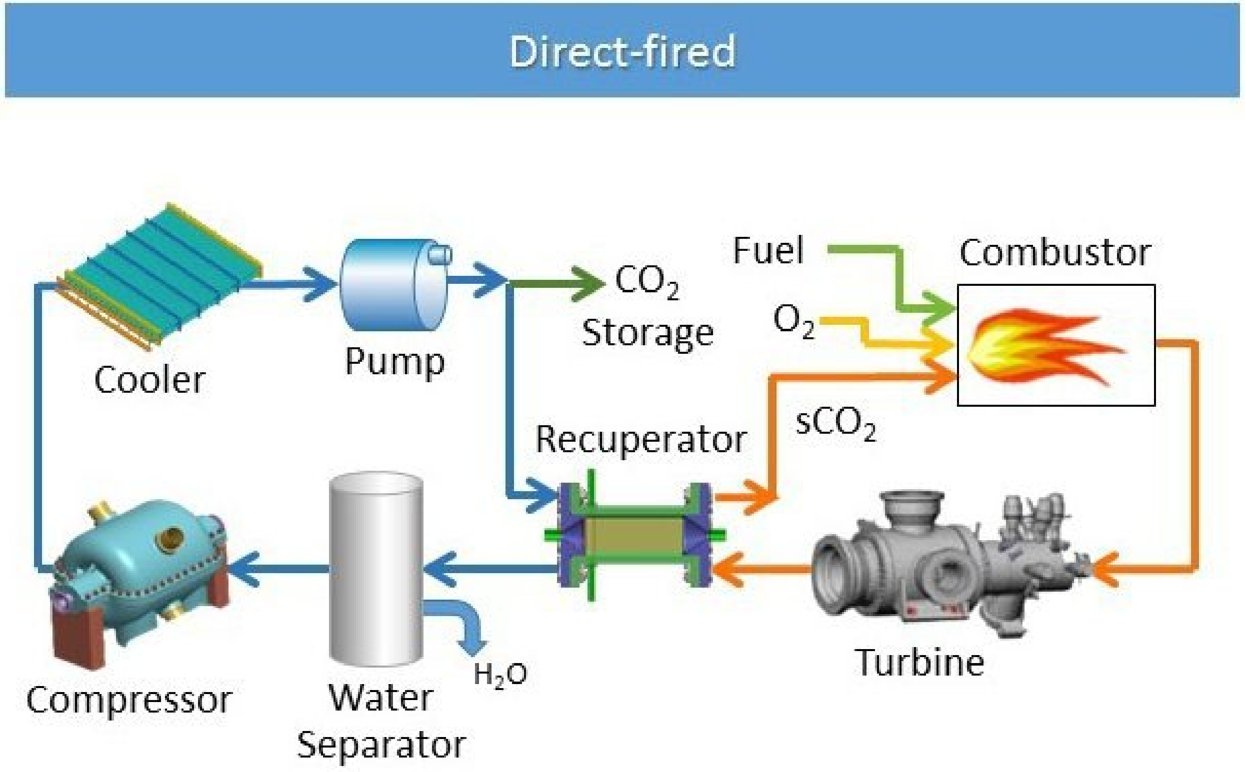
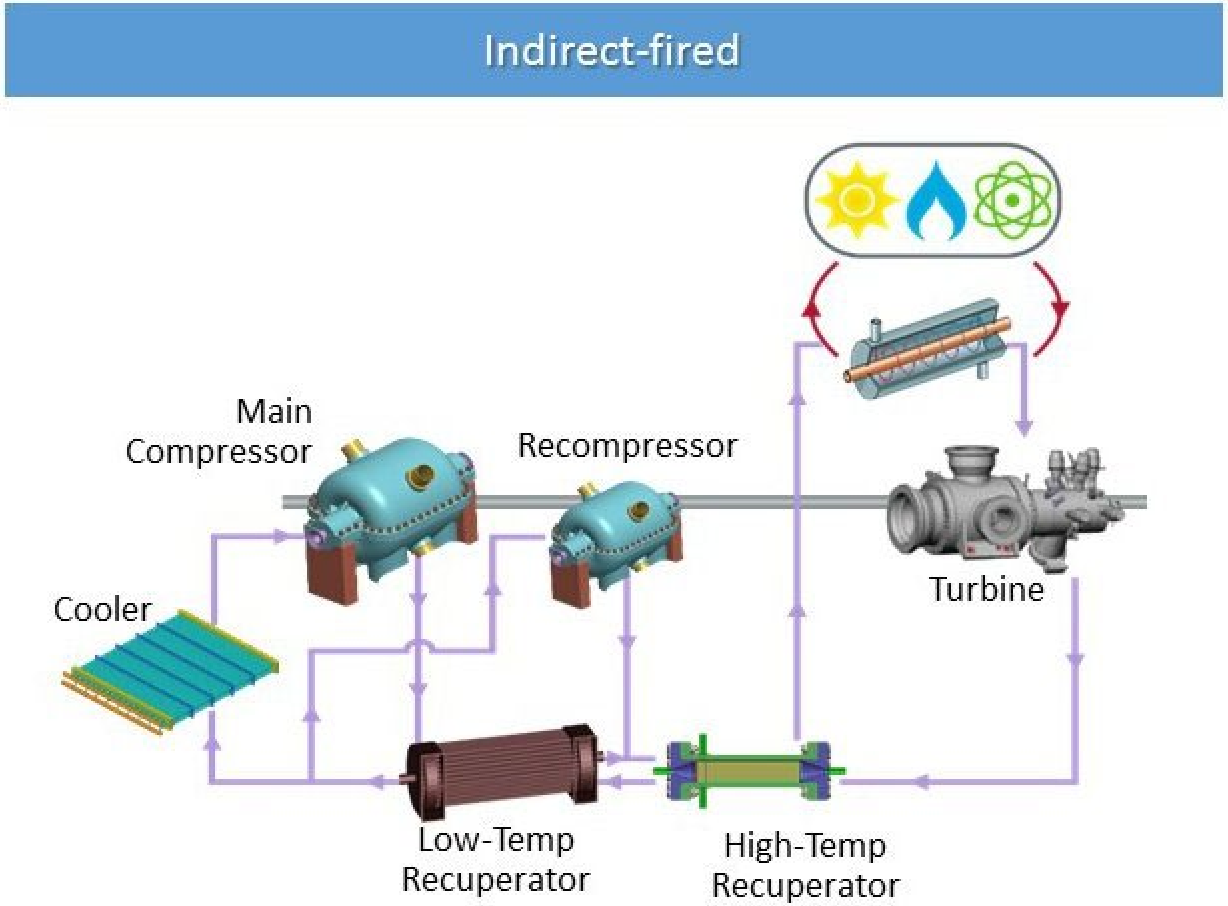
Direct-fired Oxy Combustion in sCO_2 Power Cycles

Southwest Research Institute

Direct vs Indirect-Fired sCO_2 Cycle





https://www.energy.gov/sco2-power-cycles/sco2-power-cycles-fossil-fuels

Introduction

Advantages of a direct-fired sCO2 power cycle

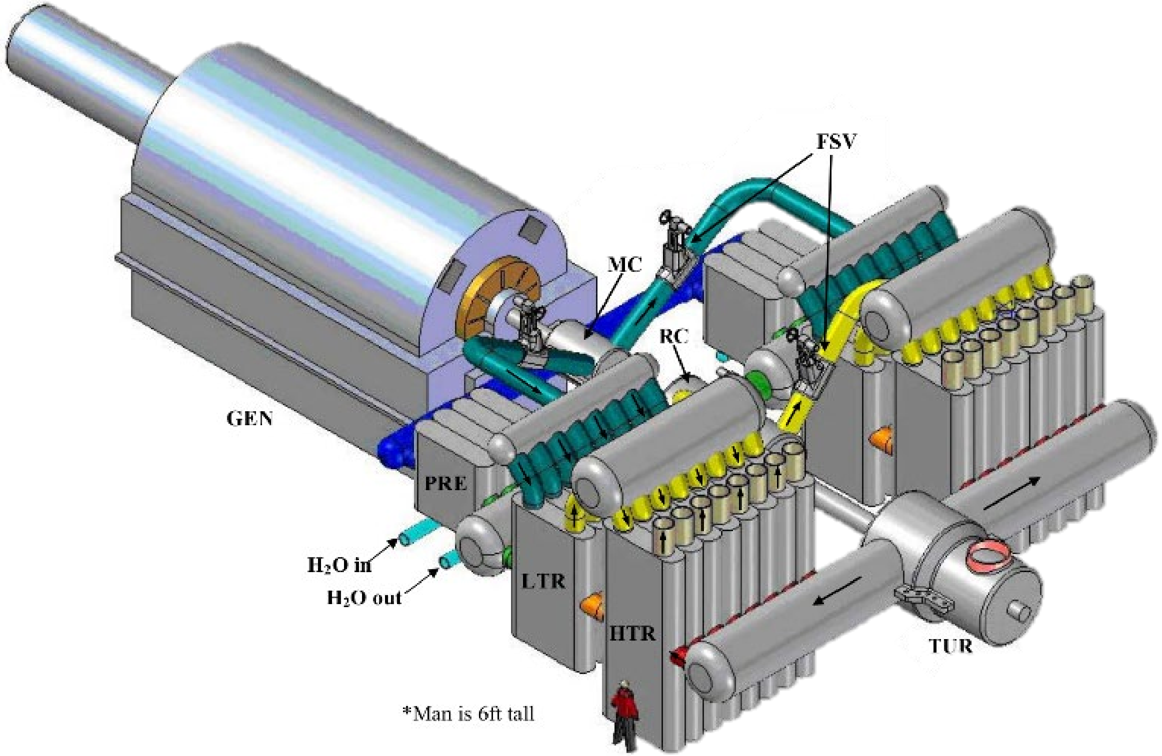
- Compact hardware
- Greater efficiency
- Nearly 100% carbon capture

Challenges

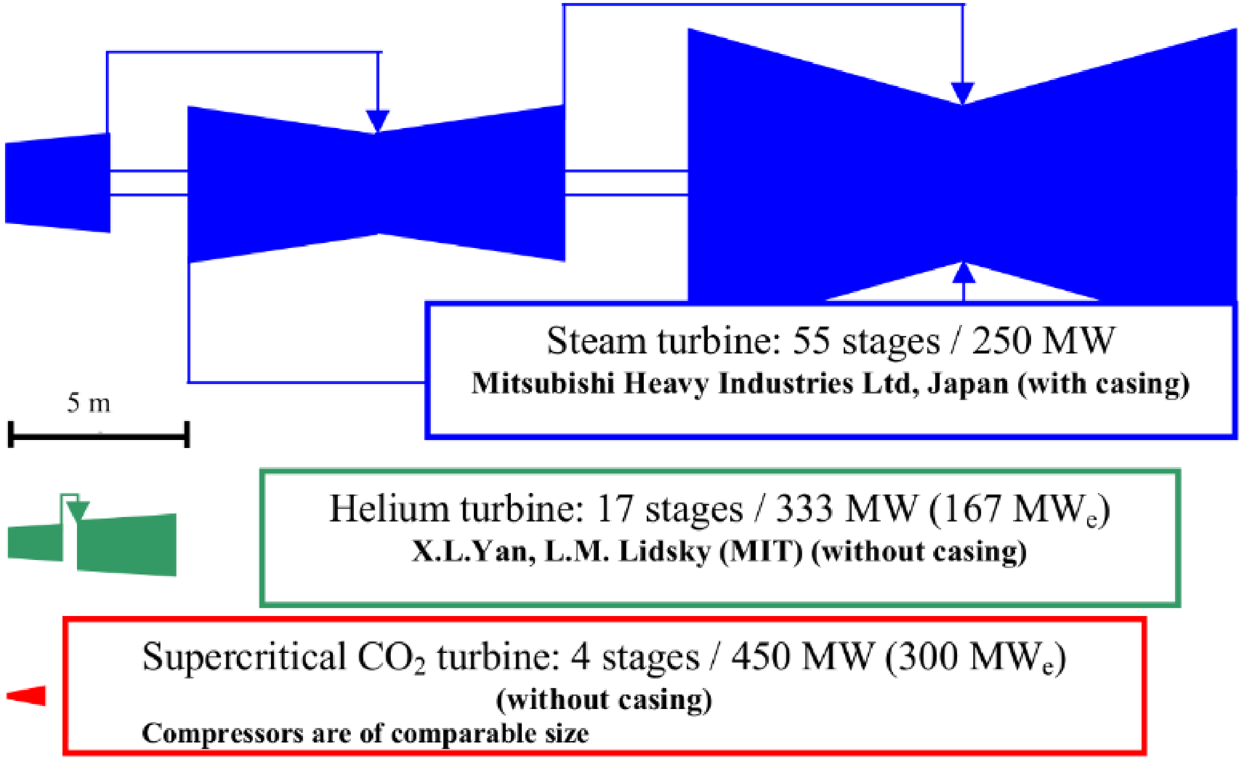
- Lack of validated combustion modeling techniques
- Combustor design best practices are still developing
- High pressure and temperatures lead to costly hardware (think rocketry)

