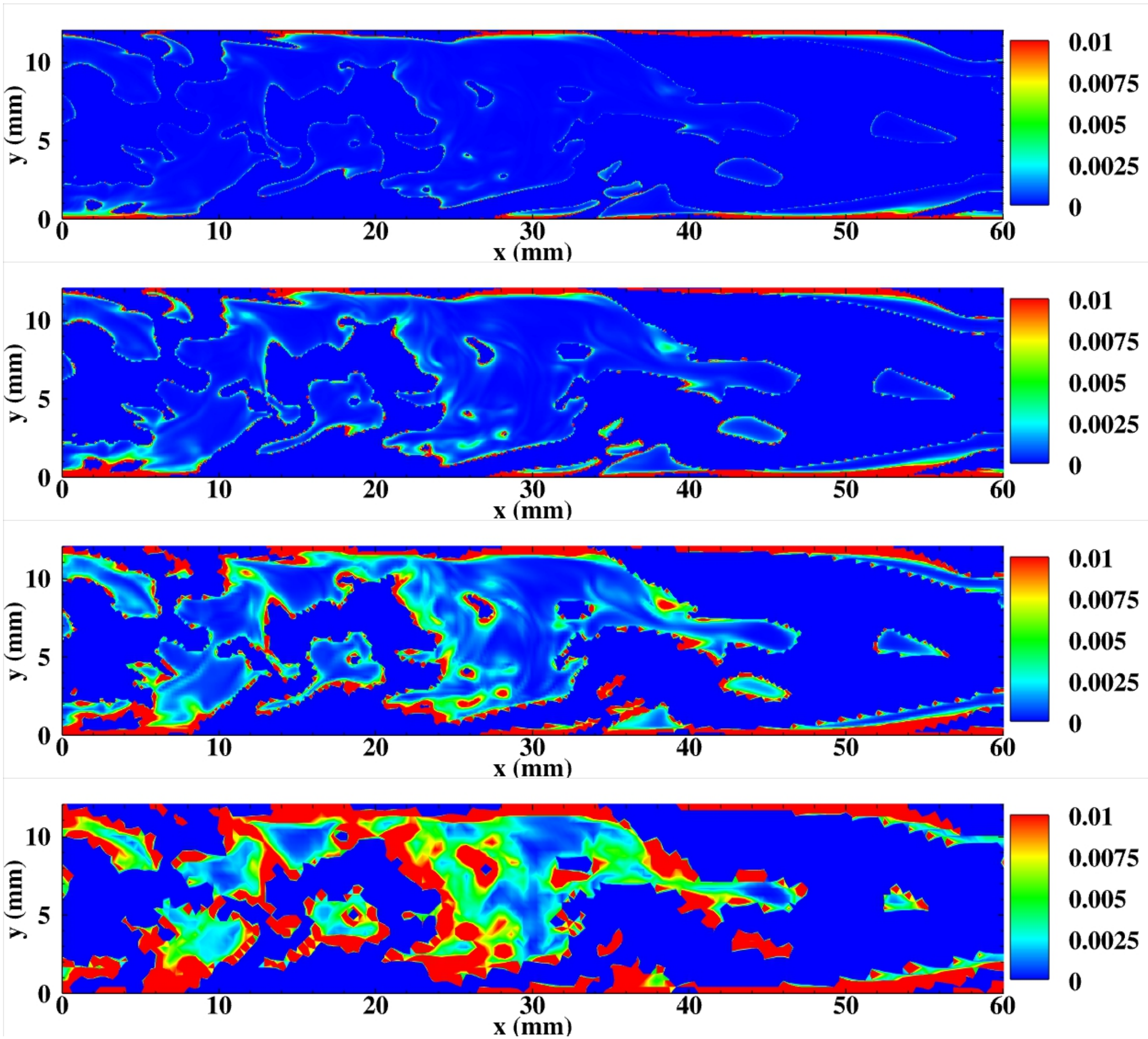
- **Petascale simulation of flame flashback in a turbulent channel flow**
  - ➡ Gruber etal., JFM, 2012





