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

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Challenges in Simulating Gas Turbines

- **Lack of appropriate physical models**
  - ➡ Unsteady dynamics, wall-flame interactions, multiple combustion regimes
- **Less than ideal validation data**
  - ➡ Diagnostic fidelity reduces with flow complexity
    - High-pressure confined environment
- **Geometric complexity**
  - ➡ Vanes, swozzles, etc.
  - ➡ Unstructured grid systems are indispensible
- **Uncertainty**
  - ➡ Boundary conditions, chemistry, operating conditions

Operating Hypotheses

- **Combined LES and RANS capabilities**
  - ➡ LES is not the solution to all problems
  - ➡ RANS has lot of unrealized potential
- **Experiments in the absence of modeling guidance is not useful for advancing predictive capability**
  - ➡ Models should capture sensitivity to parameters in a real gas turbine
  - ➡ Experiments should be designed to reproduce this sensitivity
    - Non-trivial exercise
    - Current simulation approaches cannot provide this guidance

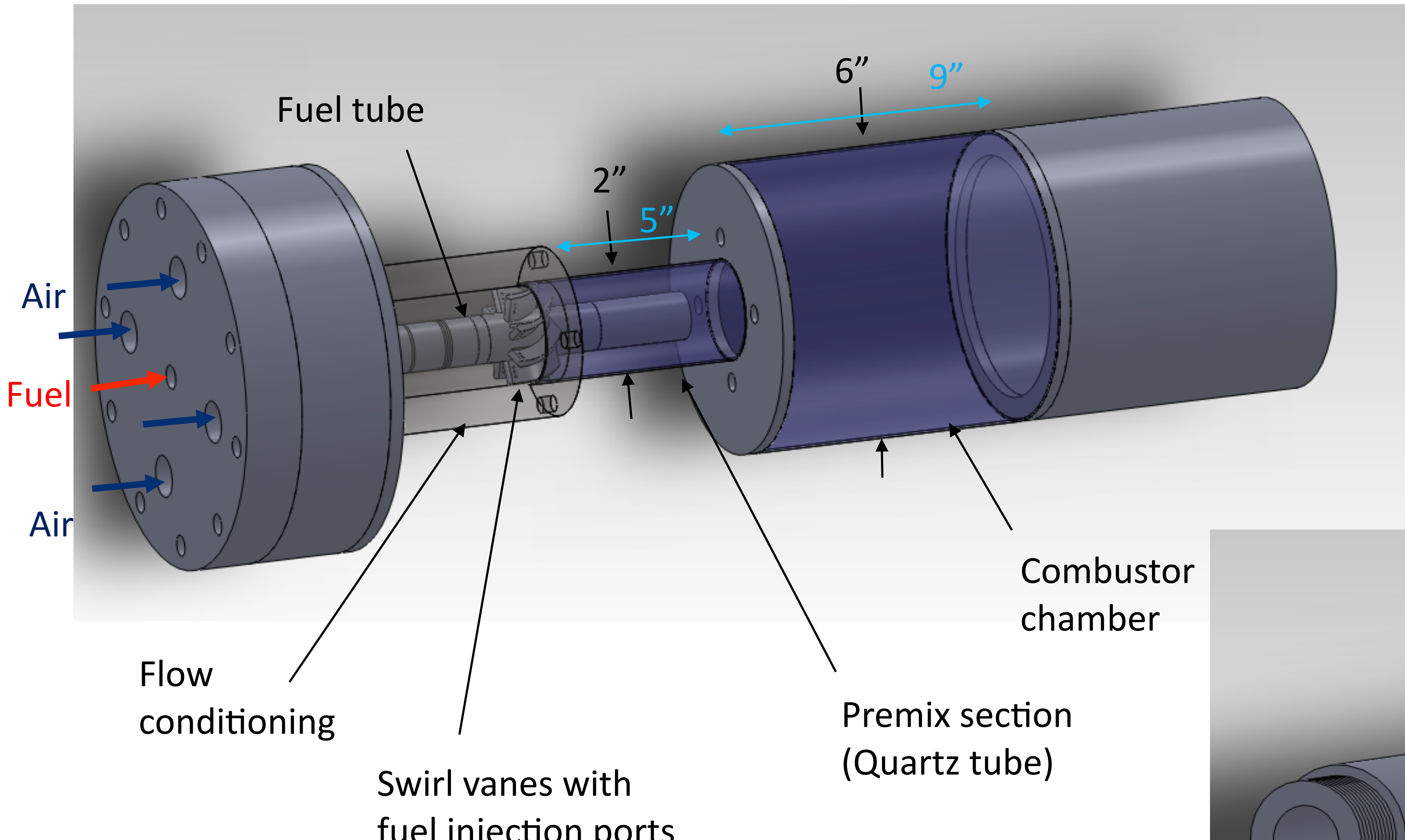
Objectives

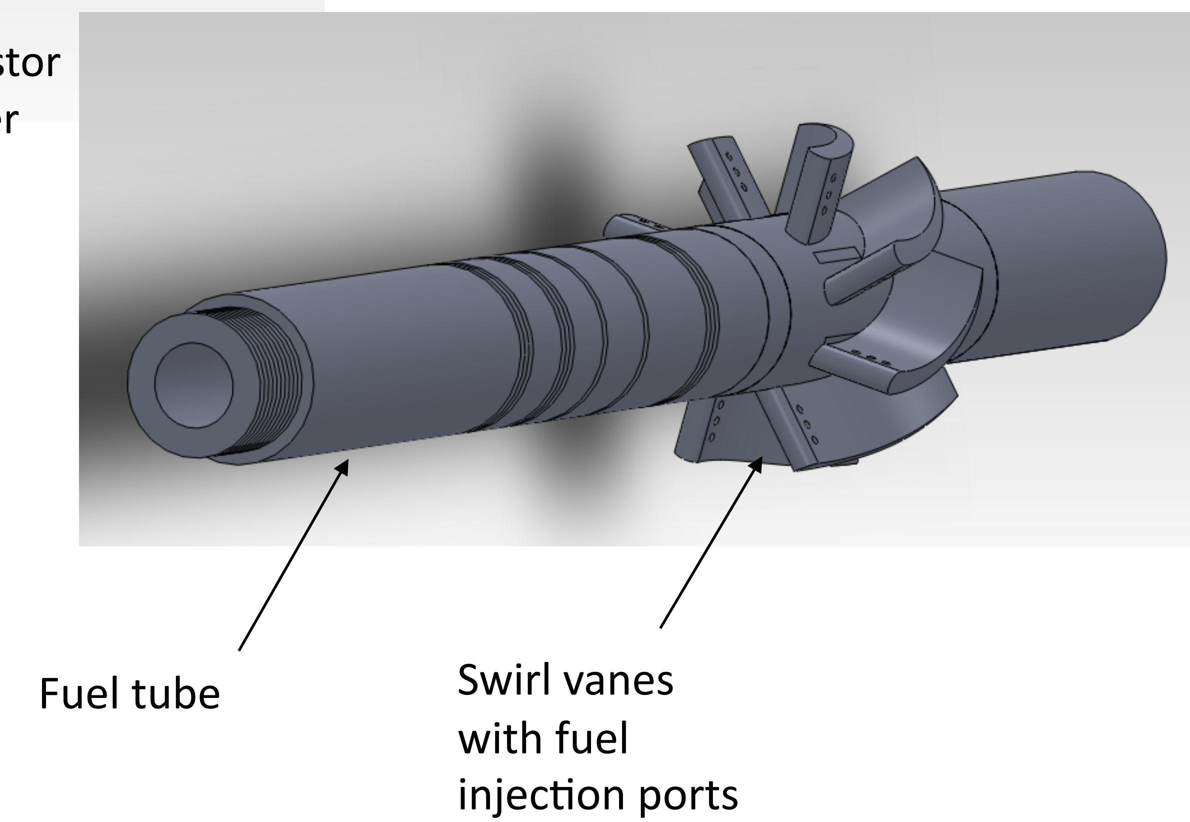
- **Integrate high and low fidelity computational models (LES, RANS) with experiments**
  - ➡ To capture unsteady dynamics in gas turbine combustors
  - ➡ Provide **predictive** insight in the design process

- **Target-based model development**
  - ➡ UT high-pressure combustor as the overarching simulation

