

# VALIDATION OF A NUMERICAL APPROACH TO MODEL HYDROGEN COMBUSTION IN GAS TURBINE ENGINES



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# Motivation

**Develop an appropriate pure hydrogen combustion modeling approach for use in broad design studies of hydrogen burners in gas turbines. The approaches should be able to accommodate all levels of premixing, while being inexpensive enough to be run for many design points.**



# Problem Definition

- Hydrogen combustion is difficult and expensive to model
- Gas turbine fuel injectors can have esoteric geometries and benefit from wide design studies with many designs
- We aimed to develop an approach that is:
  - Fast enough to run many design cases
  - Accurate enough to predict NOx and flame behavior
- Two experimental cases are selected for validation

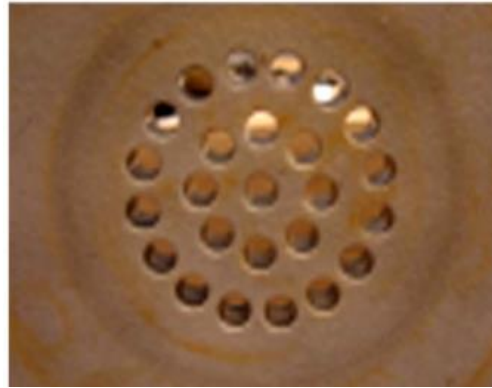


# Validation Case 1

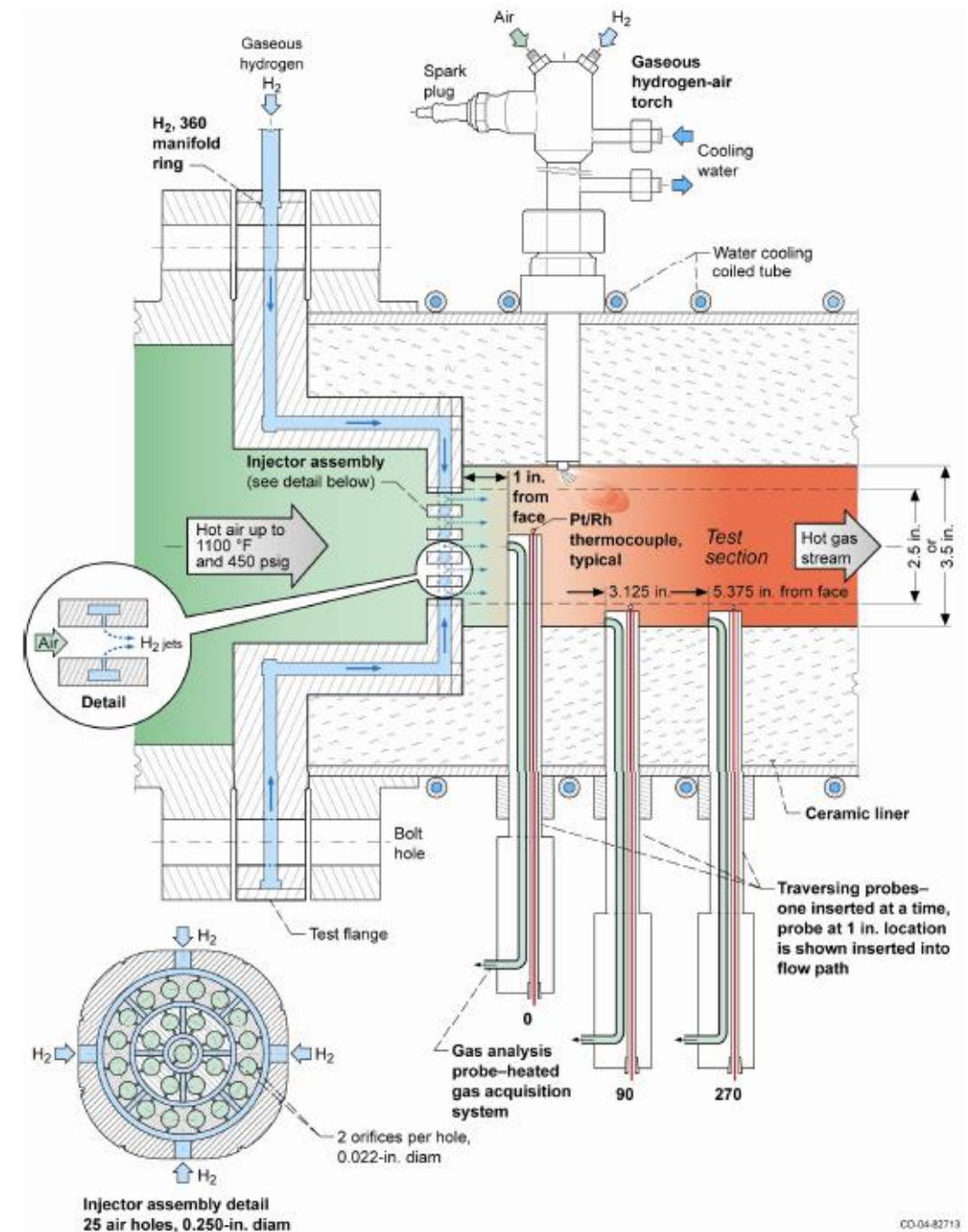
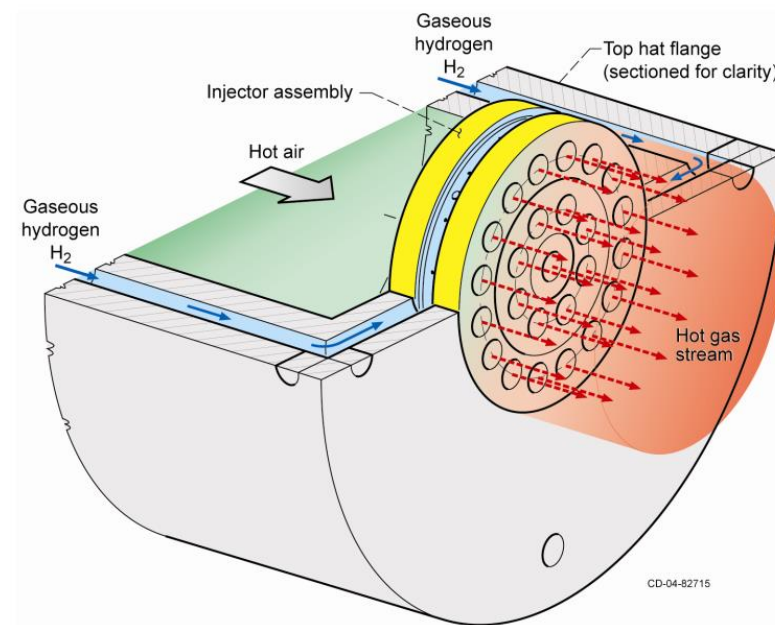


# Marek/NASA: Nozzle Design

Poorly premixed



Medium Pressure



Ref: Marek, Cecil, Timothy Smith, and Krishna Kundu. "Low emission hydrogen combustors for gas turbines using lean direct injection." *41st AIAA/ASME/SAE/ASEE joint propulsion conference & exhibit*. 2005. <https://ntrs.nasa.gov/citations/20080002274>

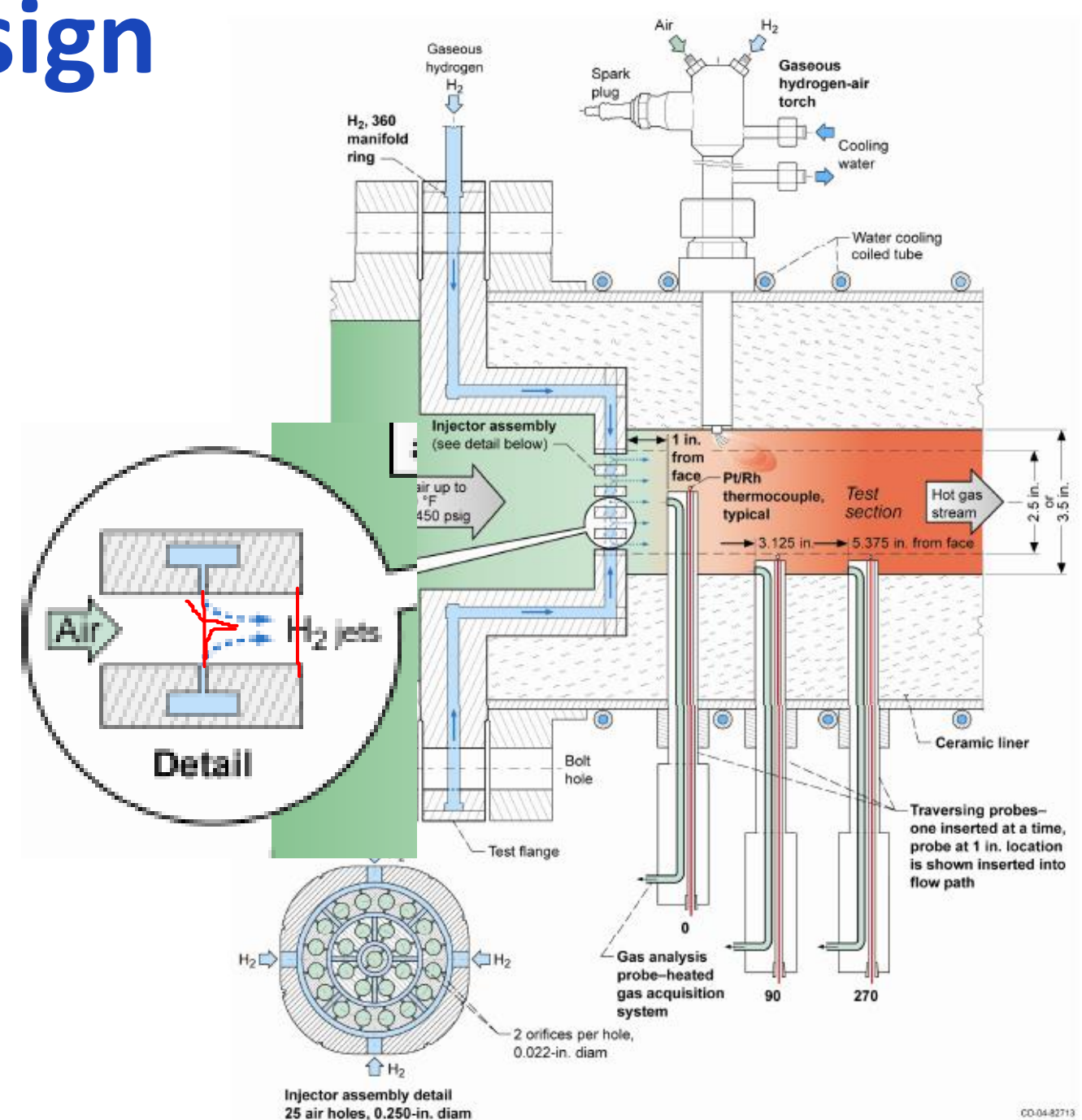
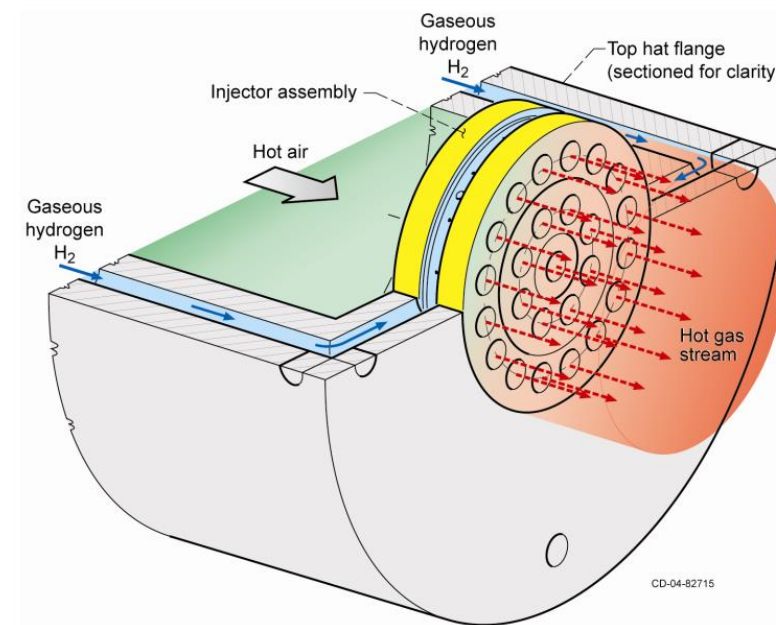


# Marek/NASA: Nozzle Design

Poorly premixed



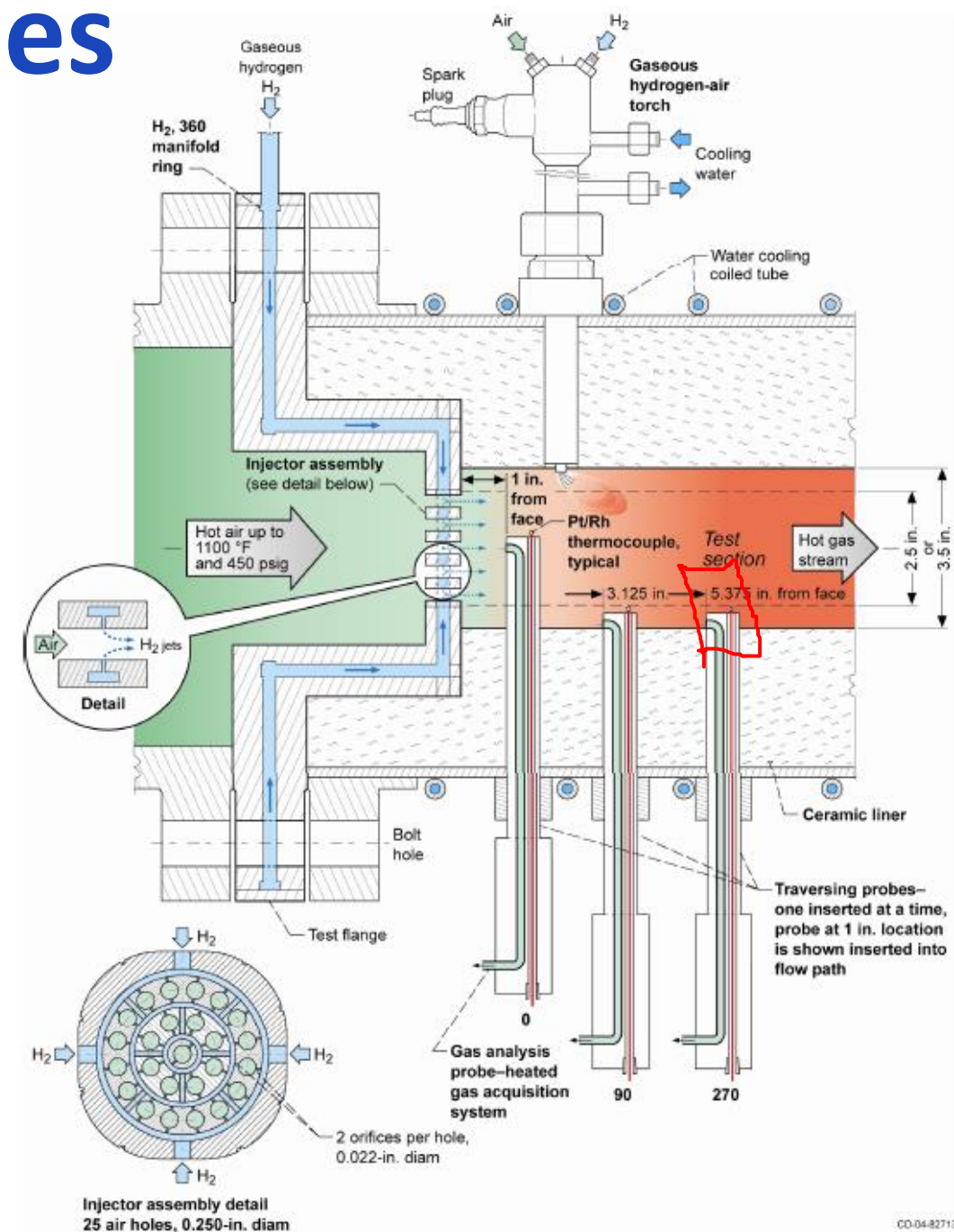
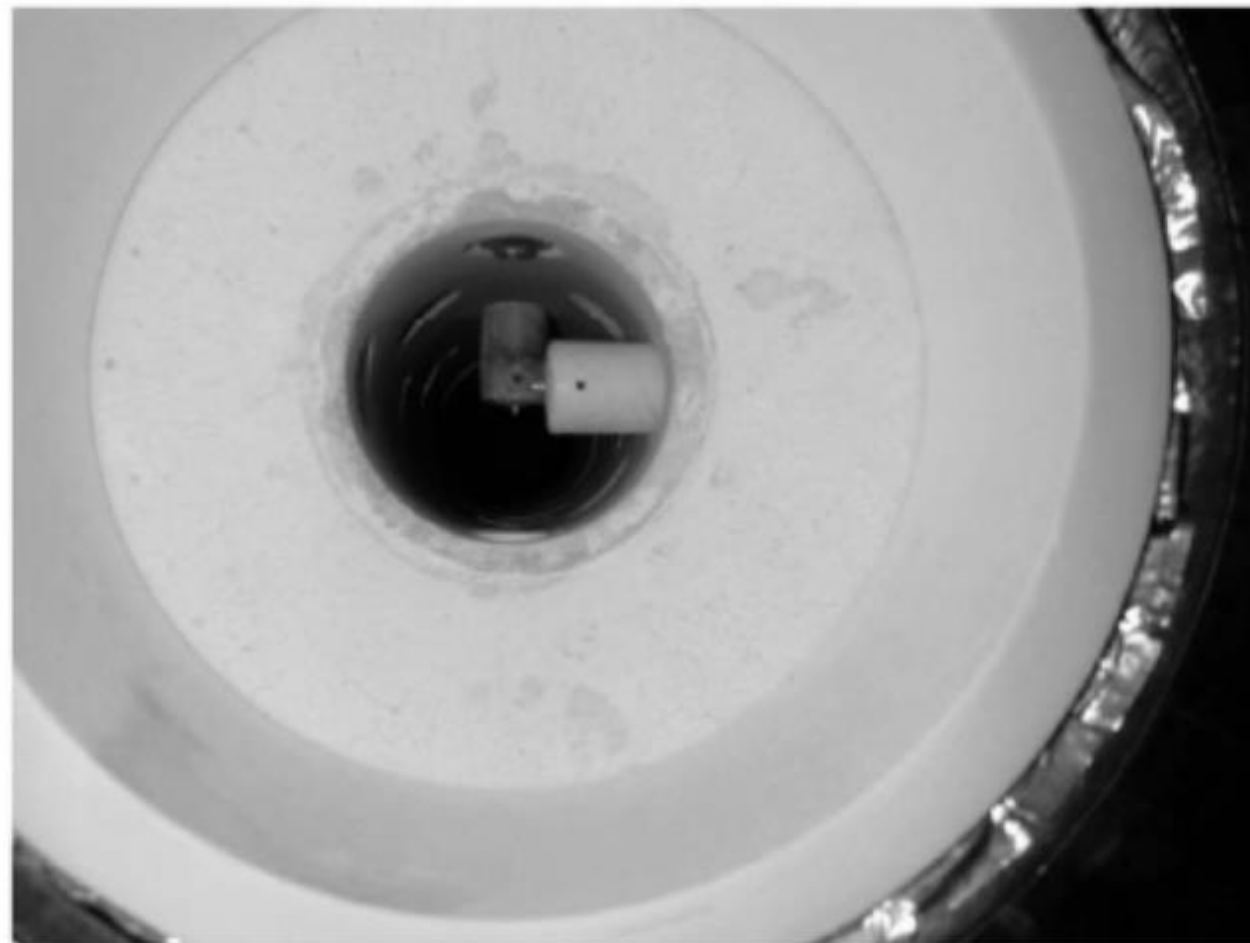
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# Marek/NASA: Emissions Probes