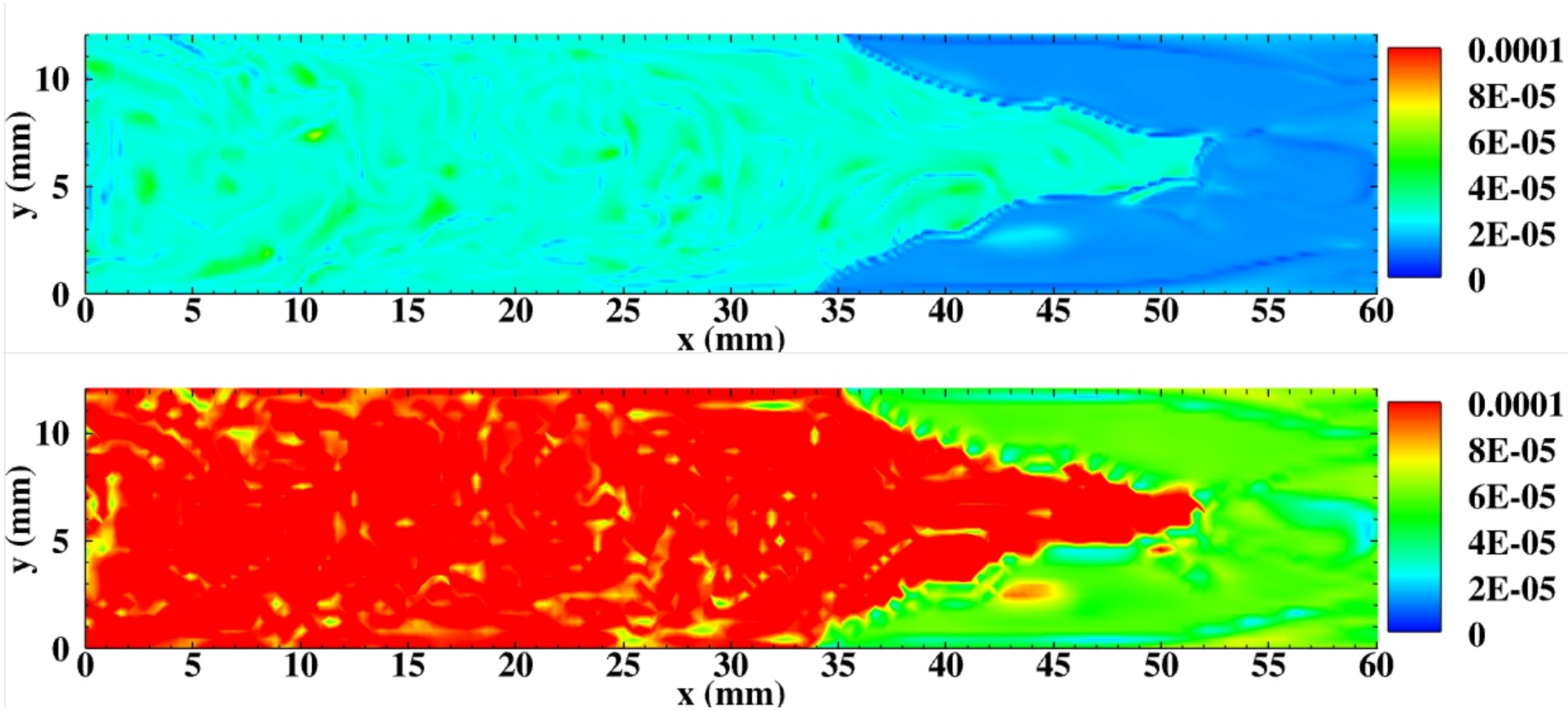
A Priori Results

- **DNS-based analysis of unresolved kinetic energy**



Decreasing LES resolution

Mixing Timescale and Kinetic Energy Production



High

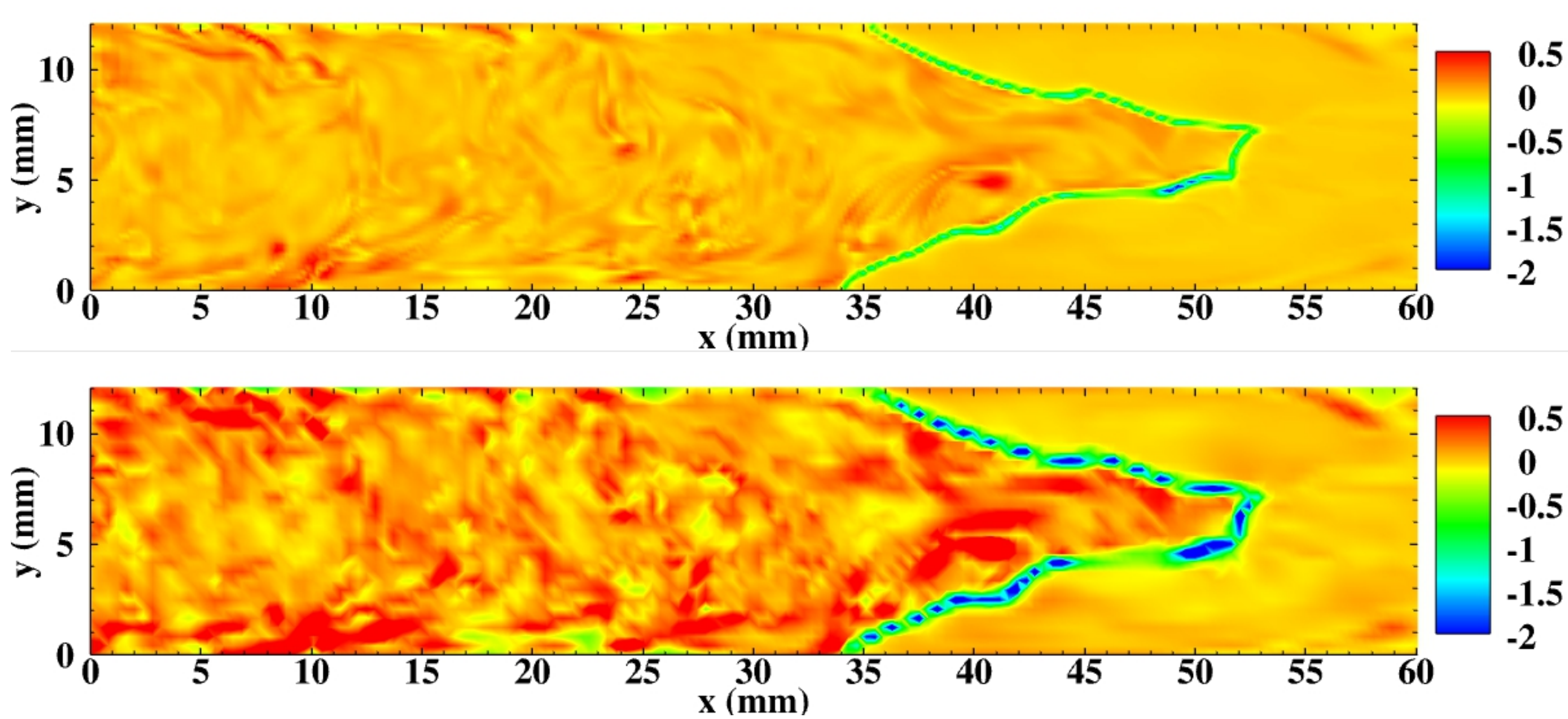
k_{sgs}/ε

Low

High

P/ε

Low



Uncertainty Quantification in Gas Turbine Simulations

Application to Chemistry Model

CFD and Predictions

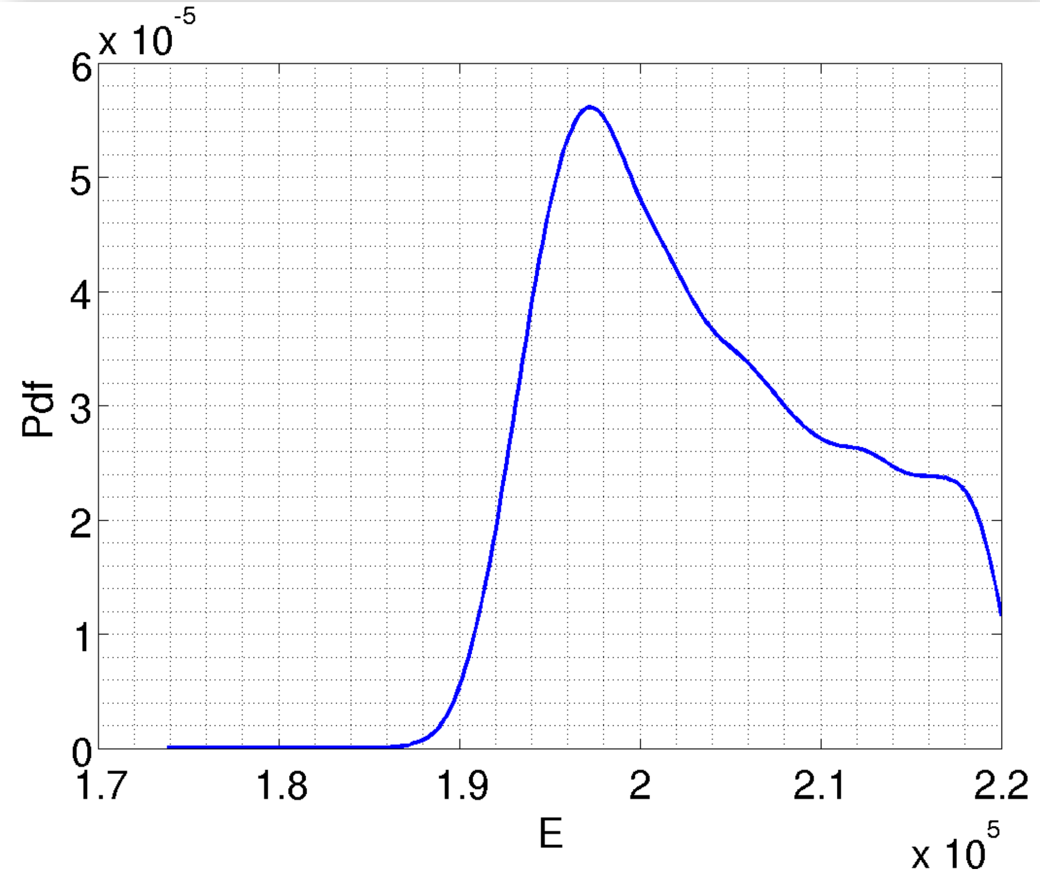
- **The goal of CFD is to issue predictions at future conditions**
  - ➡ No corroborating data exist
- **CFD models are highly imperfect**
  - ➡ Varying degree of error
- **How reliable are the predictions?**
  - ➡ Measure of prediction error is necessary
  - ➡ Termed as prediction uncertainty
  - ➡ Field of uncertainty quantification (UQ)

Uncertainty Quantification (UQ) Basics

- **Models are necessarily imperfect**
- **Measurements designed to calibrate models also contain errors**
- **Two forms of errors**
  - ➡ Model form error arising from specific model formulation
    - Example: Specific set of reactions to describe fuel combustion
  - ➡ Parametric uncertainty
    - Reaction rates cannot be determined to arbitrary precision
- **UQ theory**
  - ➡ Uses experiments (data) to develop a probabilistic estimate of the parameters and model form errors