Target System

- **UT high-pressure swirl combustor**





Key Issues

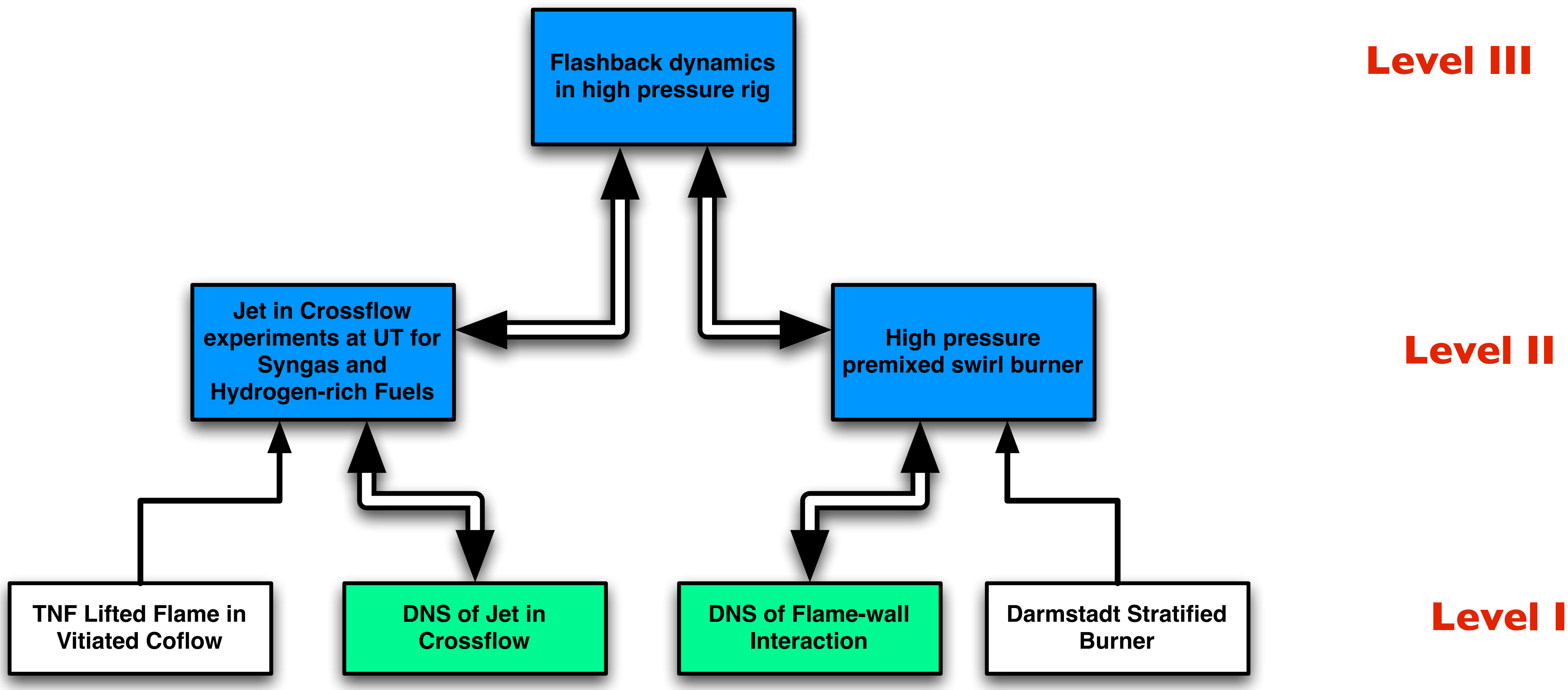
- **Fuel injection, mixing, and combustion**
  - ➡ Crossflow jet configuration
  - ➡ Flame stabilization and mixing issues

- **Flashback dynamics**
  - ➡ Flame propagation in turbulent core flow
  - ➡ Flame-wall interaction and boundary layer modulation

Key Computational Issues

- **LES-based modeling**
  - ➡ Combustion models in complex geometries
  - ➡ Flame-wall interaction modeling
  - ➡ Jet-in-crossflow anomalous behavior
- **Predictive uncertainty in RANS**
  - ➡ Highly parameter dependent turbulence models
- **Technology transfer**
  - ➡ A common platform to share advances with industry

Hierarchical Validation Pyramid

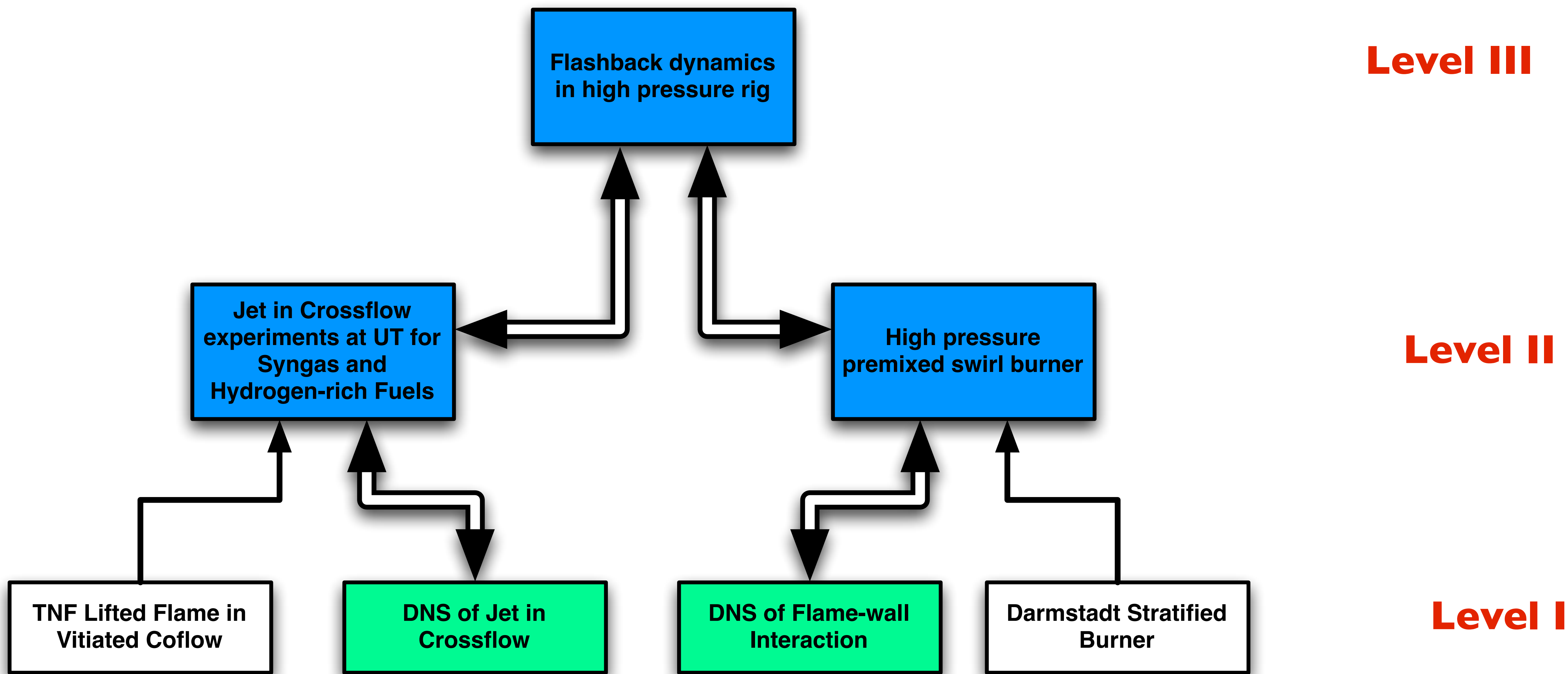


- **Level 1 - Fundamental data from legacy expts. and direct numerical simulations (DNS)**
- **Level 2 - UT re-configurable experiments designed for validation**
- **Level 3 - UT target system experiments**

Research Plan

- **UT high-pressure swirl combustor experiments**
  - ➡ Validation driven experiments
- **LES model development**
  - ➡ Eulerian probability density function (PDF) approach for complex geometries
  - ➡ Transported-equation based dissipation rate model
- **RANS accuracy improvement**
  - ➡ Calibration as a mathematical approach
  - ➡ Propagating uncertainties in chemistry and boundary conditions
- **Open source model transfer**
  - ➡ OpenFOAM based model implementation