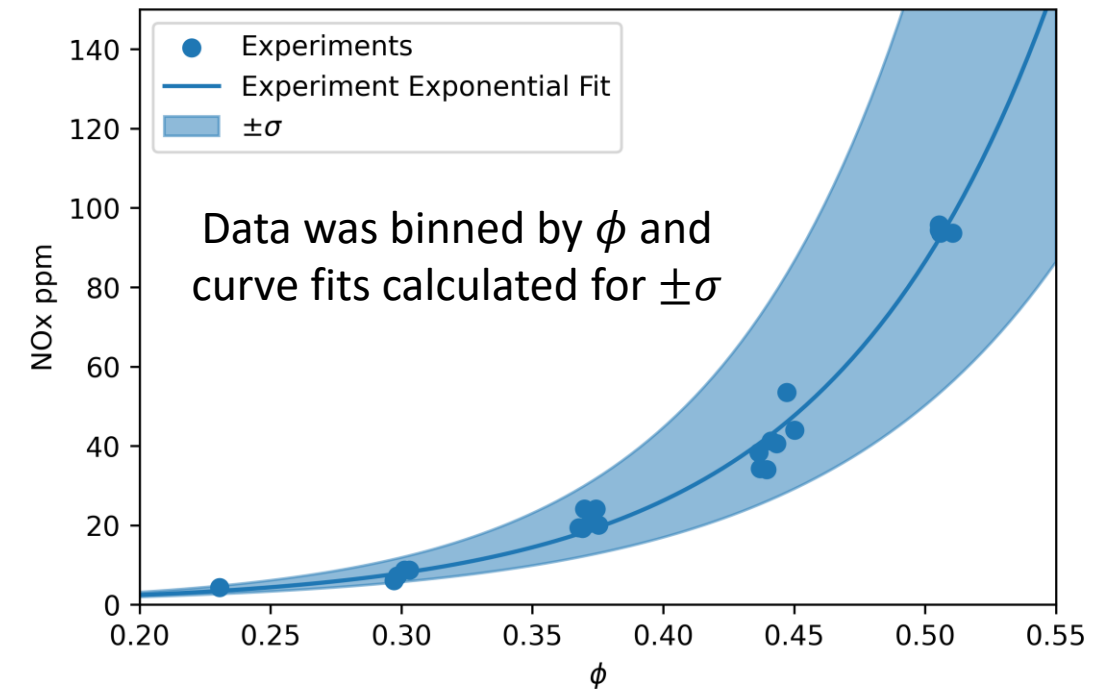
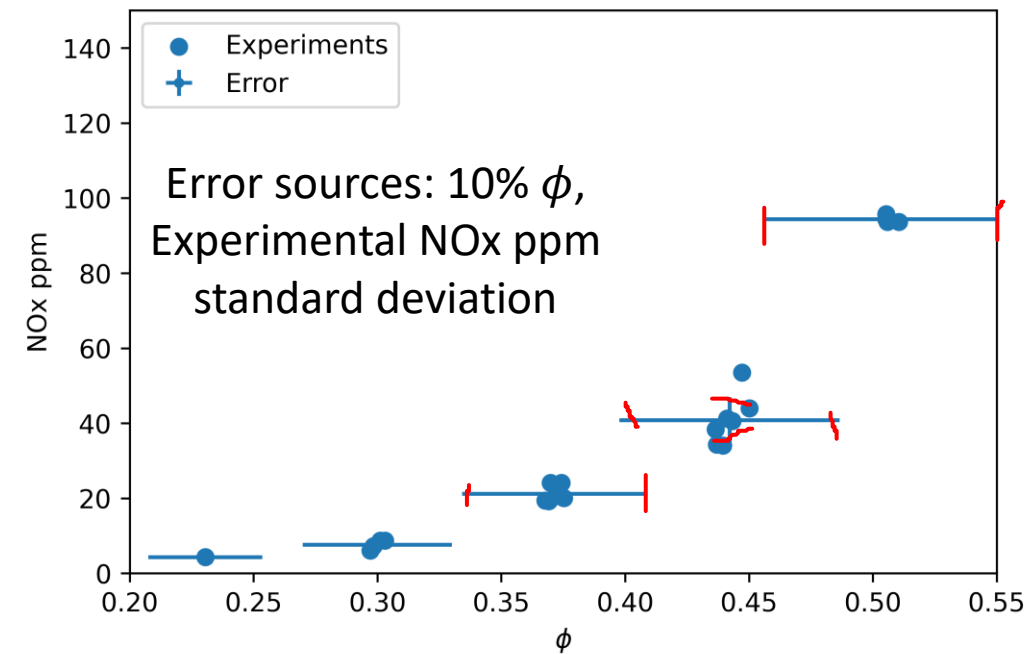
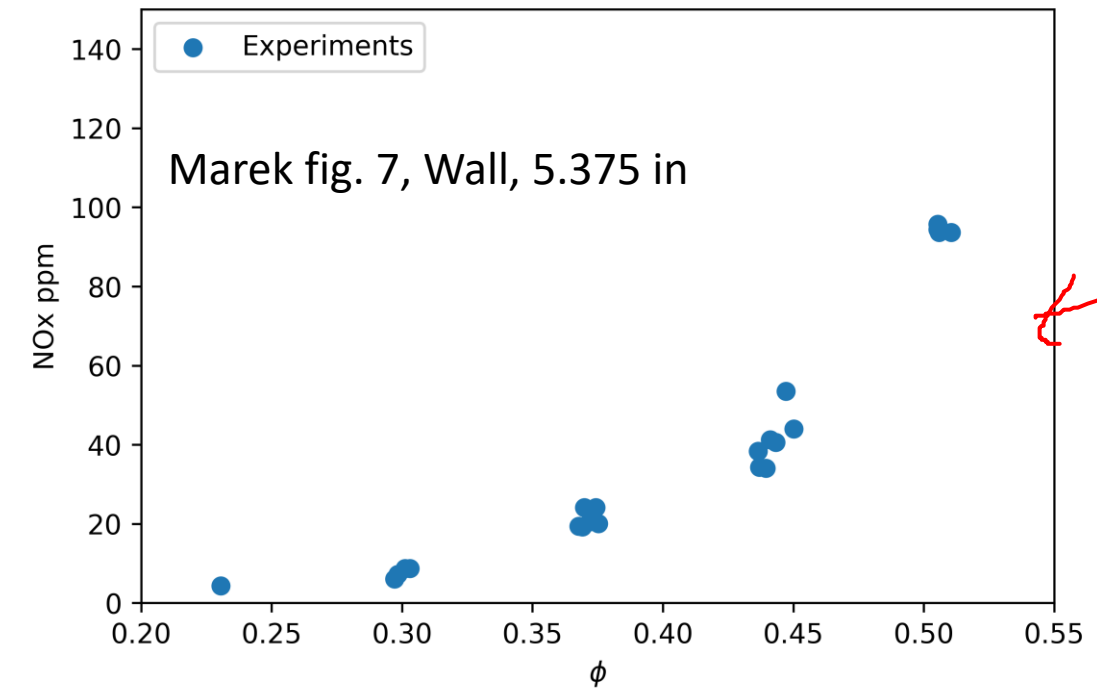
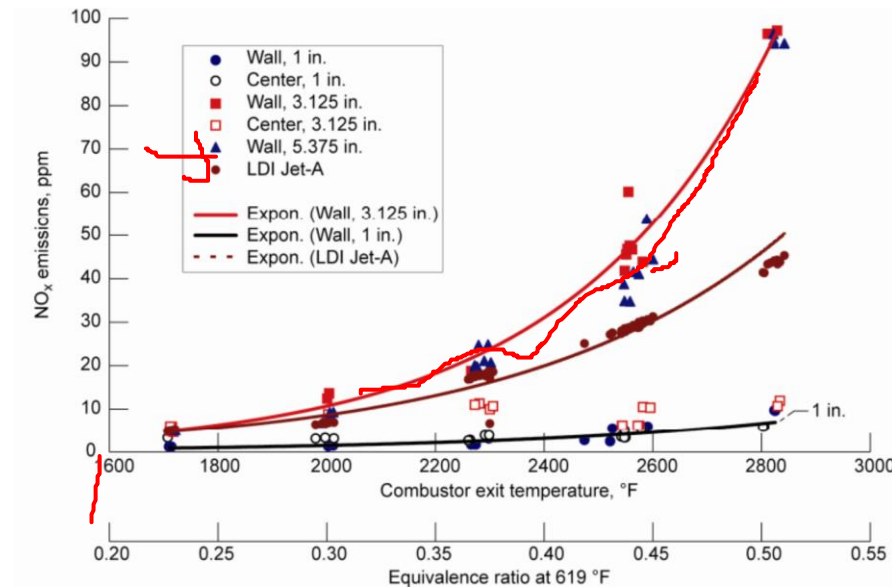


CO-04-82713

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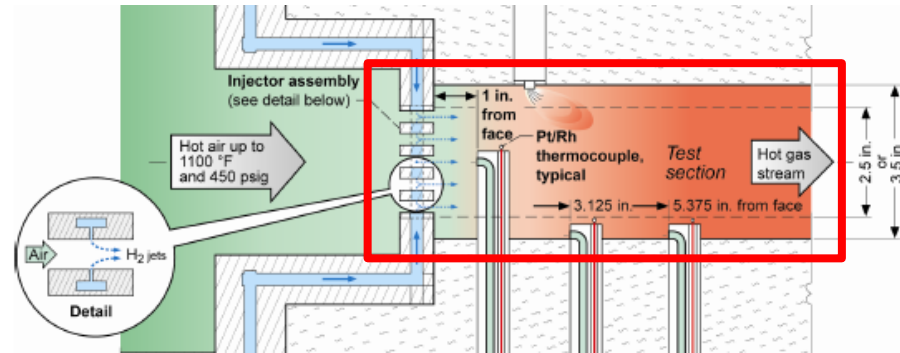
# Experimental data



# Numerical Approach



# Fluid domain

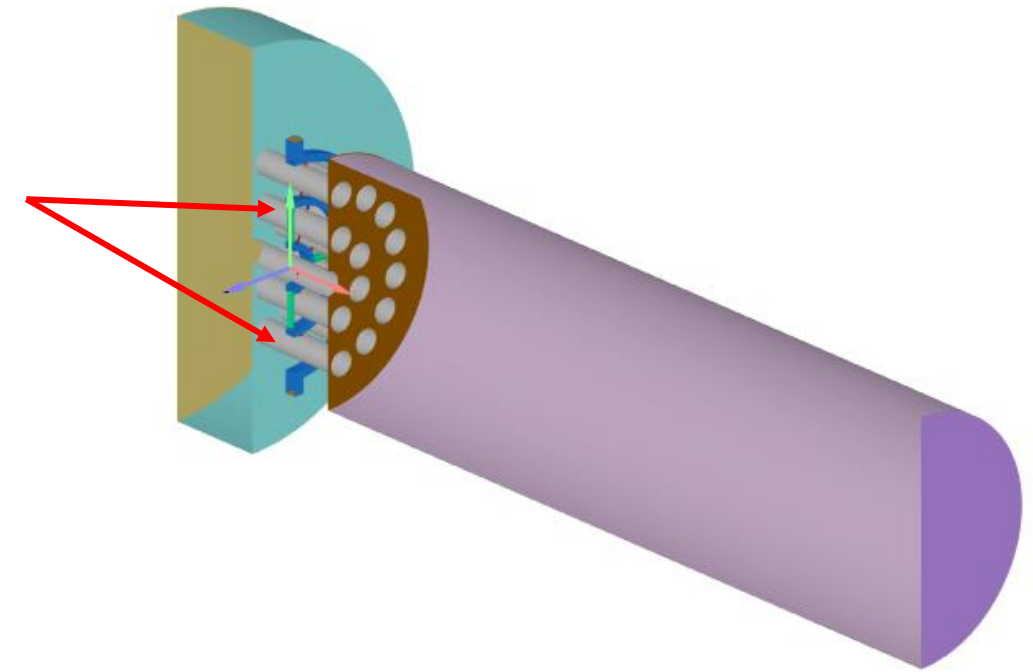


Air inlet

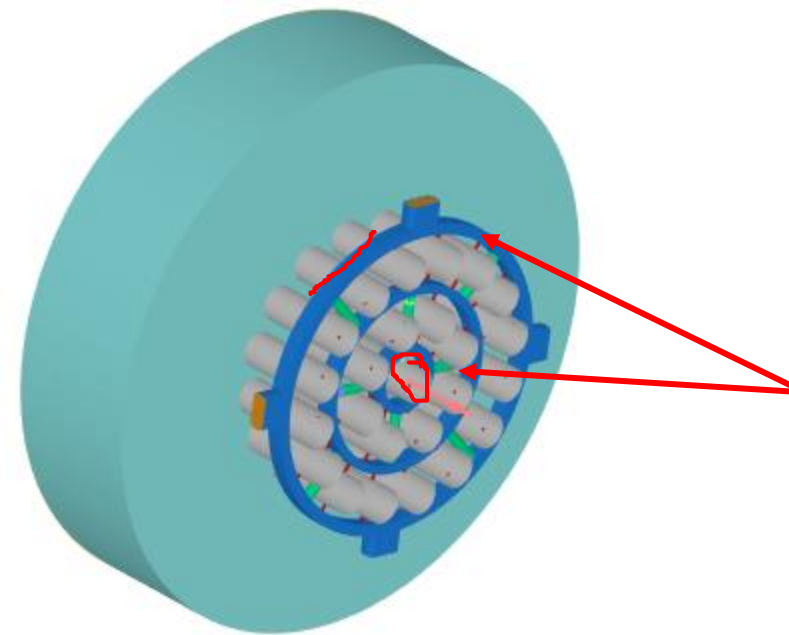
Hydrogen  
inlets

Diameter of combustor:  
0.0635 m

Air tubes



Fuel manifold  
modeled to capture  
nonuniform fuel  
distribution



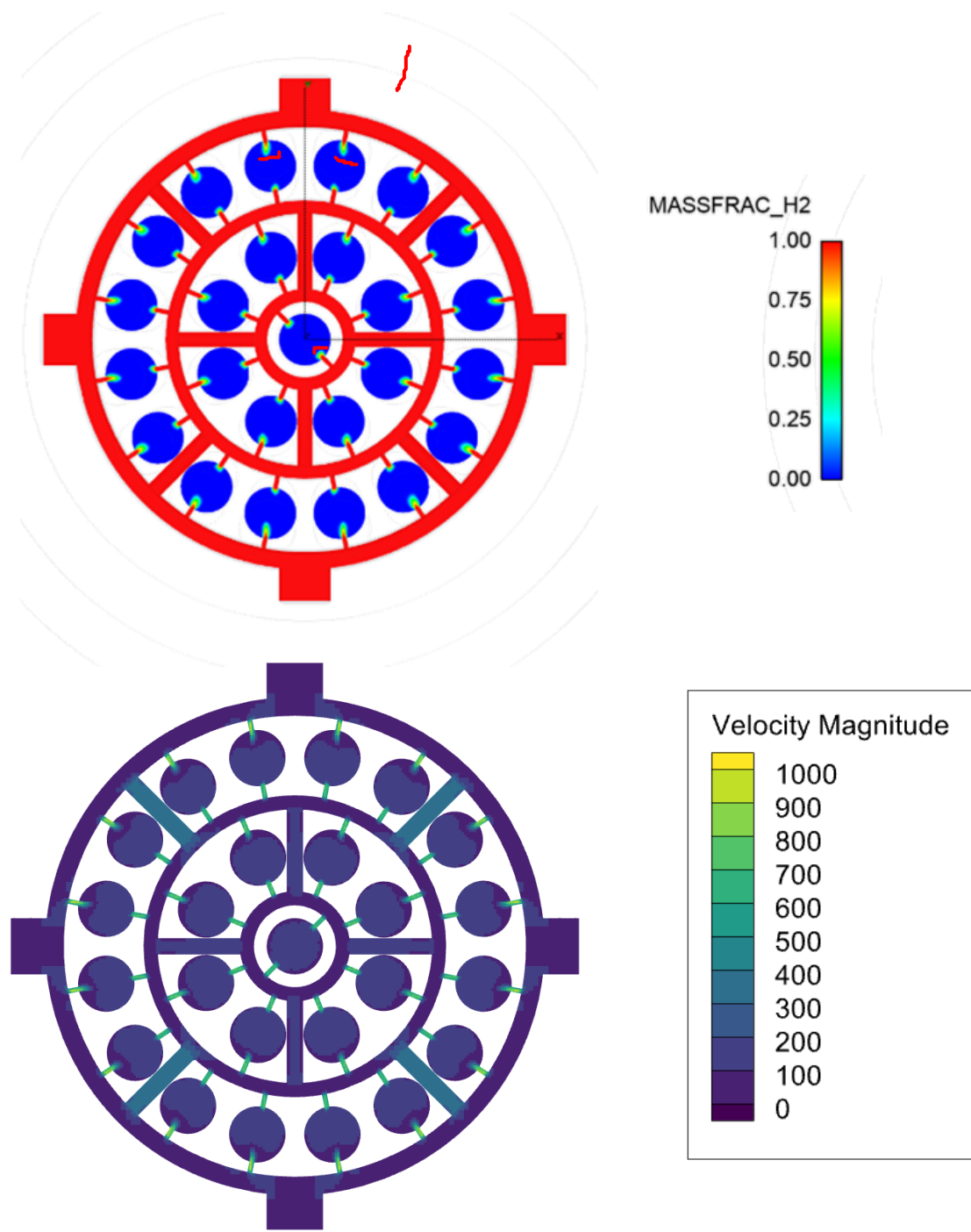
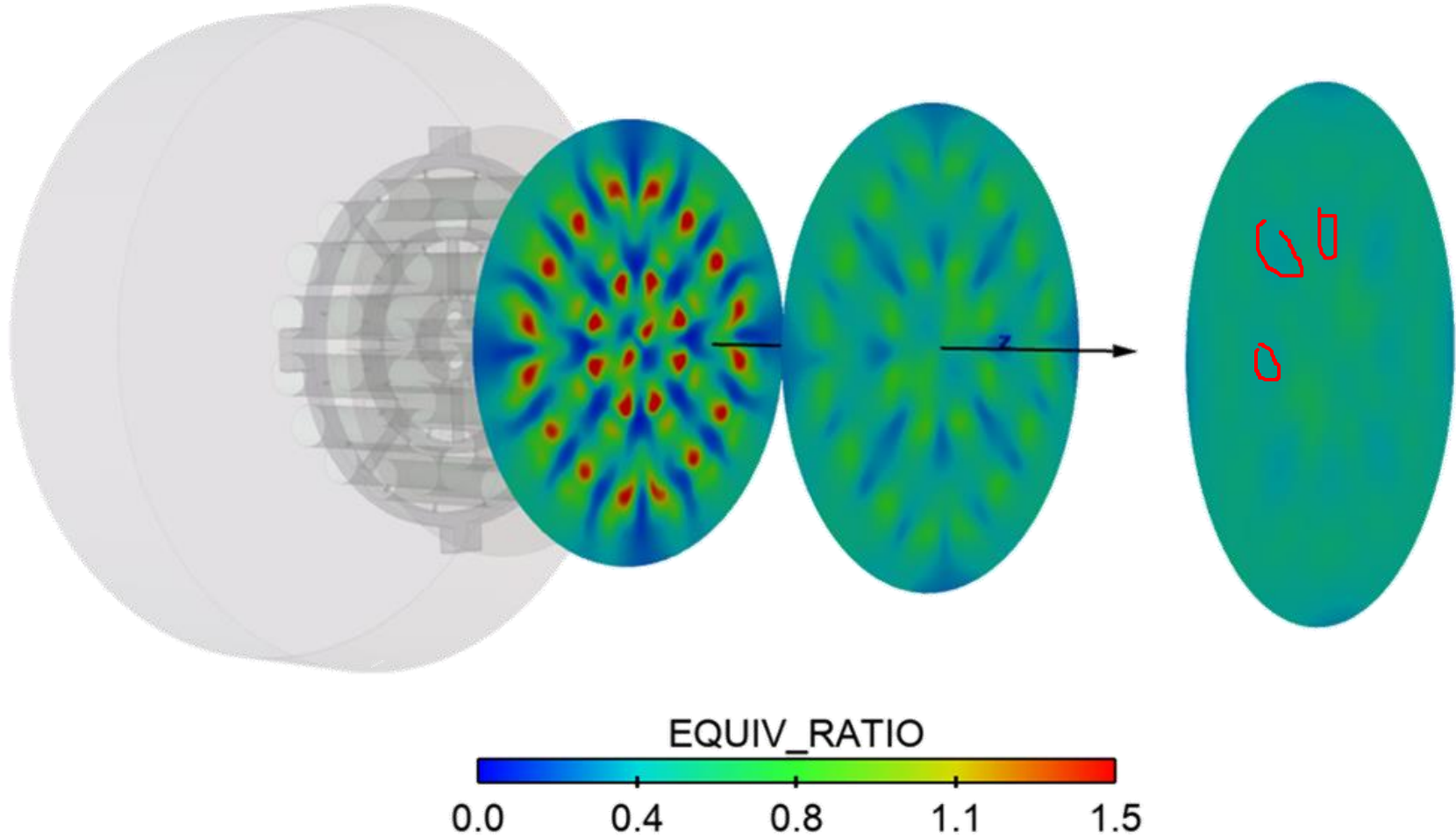
# Boundary Conditions

| Parameter                                      | Value                                        |
|------------------------------------------------|----------------------------------------------|
| Air flow rate (inflow)                         | 0.386 kg/s                                   |
| Fuel flow rate                                 | Varied to get desired equivalence ratio      |
| Air inlet temperature (inflow)                 | 600 K                                        |
| Fuel inlet temperature                         | 300 K                                        |
| Near wall treatment                            | Law of the wall model                        |
| Wall heat transfer boundary condition          | Adiabatic assumption                         |
| Outflow pressure                               | 6.894 bar                                    |
| Turbulence Model                               | Steady RANS k- $\epsilon$ (mean $y^+ = 47$ ) |
| Turbulent kinetic energy (air inlet)           | 2% turbulent intensity (CONVERGE default)    |
| Turbulent dissipation length scale (air inlet) | 0.003 m ( $\sim 1/2$ air nozzle diameter)    |
| Turbulent kinetic energy (H2 inlet)            | 2% turbulent intensity (CONVERGE default)    |
| Turbulent dissipation length scale (H2 inlet)  | 0.0003 m ( $\sim 1/2$ fuel jet diameter)     |



# Fuel air mixing

$\phi=0.375$



# Combustion Model Study



# Combustion Model Comparison: FGM

- The **Flamelet Generated Manifold (FGM)** model uses pre-generated lookup tables to model combustion.
- The FGM table was generated at 6.894 bar for  $\phi$  0.3 to 2 for both 1D premixed and 1D diffusion to match the Marek case conditions.
- The table is parameterized by
  - Mean mixture fraction
  - Mixture fraction variance
  - Reaction progress
  - Enthalpy
- Assumptions:
  - FGM models typically assume a Lewis number near unity.
  - FGM models can have difficulty accounting for hydrogen's high diffusivity.



# Combustion models: SAGE and 3pt PDF SAGE

In **SAGE**, reaction rates are calculated by direct chemistry from the chemical kinetics mechanism by CONVERGE's SAGE solver and transport equations are solved by CFD solver.

- Preferential hydrogen diffusion is used to account for hydrogen's high diffusivity
- Reaction rates in mechanism files are expressed in Arrhenius form.

$$K_{f_i} = A_i T^{\beta_i} \exp\left(\frac{-E_i}{RT}\right)$$

where

$A_i$  is the pre-exponential factor,

$\beta_i$  is the temperature exponent,

$E_i$  is the activation energy (in cal /mol),

R is the ideal gas constant

 **3pt PDF SAGE** is built on top of the SAGE model but includes these additional features:

- Temperature fluctuation is considered based on user inputs for each computational cells.
- Three fluctuation in temperature is considered for each computational cells.
- Reaction rates are calculated by SAGE three times for each computational cells.

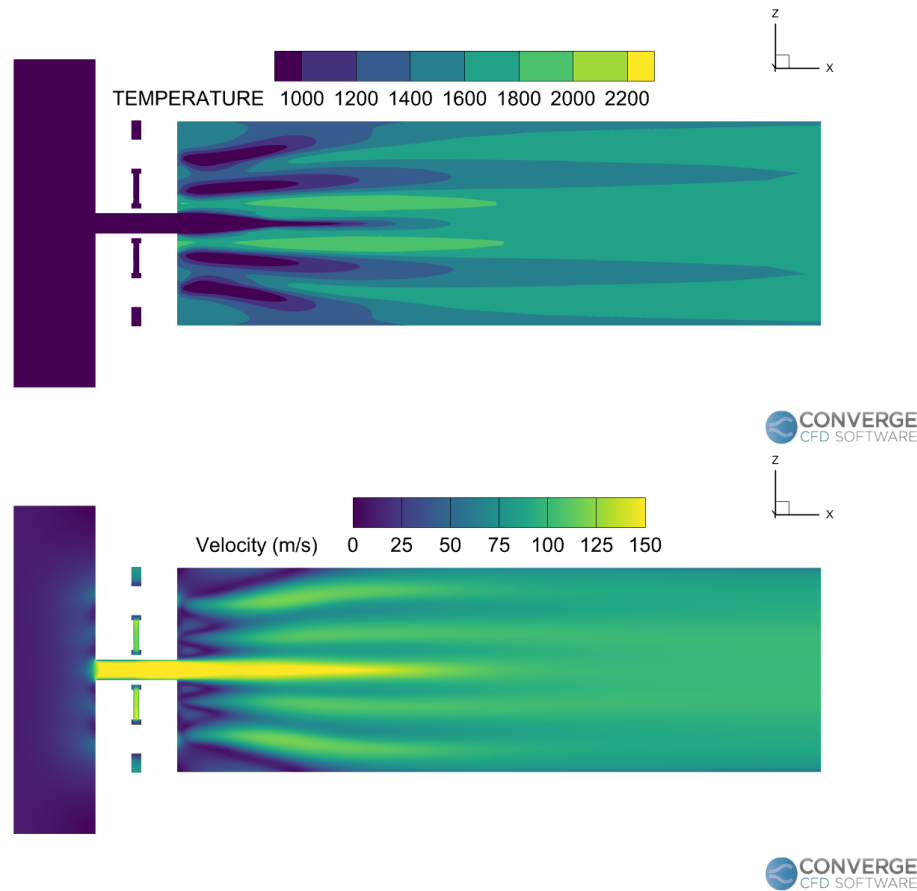


# Model parameters available in CONVERGE were selected for the computational model

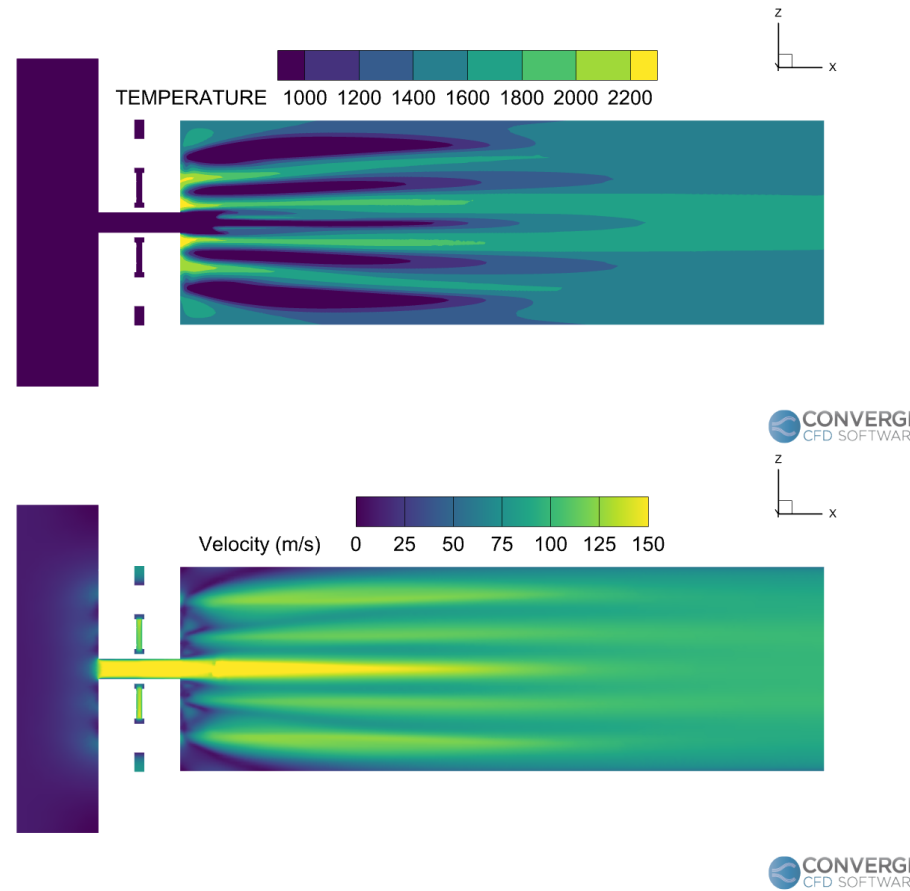
| Parameter                   | SAGE                                                                | FGM | 3pt PDF SAGE |
|-----------------------------|---------------------------------------------------------------------|-----|--------------|
| Equivalence ratio           | 0.37                                                                |     |              |
| NOx model                   | Extended Zeldovich passive                                          |     |              |
| Base grid size              | 2.24 mm                                                             |     |              |
| Smallest grid size          | 0.28 mm                                                             |     |              |
| Adaptive mesh refinement    | Based on: Temperature gradient (2.5 K)<br>Velocity gradient (1 m/s) |     |              |
| Heat transfer model         | O'Rourke and Amsden                                                 |     |              |
| Chemical kinetics mechanism | Galway mechanism                                                    |     |              |