Bayesian Theory of UQ

- **Based on assigning probabilistic values for parameters**
  - ➡ No single value but a likely range of values
- **Uncertainty in knowledge expressed through PDFs**
  - ➡ For instance, PDF of parameters
- **Use Bayes' theorem to utilize data for finding these PDFs**
  - ➡ As more data is available, PDFs change
  - ➡ Reflects a change in our knowledge of the system



PDF of activation energy obtained by using many different experiments

Bayesian Learning or Bayesian Inference

- **The basis of Bayesian inference is the Bayes theorem**
- **Consider two events A and B**
- **Bayes' theorem relates the conditional PDFs of the two events to the marginal PDFs**

Likelihood

Prior

$$P(A|B) = \frac{P(B|A)}{P(B)} P(A)$$

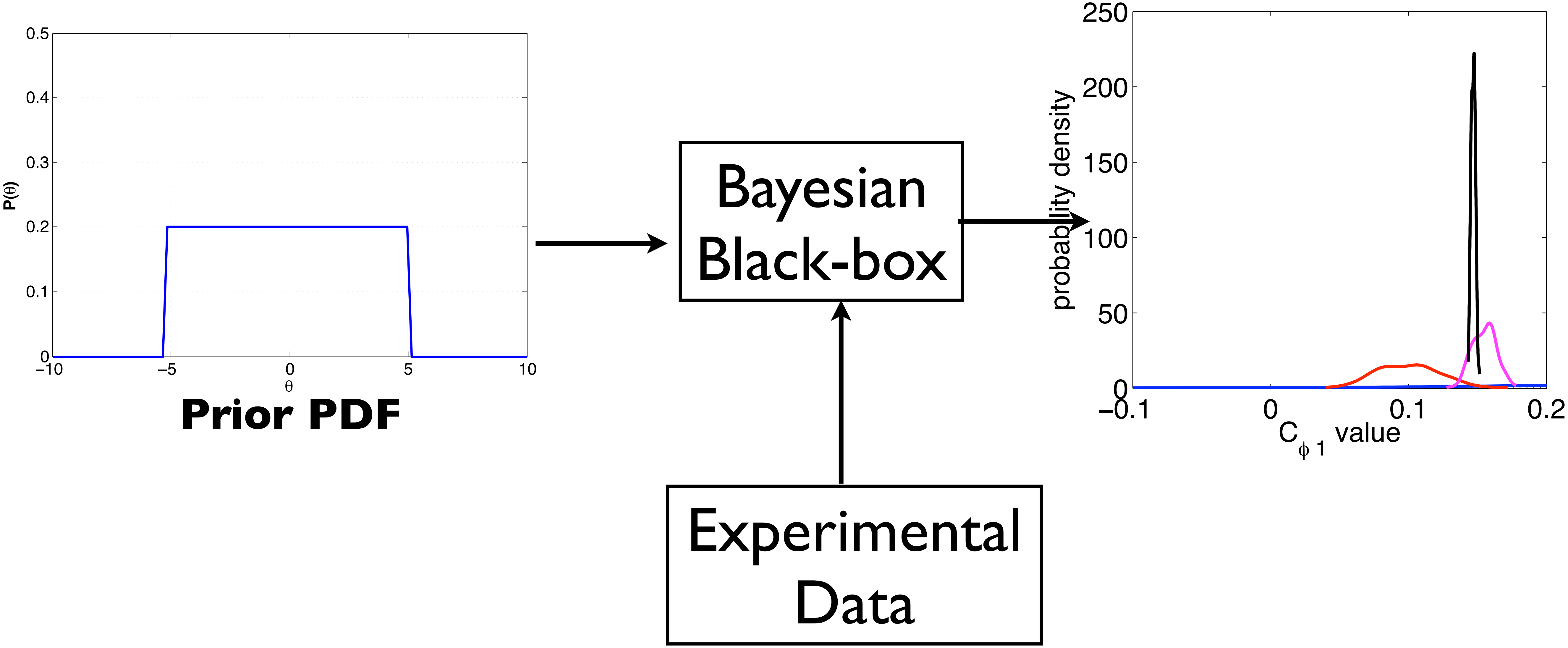
Posterior

Probability of Evidence

➡ For example, A could be the activation energy, and B will be experimental data

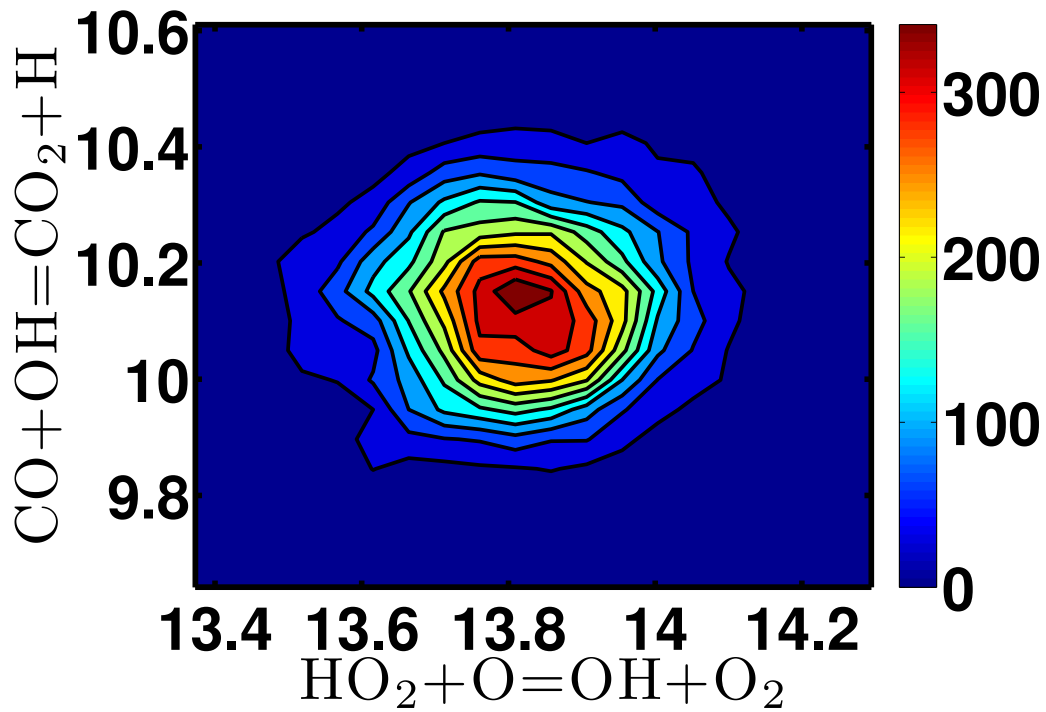
➡ The Bayes' theorem then updates the activation energy given the experimental data