Hierarchical Validation Pyramid



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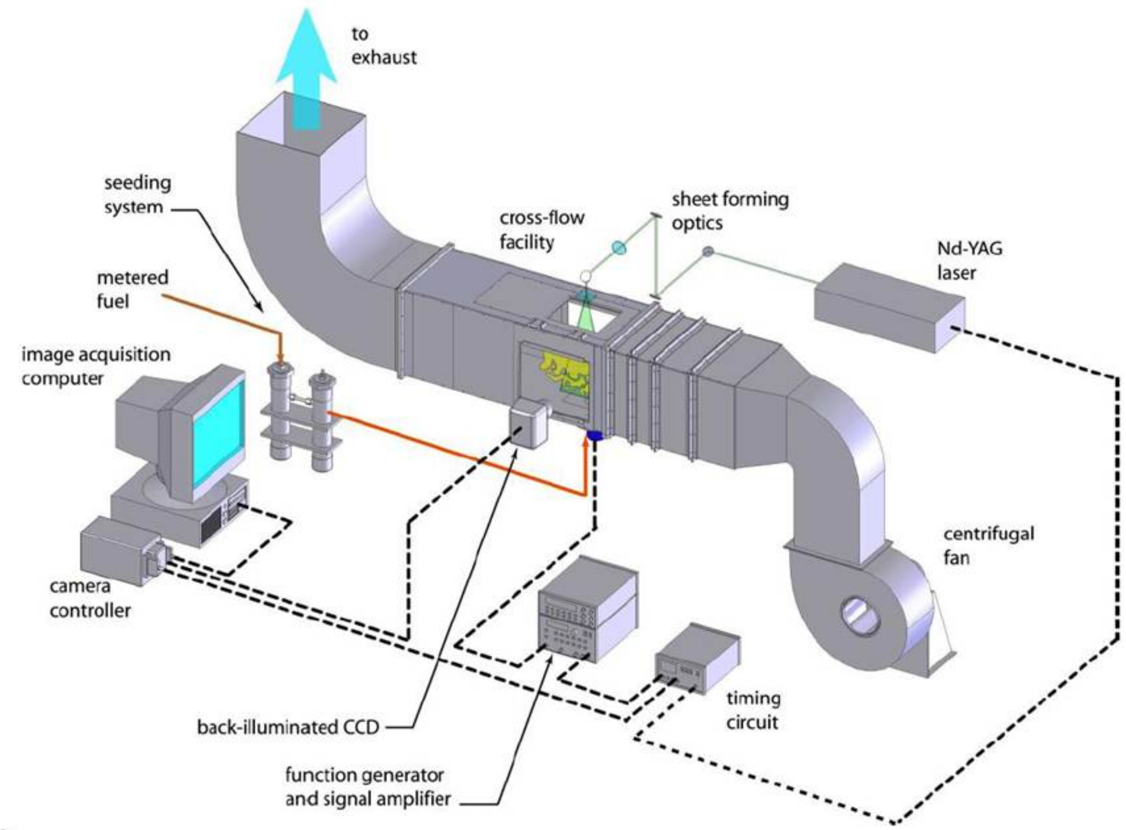
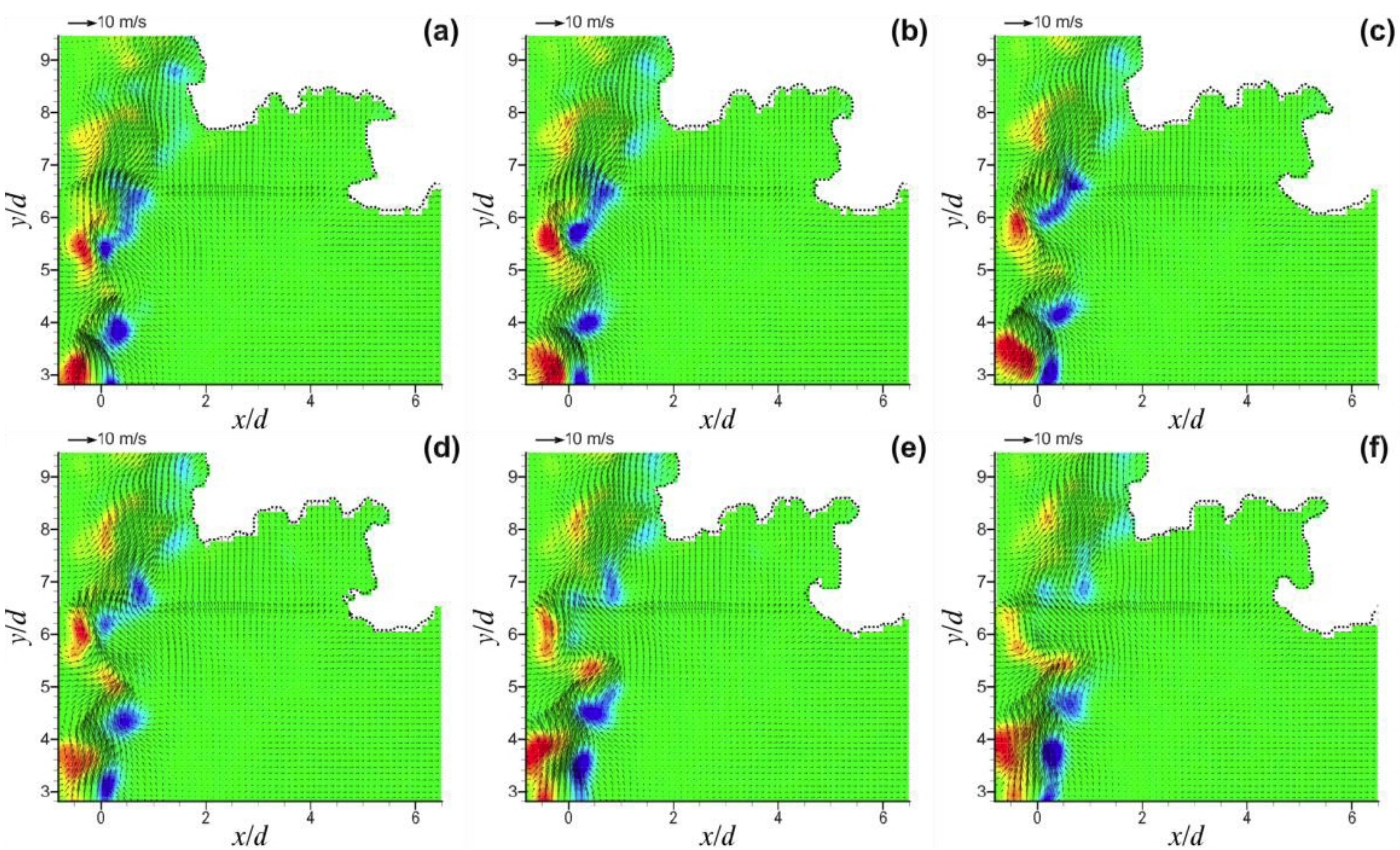
Pitched Jets in Crossflow

- **Variations in jet angle, fuel composition**

Figure 12: **Jet flames in crossflow with different levels of premixing. The fuel is 70% CH4 + 30% H2. (a) non-premixed, (b) jet fluid diluted by 25% (volume basis) with air, and (c) jet fluid diluted by 50% with air.**



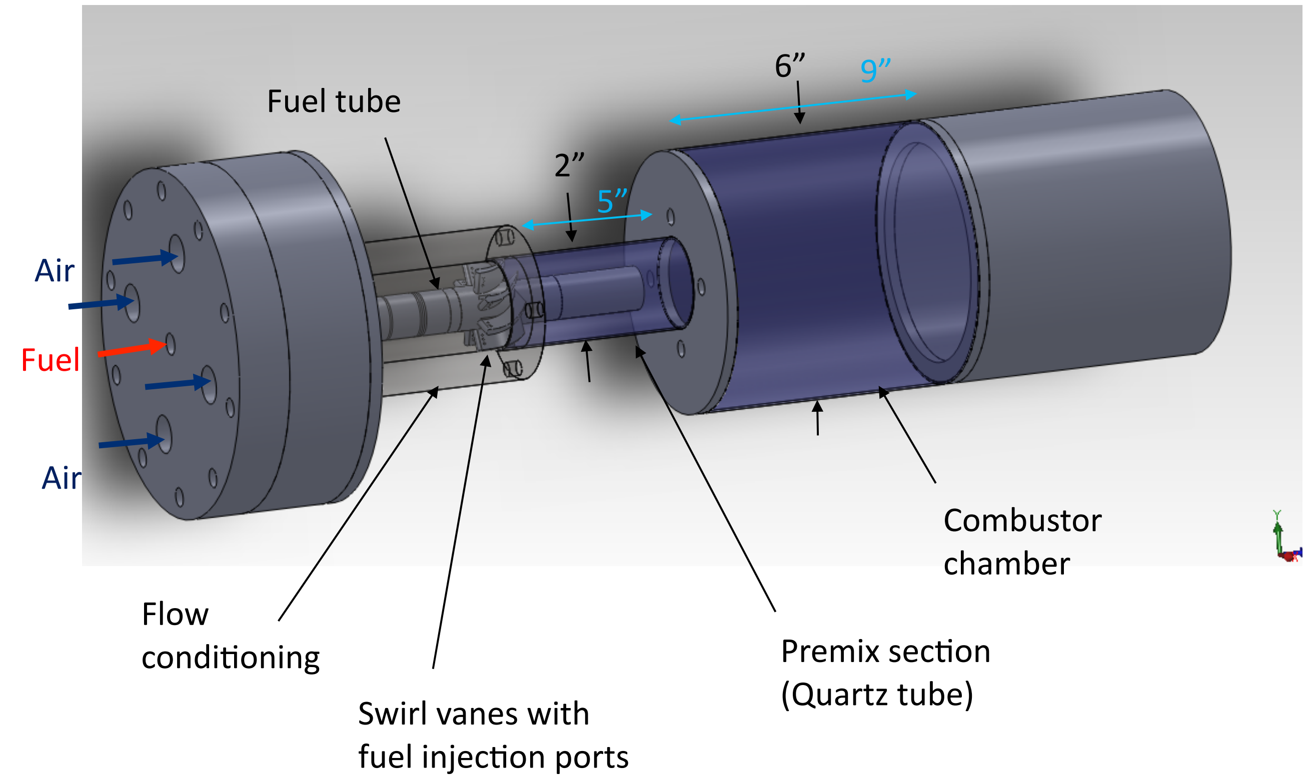


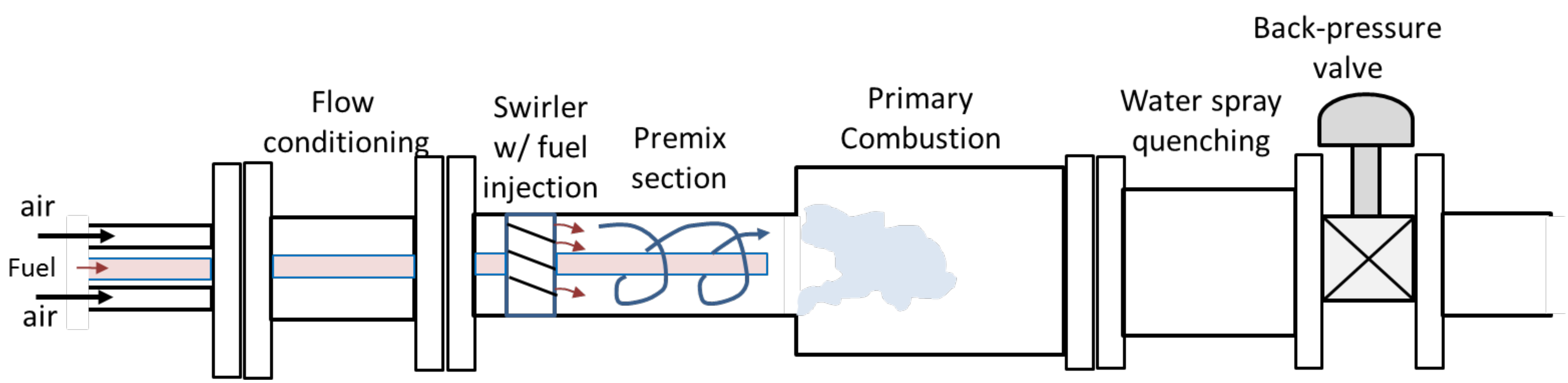
LES of JICF

Simultaneous PLIF +PIV

Flashback Dynamics

- **Fuel injection through swirl vanes**
- **Flashback induced through back-pressure valve**
- **Optical access for simultaneous velocity/scalar measurements**