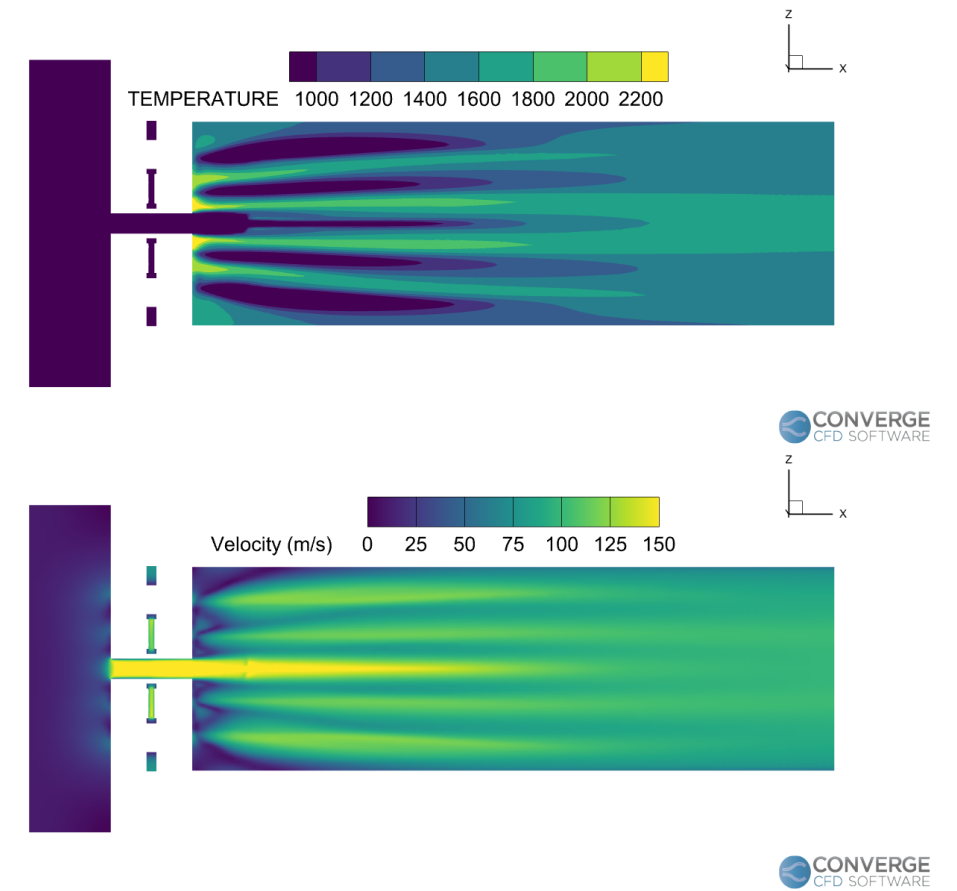
# Combustion model flow field comparison



FGM



SAGE



3pt PDF SAGE

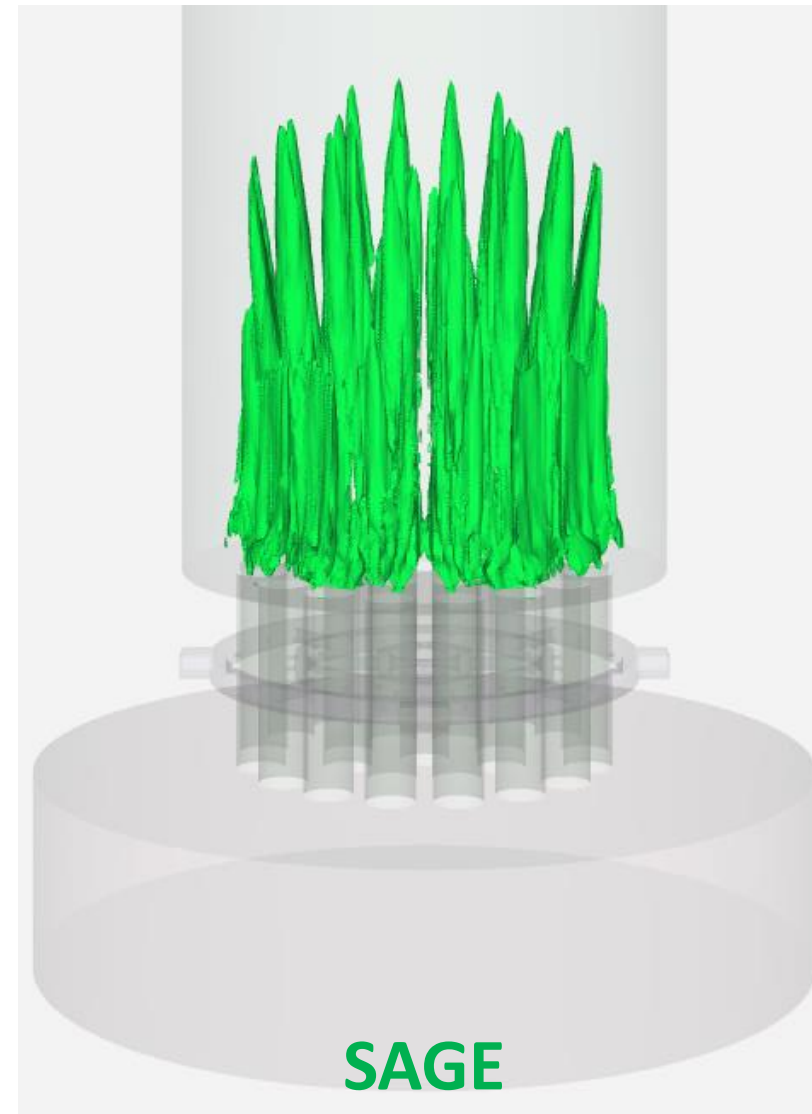


# OH- Iso-surface (0.006 mass fraction)

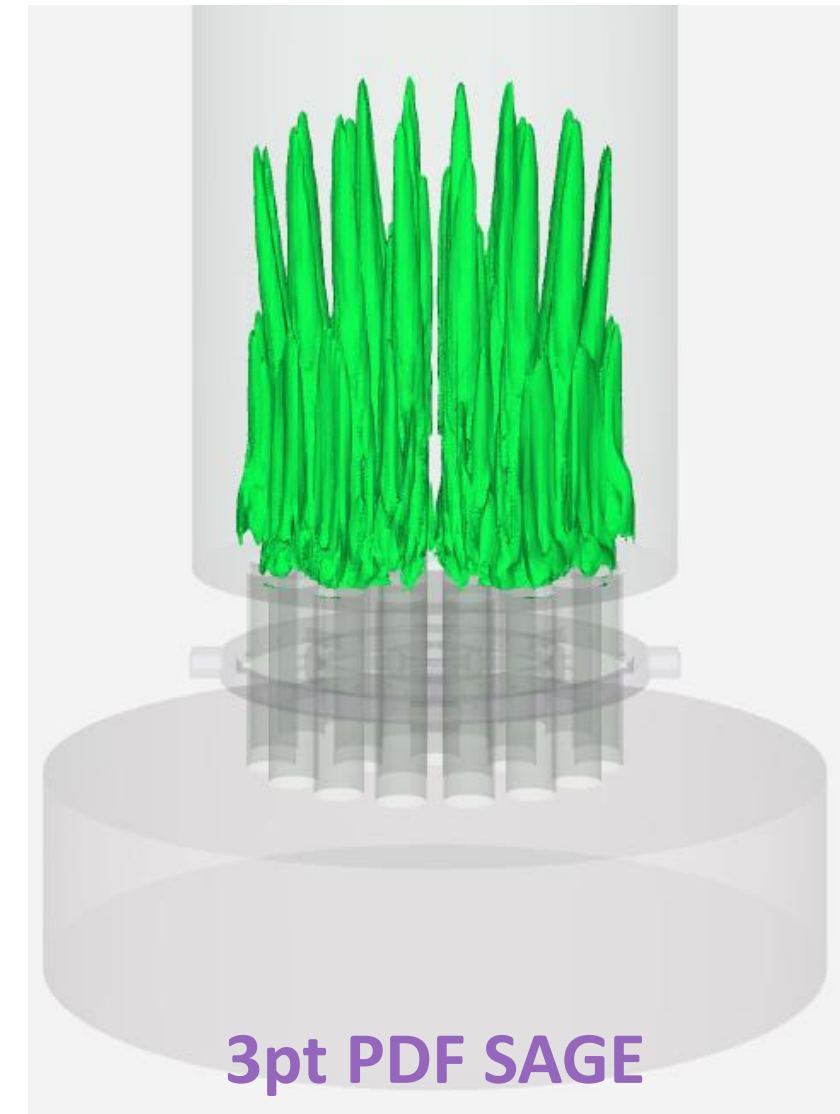
~5x faster solution



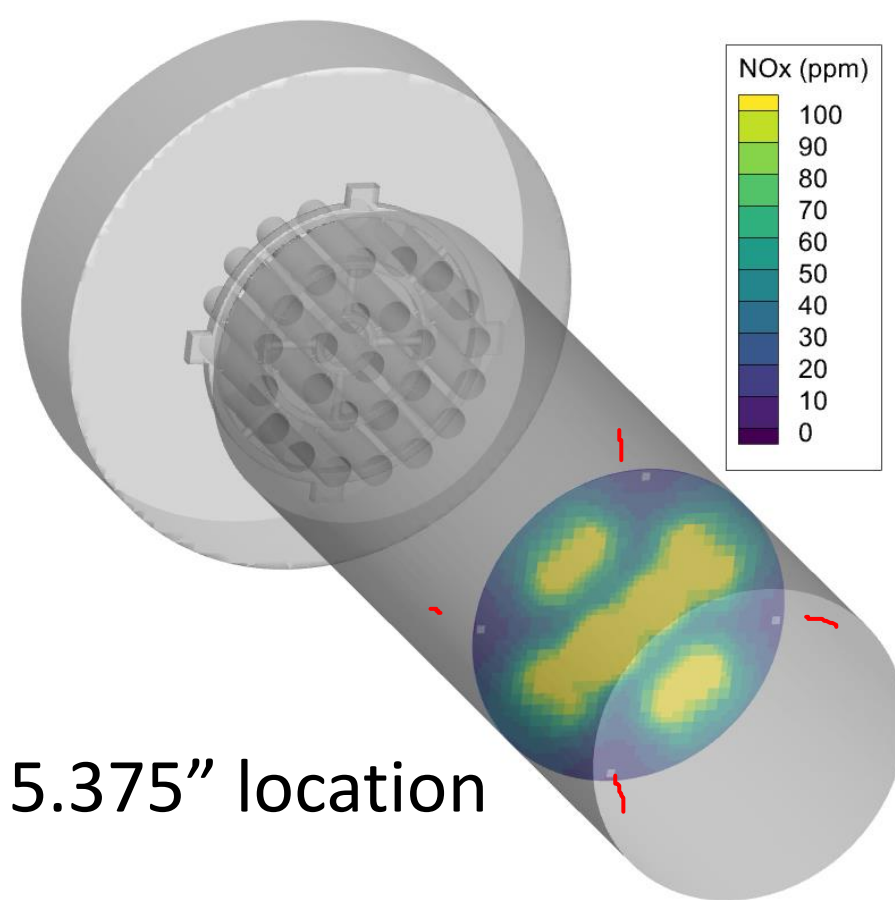
Baseline solution



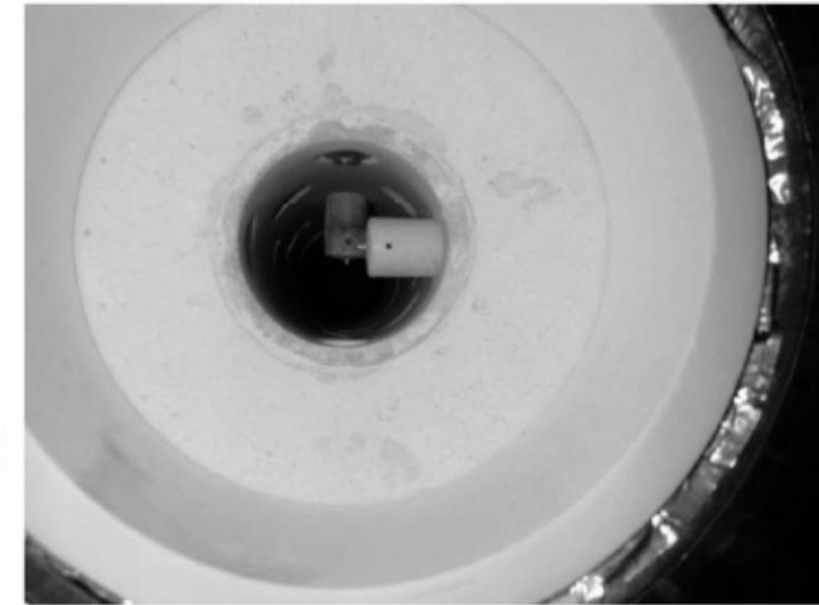
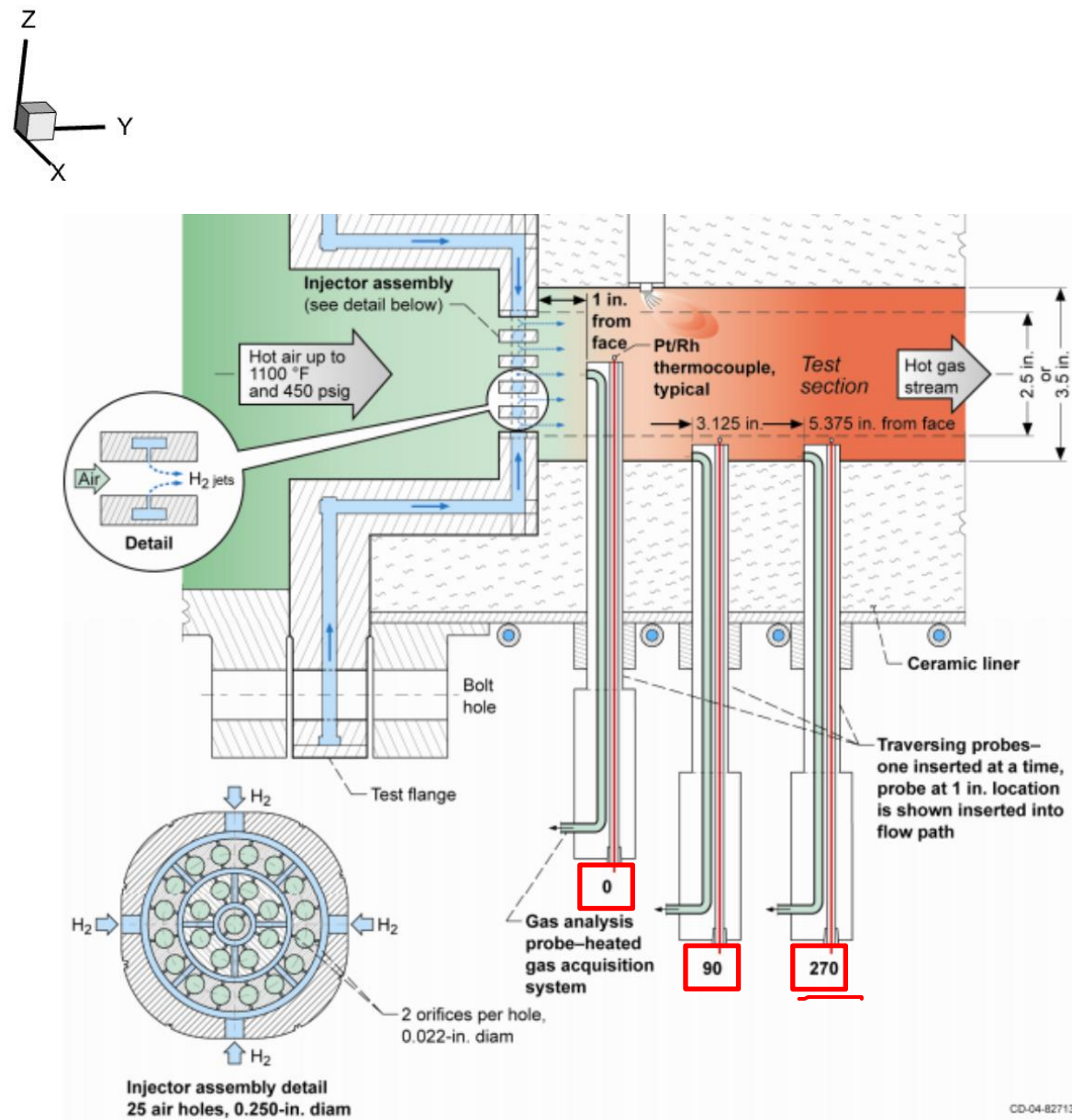
~1.2x slower solution



# Probe-matching NOx collection method



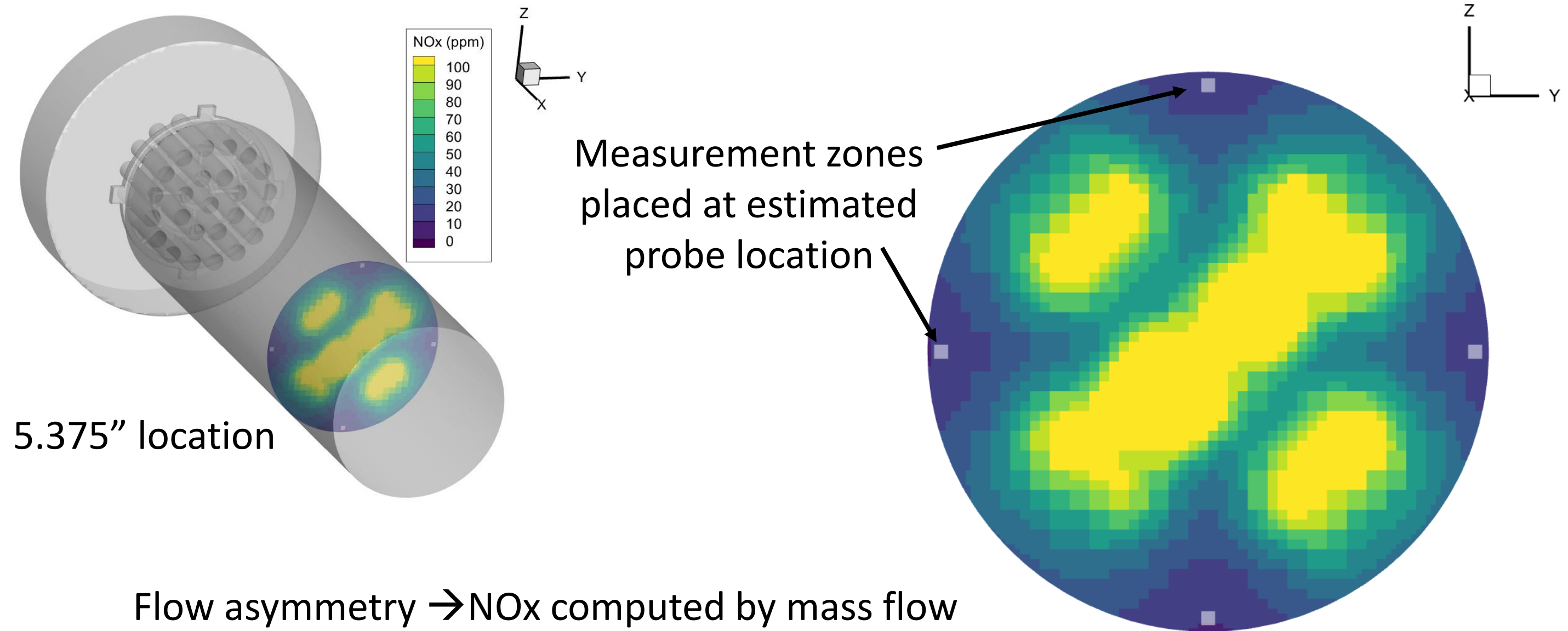
5.375" location



Probe exact location and insertion depth ambiguous, estimating from schematics



# Initial (Rejected) NOx collection method

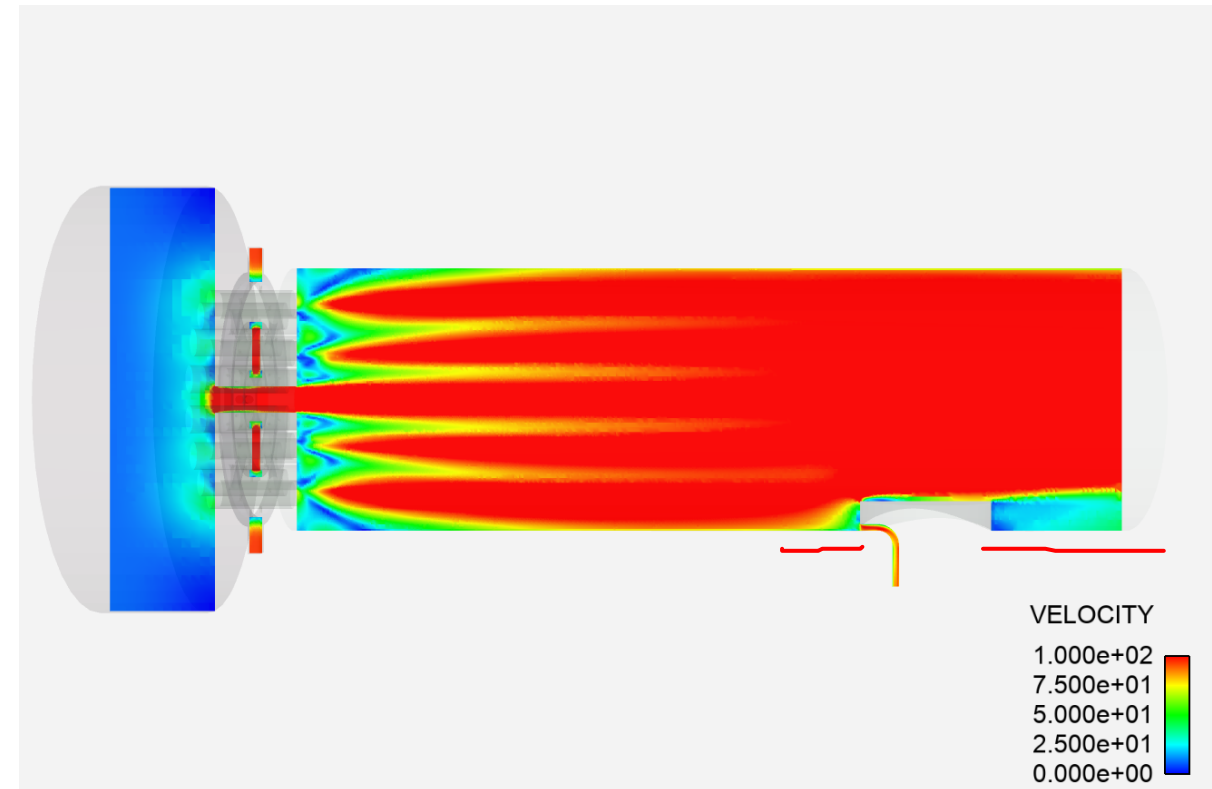
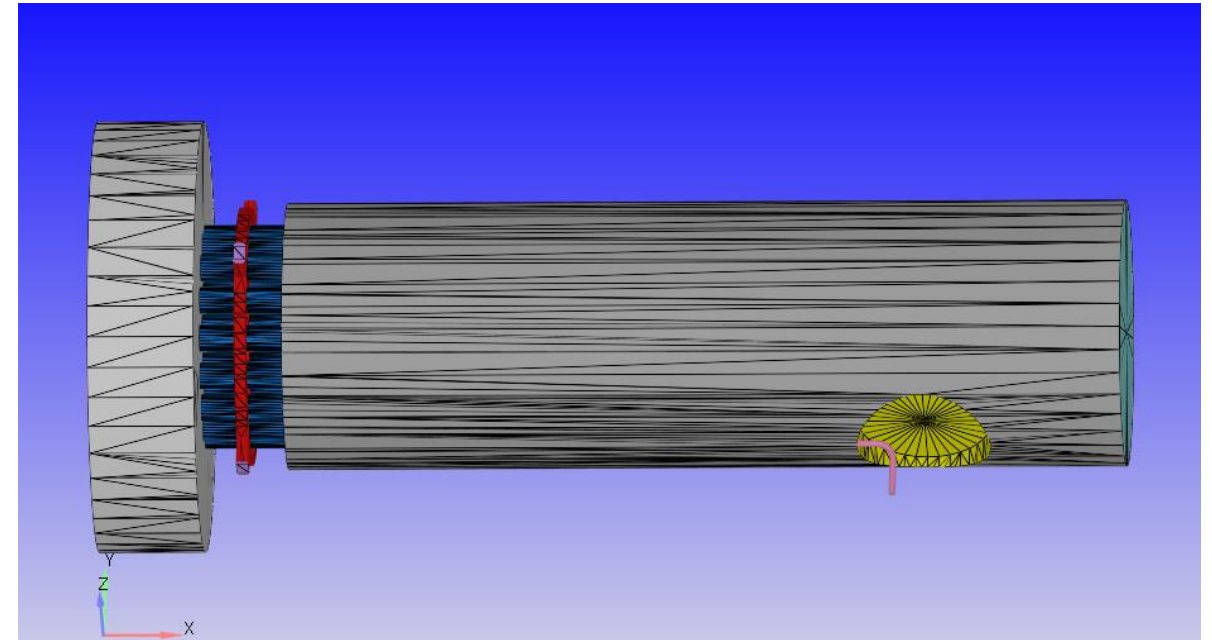