Advantages of sCO_2 Power Cycles

- High fluid densities lead to compact turbomachinery



*Man is 6ft tall



Steam turbine: 55 stages / 250 MW
Mitsubishi Heavy Industries Ltd, Japan (with casing)

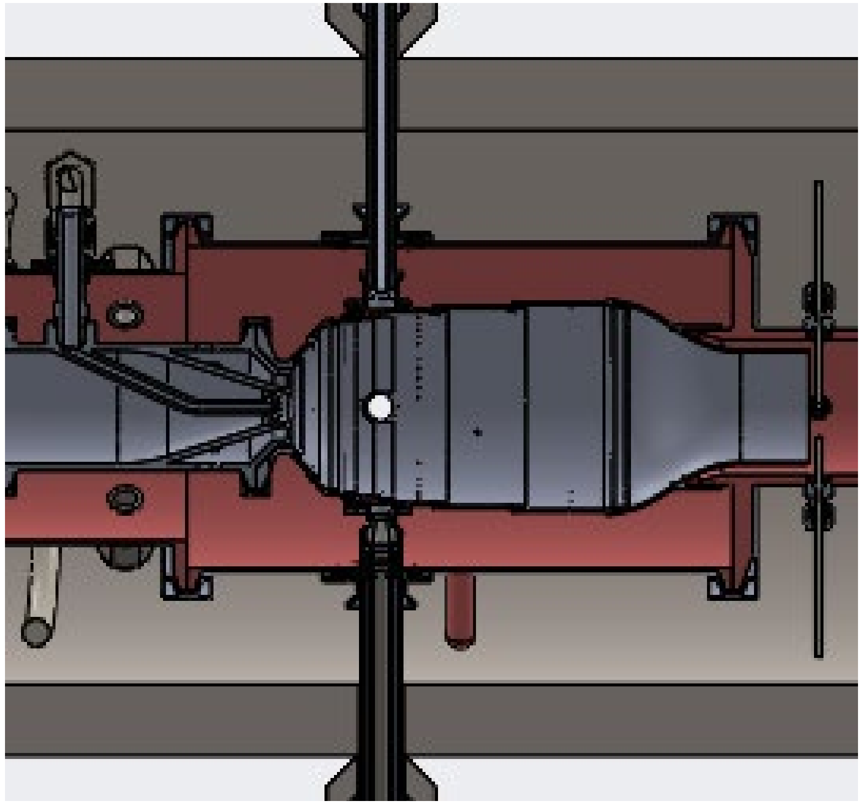
Helium turbine: 17 stages / 333 MW (167 MW_e)
X.L.Yan, L.M. Lidsky (MIT) (without casing)

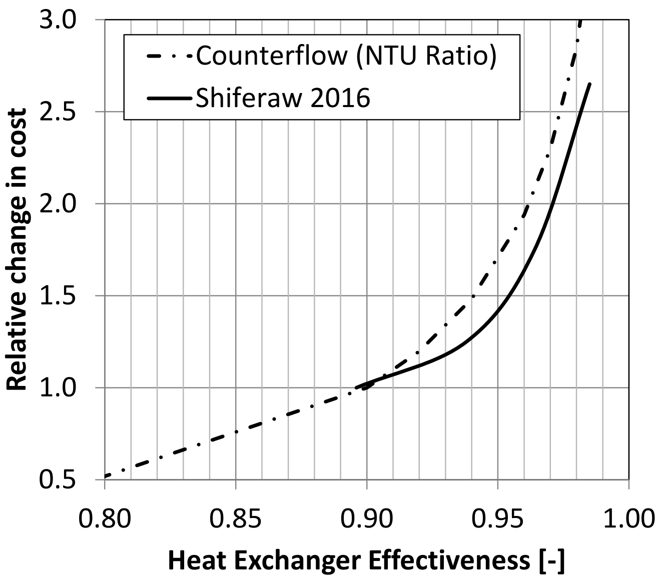
Supercritical CO_2 turbine: 4 stages / 450 MW (300 MW_e)
(without casing)
Compressors are of comparable size

Third Generation 300 MWe S-CO2 Layout from Gibba, Hejzlar, and Driscoll, MIT-GFR-037, 2006

Advantages of sCO_2 Power Cycles

- Offer +3 to +5 percentage points over supercritical steam for indirect coal fired applications



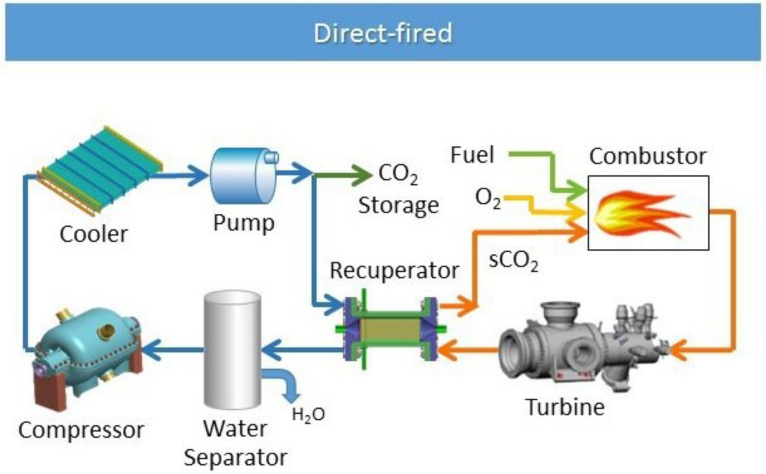


Courtesy Thar Energy, DE-FE0026273

2.5MWt Sunshot Heater
Inconel 740H Bare Tube HX

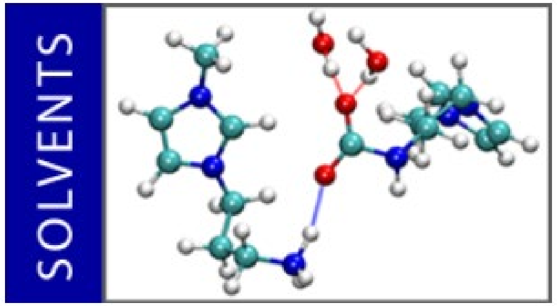
Advantages of sCO_2 Power Cycles

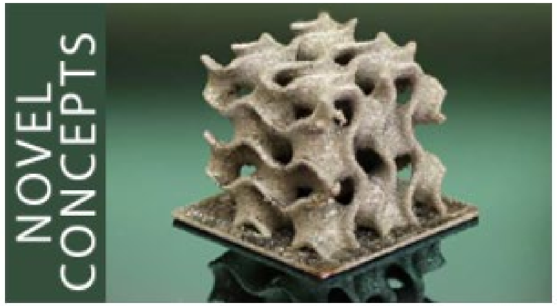
Nearly 100% carbon capture



https://www.eia.gov

Petra Nova power plant (Houston)
240 MW, 90% CC, $1 billion retrofit cost

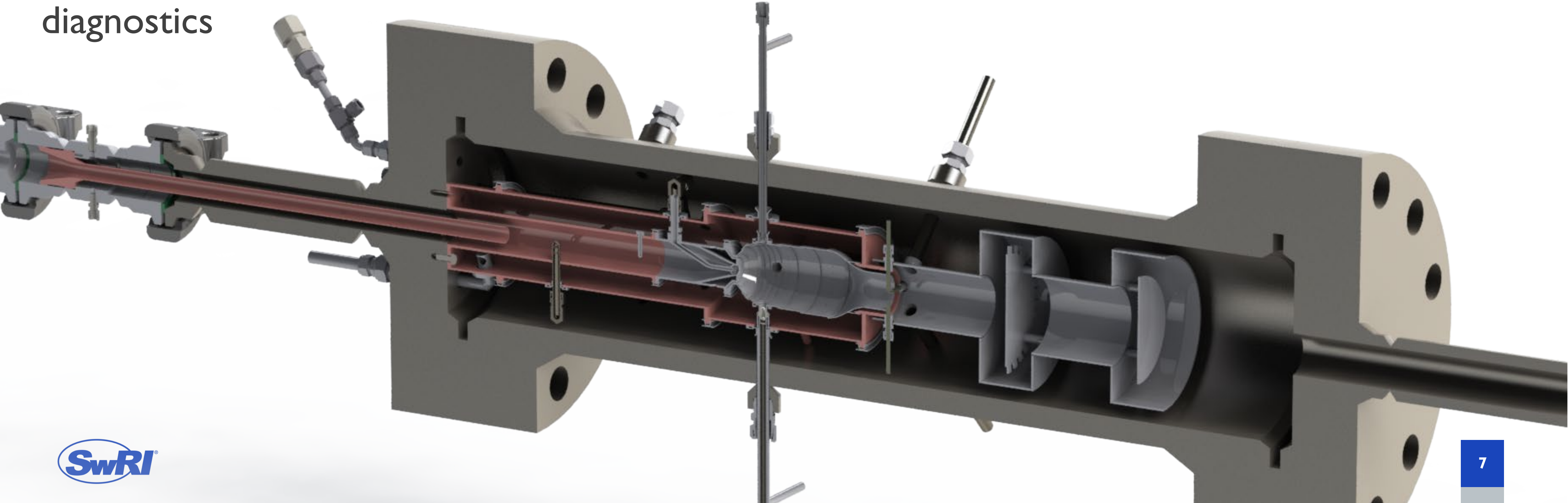




https://netl.doe.gov/coal/carbon-capture/post-combustion

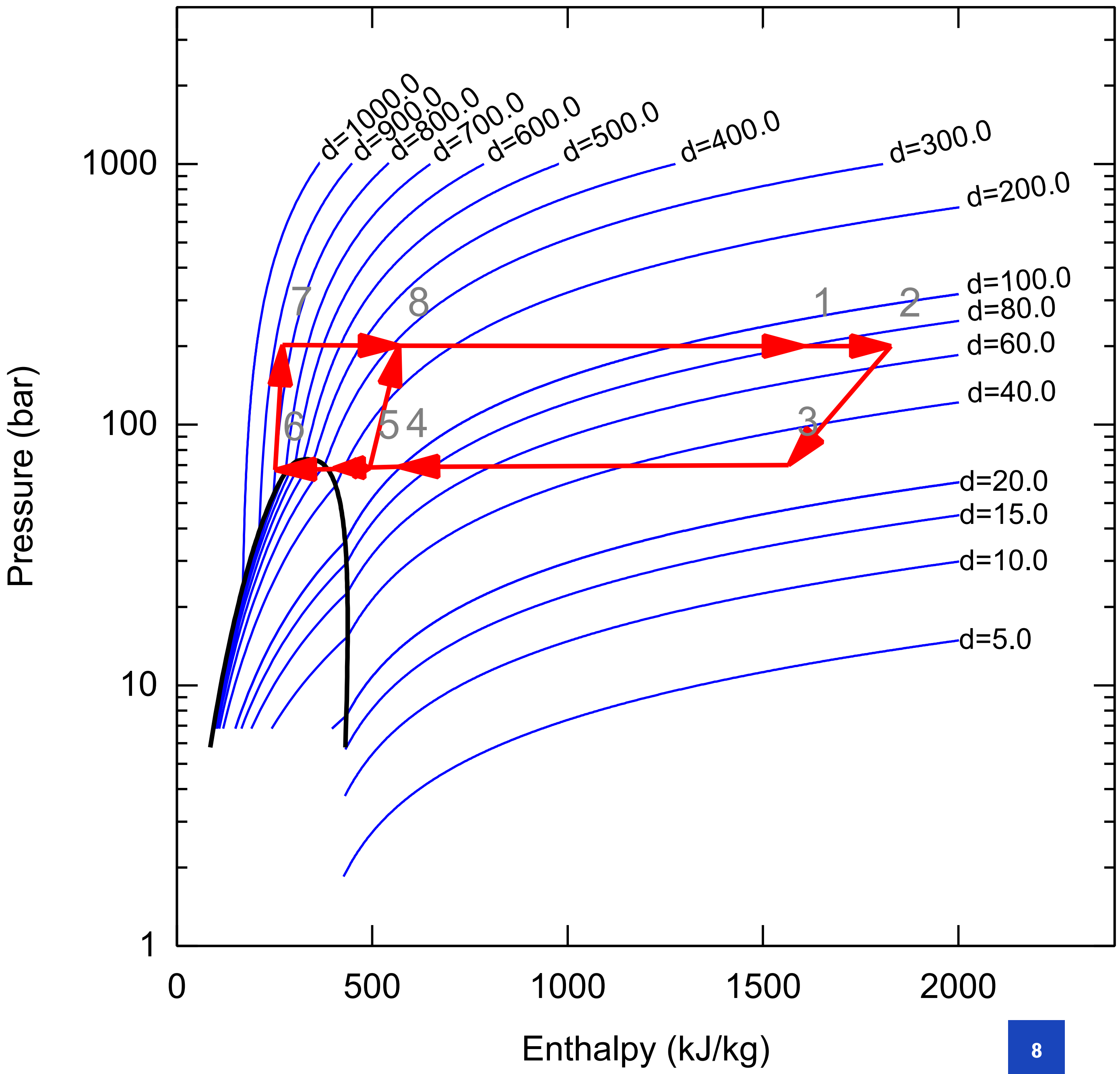
Project Objectives

- Design a 1 MW thermal oxy-fuel combustor capable of generating 1200°C outlet temperature
- Manufacture combustor, assemble test loop, and commission oxy-fuel combustor
- Evaluate and characterize combustor performance using optical access for advanced diagnostics