Modeling Approach

- **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**

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

- **PDF transport equation**

Chemical Source

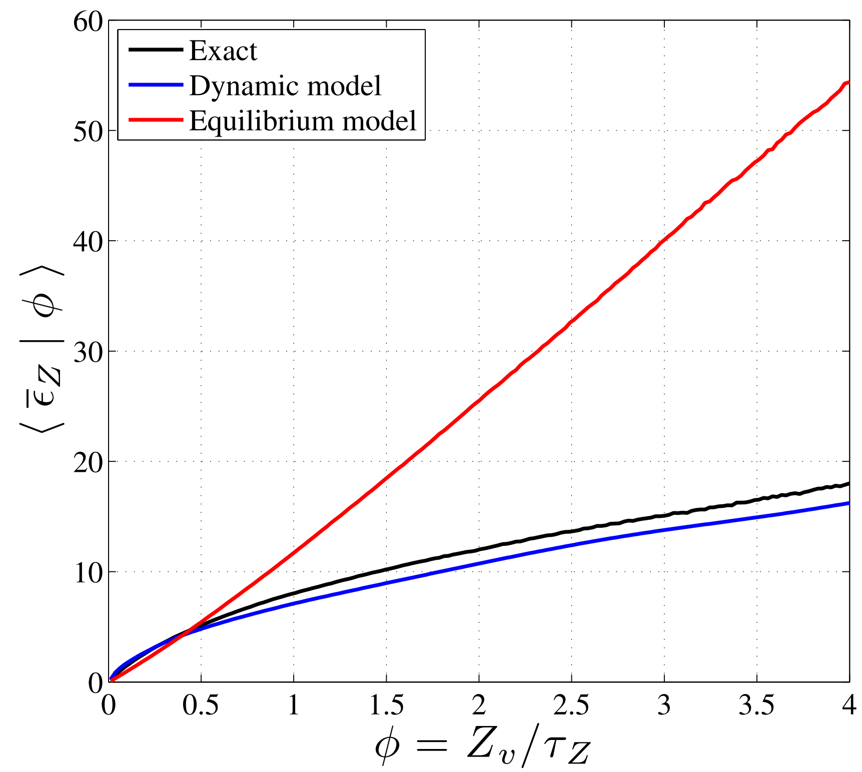
$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j}\left[P\widetilde{u_j|\boldsymbol{\zeta}}\right] = -\frac{\partial}{\partial \zeta_\alpha}\left[P\widetilde{\mathcal{M}_\alpha|\boldsymbol{\zeta}}\right] - \frac{\partial}{\partial \zeta_\alpha}\left[PS_\alpha\right]$$

Conditional Diffusion

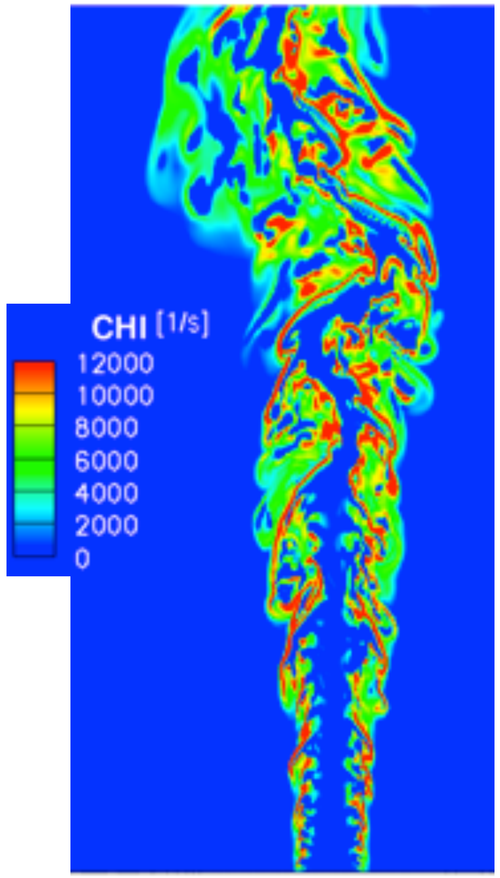
  - ➡ Condition diffusion requires a model for scalar dissipation rate

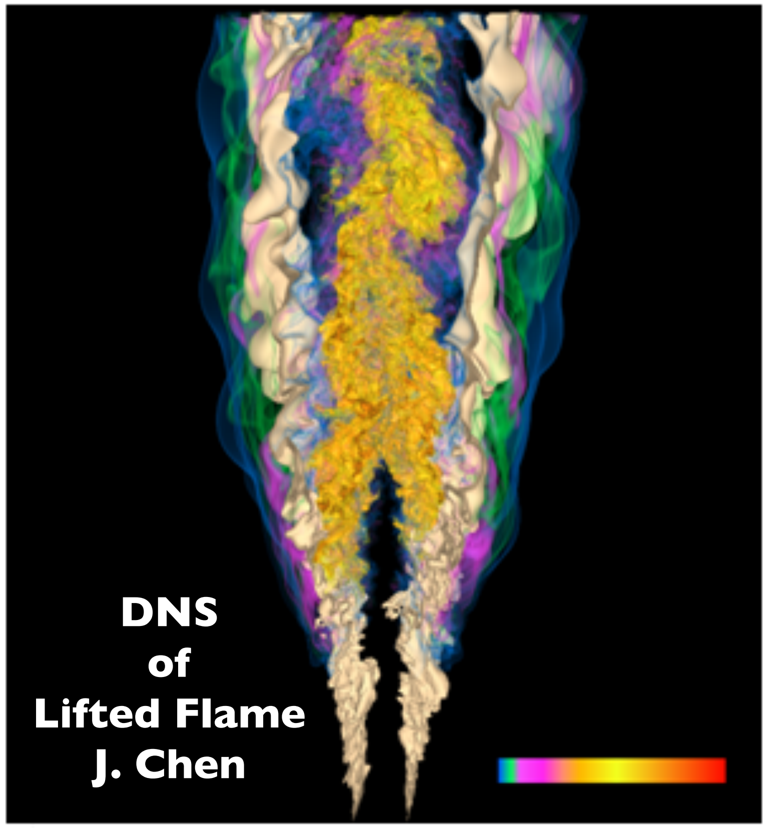
Nonequilibrium Dissipation Rate Model

- **Currently used dissipation rate models rely on equilibrium assumption**
  - ➡ Highly restrictive
  - ➡ Invalid even in homogeneous isotropic turbulence



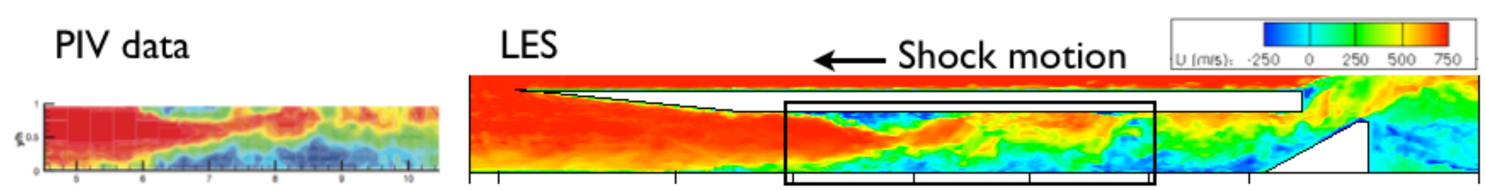
- **Transport-equation based dissipation model**
  - ➡ Incorporates spatial transport of scalar energy
  - ➡ Allows scalar and turbulence scales to be decoupled

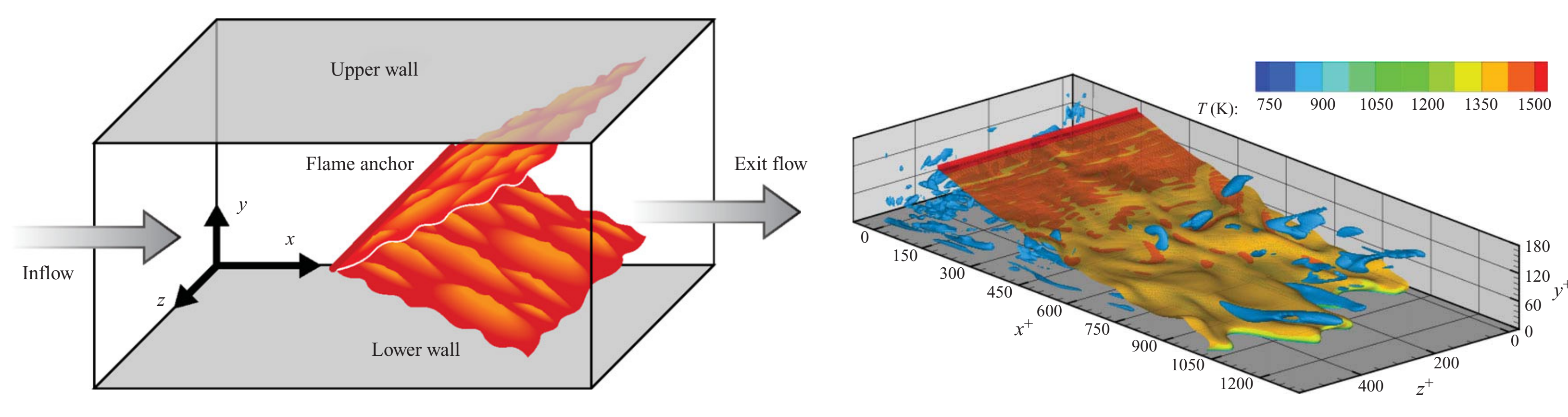




Flame-Wall Interaction

- **Propagation of flames in a boundary layer**
  - ➡ Modulates the turbulent boundary layer
  - ➡ Alters turbulent energy transport and dissipation
- **Similar to unstart propagation in scramjets**
  - ➡ Propagation of density/ pressure fronts through a separated boundary layer
- **DNS-based analysis of turbulent flux models**





DNS of J. Chen (Sandia)