Flow asymmetry → NOx computed by mass flow rate at each of the 4 locations and averaged

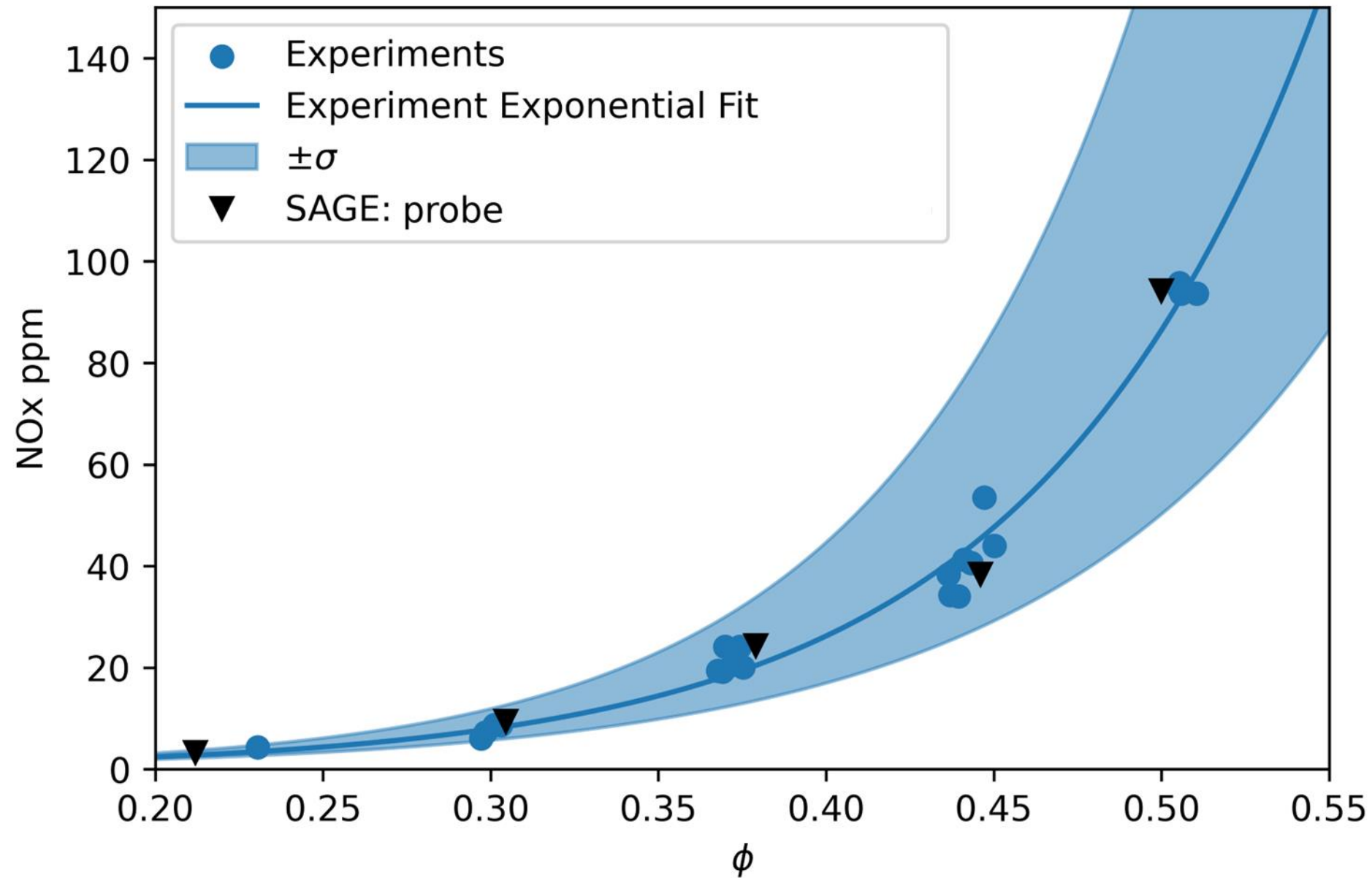


# Emissions probe model

- Marek used an emissions sampling probe to collect data.
- The probe was reconstructed given limited available data.
- The inserted probe at the 5.375" wall sampling location is shown on the right, with sampling tube shown in pink.
- The probe had a significant effect on the flow field.



# SAGE with probe matches data well



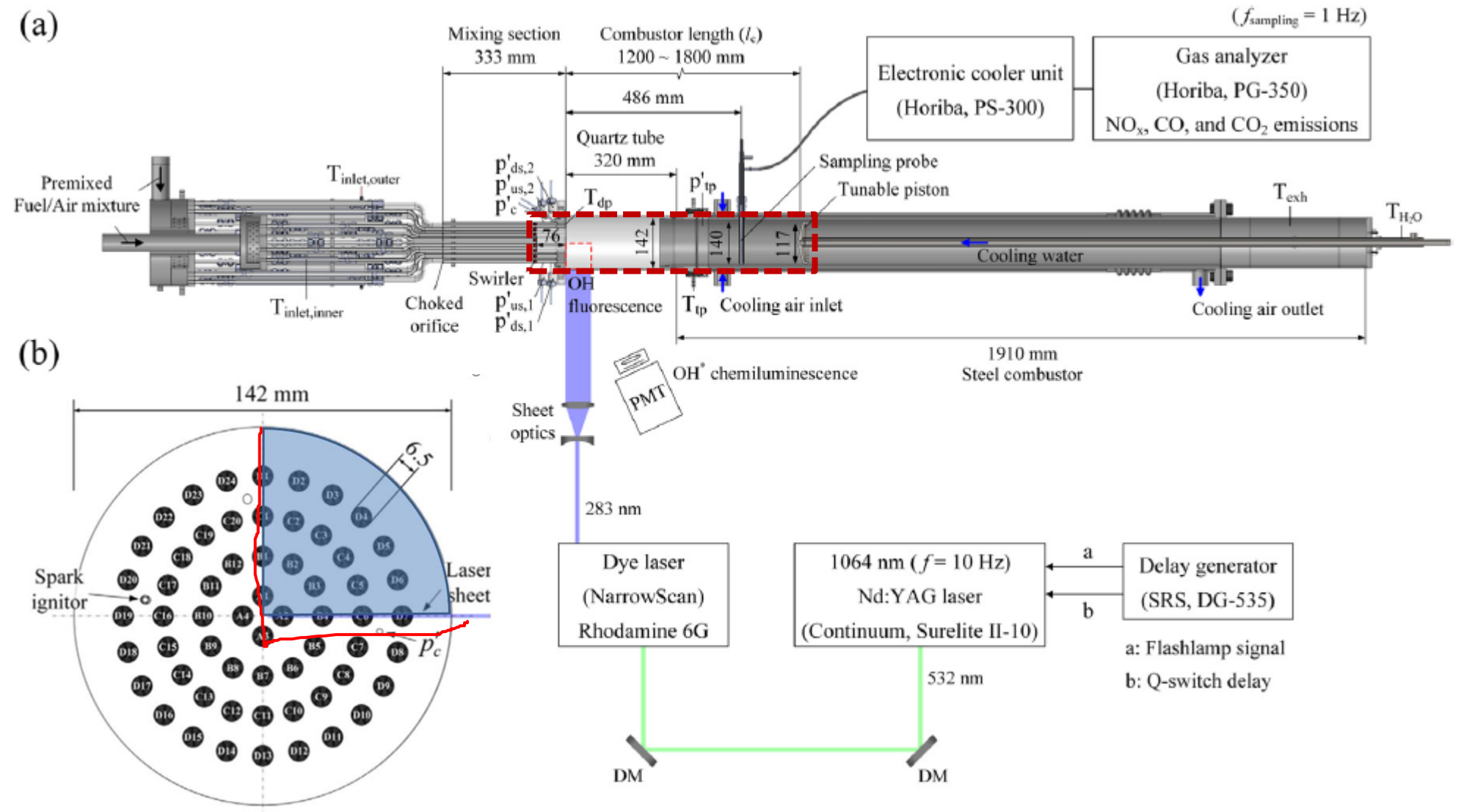
# Validation Case 2



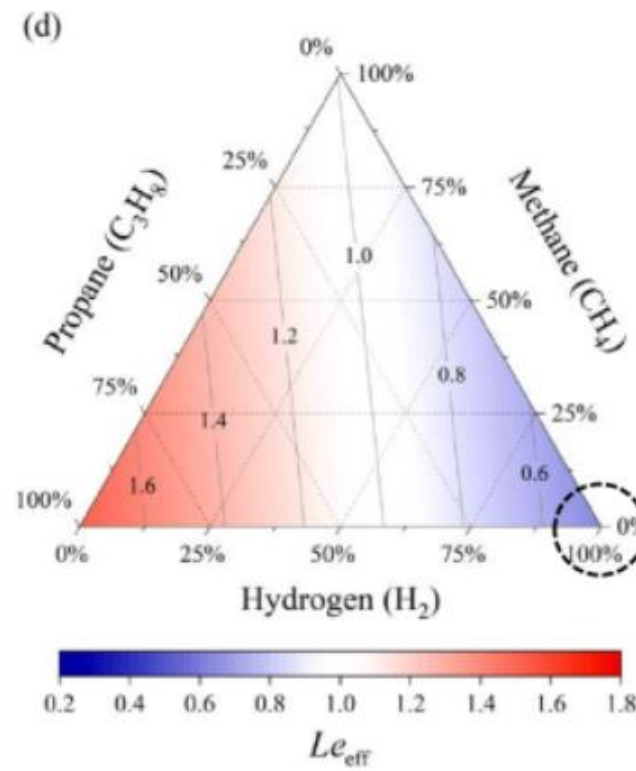
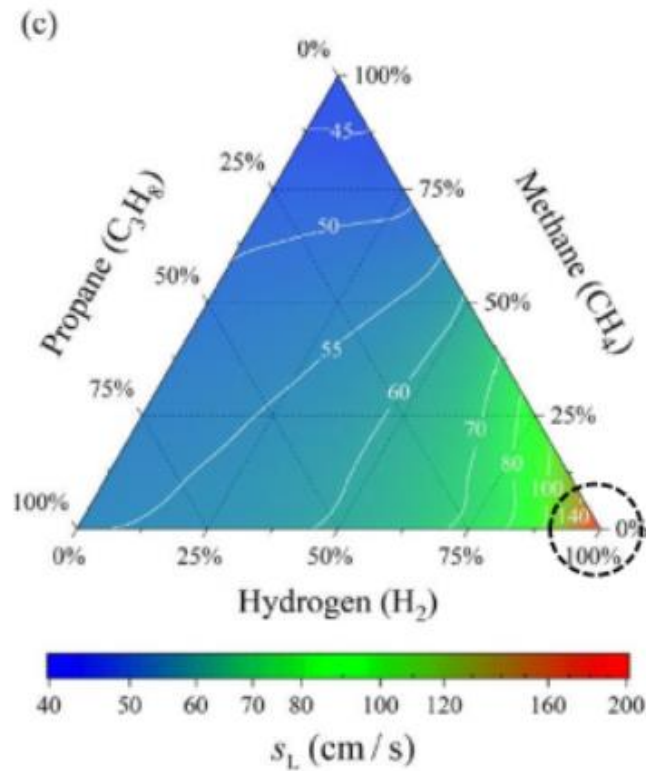
Fully premixed

Optical Access

Atmospheric



# Operating Conditions



Lewis Number = 0.5  
for pure  $H_2$

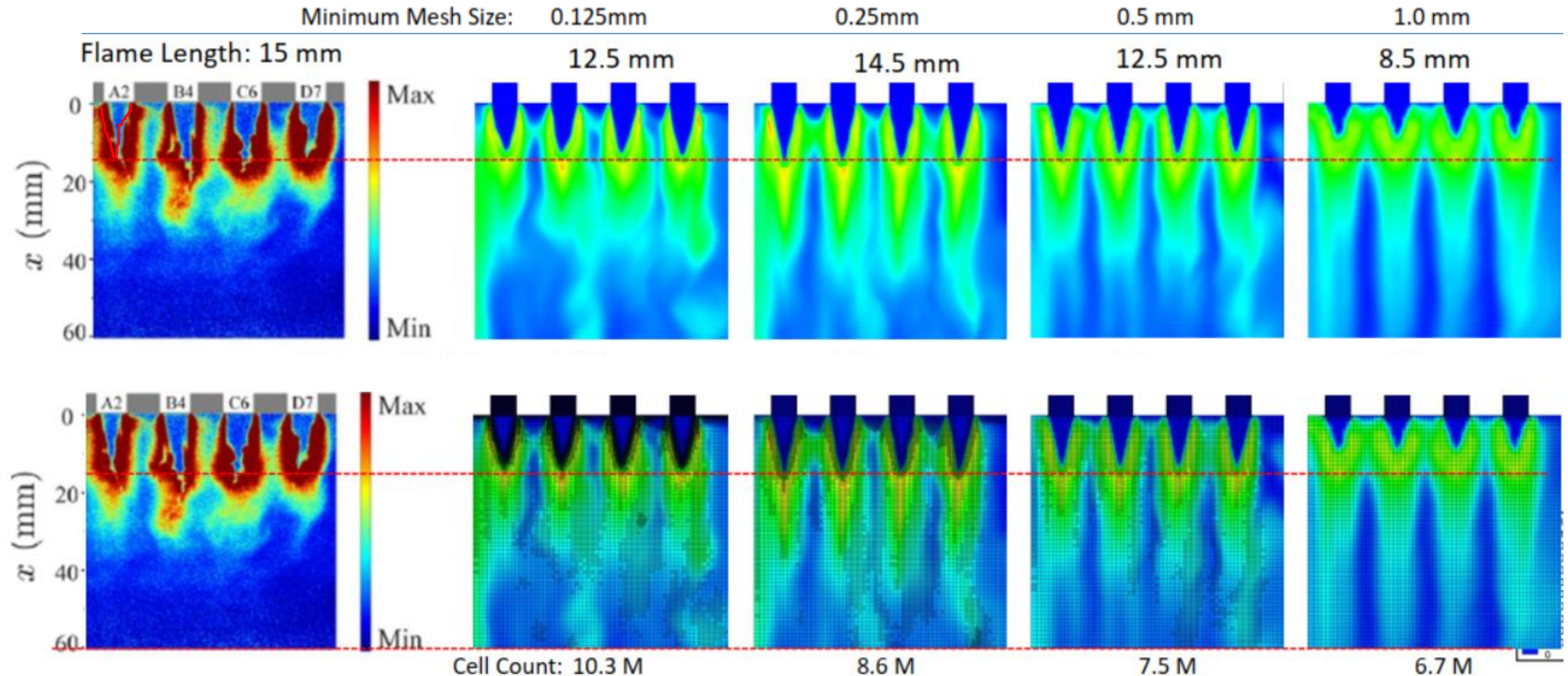
| Parameter          | Value    |
|--------------------|----------|
| Air inflow rate    | 25 m/s   |
| Equivalence Ratio  | 0.55     |
| Inflow temperature | 473 K    |
| Outflow pressure   | 1.01 bar |



# Flame Length Comparison and Mesh Study

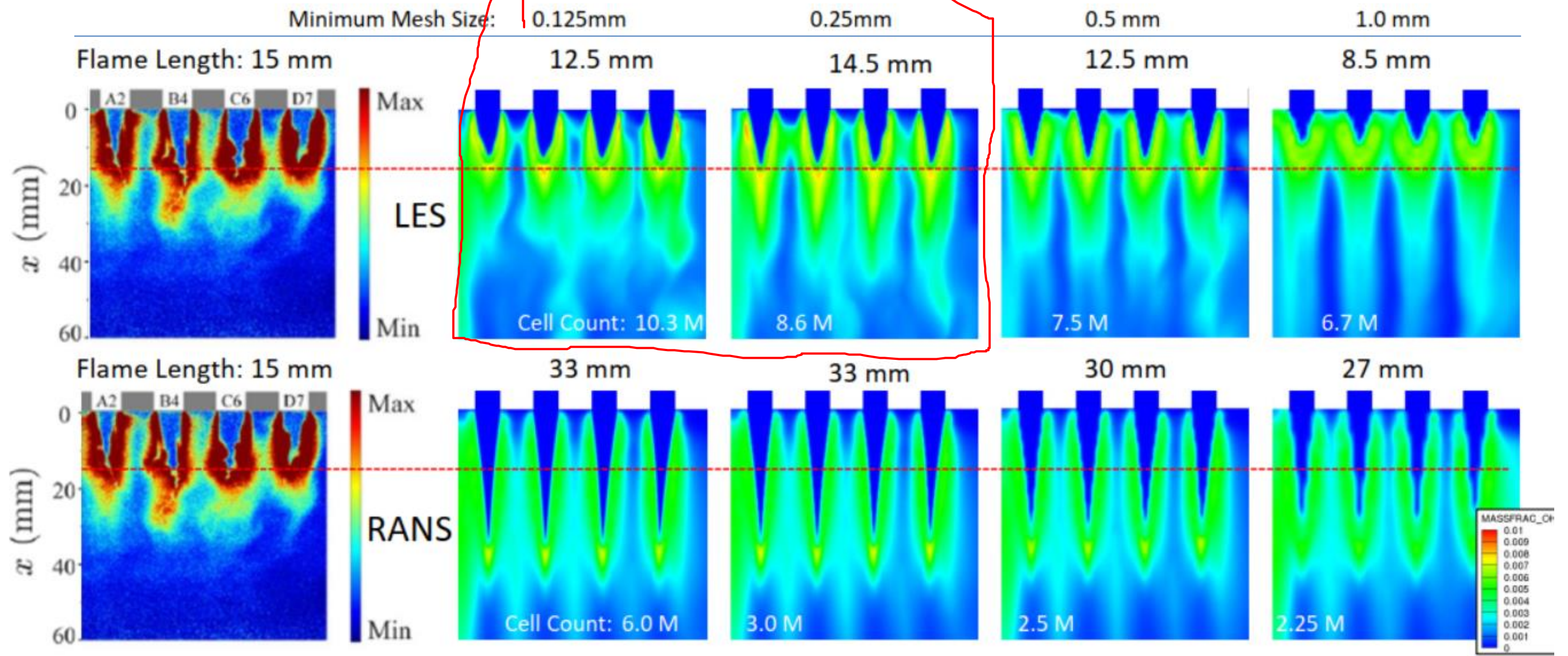
Kim Experiment

Time-average of LES



# LES vs. RANS

## Kim Experiment



# Conclusions



# Conclusions

- Poorly mixed (Marek) medium-pressure and premixed (Jin & Kim) atmospheric hydrogen combustion cases were considered to cover a range of conditions for validating a numerical approach for hydrogen combustor design.
- SAGE detailed chemistry is found to produce realistic flame structures and does not require tuning
- Steady RANS and unsteady LES approaches were compared.
  - RANS captured exponential NO<sub>x</sub> trends in Marek but failed at predicting flame length in Jin & Kim.
  - LES was found to be required to accurately capture flame length in Jin & Kim.



# Conclusions

- Poorly mixed (Marek) medium-pressure and premixed (Jin & Kim) atmospheric hydrogen combustion cases were considered to cover a range of conditions for validating a numerical approach for hydrogen combustor design.
- SAGE detailed chemistry is found to produce realistic flame structures and does not require tuning
- Steady RANS and unsteady LES approaches were compared.
  - RANS captured exponential NO<sub>x</sub> trends in Marek but failed at predicting flame length in Jin & Kim. **Design optimization** —
  - LES was found to be required to accurately capture flame length in Jin & Kim. **Detailed modeling** —



# Questions?



# Backup: Turbulence

# Turbulent Length Scale

- The RNG k-ε model requires a turbulent length scale for inflow boundary conditions
- Usually this is defined as a fraction of the diameter of the inlet
- Per the CONVERGE manual:

## Length Scale

The length scale eps boundary condition is a special case of the Dirichlet eps boundary condition. For the length scale boundary condition, the turbulent dissipation at the boundary is given by

$$\varepsilon = \frac{c_\mu^{3/4} k^{3/2}}{le}, \quad (9.20)$$

where  $c_\mu$  is a model constant,  $k$  is the turbulent kinetic energy, and  $le$  is the length scale (in meters) that you specify via `boundary_conditions > boundary > turbulence > eps > value`. You can estimate the length scale from a physical dimension in the domain (e.g., you can set the length scale to a fraction of the intake port diameter).