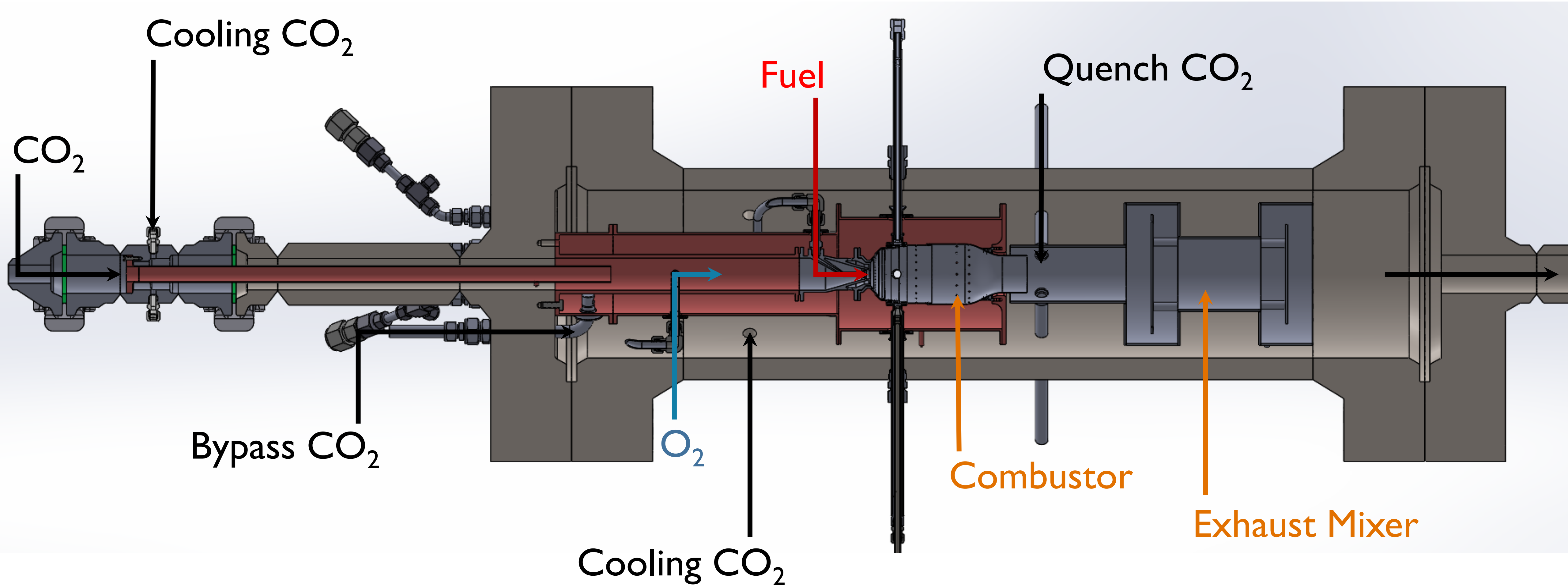


Cycle Conditions

- Combustor Inlet and Outlet temperatures dictated by reviewing previous cycle modeling work done at SwRI
- Combustor inlet temperature: 700°C at 200 bar
- Combustor outlet temperature: 1200°C
- Achieves a plant efficiency comparable to a NGCC power plant

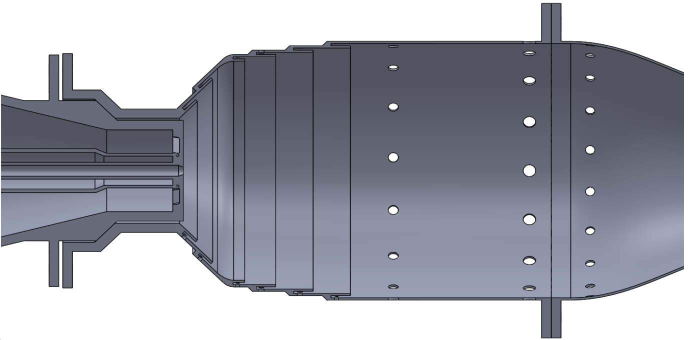


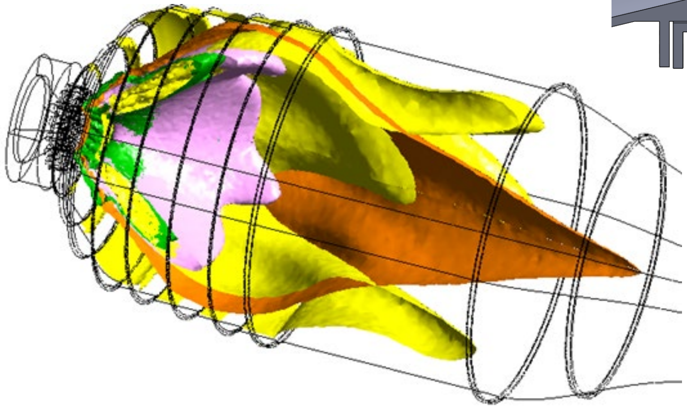
Combustor Schematic

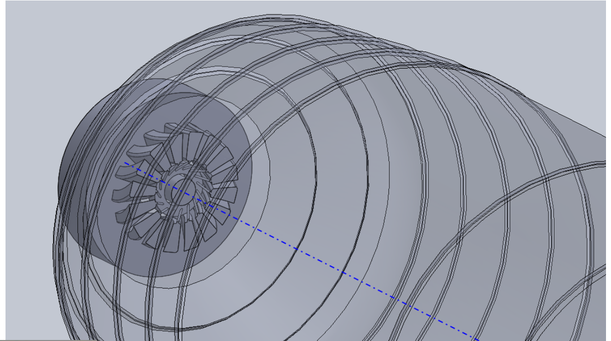


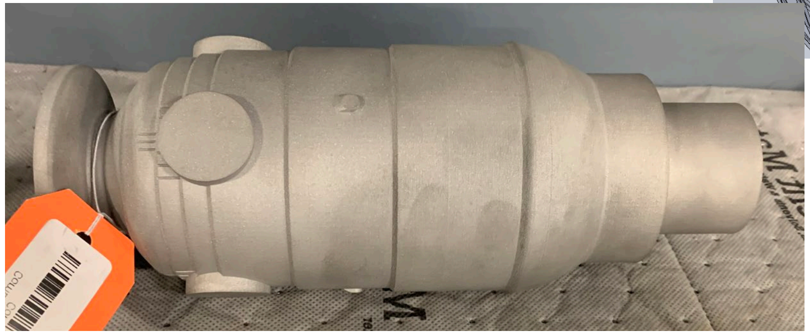
Combustor Design Key Considerations

- Mechanical casing
- Fluid flow path
- Fuel injector
- Oxygen injection
- Combustor liner thermal management
- Optical access
- Acoustic resonance
- Instrumentation
- Design for additive manufacturing



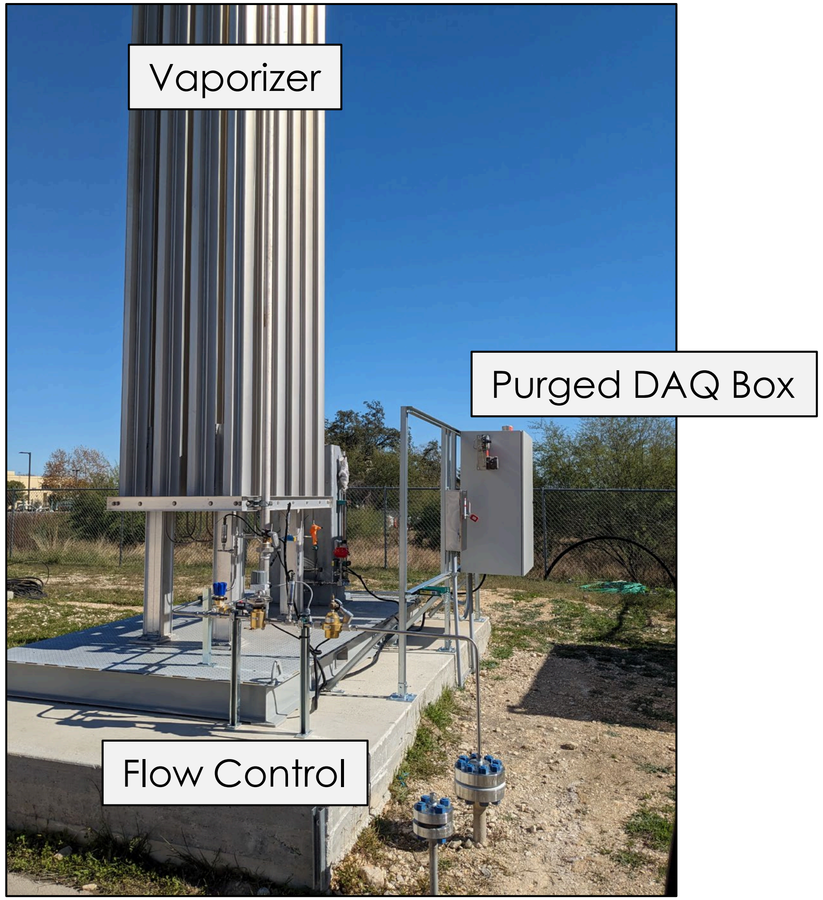


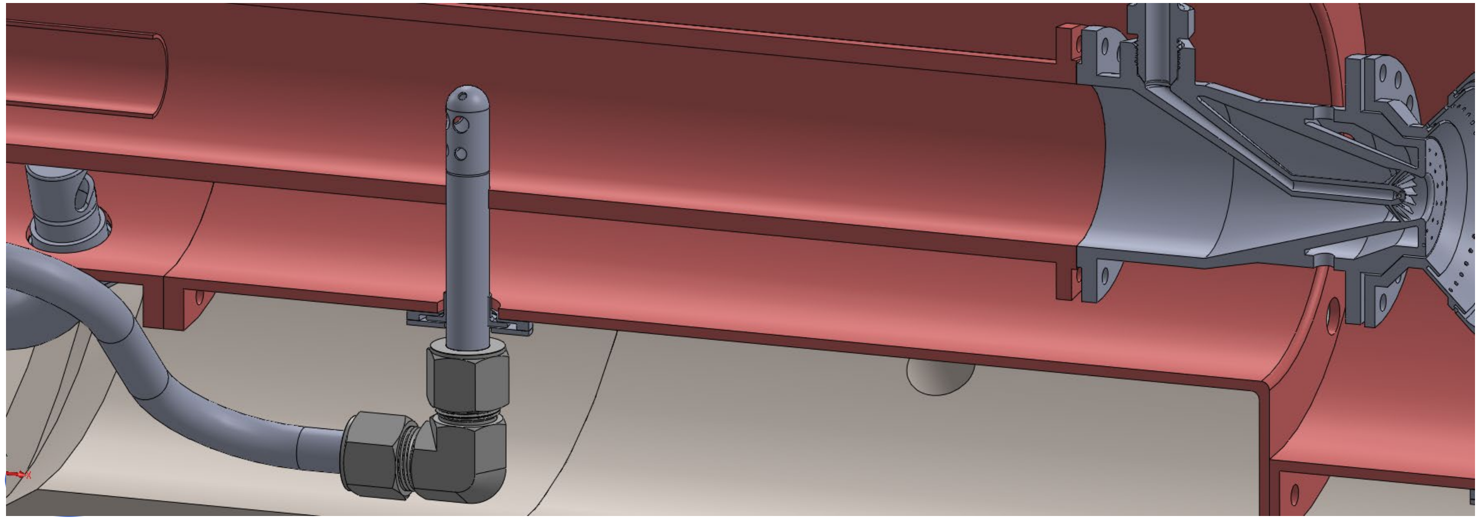


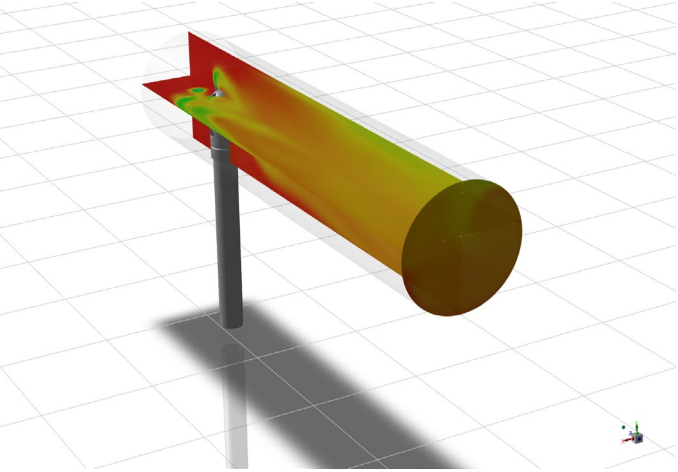


Oxygen System

- Guidance from personnel at NASA Stennis and White Sands, review from project partner Air Liquide
- LOX tank with cryogenic pump and ambient vaporizer
- Oxygen injection upstream of fuel injector