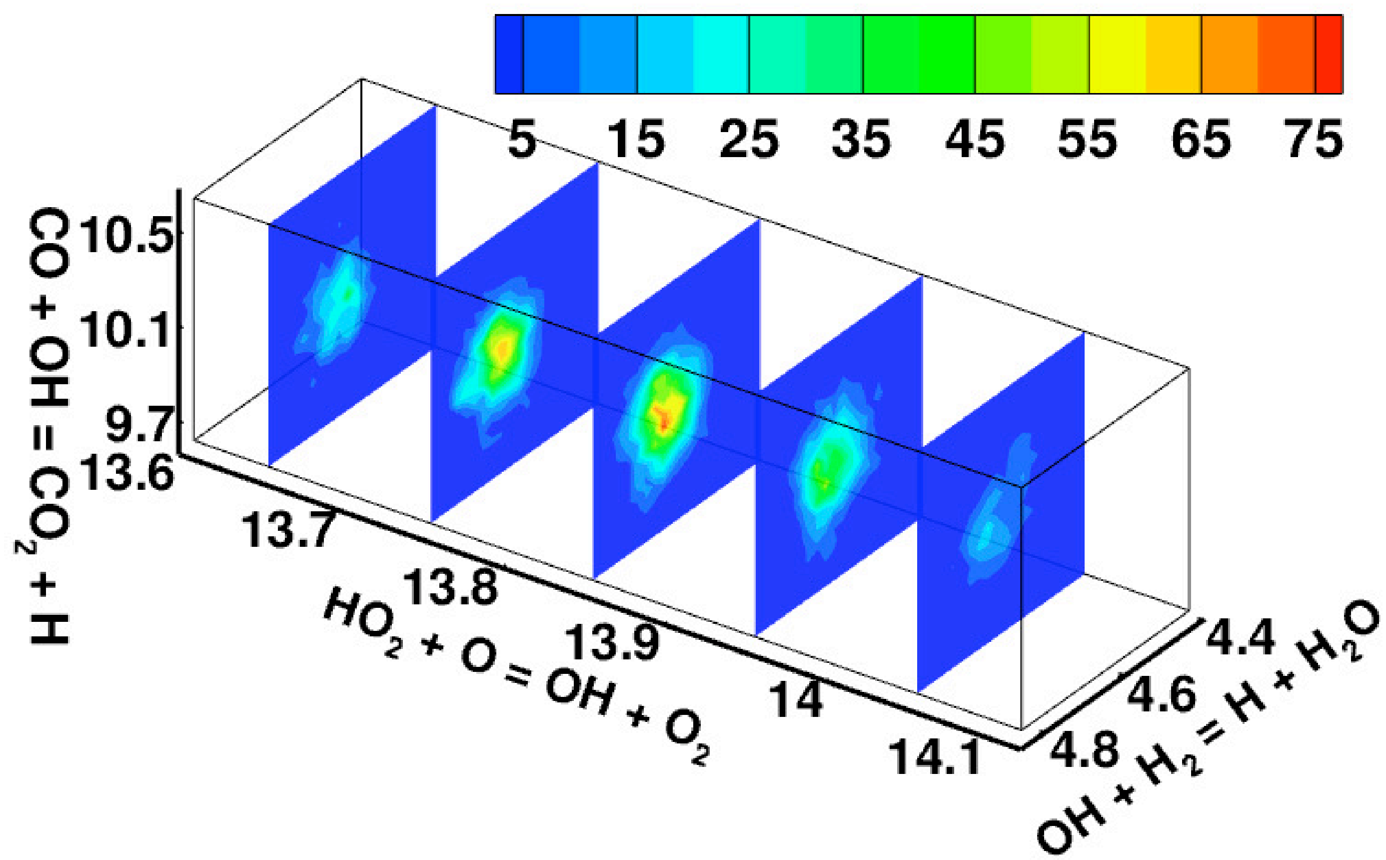
Bayesian Learning Process



Application to Syngas Chemistry Mechanism

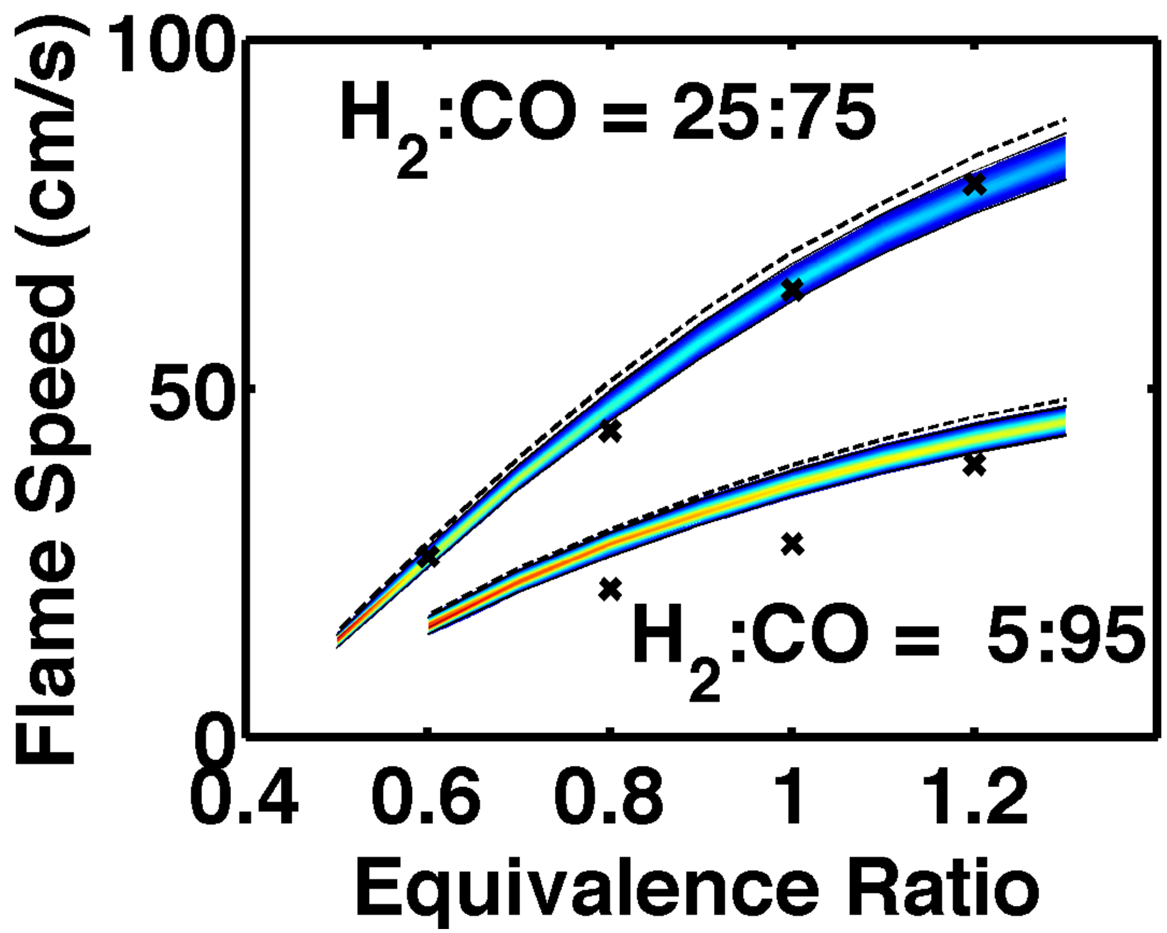
- **Several mechanisms used as starting point**
- **Calibrations carried out using experimental data**
    - ➡ >10 parameters jointly calibrated
    - ➡ PDFs are joint distribution of all variables