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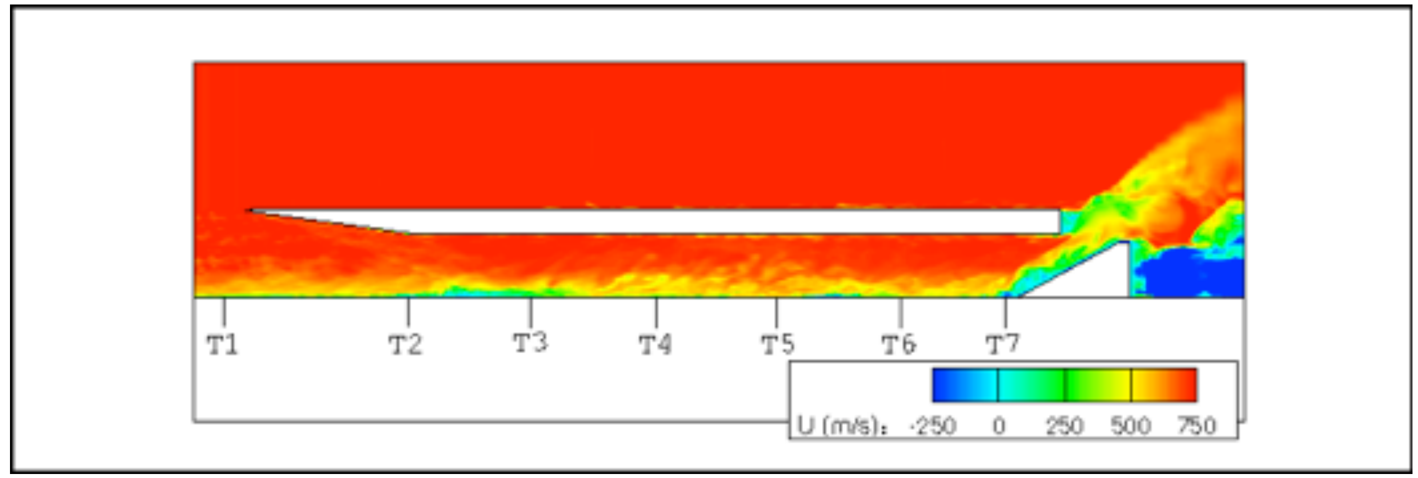
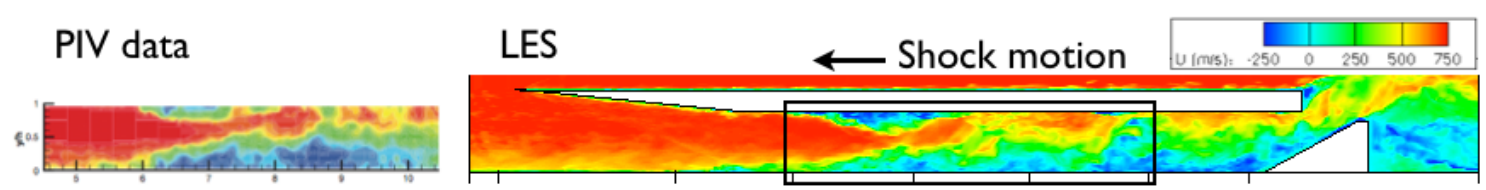
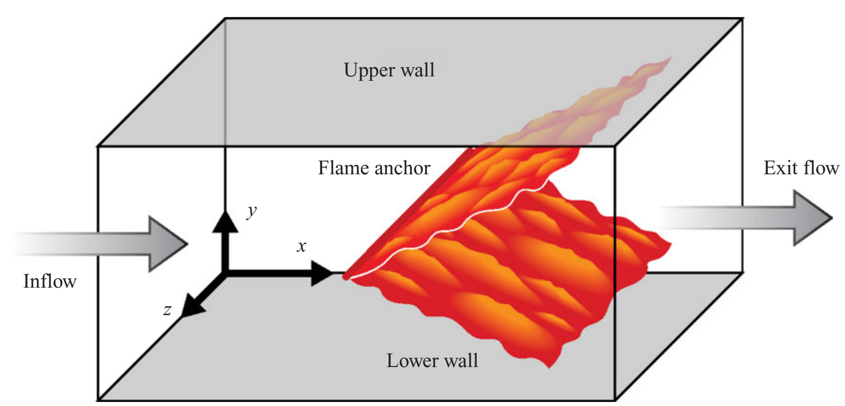
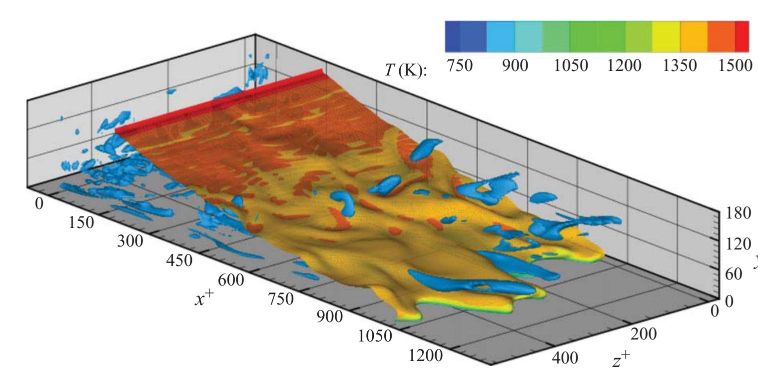








DNS of J. Chen (Sandia)

Modeling PDF Transport Equation

- **PDF transport equation**

Chemical Source

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

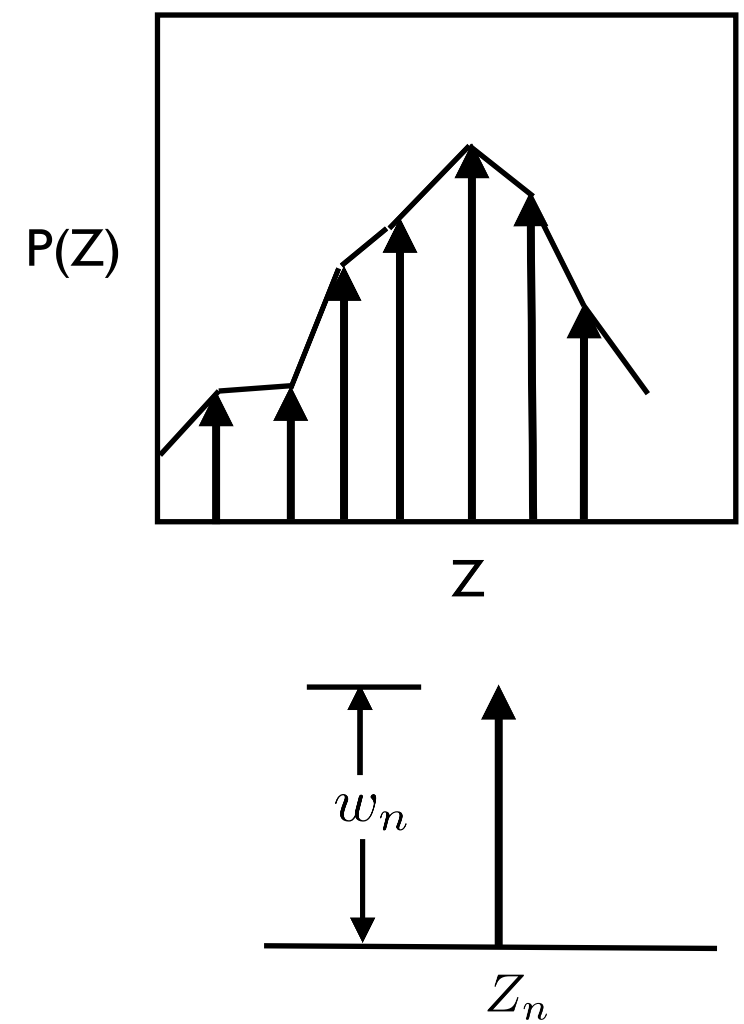
Conditional Diffusion

- **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

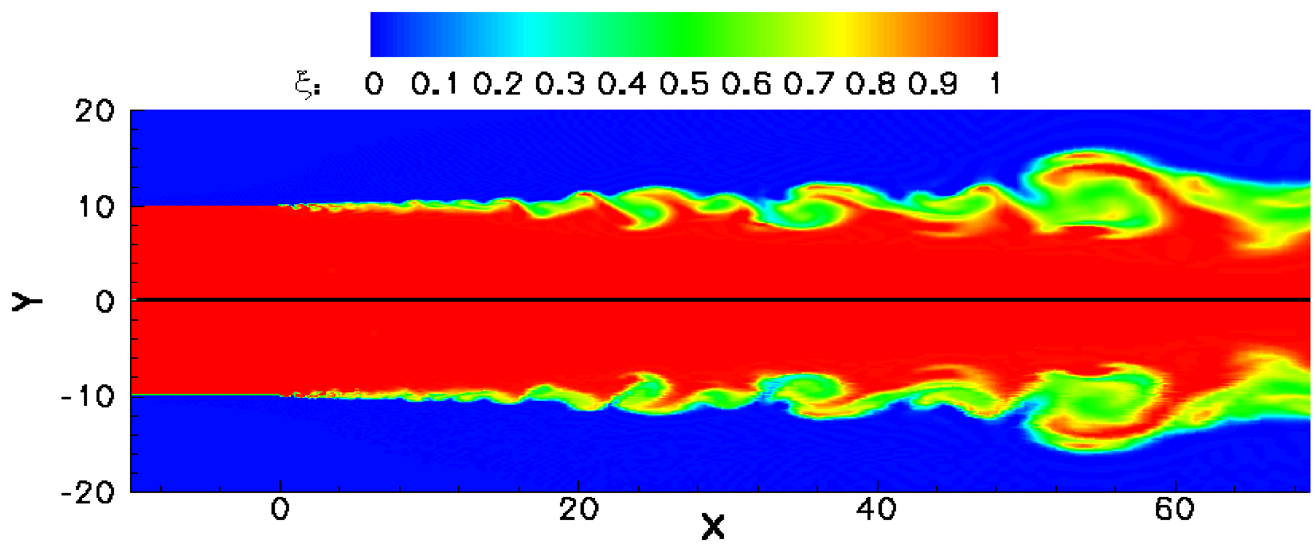
Direct-Quadrature Method of Moments (DQMOM)