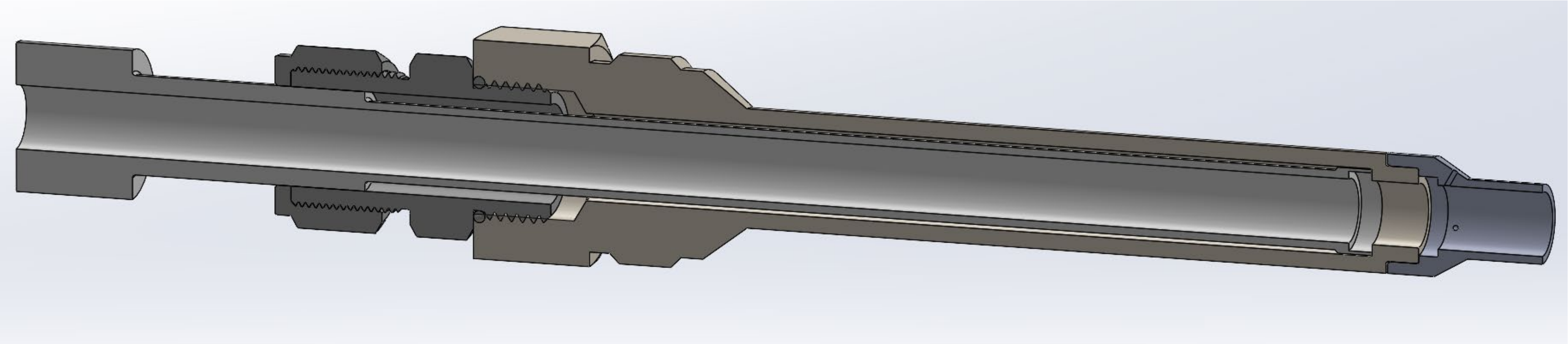




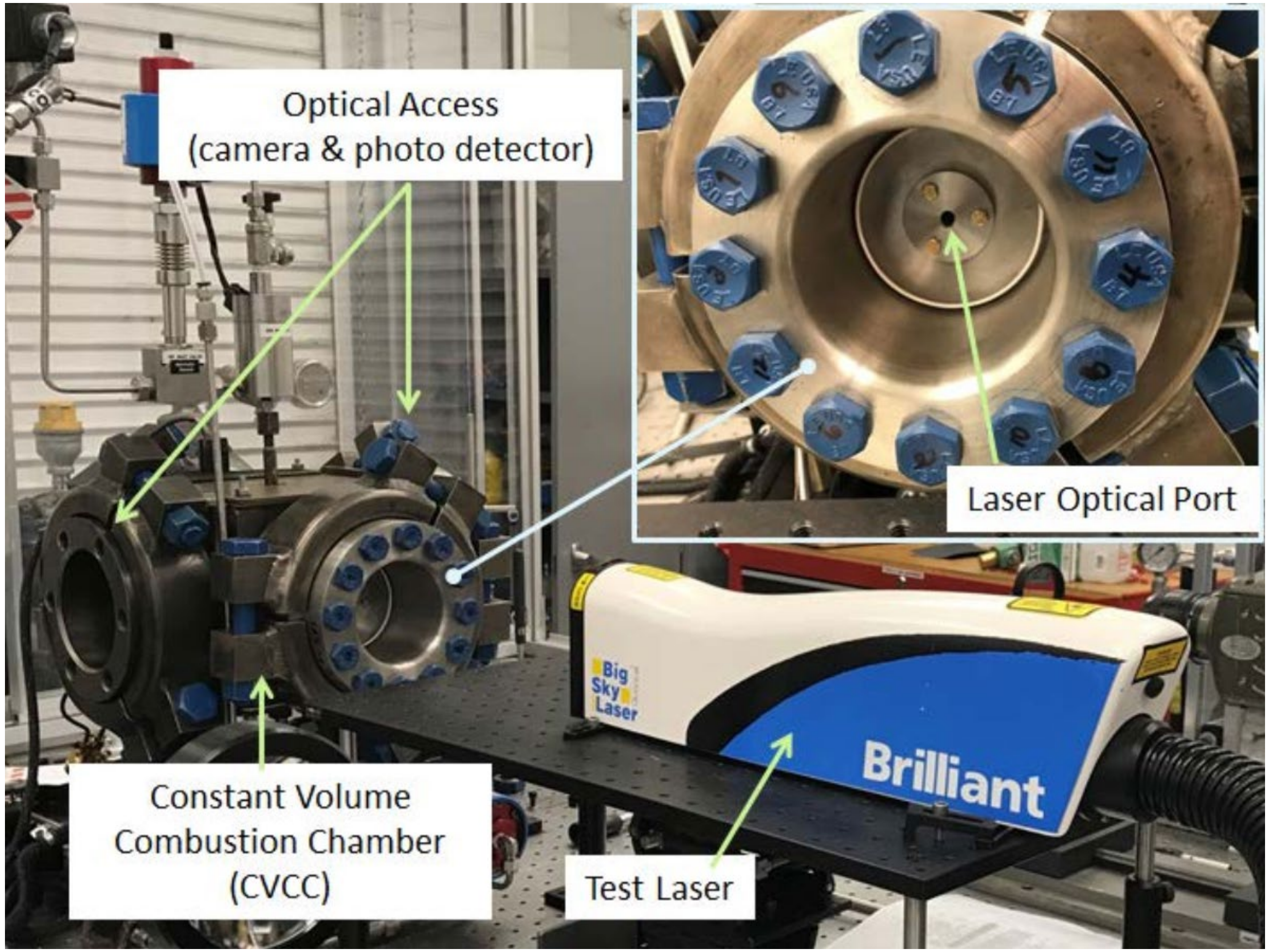


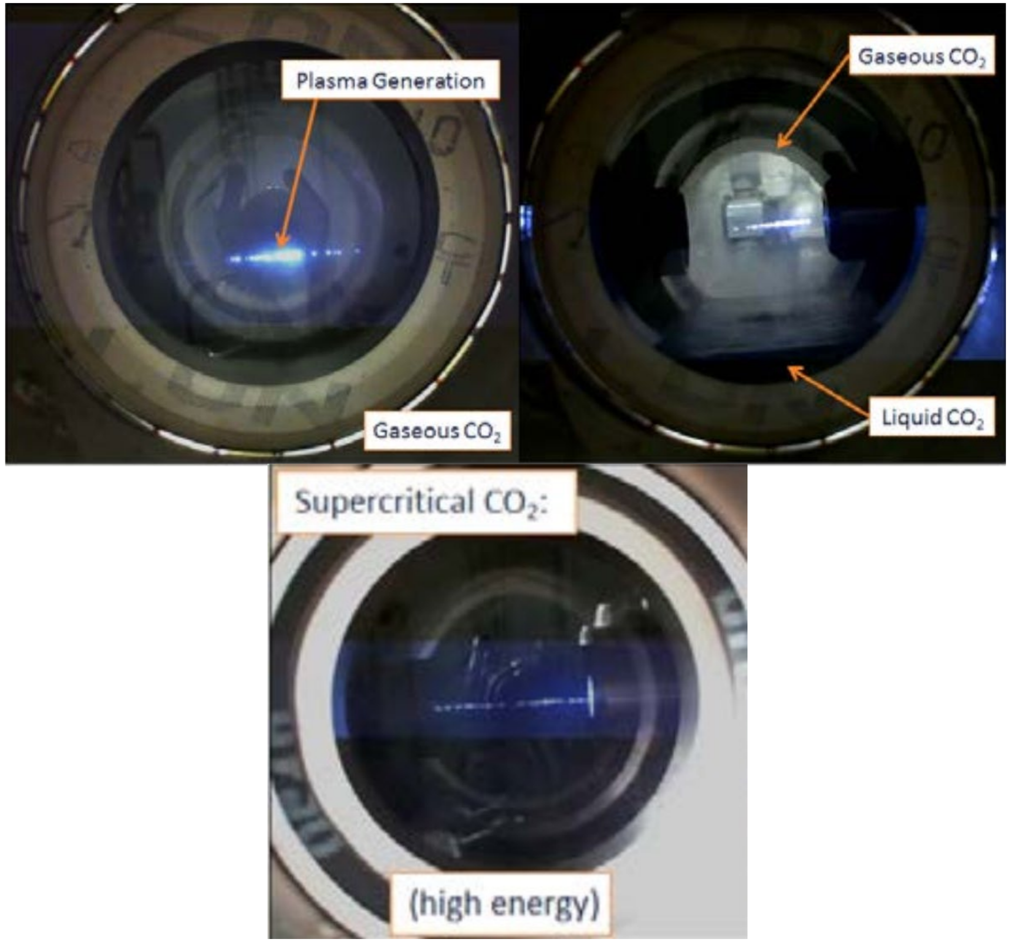
Laser Ignition System

- Class 4 Quantel Qsmart Twins
  - 2x380mJ @ 532nm, 10Hz
- Gen 2 Laser Ignition Probe – Improved lens protection & beam alignment