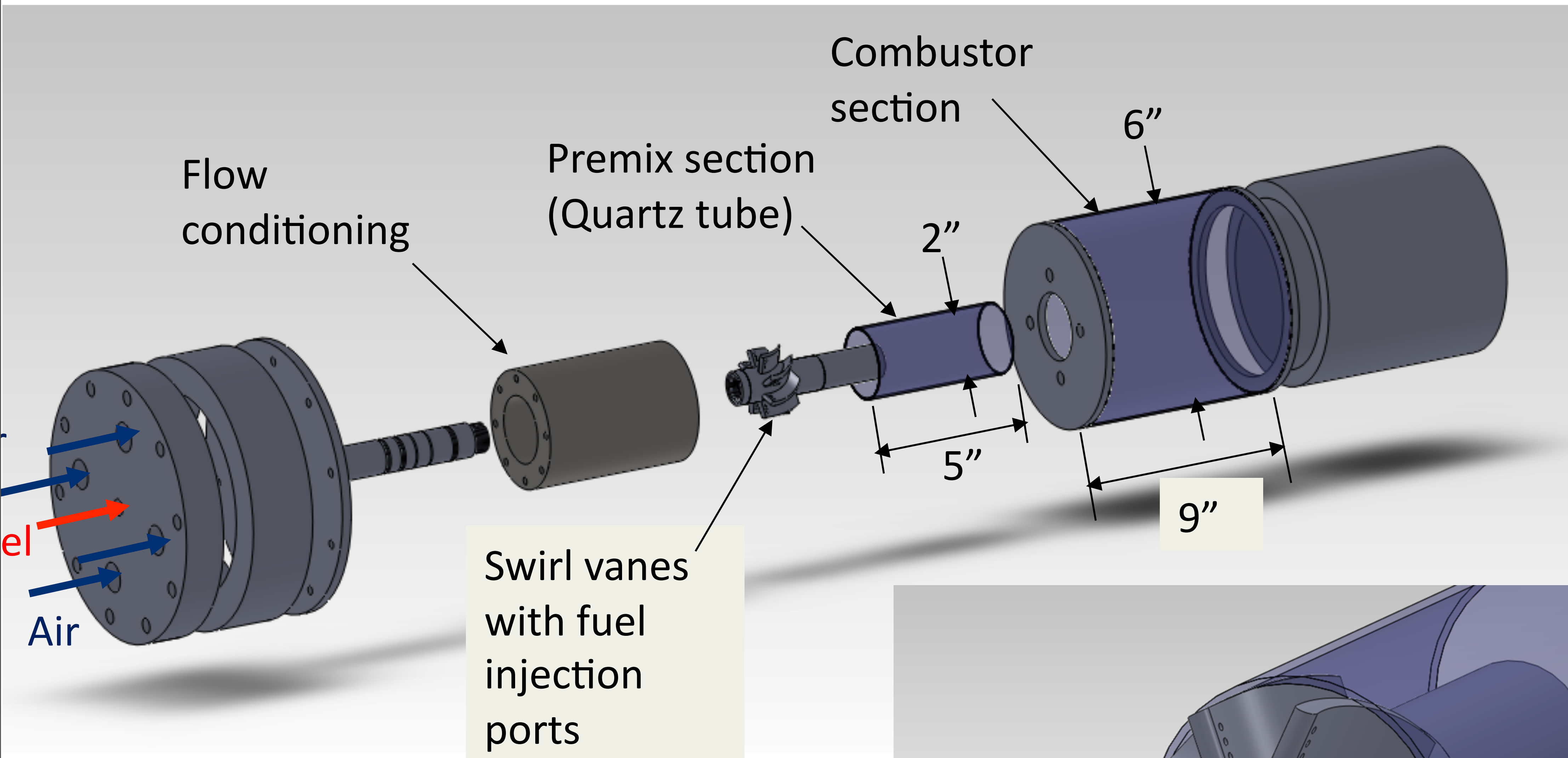
Prediction Uncertainty

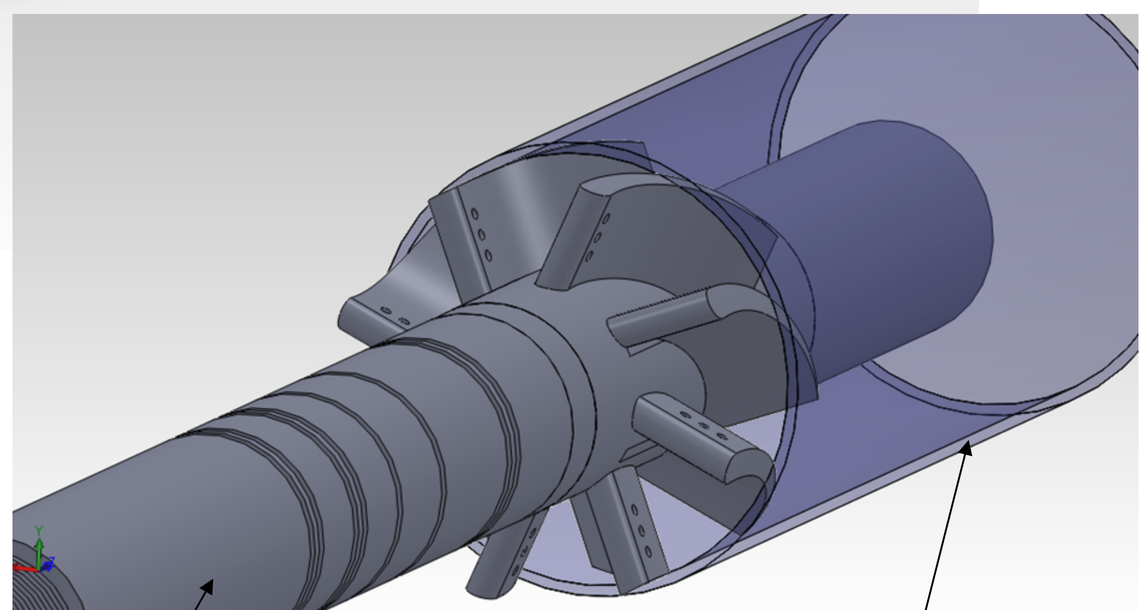
- **Calibration using 10 atm. data**
  - ➡ Prediction at 20 atm.
- **PDFs used to develop prediction uncertainty**
- **Note that experiments also contain errors**
- **Inability to match experiments**
  - ➡ Points to model failure
  - ➡ Lack of appropriate experiments needed for calibration
  - ➡ Information used to design future experiments