- **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**

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



Test case : 2-D shear layer



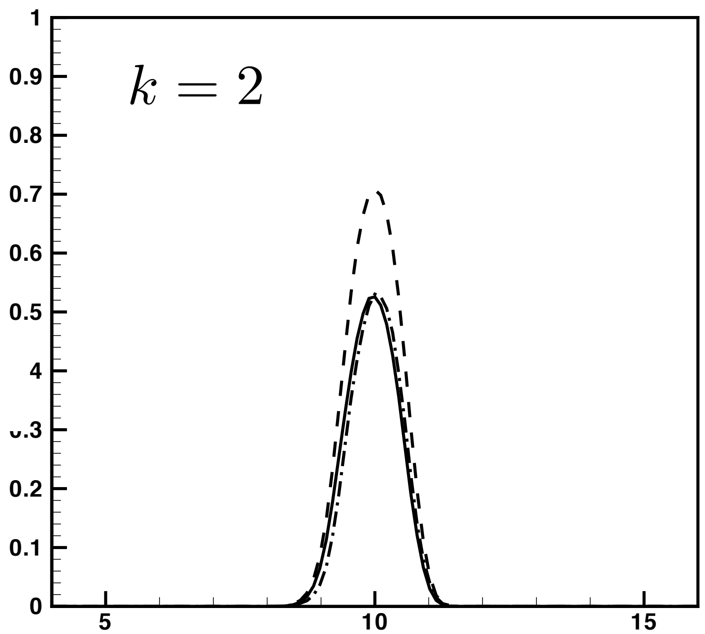
- **Flow conditions similar to the experiment of Mungal and Dimotakis (1984)**
- **Two streams at velocity of 8.8 m/s and 22 m/s**
- **Single step chemistry formulated using progress-variable and mixture fraction**

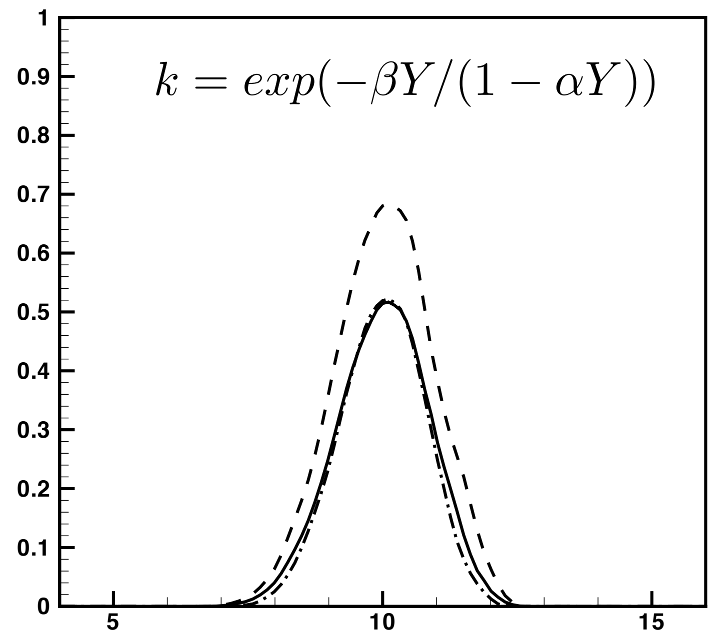
$$S(Y, Z) = k\left(\frac{Z}{Z_{st}} - Y\right)\left(\frac{1-Z}{1-Z_{st}} - Y\right)$$

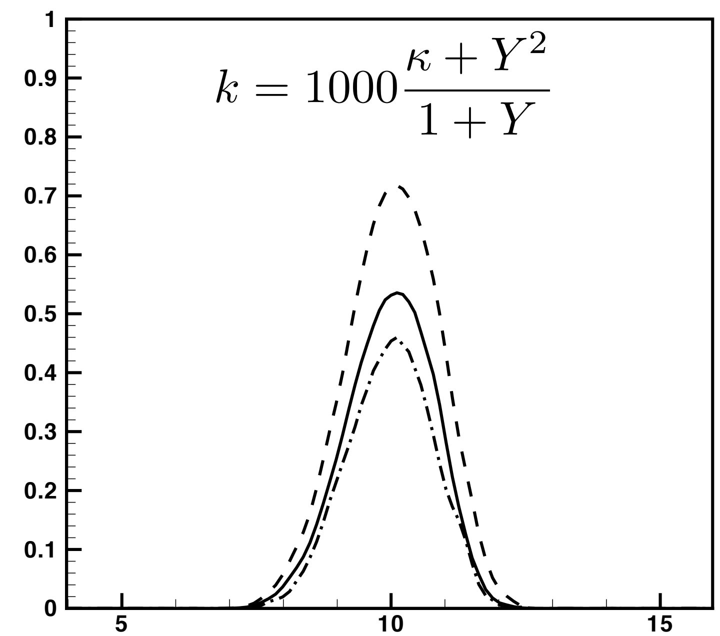
- **Test cases performed**
  - ➡ LES simulation of first moment of Y,Z and second moment of Z
  - ➡ Lagrangian simulations with IEM mixing model
  - ➡ DQMOM simulation with IEM mixing model and 2-peak formulation
  - ➡ Different functional form for rate constants