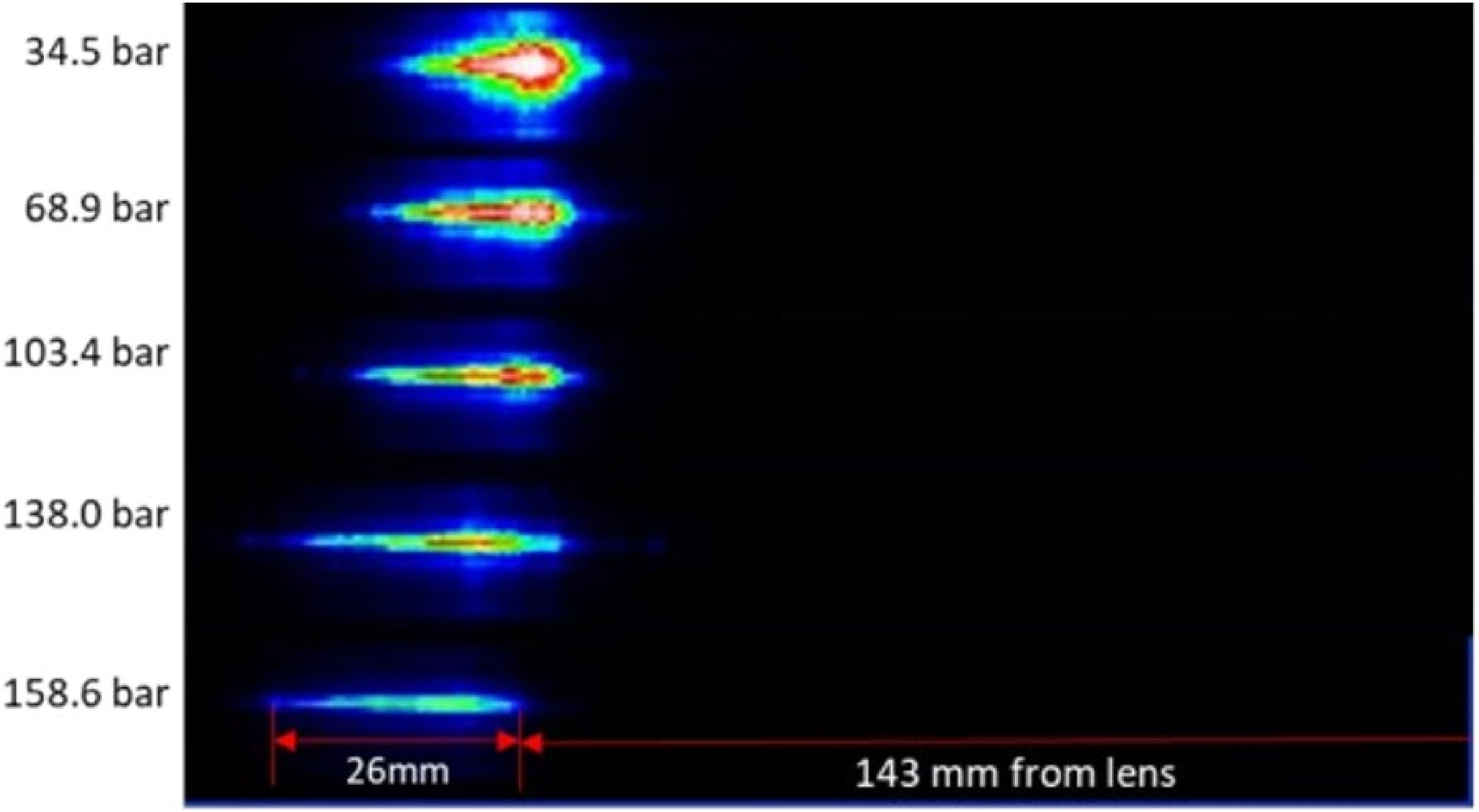
Laser Ignition tests





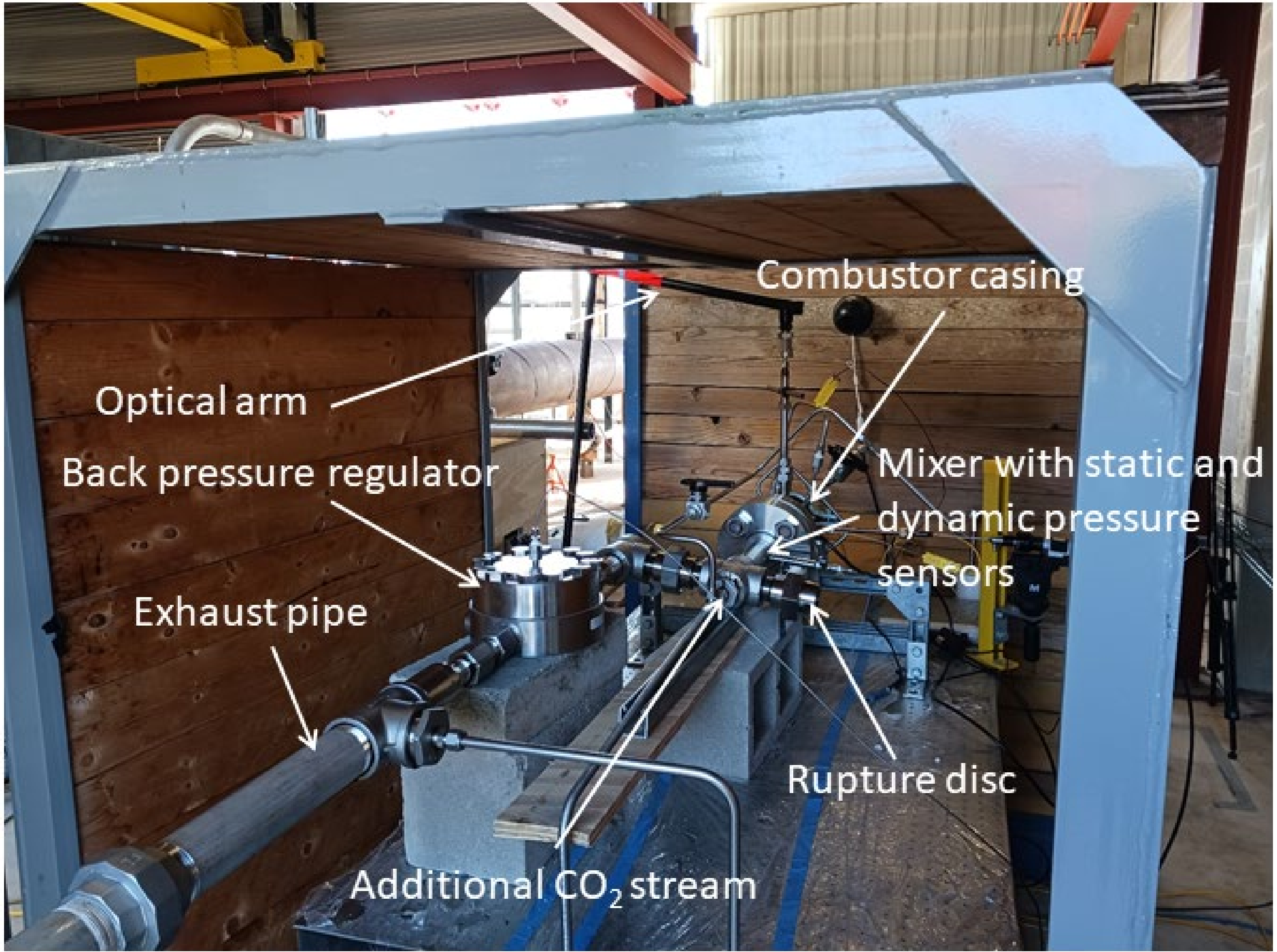
Katcher *et al.* 2019

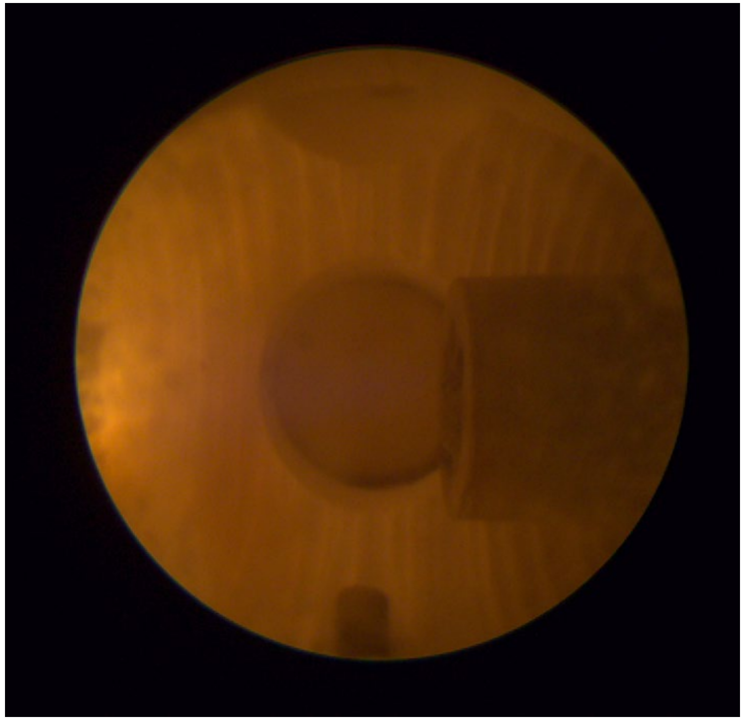
Laser Kernel Behavior in sCO_2

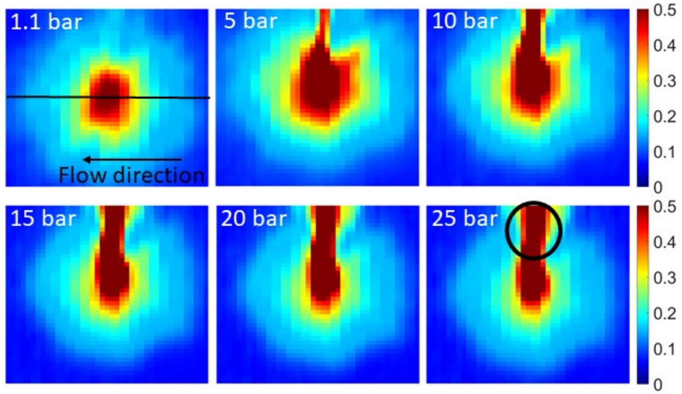


Gupta *et al.* 2022

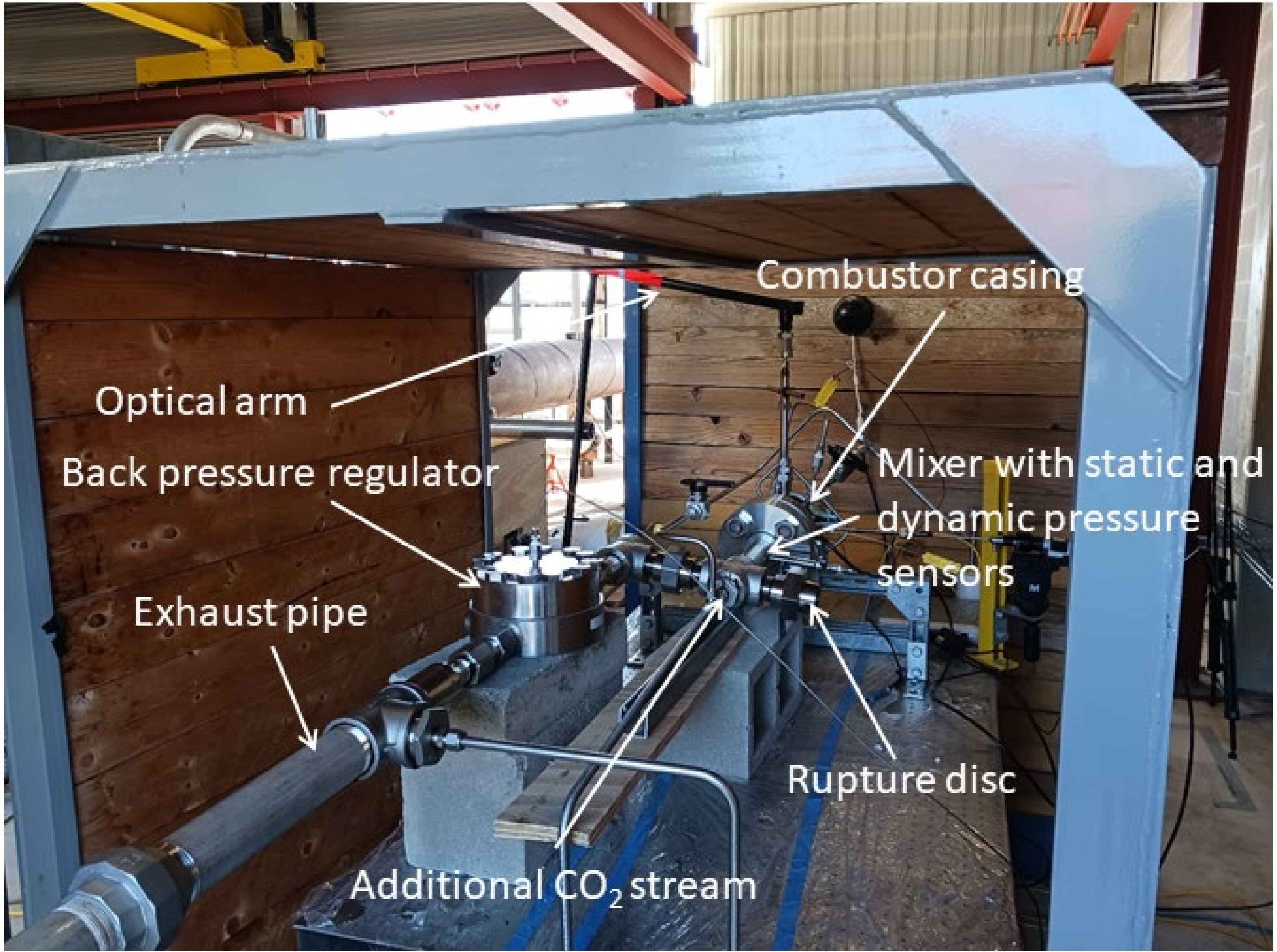
Laser Ignition tests

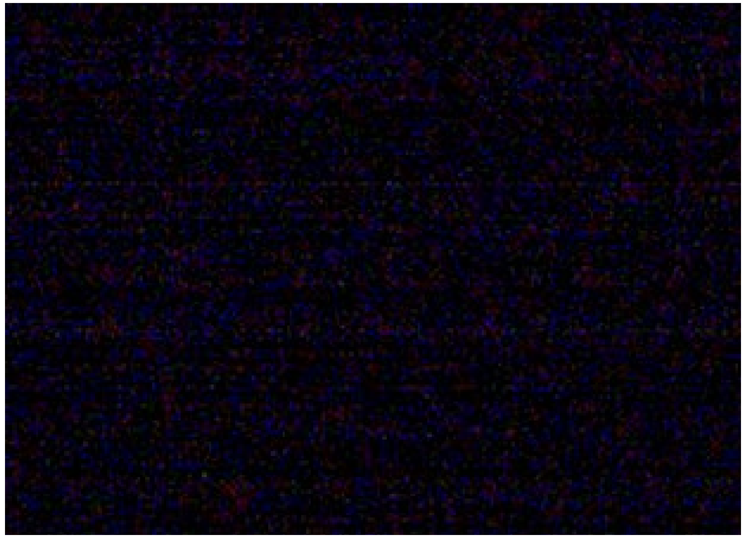


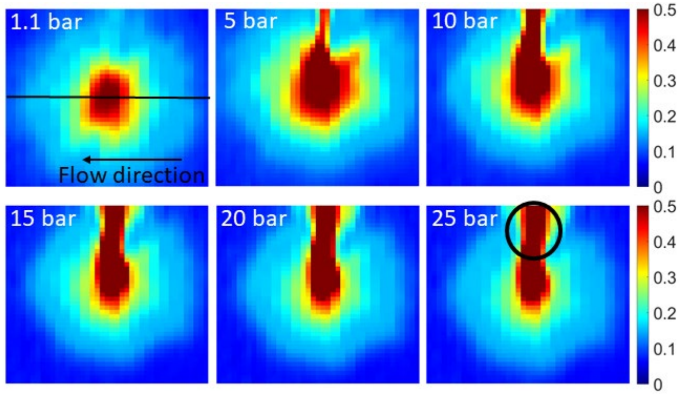




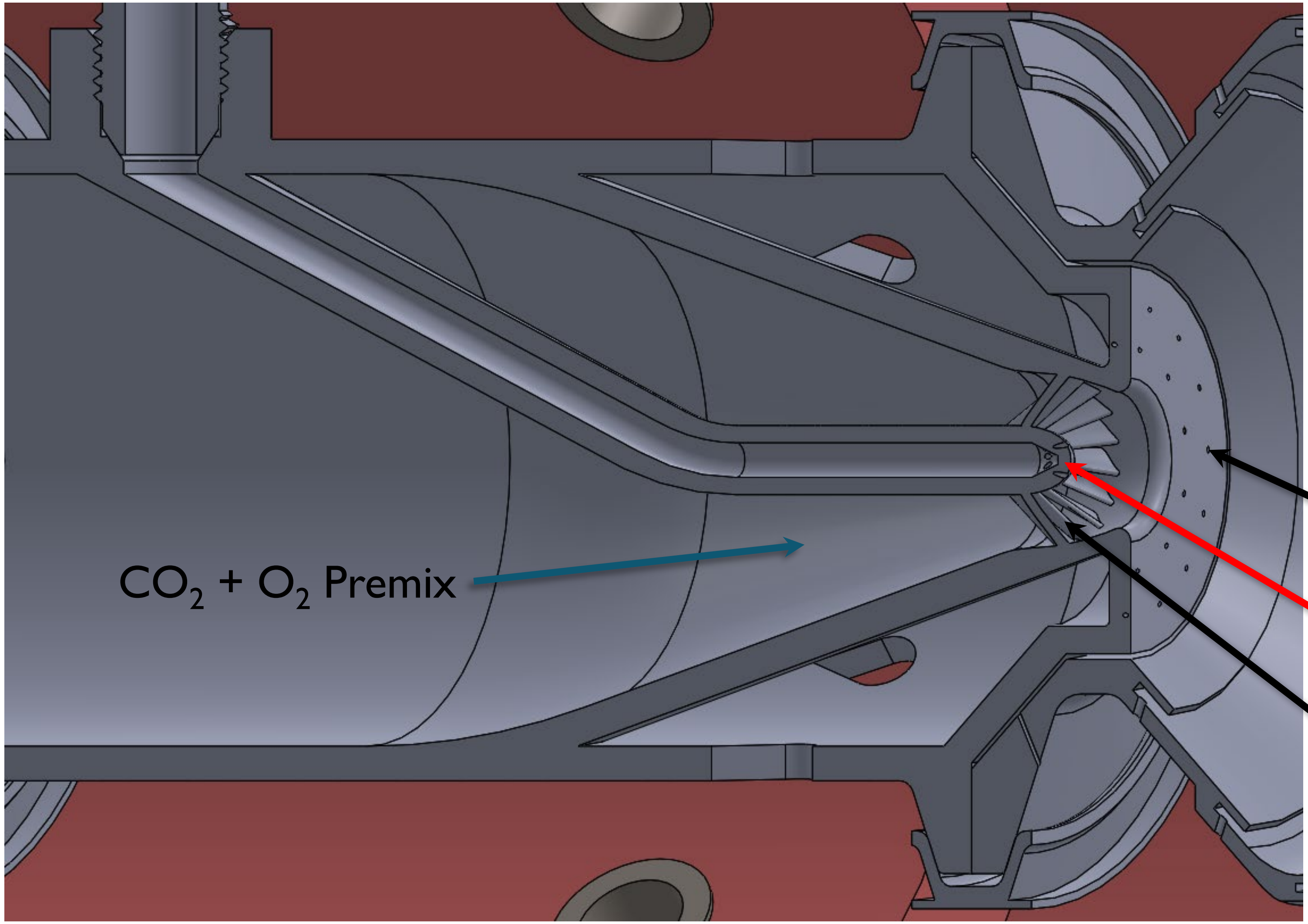
Laser Ignition tests







Fuel Injector