# Turbulence model settings

☒ Reynolds-Averaged Navier-Stokes (RANS) ☐ Detached Eddy Simulation (DES) ☐ Large Eddy Simulation (LES)

**Turbulence model:** RNG k- $\epsilon$

Wall Modeling

Von Karman's constant: 0.42 Law of the wall parameter: 5.5

Wall heat transfer model: O'Rourke and Amsden ☐ Base distance to wall on full cell size

Near wall treatment: Standard wall function

Law of the wall tke parameters:

Log-law branch: law\_ck -0.416 law\_bk 8.366

Viscous sublayer branch: law\_ceps2 1.9 law\_cvisc 11.0

RANS Constants

|                        |        |                               |       |
|------------------------|--------|-------------------------------|-------|
| $C_\mu$                | 0.0845 | $C_{\epsilon 3}$              | -1.0  |
| Reciprocal tke Prandtl | 1.39   | Reciprocal $\epsilon$ Prandtl | 1.39  |
| $C_{\epsilon 1}$       | 1.42   | $\beta$                       | 0.012 |
| $C_{\epsilon 2}$       | 1.68   | $\eta_0$                      | 4.38  |

☐ Buoyancy effects

$v^2$ -f/ $\zeta$ -f model constants

|         |      |                            |        |        |      |          |      |
|---------|------|----------------------------|--------|--------|------|----------|------|
| $C_1$   | 0.4  | $C_2$                      | 0.3    | $C_l$  | 0.36 | $C_\eta$ | 85.0 |
| $C_\mu$ | 0.22 | Reciprocal $\zeta$ Prandtl | 0.8333 | $C_2'$ | 0.65 |          |      |

Spray dissipation constant 0.0 Drop turbulent dispersion constant 0.03

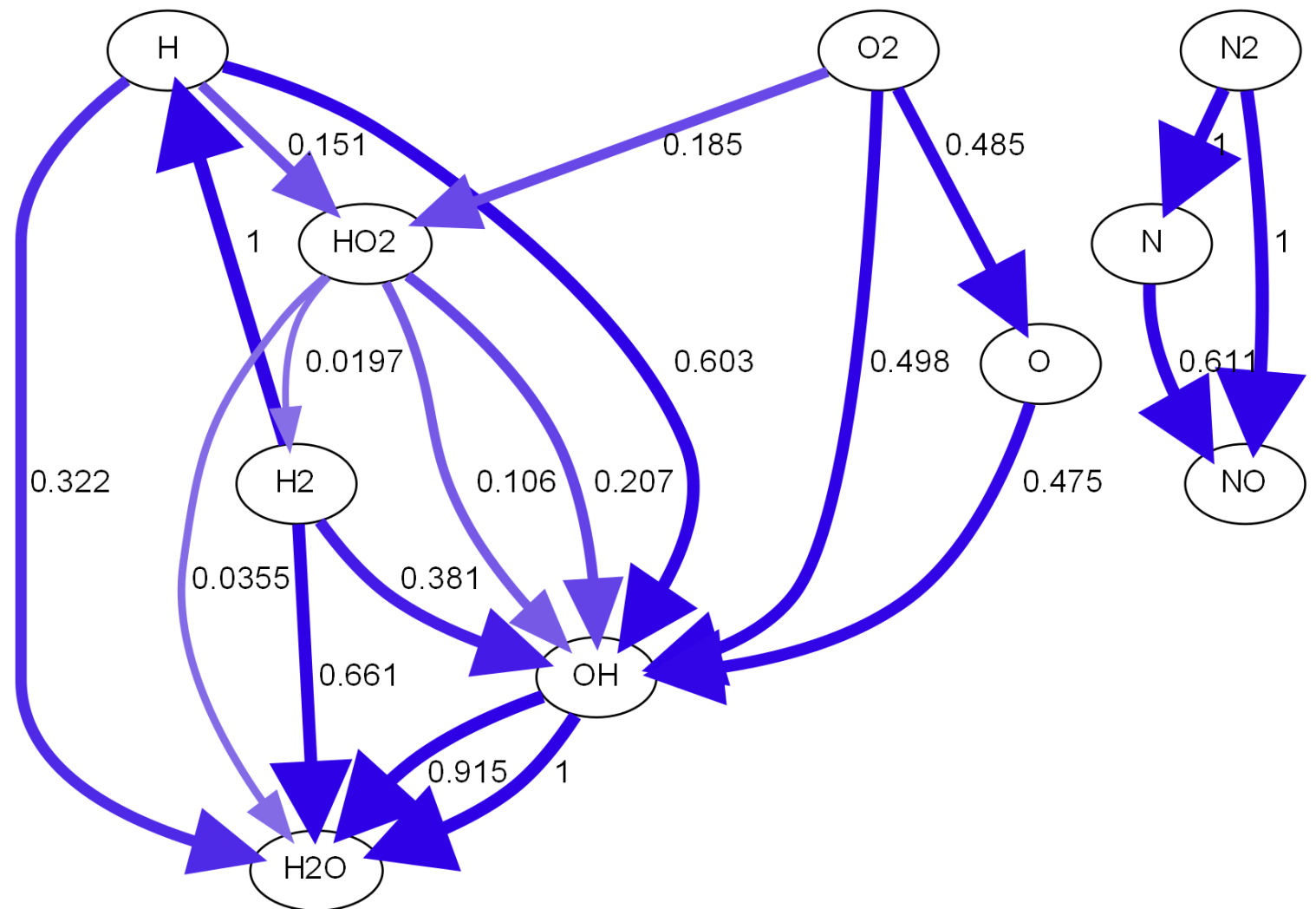
# Solver settings

| Parameter                           | Value |
|-------------------------------------|-------|
| Convection CFL number               | 30    |
| Diffusion CFL number                | 100   |
| Mach CFL number                     | 1000  |
| Solver Scheme                       | PISO  |
| P-V coupling tolerance              | 1e-3  |
| Momentum tolerance                  | 1e-5  |
| Pressure tolerance                  | 1e-8  |
| Density tolerance                   | 1e-4  |
| Energy tolerance                    | 1e-4  |
| Species tolerance                   | 1e-4  |
| Turbulence kinetic energy tolerance | 1e-3  |
| Epsilon tolerance                   | 1e-3  |

# Backup: Chemical Kinetic Mechanism

# Galway chemical mechanism

- Generated reaction path diagram from Cantera
- Just an estimate, not authoritative
- AR, CO, CO<sub>2</sub> not shown. Ar is nonreacting and CO, CO<sub>2</sub> not present in meaningful quantities
- NO $\leftrightarrow$ O relationship not shown



# Galway chemical kinetics mechanism

|                                                                     | Reaction                                                                                                                                                                                                                                       | A                     | n     | E <sub>a</sub> | Ref.        |
|---------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------|-------|----------------|-------------|
| H <sub>2</sub> /O <sub>2</sub> Chain Reactions                      |                                                                                                                                                                                                                                                |                       |       |                |             |
| 1                                                                   | $\dot{\text{H}} + \text{O}_2 = \dot{\text{O}} + \dot{\text{O}}\text{H}$                                                                                                                                                                        | $1.91 \times 10^{14}$ | 0.00  | 16.44          | [39]        |
| 2                                                                   | $\dot{\text{O}} + \text{H}_2 = \dot{\text{H}} + \dot{\text{O}}\text{H}$                                                                                                                                                                        | $5.08 \times 10^4$    | 2.67  | 6.292          | [40]        |
| 3                                                                   | $\dot{\text{O}}\text{H} + \text{H}_2 = \dot{\text{H}} + \text{H}_2\text{O}$                                                                                                                                                                    | $2.16 \times 10^8$    | 1.51  | 3.43           | [41]        |
| 4                                                                   | $\dot{\text{O}} + \text{H}_2\text{O} = \dot{\text{O}}\text{H} + \dot{\text{O}}\text{H}$                                                                                                                                                        | $2.97 \times 10^6$    | 2.02  | 13.4           | [42]        |
| H <sub>2</sub> /O <sub>2</sub> Dissociation/Recombination Reactions |                                                                                                                                                                                                                                                |                       |       |                |             |
| 5 <sup>a</sup>                                                      | $\text{H}_2 + \text{M} = \dot{\text{H}} + \dot{\text{H}} + \text{M}$                                                                                                                                                                           | $4.57 \times 10^{19}$ | -1.40 | 105.1          | [43]        |
| 6 <sup>b</sup>                                                      | $\dot{\text{O}} + \dot{\text{O}} + \text{M} = \text{O}_2 + \text{M}$                                                                                                                                                                           | $6.17 \times 10^{15}$ | -0.50 | 0.00           | [43]        |
| 7 <sup>c</sup>                                                      | $\dot{\text{O}} + \dot{\text{H}} + \text{M} = \text{OH} + \text{M}$                                                                                                                                                                            | $4.72 \times 10^{18}$ | -1.00 | 0.00           | [43]        |
| 8 <sup>d,e</sup>                                                    | $\dot{\text{H}} + \dot{\text{O}}\text{H} + \text{M} = \text{H}_2\text{O} + \text{M}$                                                                                                                                                           | $4.50 \times 10^{22}$ | -2.00 | 0.00           | [43] × 2.0  |
| Formation and consumption of HO <sub>2</sub>                        |                                                                                                                                                                                                                                                |                       |       |                |             |
| 9 <sup>f,g</sup>                                                    | $\dot{\text{H}} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$                                                                                                                                                                              | $3.48 \times 10^{16}$ | -0.41 | -1.12          | [44]        |
|                                                                     | $\dot{\text{H}} + \text{O}_2 = \text{HO}_2$                                                                                                                                                                                                    | $1.48 \times 10^{12}$ | 0.60  | 0.00           | [45]        |
| 10                                                                  | $\text{HO}_2 + \dot{\text{H}} = \text{H}_2 + \text{O}_2$                                                                                                                                                                                       | $1.66 \times 10^{13}$ | 0.00  | 0.82           | [6]         |
| 11                                                                  | $\text{HO}_2 + \dot{\text{H}} = \dot{\text{O}}\text{H} + \dot{\text{O}}\text{H}$                                                                                                                                                               | $7.08 \times 10^{13}$ | 0.00  | 0.30           | [6]         |
| 12                                                                  | $\text{HO}_2 + \dot{\text{O}} = \dot{\text{O}}\text{H} + \text{O}_2$                                                                                                                                                                           | $3.25 \times 10^{13}$ | 0.00  | 0.00           | [46]        |
| 13                                                                  | $\text{HO}_2 + \dot{\text{O}}\text{H} = \text{H}_2\text{O} + \text{O}_2$                                                                                                                                                                       | $2.89 \times 10^{13}$ | 0.00  | -0.50          | [46]        |
| Formation and Consumption of H <sub>2</sub> O <sub>2</sub>          |                                                                                                                                                                                                                                                |                       |       |                |             |
| 14 <sup>h</sup>                                                     | $\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$                                                                                                                                                                                | $4.2 \times 10^{14}$  | 0.00  | 11.98          | [47]        |
|                                                                     | $\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$                                                                                                                                                                                | $1.3 \times 10^{11}$  | 0.00  | -1.629         | [47]        |
| 15 <sup>i,f</sup>                                                   | $\text{H}_2\text{O}_2 + \text{M} = \dot{\text{O}}\text{H} + \text{OH} + \text{M}$                                                                                                                                                              | $1.27 \times 10^{17}$ | 0.00  | 45.5           | [48]        |
|                                                                     | $\text{H}_2\text{O}_2 = \dot{\text{O}}\text{H} + \text{OH}$                                                                                                                                                                                    | $2.95 \times 10^{14}$ | 0.00  | 48.4           | [49]        |
| 16                                                                  | $\text{H}_2\text{O}_2 + \dot{\text{H}} = \text{H}_2\text{O} + \dot{\text{O}}\text{H}$                                                                                                                                                          | $2.41 \times 10^{13}$ | 0.00  | 3.97           | [43]        |
| 17                                                                  | $\text{H}_2\text{O}_2 + \dot{\text{H}} = \text{H}_2 + \text{HO}_2$                                                                                                                                                                             | $6.03 \times 10^{13}$ | 0.00  | 7.95           | [43] × 1.25 |
| 18                                                                  | $\text{H}_2\text{O}_2 + \dot{\text{O}} = \dot{\text{O}}\text{H} + \text{HO}_2$                                                                                                                                                                 | $9.55 \times 10^{06}$ | 2.00  | 3.97           | [43]        |
| 19 <sup>h</sup>                                                     | $\text{H}_2\text{O}_2 + \dot{\text{O}}\text{H} = \text{H}_2\text{O} + \text{HO}_2$                                                                                                                                                             | $1.0 \times 10^{12}$  | 0.00  | 0.00           | [50]        |
|                                                                     | $\text{H}_2\text{O}_2 + \dot{\text{O}}\text{H} = \text{H}_2\text{O} + \text{HO}_2$                                                                                                                                                             | $5.8 \times 10^{14}$  | 0.00  | 9.56           | [50]        |
| a                                                                   | Efficiency factors are: H <sub>2</sub> O=12.0; H <sub>2</sub> =2.5;                                                                                                                                                                            |                       |       |                |             |
| b                                                                   | Efficiency factors are: H <sub>2</sub> O=12; H <sub>2</sub> =2.5; Ar = 0.83; He = 0.83;                                                                                                                                                        |                       |       |                |             |
| c                                                                   | Efficiency factors are: H <sub>2</sub> O=12; H <sub>2</sub> =2.5; Ar = 0.75; He = 0.75;                                                                                                                                                        |                       |       |                |             |
| d                                                                   | Original pre-exponential A factor is multiplied by two here.                                                                                                                                                                                   |                       |       |                |             |
| e                                                                   | Efficiency factors are: H <sub>2</sub> O=12; H <sub>2</sub> =0.73; Ar = 0.38; He = 0.38;                                                                                                                                                       |                       |       |                |             |
| f                                                                   | Troe parameters; reaction 9: $\alpha = 0.5$ , $T^{***} = 1.0 \times 10^{-30}$ , $T^* = 1.0 \times 10^{+30}$ , $T^{**} = 1.0 \times 10^{+100}$<br>reaction 15: $\alpha = 0.5$ , $T^{***} = 1.0 \times 10^{-30}$ , $T^* = 1.0 \times 10^{+30}$ . |                       |       |                |             |
| g                                                                   | Efficiency factors are: H <sub>2</sub> =1.3; H <sub>2</sub> O=14; Ar = 0.67; He = 0.67;                                                                                                                                                        |                       |       |                |             |
| h                                                                   | Reactions 14 and 19 are expressed as the sum of the two rate expressions.                                                                                                                                                                      |                       |       |                |             |
| i                                                                   | Efficiency factors are: H <sub>2</sub> O=12; H <sub>2</sub> =2.5; Ar = 0.45; He = 0.45;                                                                                                                                                        |                       |       |                |             |

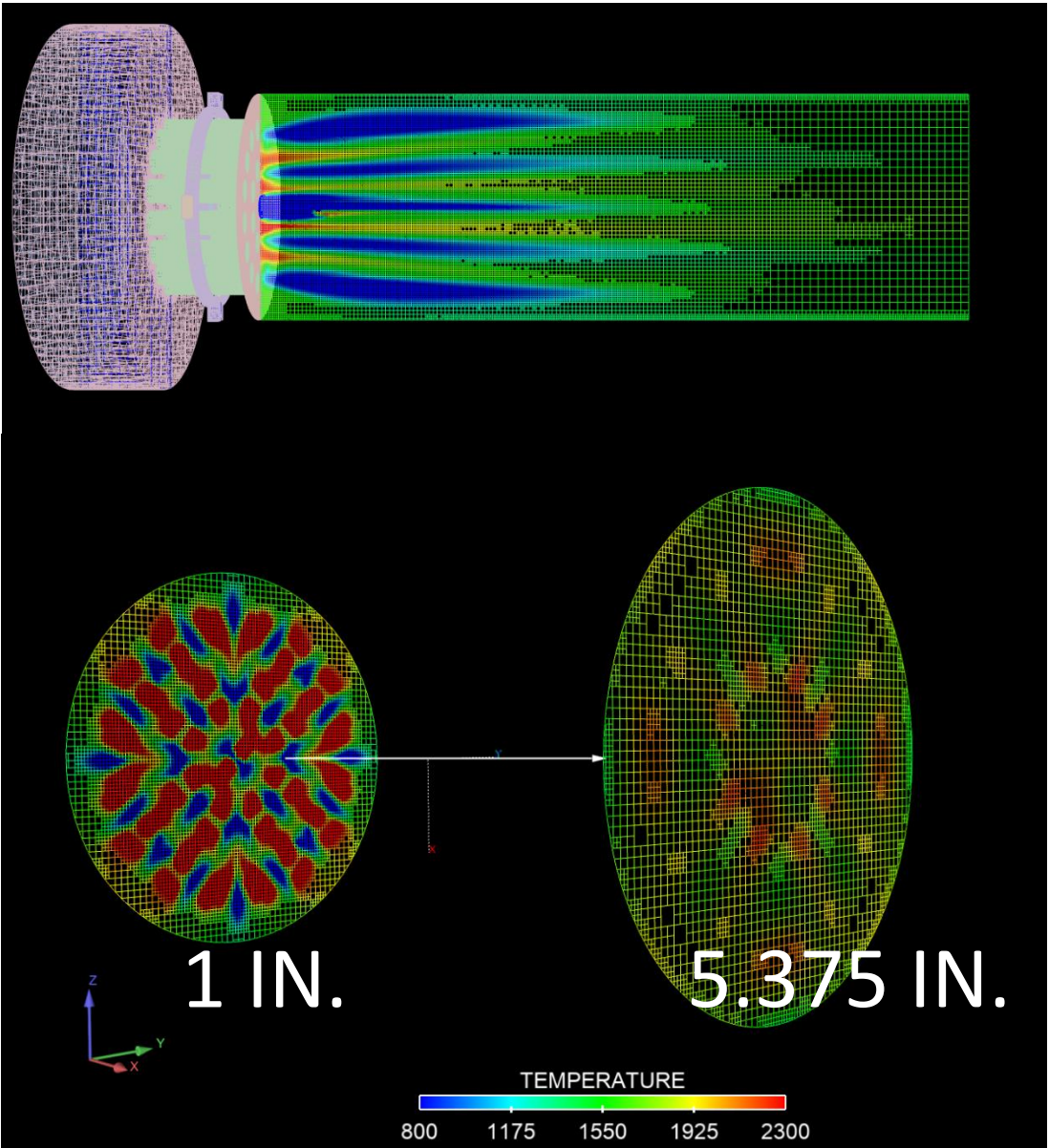
Table 1: Revised H<sub>2</sub>/O<sub>2</sub> reaction mechanism. Units: cm<sup>3</sup>, mol, s, kcal, K.

NO<sub>x</sub> and unused CO, CO<sub>2</sub>  
mechanisms adapted from  
GRI Mech 3.0

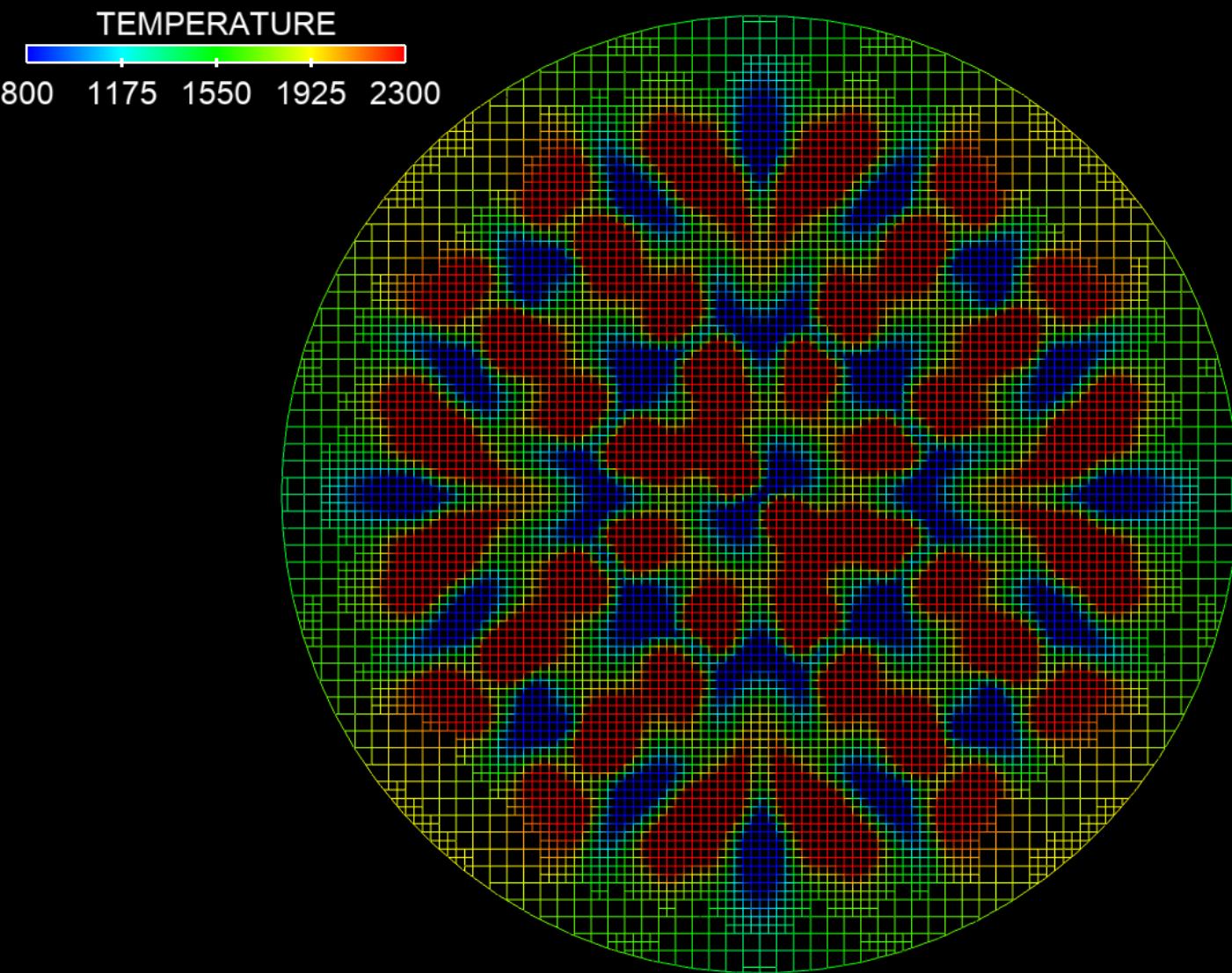
# Backup: Mesh Refinement

# Mesh Refinement Study

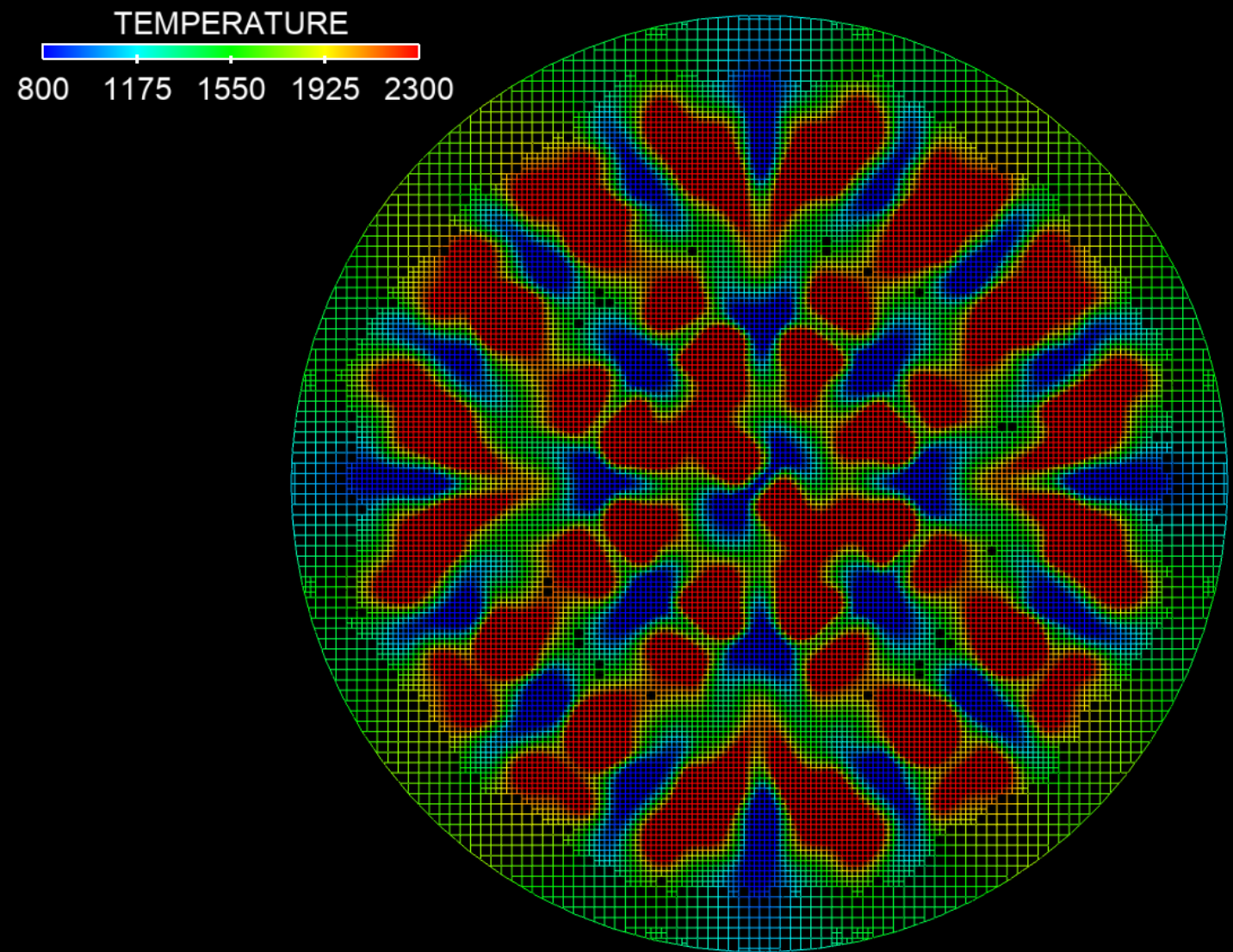
| Parameter                   | Value                                                                   |         |
|-----------------------------|-------------------------------------------------------------------------|---------|
| CFD software                | CONVERGE 3.1.4                                                          |         |
| Combustion model            | SAGE                                                                    |         |
| NOx model                   | Extended Zeldovich passive                                              |         |
| Base grid size              | 1.4 mm                                                                  |         |
| Combustor minimum grid size | 0.28 mm                                                                 | 0.18 mm |
| Plenum minimum grid size    | 0.14 mm                                                                 | 0.09 mm |
| Adaptive mesh refinement    | Temperature – 2.5 K across the cell<br>Velocity – 1 m/s across the cell |         |
| Wall heat transfer          | Adiabatic                                                               |         |
| H2 reaction mechanism       | Galway mechanism                                                        |         |
| Turbulence model            | RNG k-ε with law of the wall                                            |         |