Test results

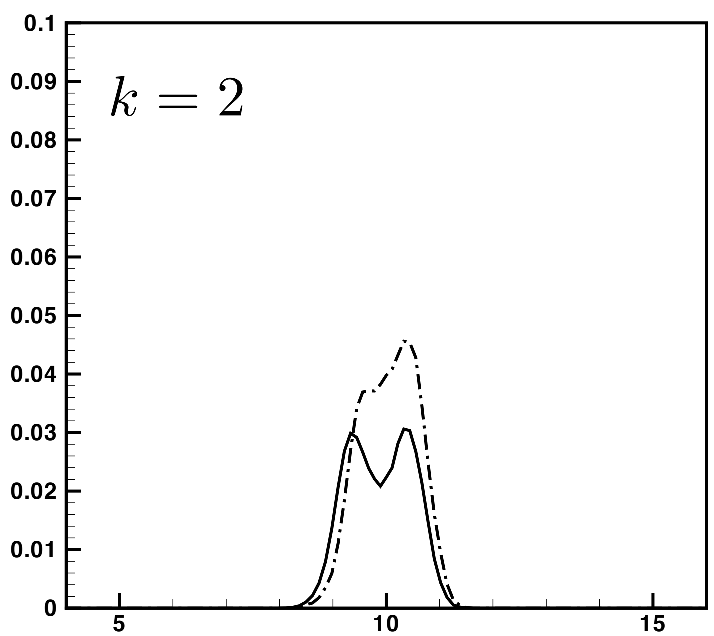
Progress variable mean

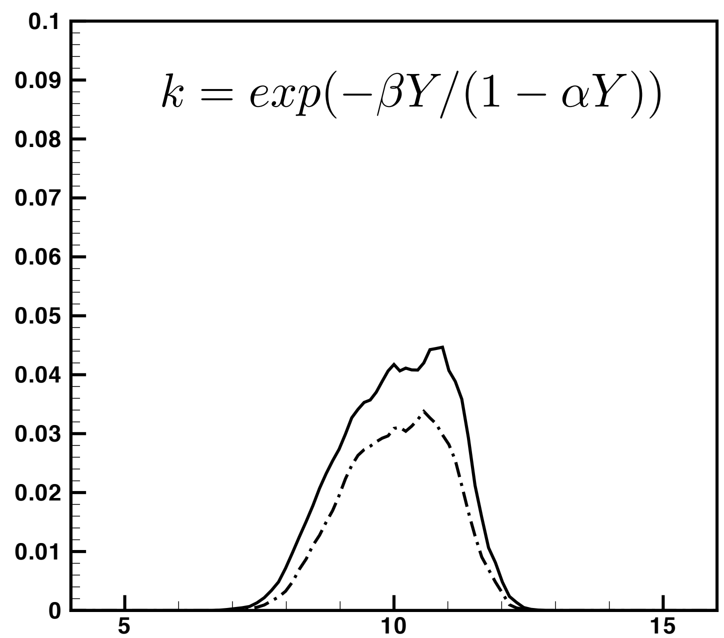


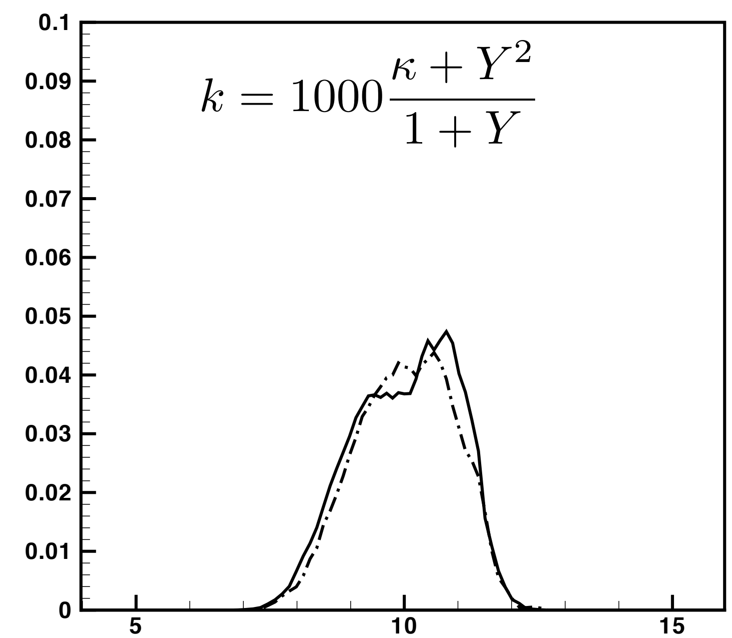




Progress variable variance







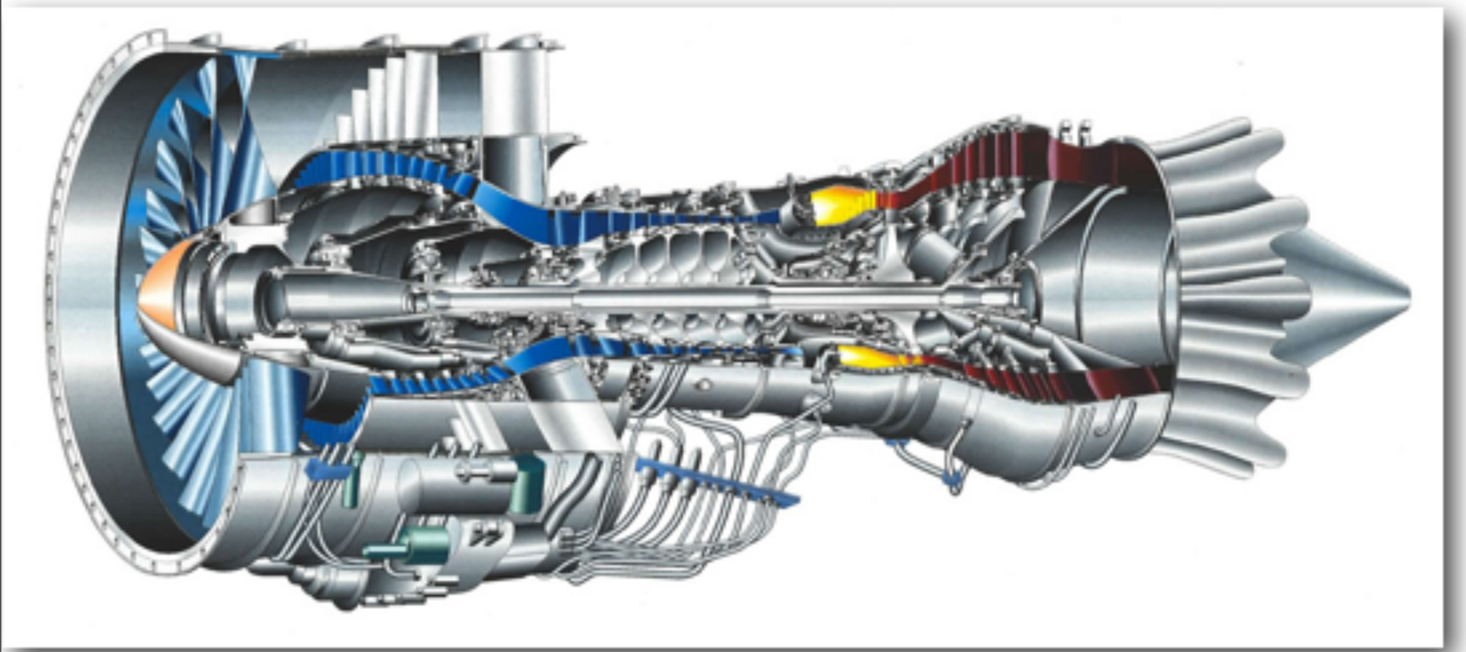
Solid - DQMOM : Dash-dotted - Lagrangian : Dashed - No subgrid model

Decision Making, Risks, and CFD

- **CFD is a vital tool for understanding practical engineering devices**
- **CFD models are also highly unreliable**
  - ➡ Modeling is as much an art as science
- **Can we rely on CFD results to make critical decisions?**

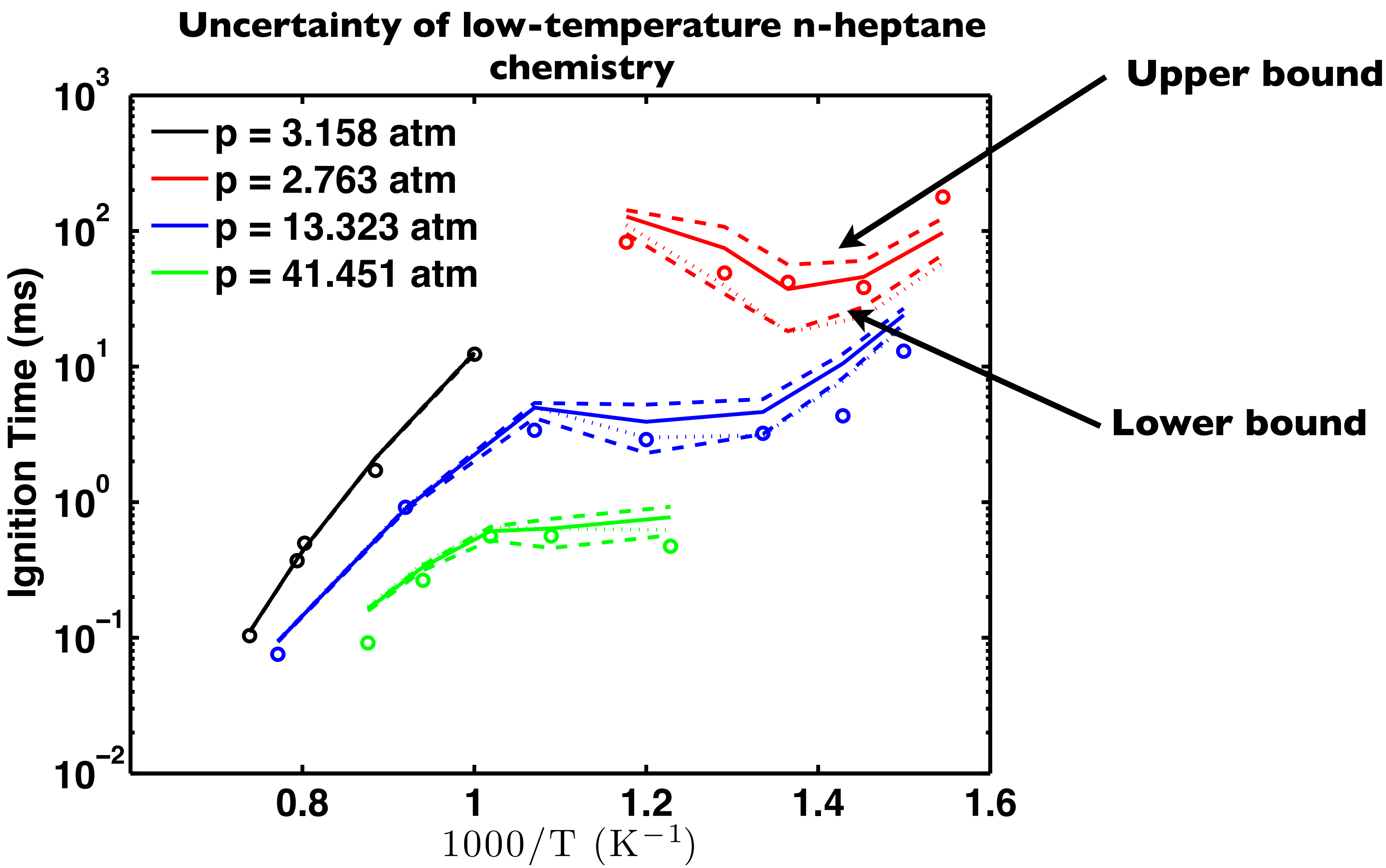
DOE interest

Our interest



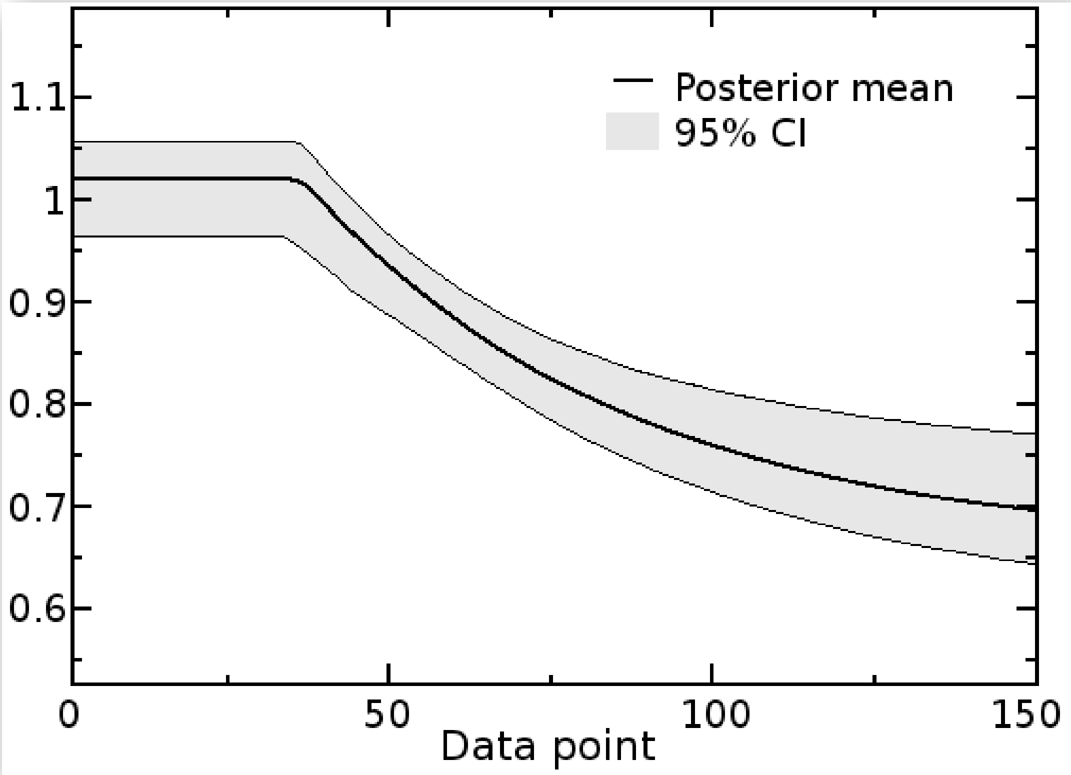
DOE Predictive Science Academic Alliance Program

- **PECOS Center at UT Austin focuses on estimating uncertainties**
- **Quantifying uncertainties**
  - ➡ Use experiments and models to determine simulation error bars