$CO_2 + O_2$ Premix

CO_2 Face Cooling

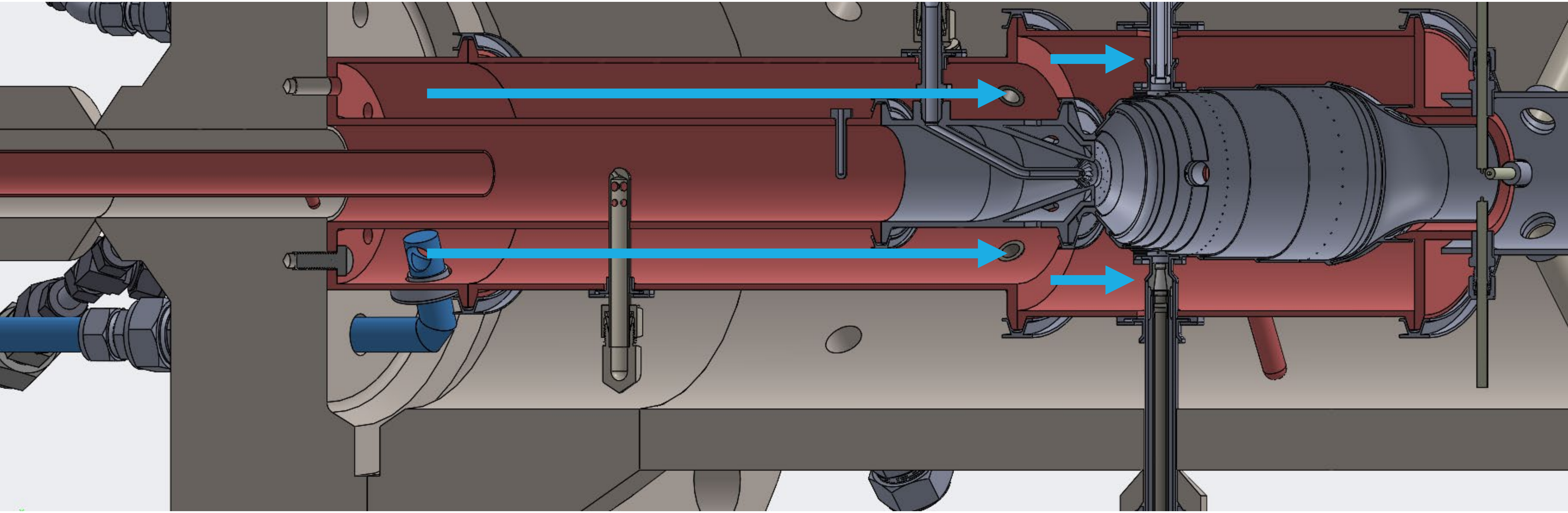
Methane Fuel Injection Point

Swirling Vanes

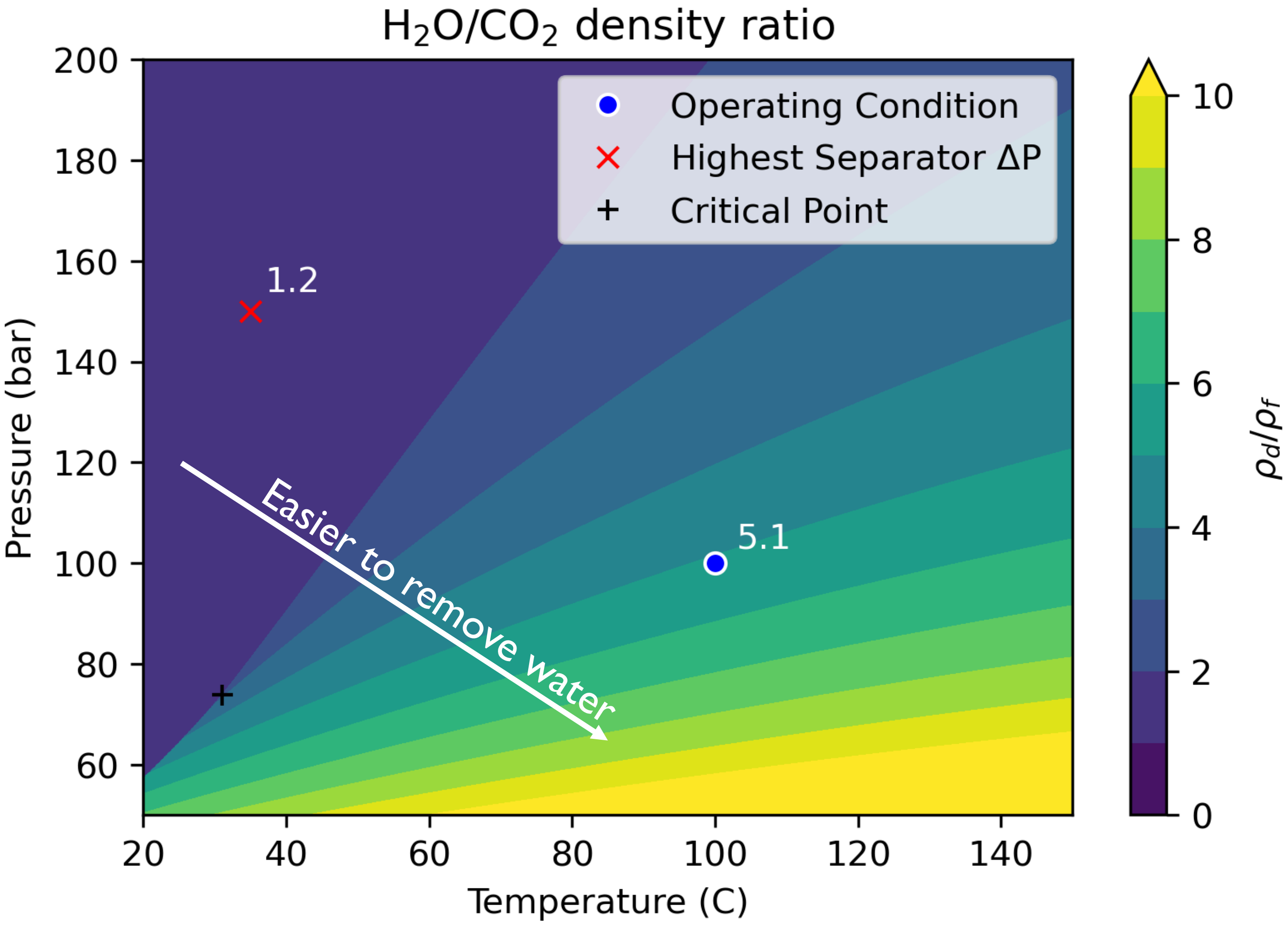
- Additively manufactured Haynes 282
- 32° swirl angle of inlet vanes chosen after literature review and CFD simulations

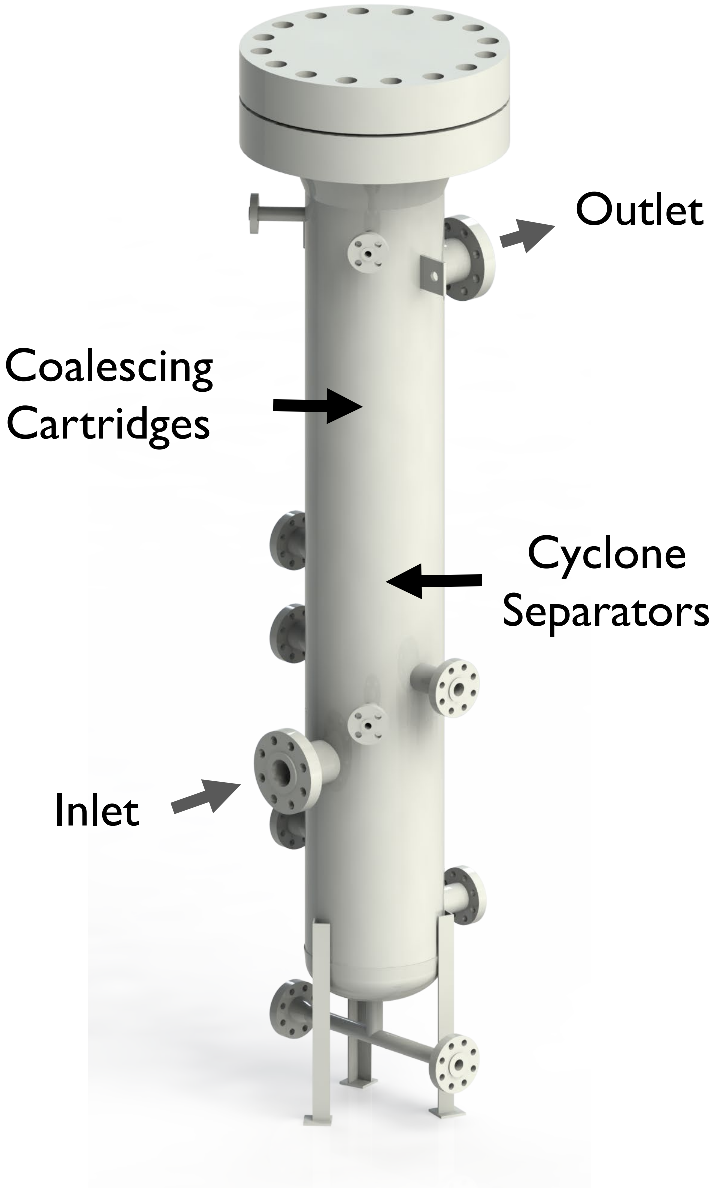
Combustor Cooling

CO_2 bypass gas enters annulus from a dedicated line (highlighted in blue) with flow control, allowing remote manipulation of combustor liner temperatures