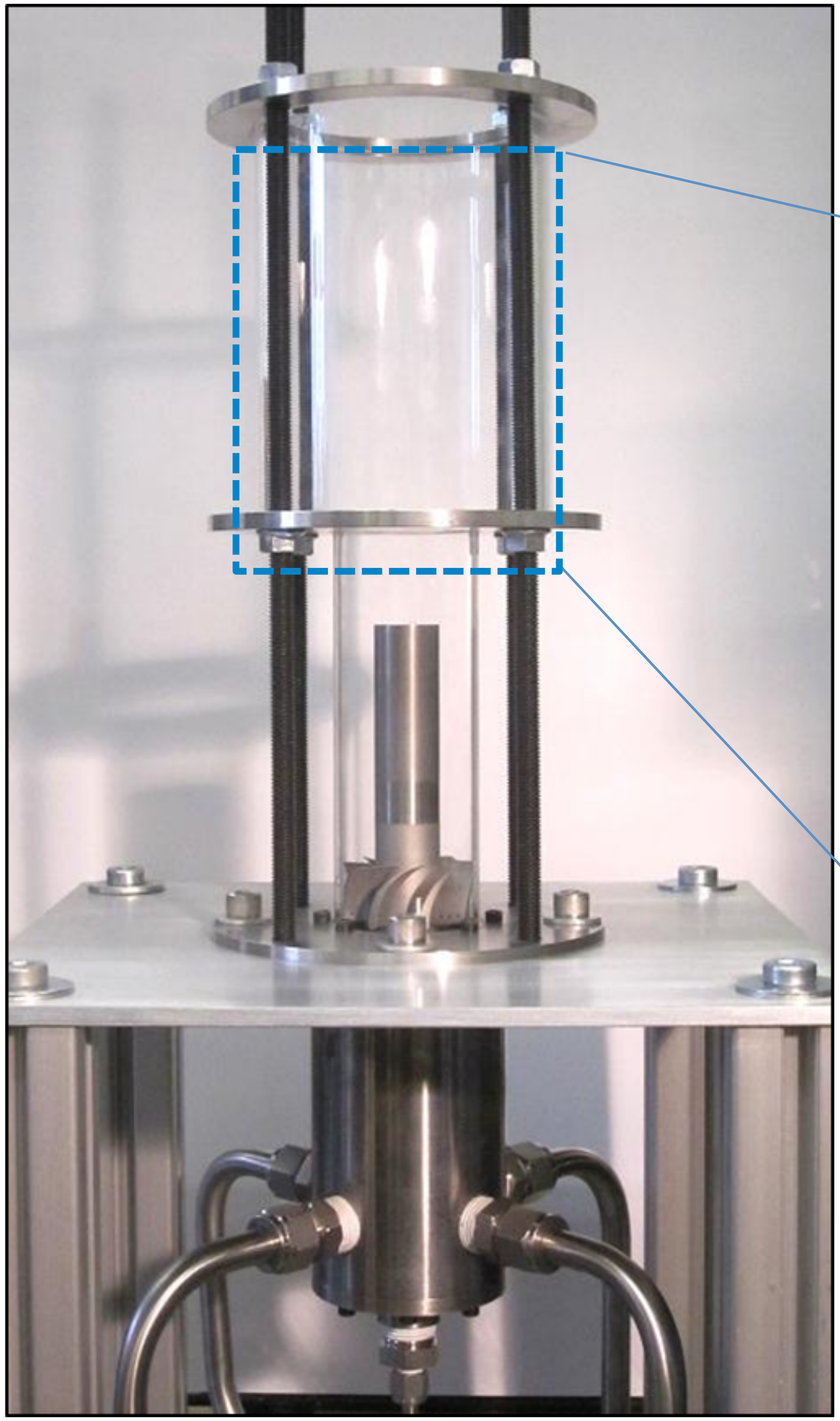
UT Swirl Burner Studies

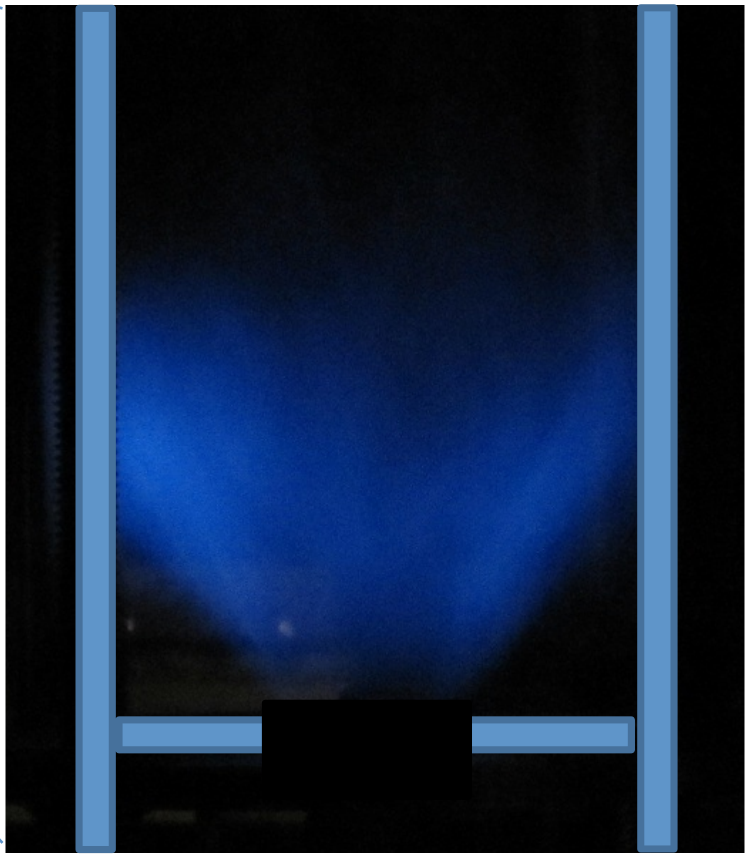
Swirl Burner Design





Burner Operation

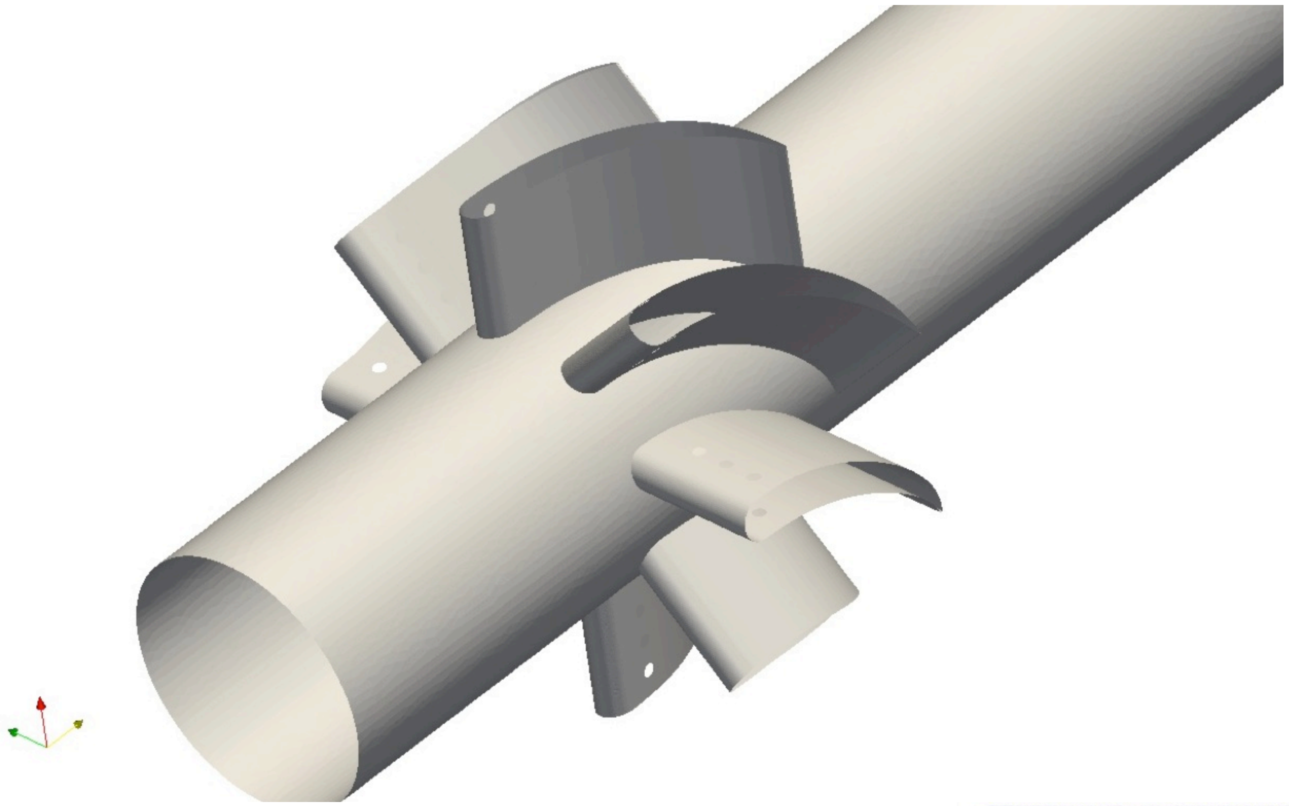




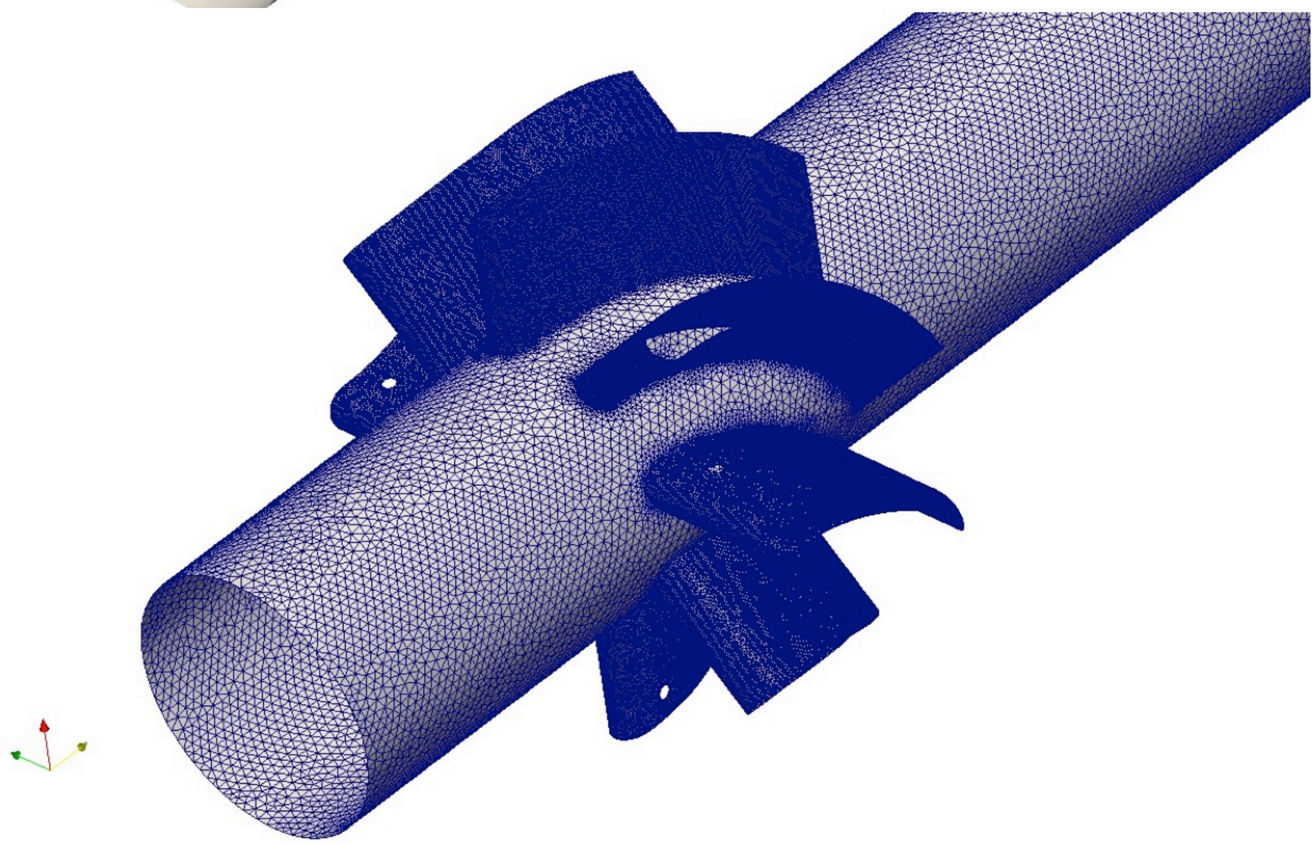
Lean-premixed ($\phi = 0.6$) methane-air swirl flame

CFD for Burner Design and Operation

- **Use high-fidelity simulations to determine relevant experimental conditions**
  - ➡ Minimizes experimental testing
  - ➡ Better suited for model validation