Uncertainty Quantification (UQ)

- **Since models will always incur errors, the best strategy is to quantify the errors**
  - ➡ In a simple sense, compute error bars for the solution
  - ➡ More broadly, CFD results are no longer deterministic "plots" but probabilistic distributions



- **The quantifiable error in the computations is termed uncertainty**
  - ➡ Expressed in terms of confidence in results, which are also computed

RANS Models for Scalar Flux

- **RANS scalar transport equation**

Chemical source term

$$\frac{\partial \overline{\rho}\widetilde{\phi}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_j\widetilde{\phi}}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\overline{\rho} D \frac{\partial \widetilde{\phi}}{\partial x_j}\right) = -\frac{\partial \overline{\rho}\widetilde{u_j'\phi'}}{\partial x_j} + \widetilde{S(\phi)}$$

Scalar flux

➡ Closures for the scalar flux needed

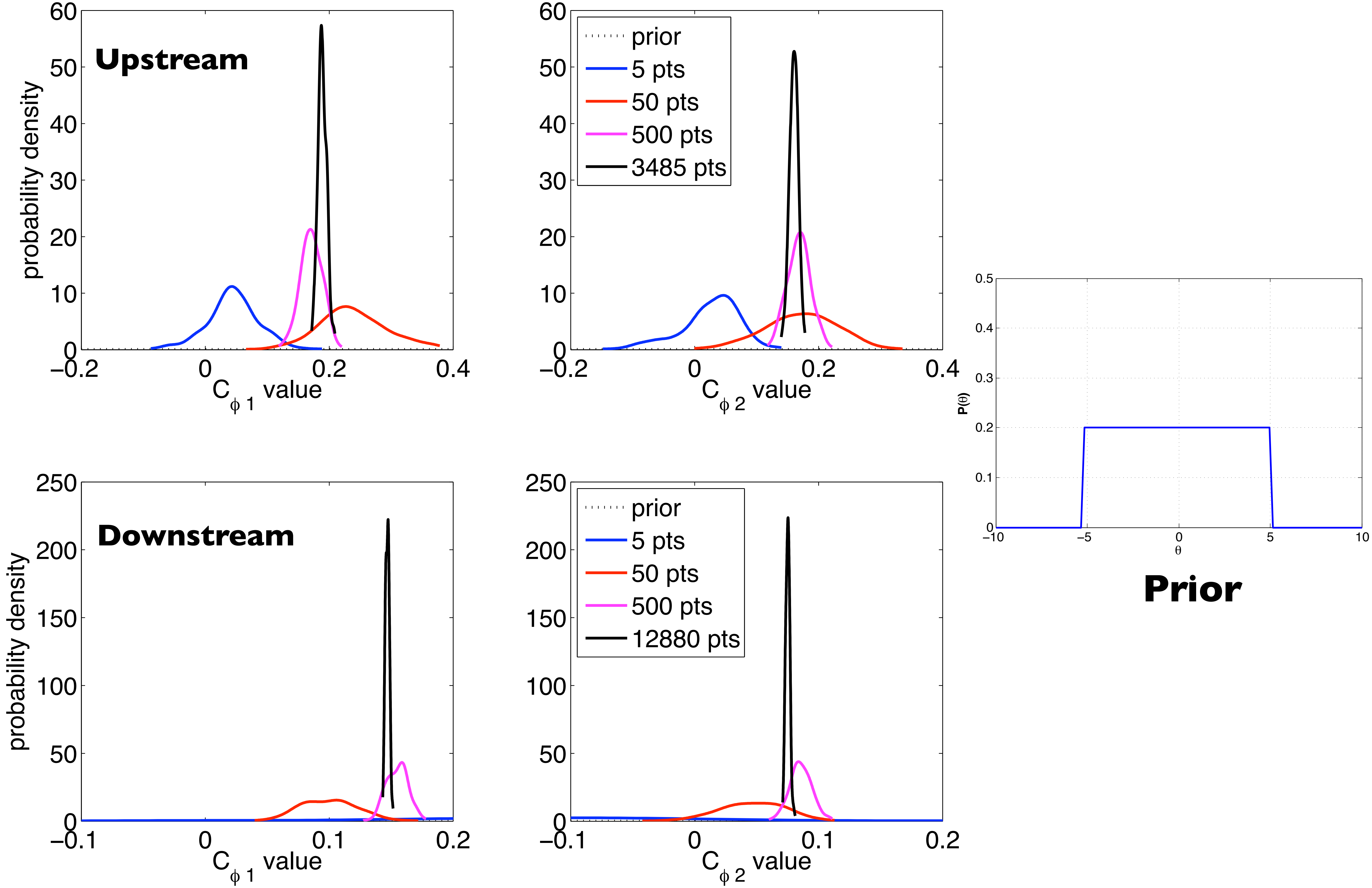
- **Several models considered**

➡ E.g., Combination generalized gradient diffusion model

$$\widetilde{u_i'\phi'} = -\tau_T \left(C_{\phi 1}\widetilde{u_i'u_j'} + C_{\phi 2}\frac{\widetilde{u_i'u_k'}\,\widetilde{u_k'u_j'}}{k}\right)\frac{\partial \widetilde{\phi}}{\partial x_j}$$

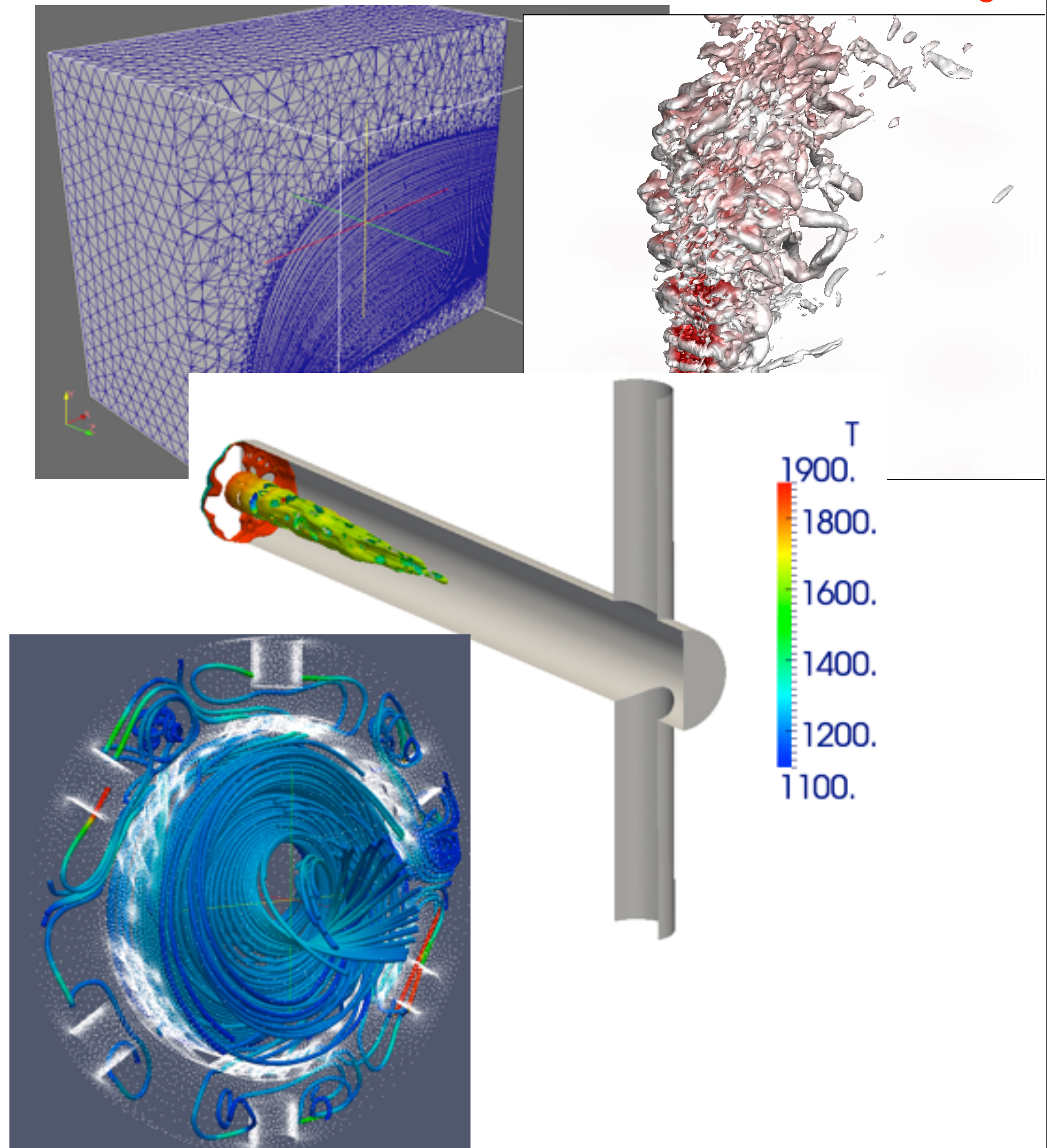
➡ Model coefficients ($C_{\phi 1}, C_{\phi 2}$) need to be determined

Probabilistic Description of RANS Model Constants



Technology Transfer Using OpenFOAM

- **Open source software**
- **Large-scale code modification**
  - ➡ Numerics changed to accommodate LES computations
  - ➡ New flow solvers for turbulent combustion problems
  - ➡ Arbitrary chemistry inclusion with chemkin-compatible interface



UT Gas Turbine Program

- **LES/RANS combined modeling approach**
  - ➡ LES for unsteady dynamics
  - ➡ Calibration-based RANS for parametric studies
- **Well-characterized experimental setup**
  - ➡ Simultaneous PIV/PLIF measurements under high pressure conditions
  - ➡ Pitched jets in crossflow with varying fuel compositions
- **Open source technology transfer**
  - ➡ OpenFOAM based transfer of models