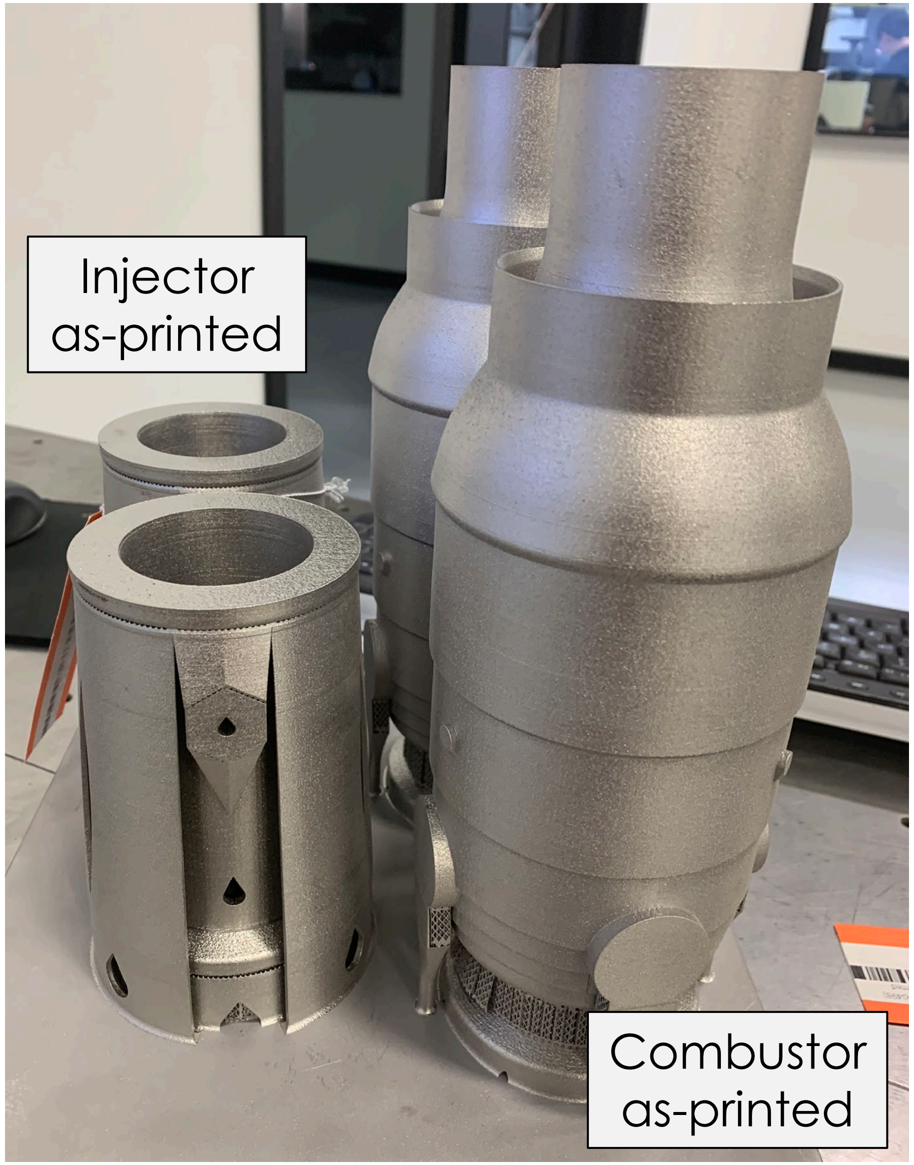
Water Separator

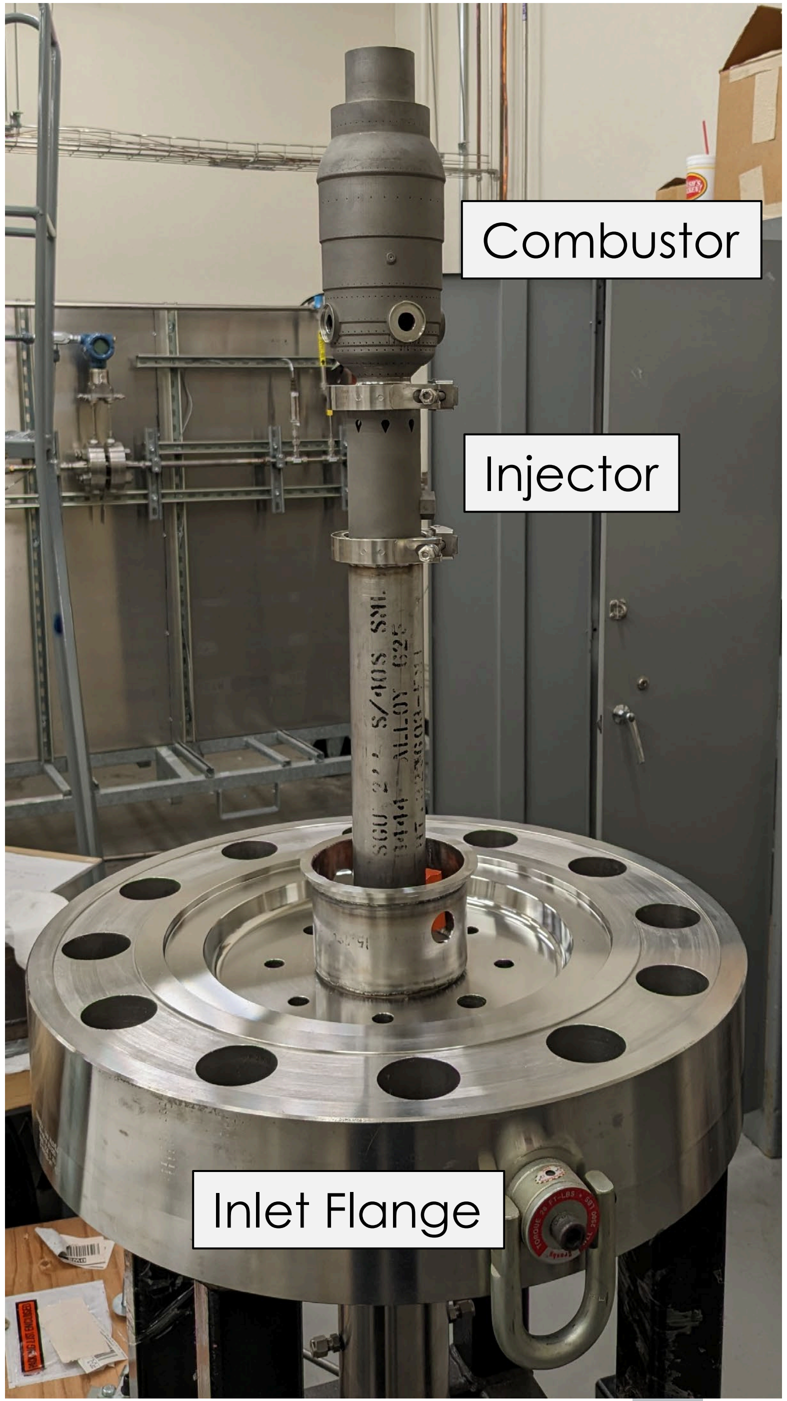




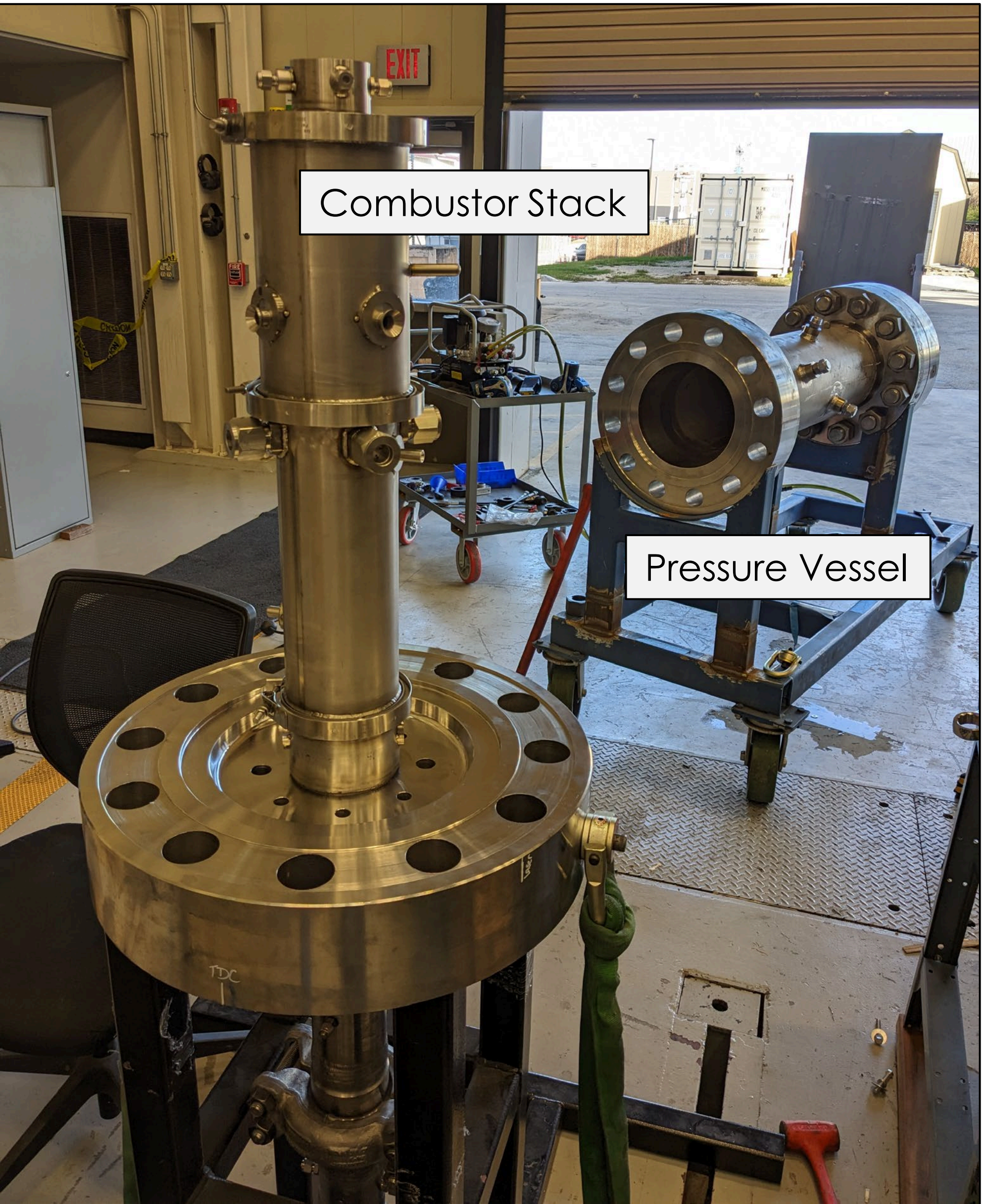
Other contaminants like carbonic acid need to be sensed and removed as well!