# Mesh refinement comparison



**Smallest grid size  
=0.14 mm**



**Smallest grid size  
=0.09 mm**

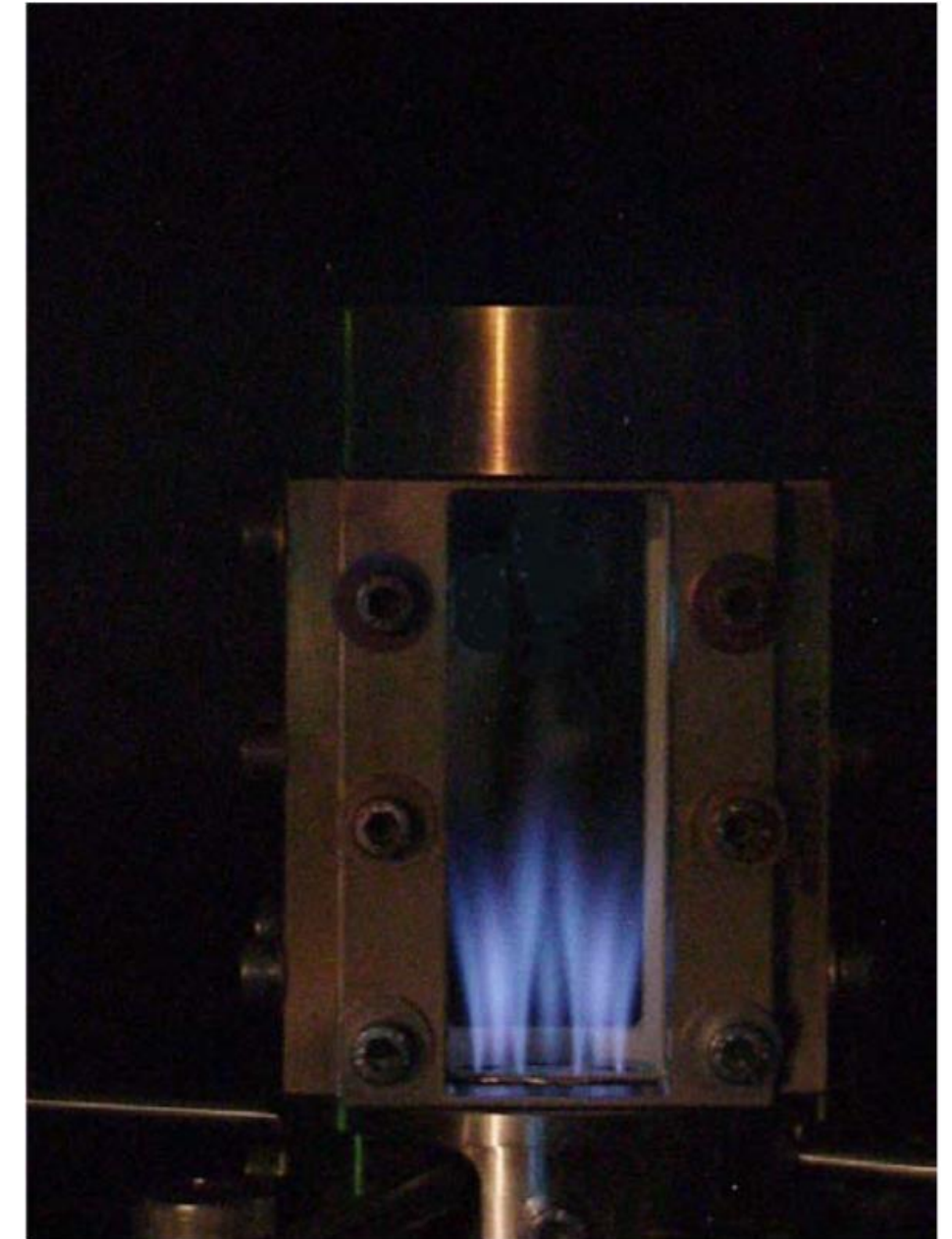
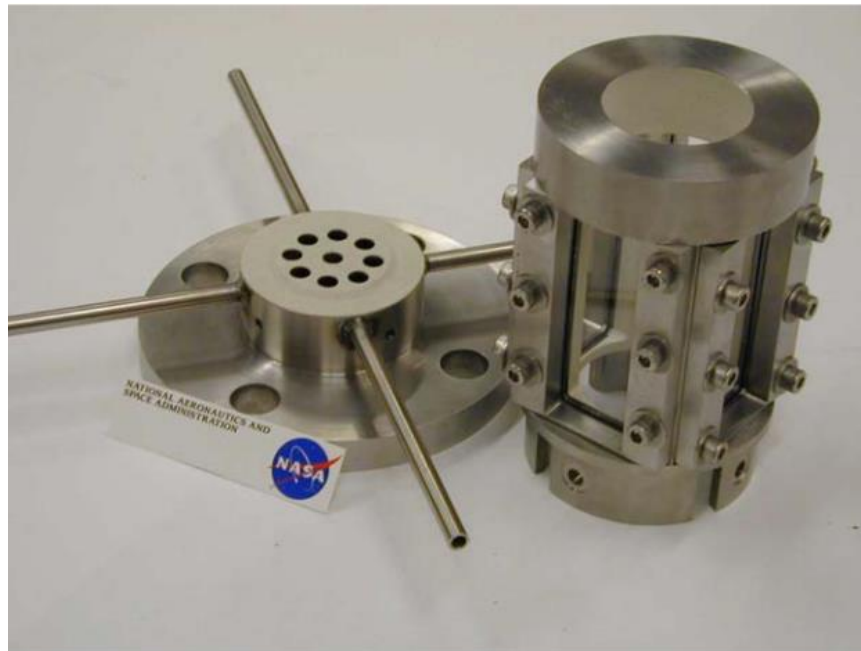
# NOx: Comparison at different locations

| Parameter                               | Combustor minimum grid size<br>=0.14 mm | Combustor minimum grid size<br>=0.09 mm |
|-----------------------------------------|-----------------------------------------|-----------------------------------------|
| Adiabatic flame temperature             | 1788 K                                  |                                         |
| Mean combustor temperature<br>by volume | 1669 K                                  | 1659 K                                  |
| Average NOx@1 in.                       | 36 ppm                                  | 34 ppm                                  |
| Average NOx@3.125 in.                   | 122 ppm                                 | 125 ppm                                 |
| Average NOx@5.375 in.                   | 128 ppm                                 | 132 ppm                                 |
| Average NOx@exit plane                  | 129 ppm                                 | 133 ppm                                 |

# Backup: Sandia Flame Studies

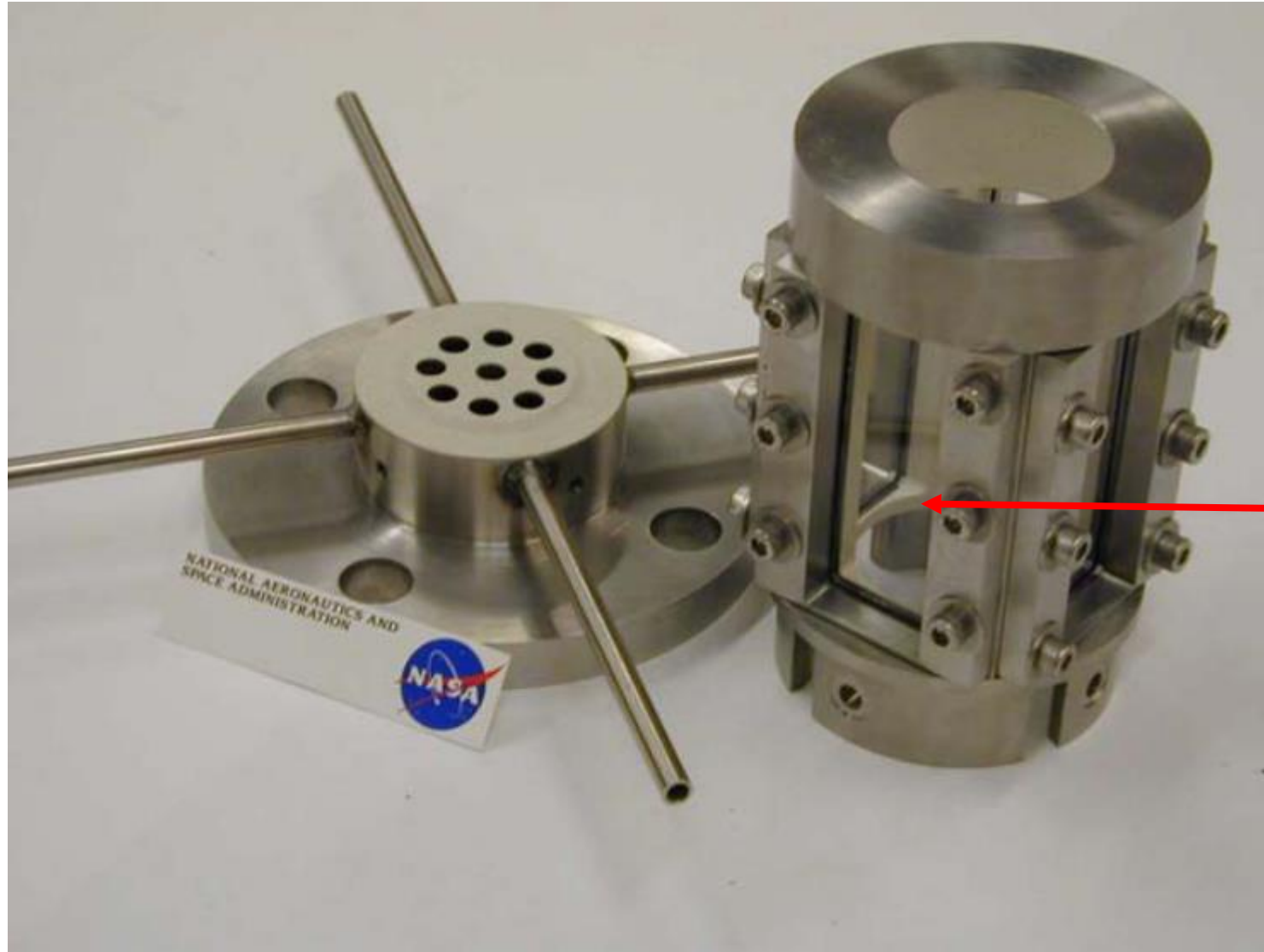
# Sandia hydrogen flame studies

- Separate H<sub>2</sub> flame characterization study performed by Sandia on similar nozzle.
- Similar to Marek/NASA, but different: atmospheric outlet, different dimensions, no outer ring of nozzles.
- Useful for assessing ability of numerical approach to predict flame holding.



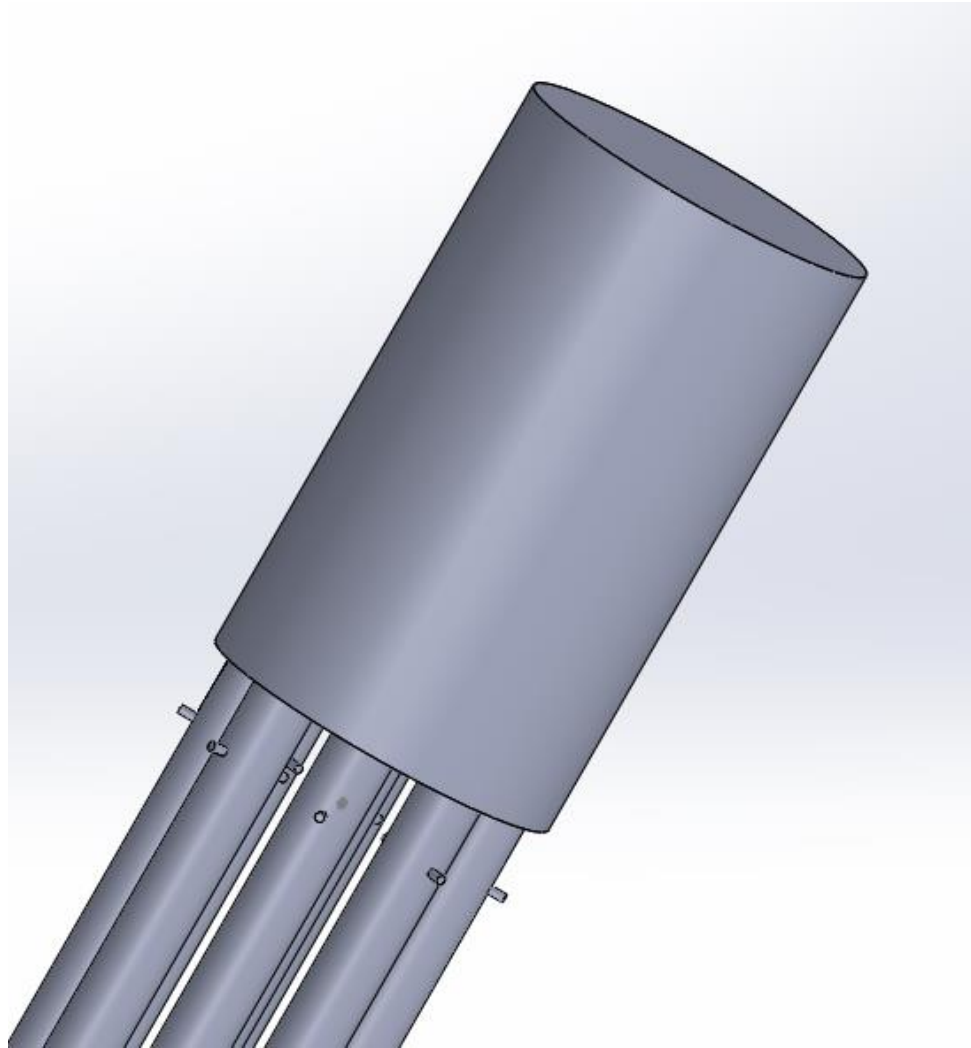
Schefer, R., *et al.*, 2003. <https://www.osti.gov/servlets/purl/811192>

# Sandia experimental quirks

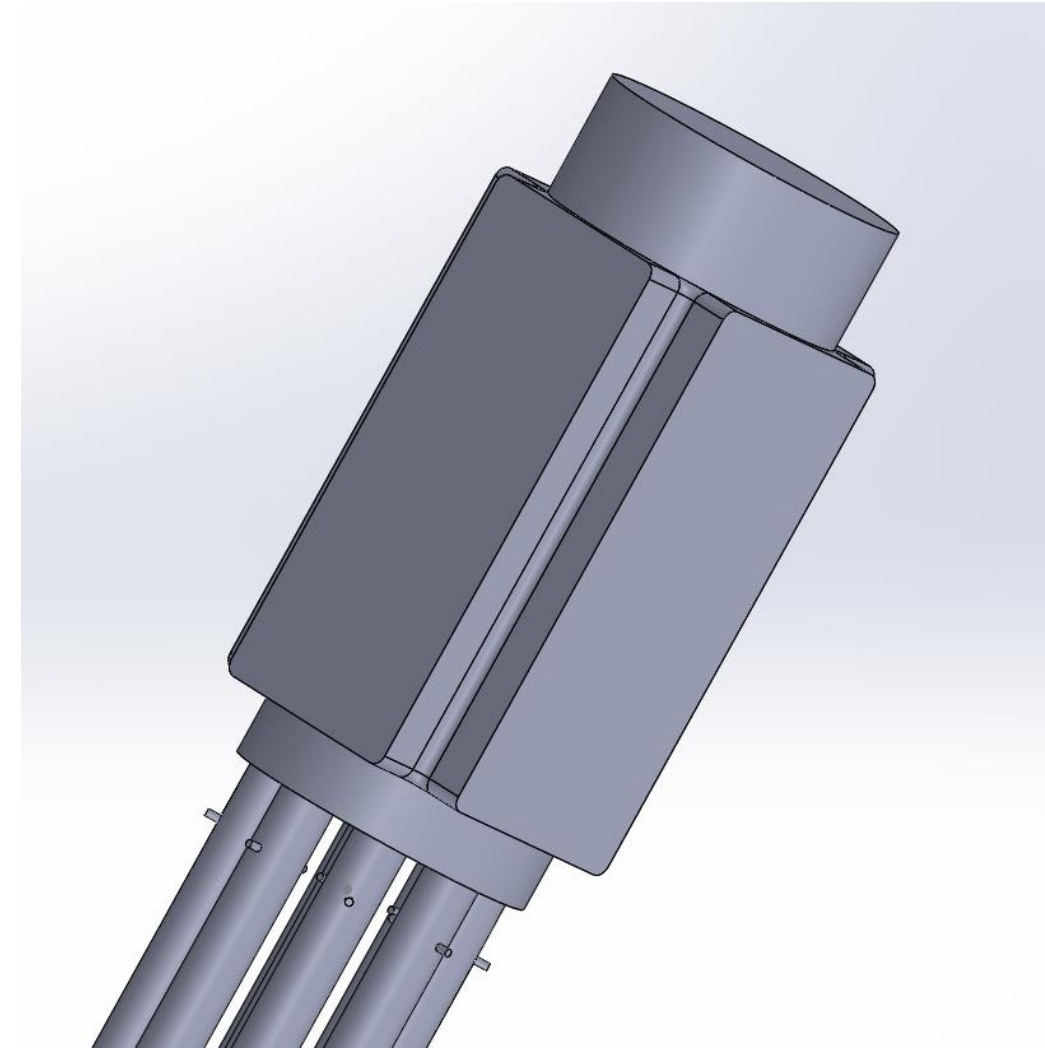


- Schefer used flat windows, so there are features inside that affect the flow field significantly.
- The flow cross-section transitions from circular to rectangular. Reinforced corners are needed to affix the windows.
- Making an accurate view of the interior is difficult.

## Initial Schefer interior CAD

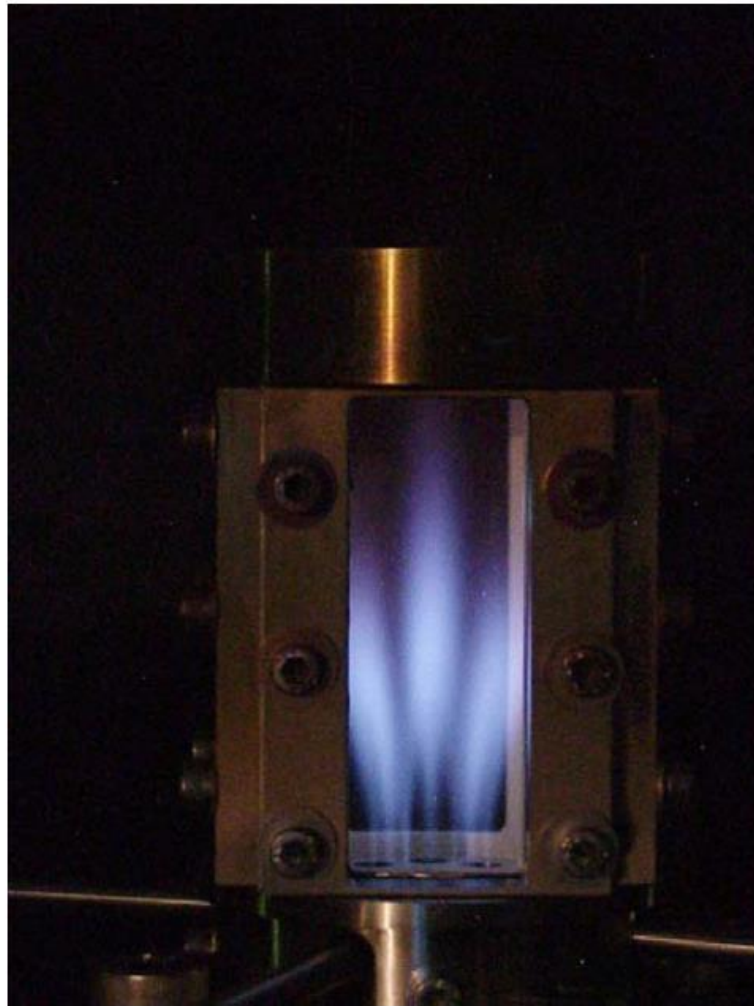


## New Schefer CAD

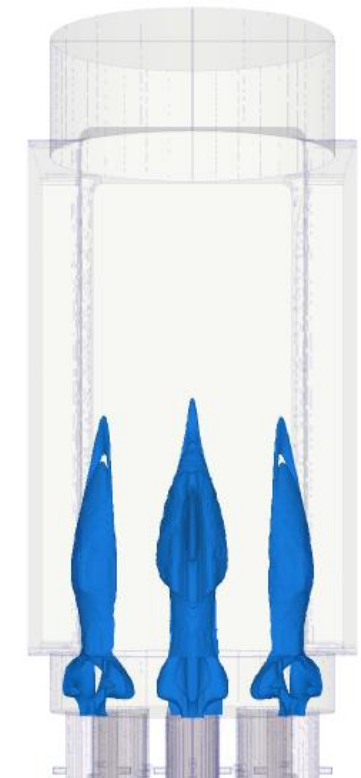
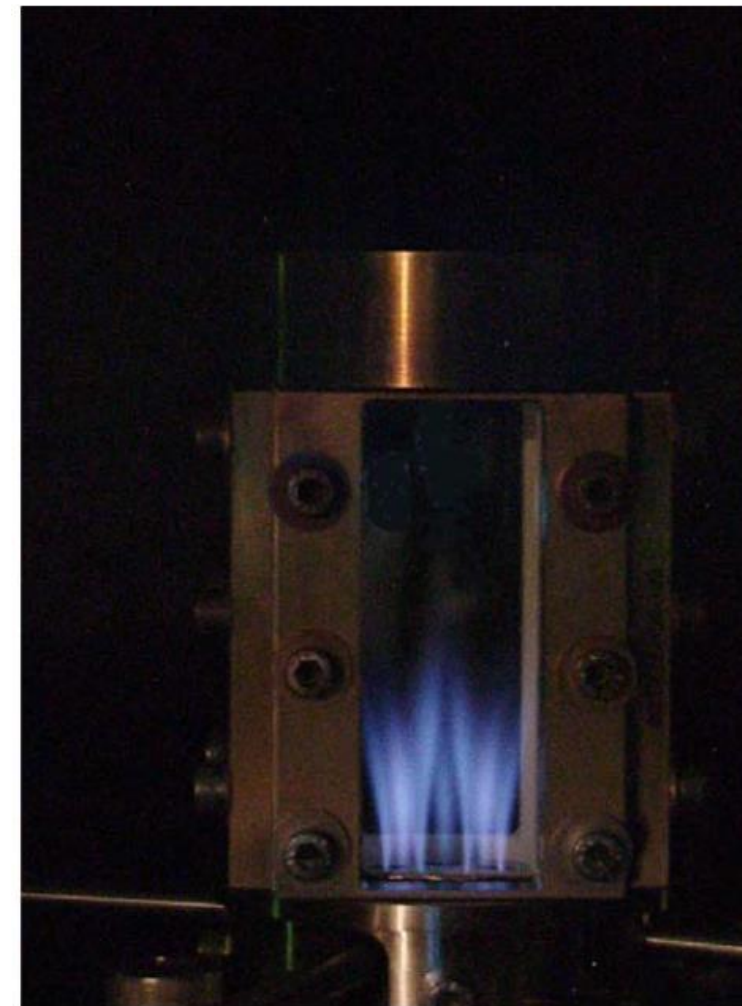