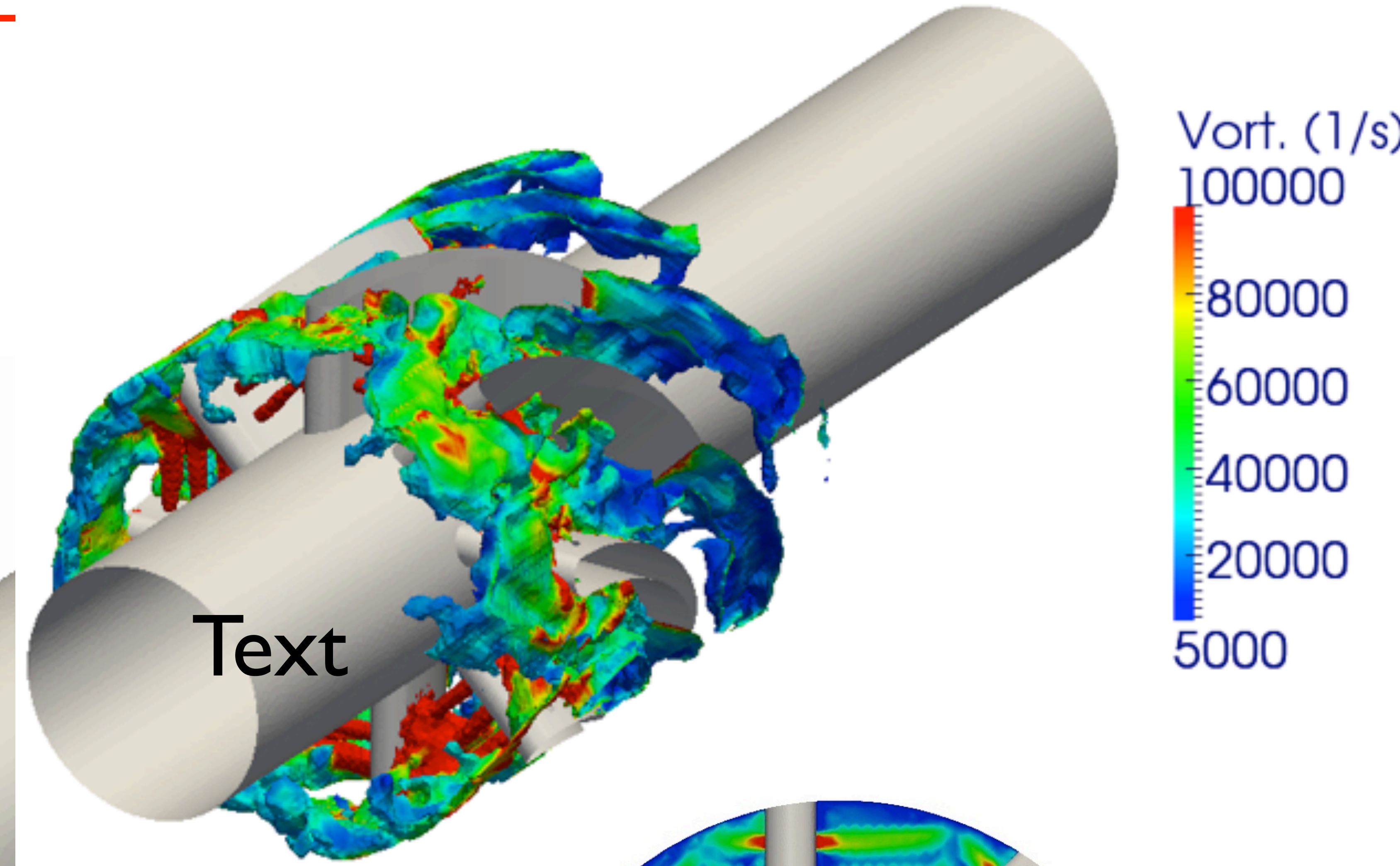


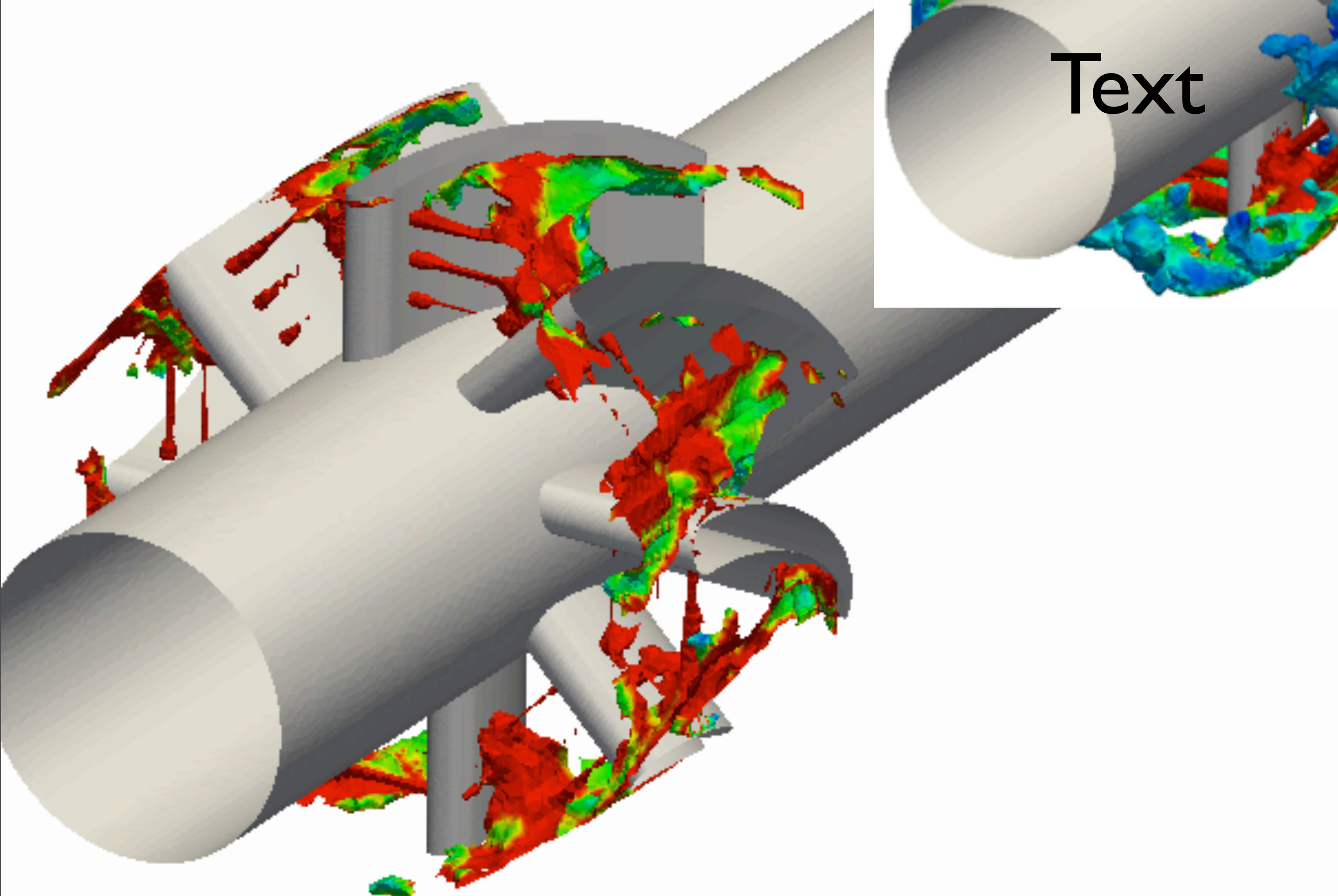
- **OpenFOAM based LES modeling of mixing**
  - ➡ To understand the role of jet-jet interaction in vane-based injection
  - ➡ Effect of hydrogen addition in methane jet

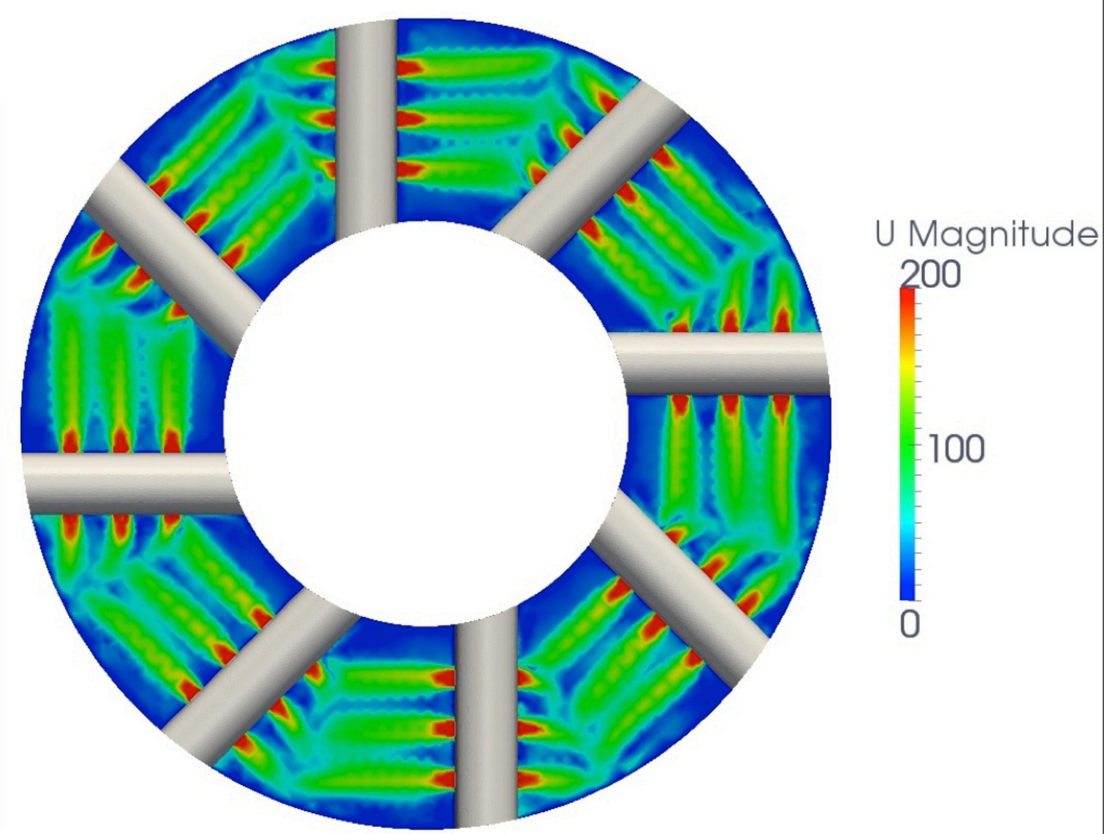


Preliminary Results

- Hydrogen Jet: 200 m/s
- Crossflow at 10 m/s
- 6 injection holes/vane







Status

- **JICF studies**
  - ➡ UT experiments ramping up; Initial data being analyzed
  - ➡ UT simulations being performed
  - ➡ OpenFOAM implementation being transferred to Siemens
    - (Open to other industrial partners)
- **UQ Computations**
  - ➡ Chemistry UQ completed
  - ➡ Transition to full CFD computations
- **UT swirl burner**
  - ➡ Design, fabrication, and initial runs complete
  - ➡ Experimental conditions being optimized using LES computations