The Schefer experimental apparatus is poorly documented. Feature type and dimensions are estimated from limited photos. Flat window mounting likely creates large recirculation regions in the flow.

$$\phi=0.3$$

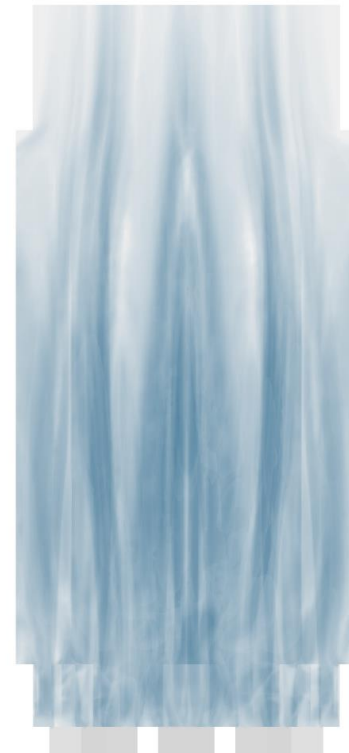
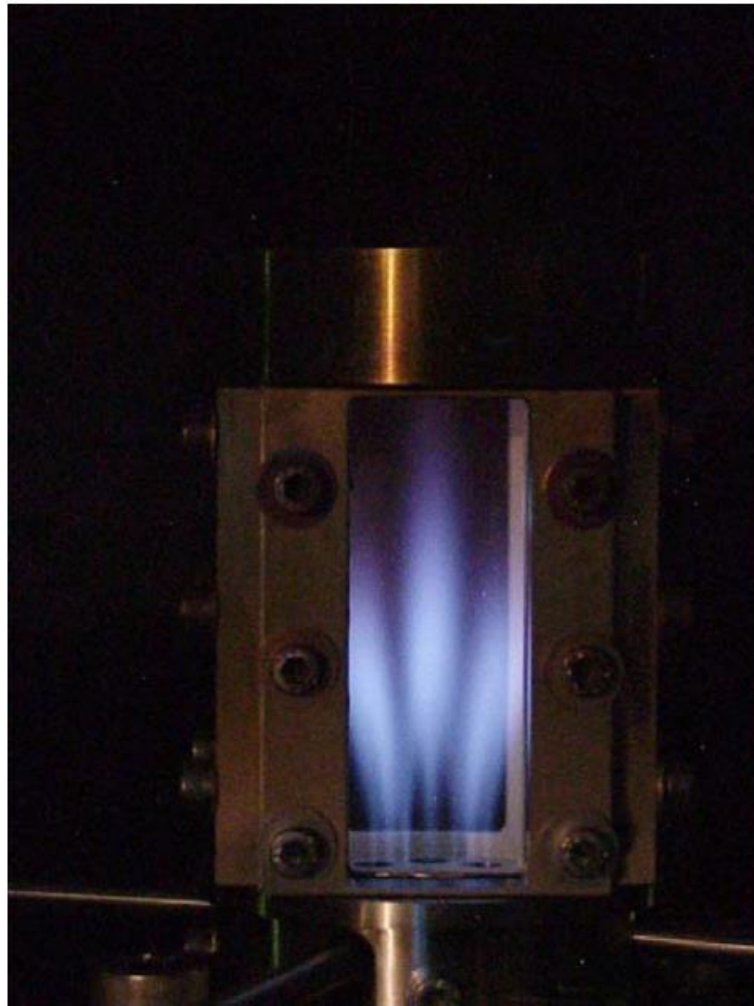


$$\phi=0.15$$

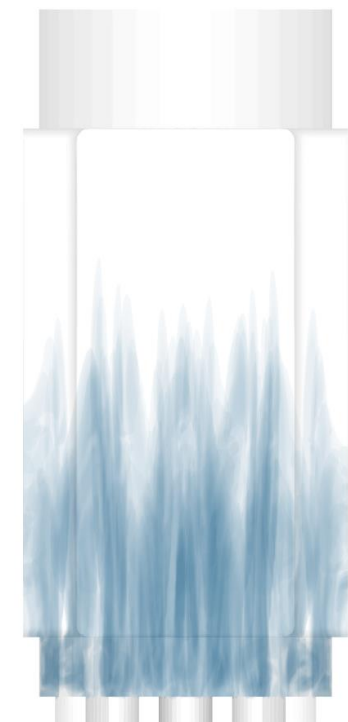
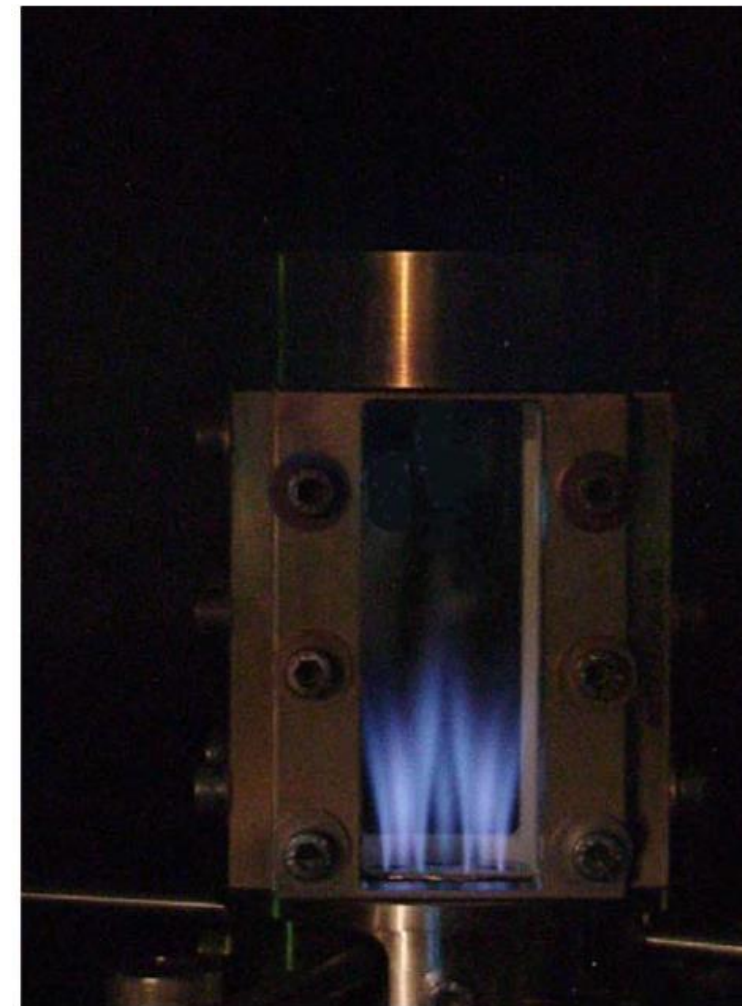


Flame length matching is excellent for frontmost isosurfaces of constant OH, shape is comparable

$$\phi=0.3$$

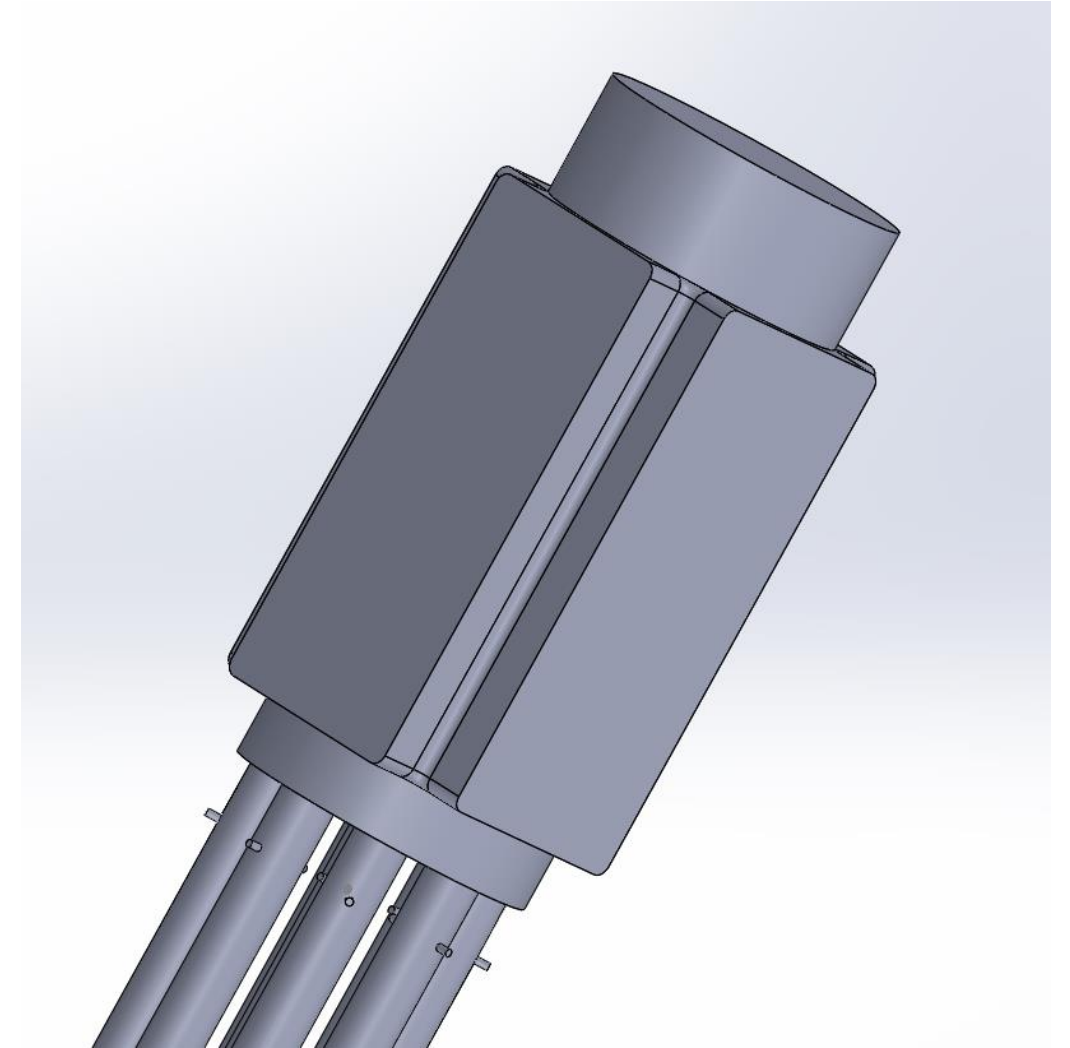
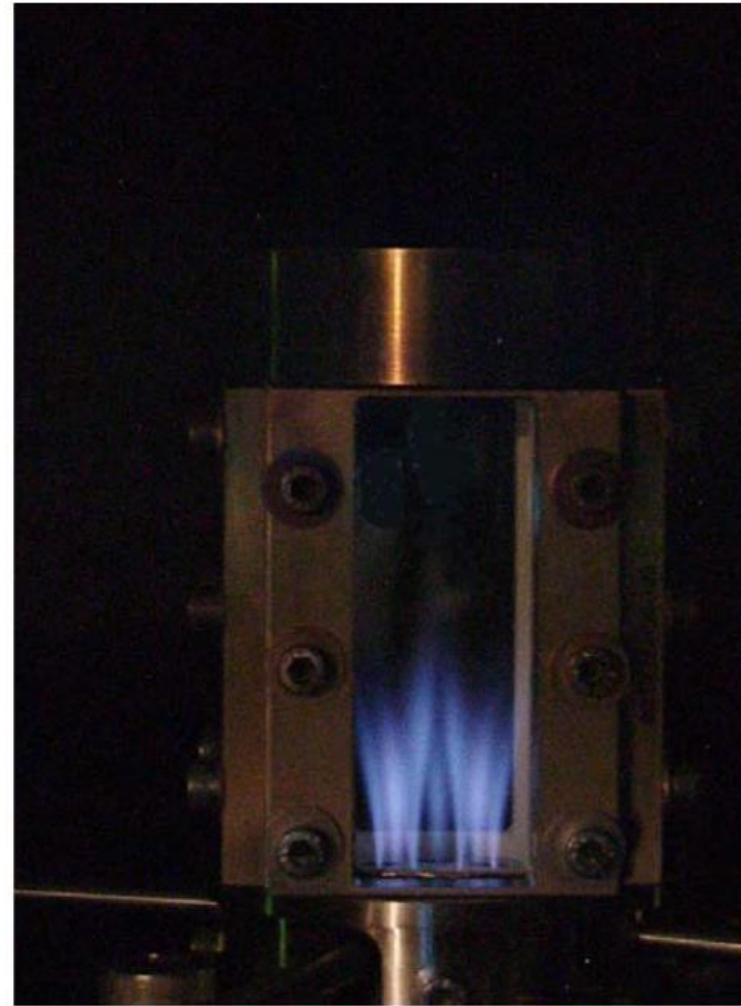
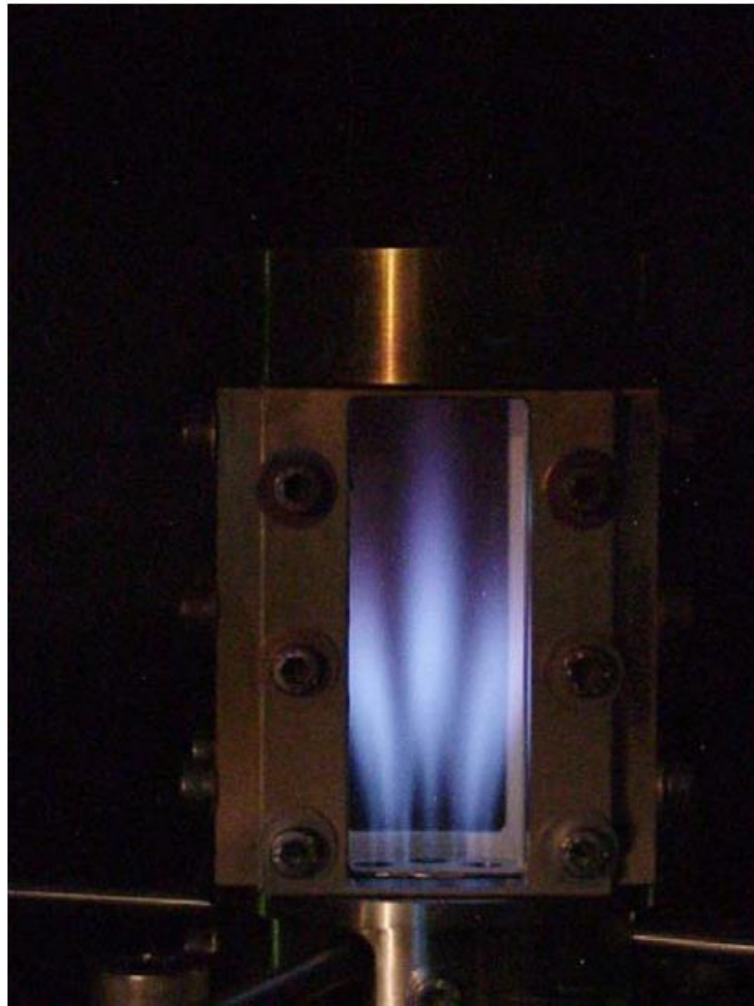


$$\phi=0.15$$



Volumetric view of spatial gradient of OH qualitatively matches flame shape

# Flame shape caveats

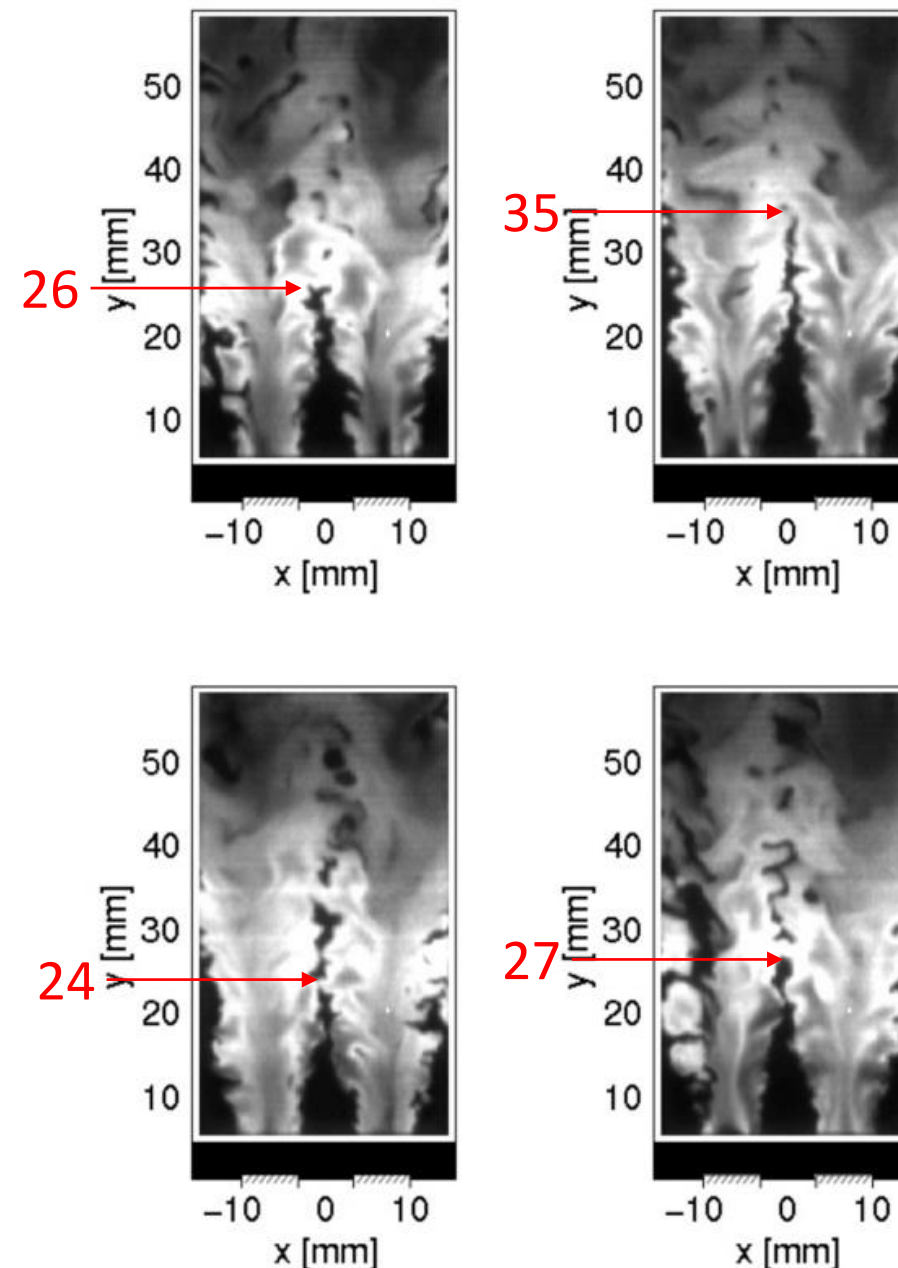


Images suggest larger recirculation regions, more prominent backwards facing step than CAD

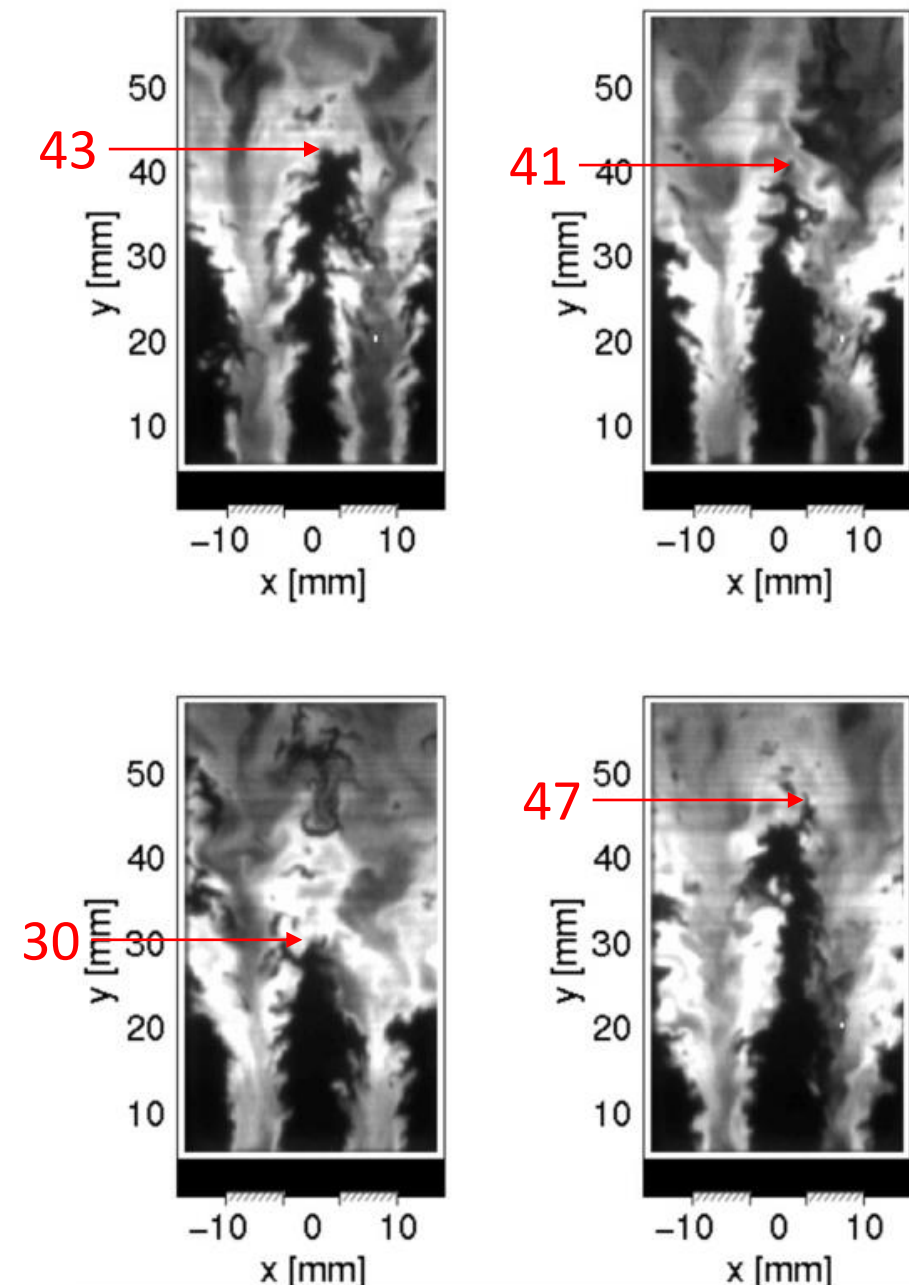
# Flame length

- Numerical results show good qualitative agreement with flame length and shape.
- The experimental apparatus is ambiguous. Large recirculation regions and the possibility of combustion downstream of the atmospheric outlet make exact replication of the experiment difficult.
- Attempted to extract instantaneous flame lengths from provided images

$\phi = 0.15$   
Avg= 28.0 mm



$\phi = 0.33$   
Avg = 40.25 mm



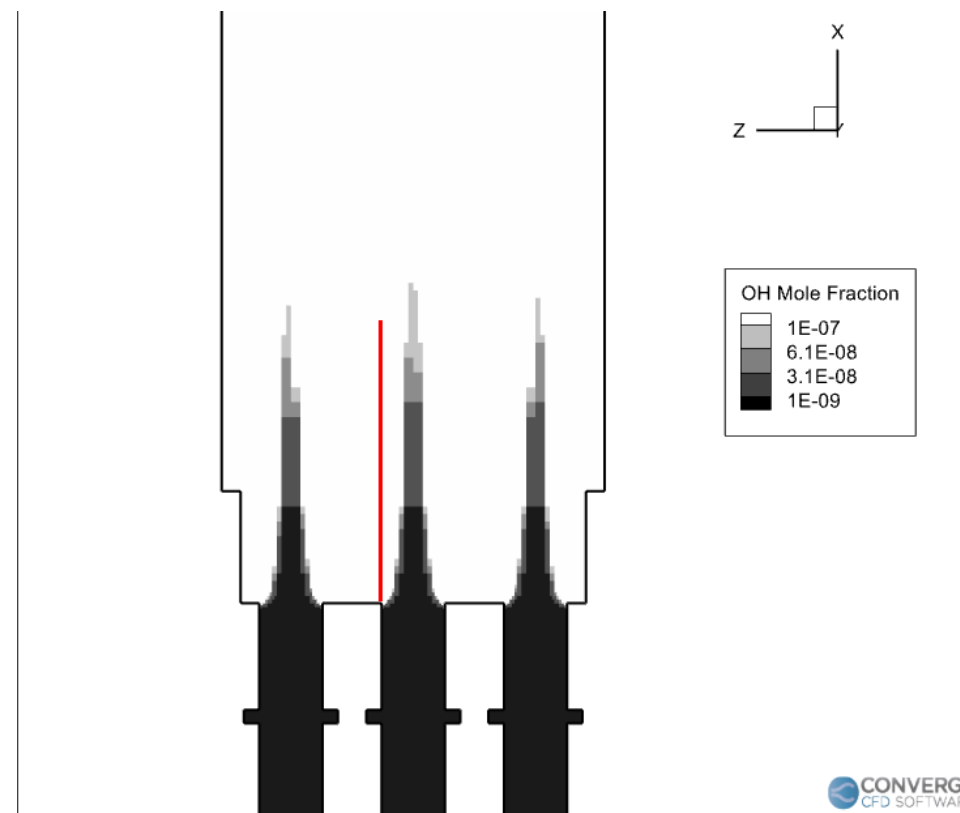
# Flame length comparison

- Extracted center plane OH contours from runs of both equivalence ratios, averaged experimental flame lengths marked in **red**.
- Numerical flame length sensitive to chosen OH isocontour.
- $1e-7$  is a reasonable upper limit, as below that there is almost no OH, but without knowing experimental sensitivities a complete comparison is difficult.

$$\phi = 0.15$$

Experimental: 28.0 mm

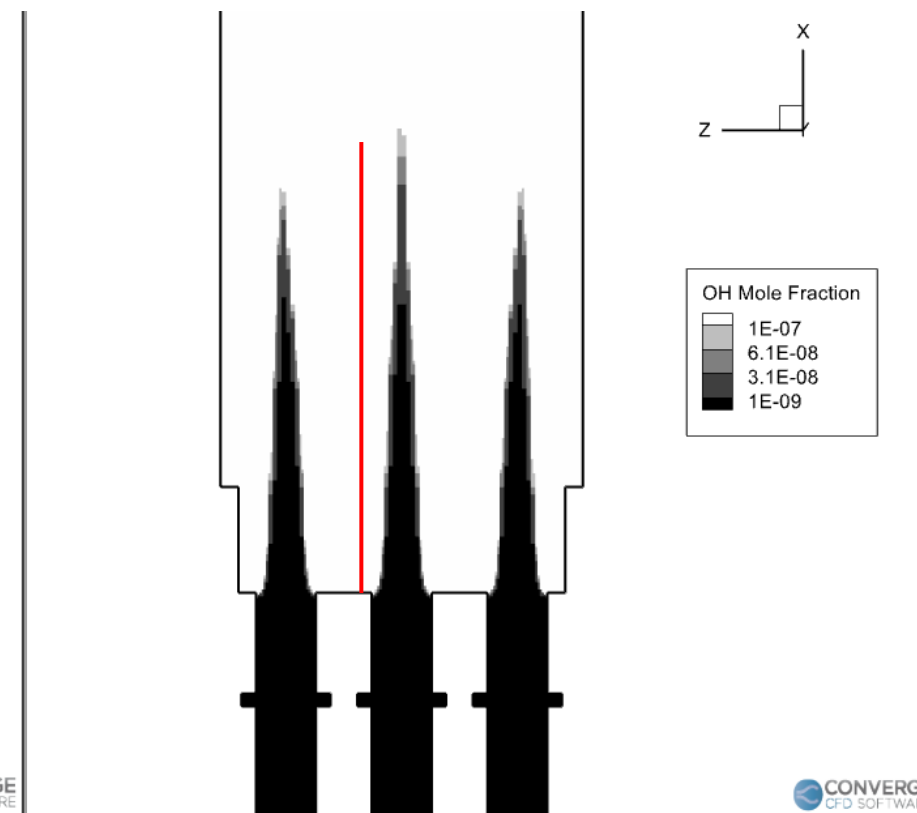
Numerical: 31.78 mm



$$\phi = 0.33$$

Experimental: 40.25 mm

Numerical: 40.54 mm



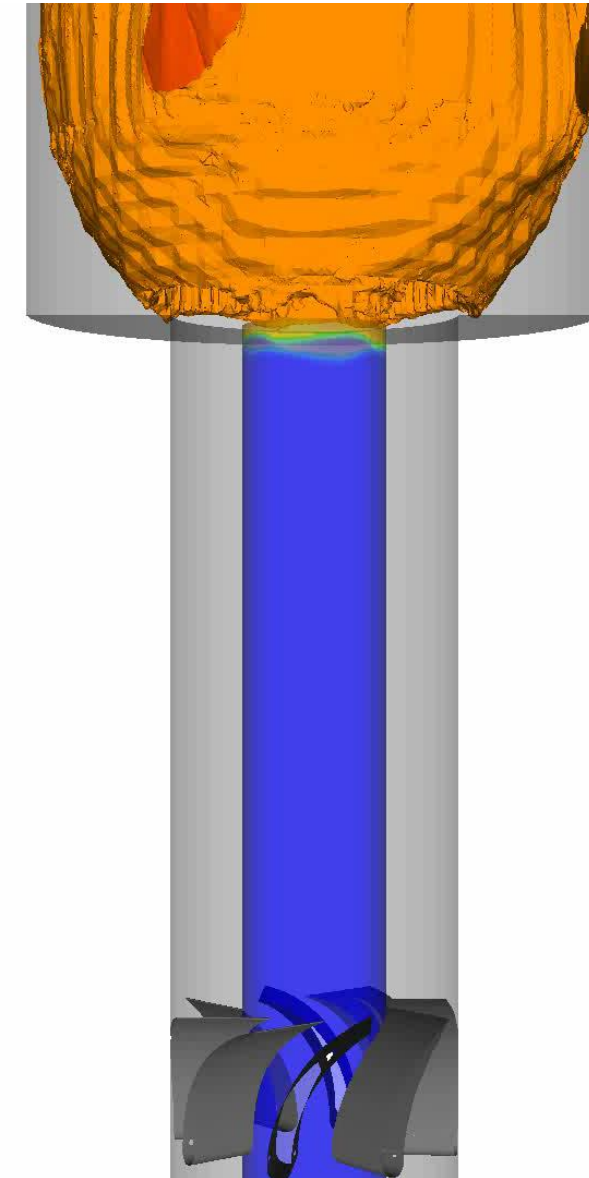
# Backup: Flashback and LBO

# Flashback and LBO

- CSI claims that CONVERGE can model flashback in LES mode.
- They demonstrated boundary layer flashback, but costly.
- Determining precise LBO and flashback limits for each nozzle design using high fidelity CFD is extremely costly for a design space exploration.
- Because the current project specifies a single, full-load operating condition, LBO exploration is beyond scope.
- CSI claims to have demonstrated LBO and it could be investigated, but would require a contract modification or separate project.



Ebi & Clemons, 2014



Kumar, 2022

# Flashback mechanisms and prediction models

- RANS alone is inadequate to predict flashback
- Literature models will be used as part of the 1-D design tool to prevent simulating cases that would be near the flashback limit or would obviously blow off
- Flashback types considered (per Benim & Syed, 2015):
  - Autoignition
  - Combustion instabilities
  - Turbulent flame propagation in core flow and within boundary layer
  - Combustion induced vortex breakdown (CIVB)

# Autoignition

**Condition:**  $\tau_{\text{autoignition}} < \tau_{\text{residence}}$

**Description:** The fuel-air mixture autoignites before it exits the nozzle

**Mitigation:** The 1-D design code will estimate flow residence time for a given nozzle geometry and give a factor of safety. Estimated autoignition time will be computed by the Galway chemical mechanism. RANS will provide a residence time check by comparing the path-integrated autoignition time to the maximum flow residence time. LES will provide a residence time check by comparing the path-integrated autoignition time to the maximum flow residence time. Certain types of mixing like cavity injection may be discarded during initial selection due to their long flow residence times. The risk of autoignition is deemed low for the present design approach.

# Combustion instabilities

**Condition:**  $u'_{\text{low-frequency pressure}} > u$

**Description:** Unsteady low-frequency pressure oscillations cause a temporary flow reversal into the nozzle. For example:  $u'_{\text{low-frequency pressure}} \approx \frac{p'}{\rho a}$  for a rearward-facing step flameholder (Keller, 1982, Thibaut & Candel, 1998).  $p'$  is difficult to predict, as high-order models are required to capture thermoacoustic instabilities.

**Mitigation:** LES will allow frequency analysis of unsteady flow features, for example vortex shedding from shear layers. These frequencies will be compared to the natural frequencies of the chamber, nozzles, etc. as a preliminary check on resonance before testing. Generally, acoustic and thermoacoustic instabilities are first detected during testing and accurate prediction is beyond scope for this phase. LMS Virtual.Lab software from Siemens being investigated for more accurate noise/resonance predictions.

# Turbulent flame propagation in core and BL

**Condition:**  $S_T > u$

**Description:** Turbulent flame speed locally exceeds the flow velocity, causing the flame front to propagate upstream. Flashback can occur within the core flow as well as in the boundary layer, with different physical mechanisms for each.

For boundary layer flashback, a critical velocity gradient,  $g_c$ , is a widely-used approach to gauge the extent of upstream flame propagation. This is also an area of active research, though the complications of turbulence are slightly more tractable in wall-bounded flows.

For core flow flashback, an example simple empirical correlation for a planar flame (which neglects quenching effects of high turbulence) is:  $\frac{S_T}{S_L} = 1 + 0.435 \text{ Re}^{0.44}$  (Liu, 1991). Many of these simple relationships rely on positive Markstein lengths (related to the local curvature of the flame front) while, unfortunately, lean  $\text{H}_2$ /air combustion generally has a negative Markstein length.

# Turbulent flame propagation in core and BL cont.

**Description continued:** Many formulations for  $S_T$  are available but are highly conditions specific. For example, Daniele & Jansohn, 2012 was performed at very near the present operating conditions but with 40% H<sub>2</sub>-40%CO-20%N<sub>2</sub> and did not measure tip temperature. Goulier *et al*, 2017 relies on pressure scaling. For a more general model of turbulent flame speed for lean premixed H<sub>2</sub>/air, there is significant disagreement in the literature. Additionally, it is not sufficient to increase the flow velocity without limit, as that can lead to blow off.

# Turbulent flame propagation in core and BL cont.

**Mitigation:** Kalantari *et al.* 2016 developed an empirical correlation based on Da to calculate the injector critical velocity,  $u_c$ , to avoid flashback:

$$Da = e^{-12.06} Le^{1.68} Pe_f^{1.91} \left(\frac{T_3}{T_0}\right)^{2.57} \left(\frac{T_{tip}}{T_0}\right)^{-0.49} \left(\frac{P_3}{P_0}\right)^{-2.1}$$

$$g_c = \frac{S_L^2}{\alpha Da} \qquad g_c = \frac{0.03955 u_c^{1.75} \rho_3^{0.75}}{\mu_3^{0.75} D^{0.25}}$$

Solving the above for  $u_c$  gives the critical velocity for the core flow which will be imposed by the 1-D design code. A core flow flashback prediction model for premixed hydrogen is given by Dinkelacker, 2011 is:

$$S_t = S_L \left( 1 + \frac{0.46}{Le} Re^{0.25} \left(\frac{u'}{S_L}\right)^{0.3} \left(\frac{p}{p_0}\right)^{0.2} \right)$$

This model incorporates Lewis number scaling and should be appropriate for pure H<sub>2</sub> and some fuel blends.

# Combustion induced vortex breakdown (CIVB)

CIVB is where a vortex ring produced by the nozzle is disturbed by combustion and penetrates upstream:

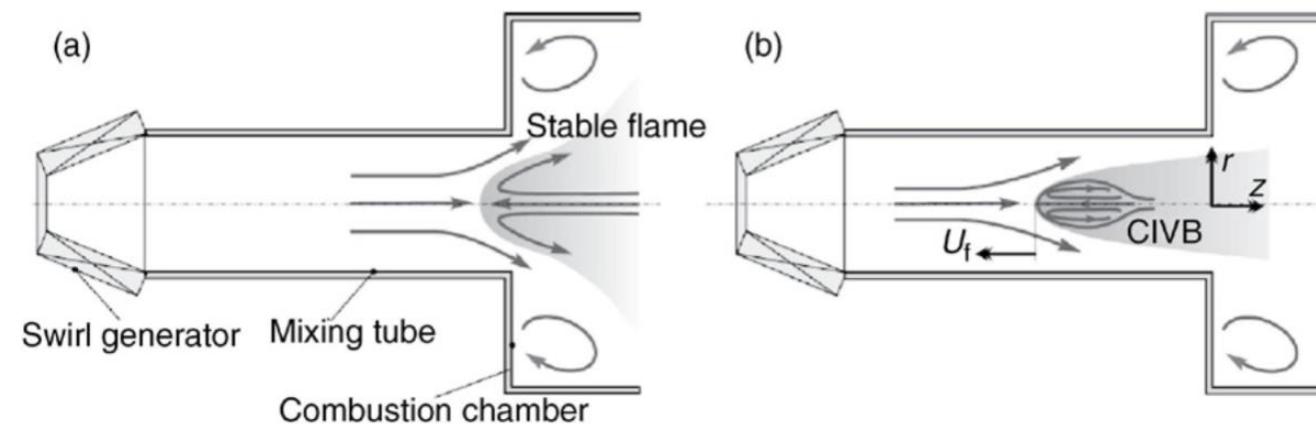


Fig. 9.2. Sketch of premixed swirl burner flow patterns for a (a) stable flame; (b) flame with flashback due to CIVB (Kröner et al., 2007).

Because this flashback mechanism relies on fluid physics downstream of the dump plane, it will be addressed later in the design process. The final nozzle configuration will be designed to prevent the formation of strong, stable vortex rings which could be reingested. This is not likely for our current approach.

# Flashback nomenclature

$\alpha$ : speed of sound  
 $D$ : Nozzle diameter  
 $Da$ : Damköhler number  
 $g$ : velocity gradient  
 $Le$ : Lewis number  
 $Pe$ : Péclet number  
 $S$ : flame speed  
 $T$ : Temperature  
 $u$ : velocity  
 $u'$ : velocity fluctuation

## Greek

$\alpha$ : thermal diffusion coefficient  
 $\mu$ : viscosity  
 $\rho$ : density  
 $\tau$ : characteristic time

## Subscripts

0: atmospheric station  
3: combustor entrance station  
auto: autoignition  
 $c$ : critical  
 $f$ : flame  
low-frequency pressure: phenomena driven by low-frequency pressure oscillations  
 $L$ : laminar  
residence: residence time inside the nozzle  
 $T$ : turbulent  
tip: at the burner tip

# Core flow flashback

- Core flow flashback (Dinkelacker, 2011):

$$S_T < v_{\text{nozzle}}$$

Where

$$S_T = S_L \left( 1 + \left( \frac{0.46}{Le} \right) Re_{\text{nozzle}}^{0.25} \left( \frac{v'_{\text{nozzle}}}{S_L} \right)^{0.3} \left( \frac{p_{t,in}}{p_0} \right)^{0.2} \right)$$

- Turbulence intensity and nozzle Reynolds number drive the turbulent flame speed. VGs, fuel injection jets, and nozzle diameter are free design variables that affect these.
- $Re_{\text{nozzle}}$  can be calculated from design variables  $D$  and  $v$  as well as the operating conditions. Cases were postprocessed to calculate turbulent velocity fluctuations,  $v'_{\text{nozzle}}$ . In RANS, this is computed from the subgrid isotropic turbulence intensity. In LES, we add the resolved turbulent fluctuations calculated by adding the time-resolved velocity fluctuations to the subgrid fluctuation values.

# Boundary layer flashback

- BL flashback (Kalantari, 2016):

$$v_c < v_{\text{nozzle}}$$

Where

$$\text{Da} = e^{-12.06} \text{Le}^{1.68} \text{Pe}_f^{1.91} \left( \frac{T_3}{T_0} \right)^{2.57} \left( \frac{T_{\text{tip}}}{T_0} \right)^{-0.49} \left( \frac{p_{t,in}}{p_0} \right)^{-2.1} \quad g_c = \frac{s_L^2}{\alpha \text{Da}} \text{ or } \frac{S_T}{y_{@v=S_T}}$$

$$g_c = \frac{0.03955 v_c^{1.75} \rho_3^{0.75}}{\mu_3^{0.75} D^{0.25}}$$

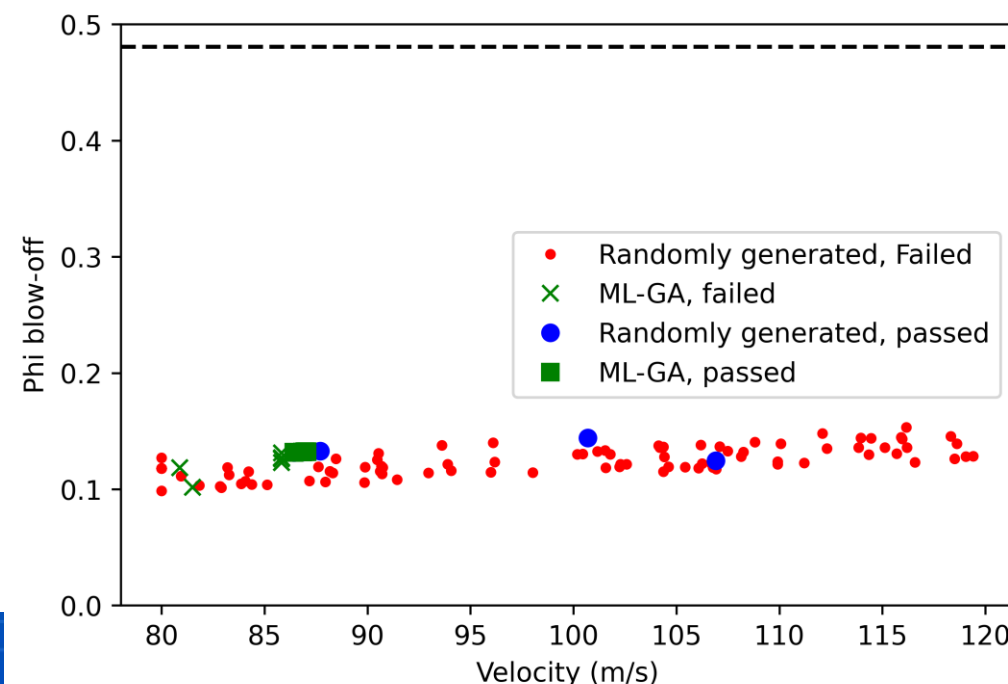
- BL flashback can occur when the critical velocity gradient ( $g_c$ ) exceeds a certain value. This is especially dangerous when flow separation occurs or is incipient.
- $T_{\text{tip}}$  can only be estimated from combustion cases, assumed 800 C for cold-flow cases
- Note: BL flashback model was fairly insensitive to operating conditions, LES will be monitored for adverse pressure gradients

# A note on flame blow-off and autoignition

- Autoignition will be captured by CFD model, 1-D tool predicts >10x factor of safety for all cases.
- If bulk flow velocity is too high, flame blow-off can occur.
- Present blow-off model is taken from Driscoll & Rasmussen 2005, and while it is designed for scramjets with a flameholding cavity at Mach 2-3, the principles are similar. This is a useful first order look. Additionally, the RANS and LES combustion cases should be more than capable of modeling flame blow-off.
- Schefer 2003 from validation case saw blow-off near  $\phi \sim 0.1$
- Rasmussen & Driscoll's model predicts blow-off near  $\phi \sim 0.1 - 0.15$
- Flame blow-off was not used as a constraint in the present study as it would be obvious from combustion results.

$$Da = \frac{H/U_{\infty}}{\left(\frac{a_0}{S_{L0}}\right) \left(\frac{1 \text{ atm}}{p}\right)^n \left(\frac{300 \text{ K}}{T}\right)^m}$$

For best correlation of the data, n and m were found to be 1.0. H is the cavity height,  $U_{\infty}$  is the free stream velocity and T is the free stream static temperature. The lean blowout limits for the case of aft wall fuel injection was found to be correlated by the relation:  $\phi_0 = 0.0043 Da^{-0.26}$ , where  $\phi_0$  is the overall equivalence ratio that is based on the properly defined characteristic air mass flow rate. For the floor fuel injection cases, the lean blowout limit was correlated by:  $\phi_0 = 0.0028 Da^{-0.80}$ . The correlations are valid over a range of conditions, including Mach numbers from 2-3, four fuel types (hydrogen, ethylene, methane, acetylene having different laminar flame speeds  $S_{L0}$ ), and static pressures (p) from 0.5 to 1.0 atm.



Rasmussen and Driscoll, "Blowout Limits of Flames in High-Speed Airflows: Critical Damkohler Number", AIAA Joint Propulsion Conference 2008

# Flashback and autoignition checks

| Phenomena                | 1-D tool pre-simulation checks                                                                                                                 | Cold-flow RANS                                                                             | Combustion RANS                                   | Combustion LES                                                                                                       |
|--------------------------|------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|---------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|
| Autoignition             | Factor of safety calculated based on estimated flow-through time of each nozzle. Autoignition >10x slower than flow through time for all cases | Not checked                                                                                | Chemical kinetics model would detect autoignition | Chemical kinetics model would detect autoignition                                                                    |
| Core flow flashback      | Flashback not directly checked, but upper limit on acceptable turbulence intensity calculated, near 5% for most cases                          | Turbulence at outlet used to compute turbulent flame speed and compare to core flow speed. | Not checked                                       | Model should accurately capture core turbulent flame speed                                                           |
| Boundary layer flashback | Estimated from critical velocity gradient                                                                                                      | Not checked                                                                                | Severe, obvious flashback would be detected       | Severe, obvious flashback would be detected. Refined boundary layer required for high-fidelity flashback prediction. |