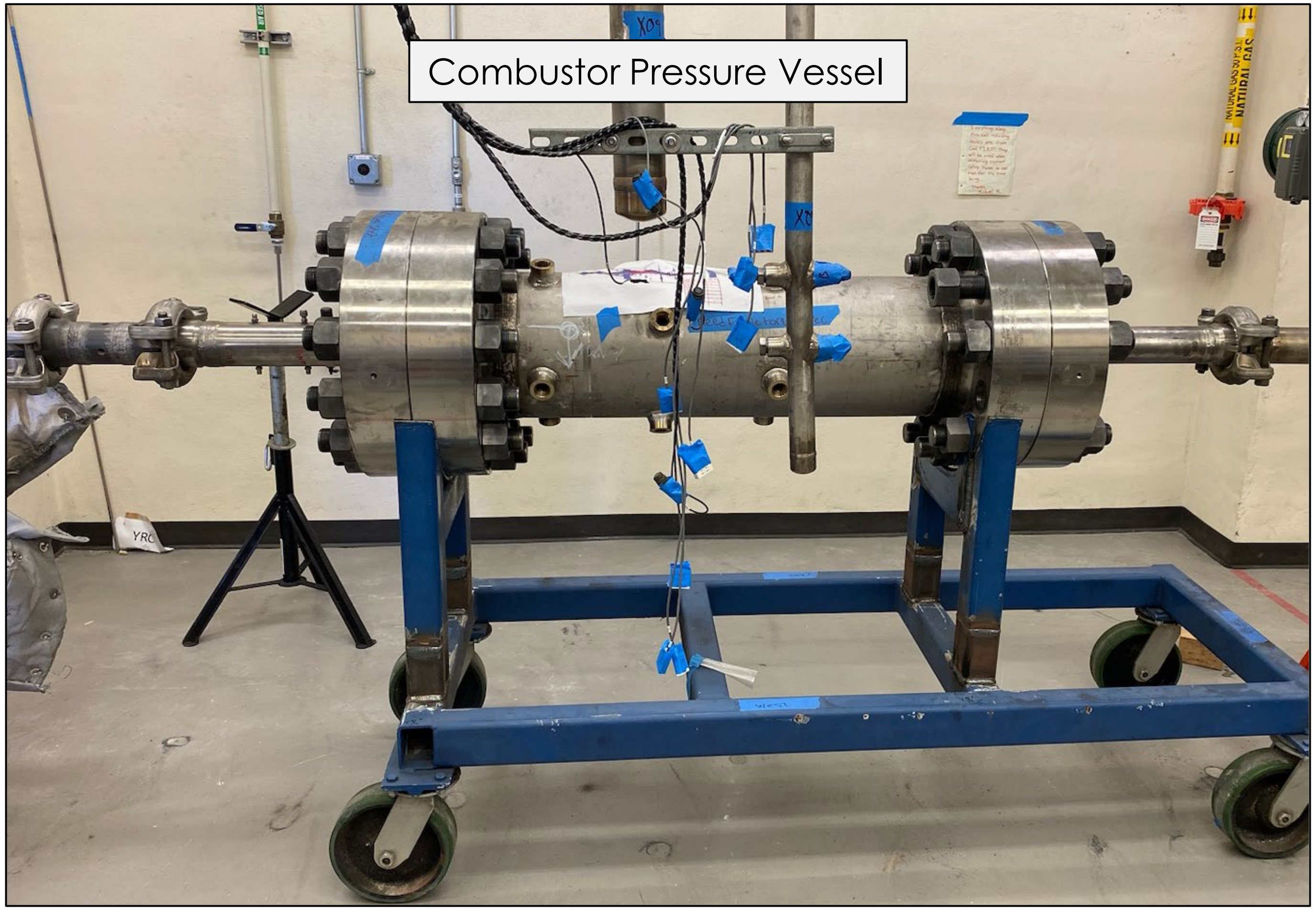
Combustor Fabrication

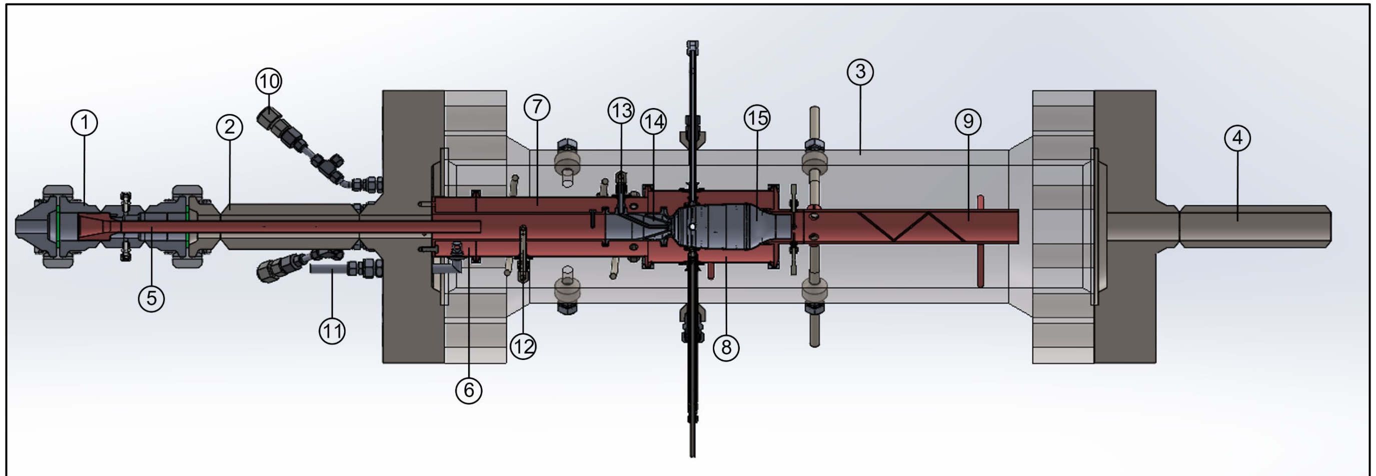




Combustor Rig

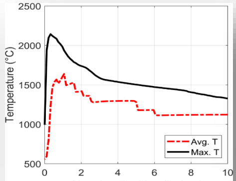


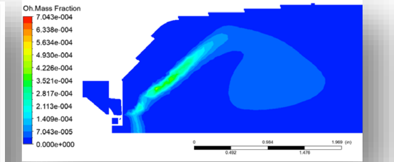




CFD Design

Heat Release And Flame Holding





Cooling/Recirculation Schemes

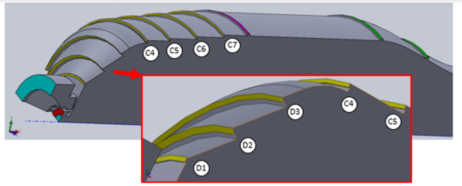


Figure 1-7. Details of the Fluid Inlets, Purposed Indicated by Face Color: CO_2+O_2 Inlet (Teal), Fuel Inlet (Red), Wall Cooling (Yellow), Recirculation Control (Magenta), and Dilution (Bright Green)

Injection and Swirl

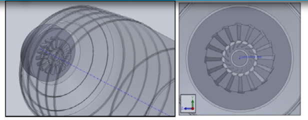


Figure 1-8. Separated Fuel Injection Scheme. Left: Isometric View with Chamber Walls Visible in Wireframe. Right: View of Injection Plane from Combustor Exit

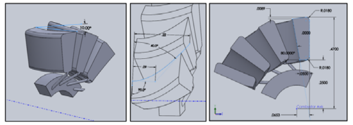
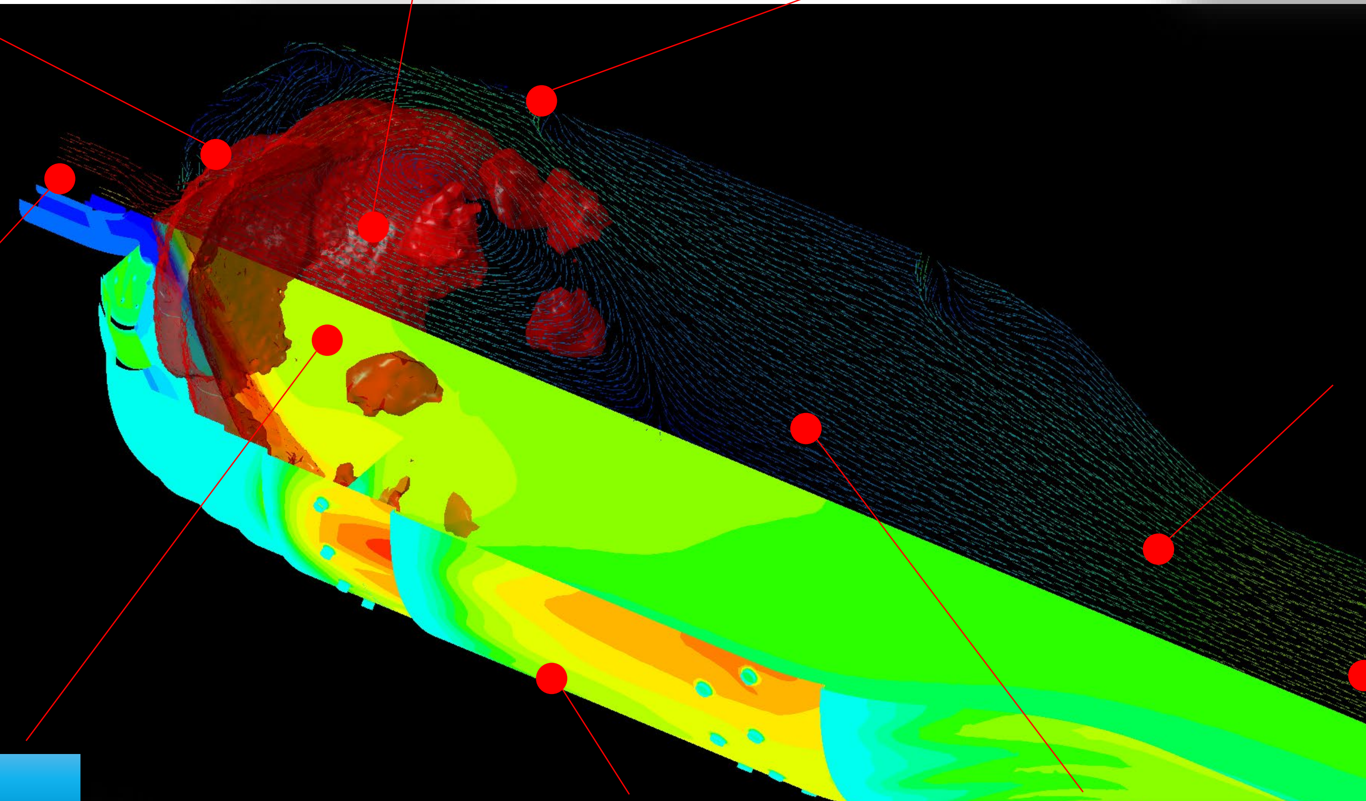


Figure 1-9. Details of the Swirling and Fuel Injection Schemes. Left: 10° Swirling Down Angle; Center: 40° Swirl Angle and Facial Sweep; Right: Swirler Inlet Facial Features



Startup Conditions

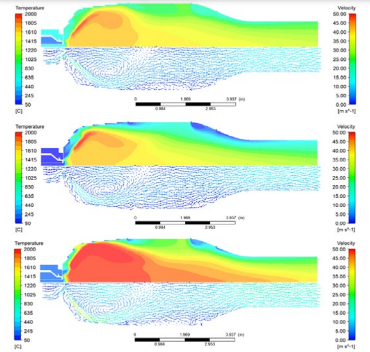
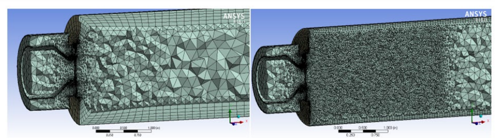
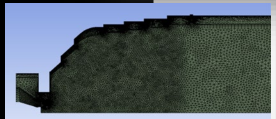


Figure 1-16. Comparison of Temperature Contours and Velocity Vectors for the Three Operating Condition Cases: Design Conditions (Top), Cold Start (Middle), Fast Start (Bottom)

Mesh Sensitivity





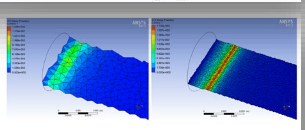


Figure 1-13. CO Mass Fractions Contoured to Show the Grid Resolution of the Combustion Reaction. Coarse Grid (left) and Fine Grid (right)

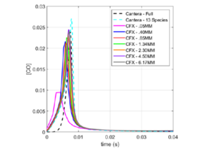
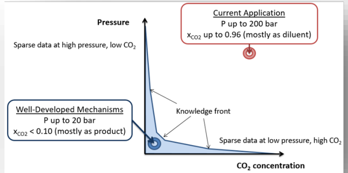


Figure 1-12. Predicted Mole Fraction of CO Versus Time Results for Various Resolutions

Chemical Kinetics

Kinetics Knowledge Base

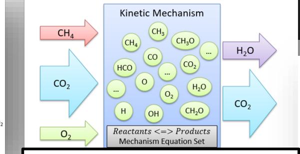


Georgia Tech

Chemical Reaction Kinetics

Overall Reaction: $CH_4 + 2O_2 \rightarrow 2H_2O + CO_2$

Actual reaction is made of hundreds of intermediate chemical reactions with dozens of intermediate chemical species.



Reactants <=> Products
Mechanism Equation Set

$$0.95\,CH_4 + 0.05\,C_2H_6 + 1.55\,O_2 \rightarrow 2.05\,H_2O + 1.05\,CO$$

$CO + 0.5\,O_2 \rightarrow CO_2$ → 41 equations from the skeletal model involving H, H_2, O, O_2, H_2O, H_2O_2, HO_2, OH, HCO, CO, and CO_2

Figure 1-2. The Conversion of the 6-Species Kinetic Model to a 13-Species Kinetic Model

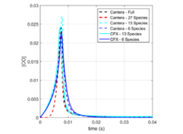
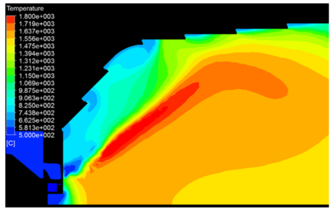


Figure 1-7. Predicted Mole Fraction CO Versus Time Results

Wall Temperatures



Equation of State and Turbulence

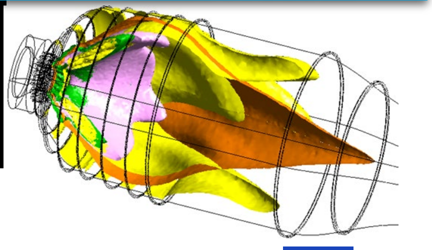
Steady State vs. Transient

$k - \varepsilon$
RANS

ANSYS FLUENT

Real gas effects

Unreacted Products



Chemical Kinetics

Georgia Tech and University of Central Florida each created combustion mechanisms for the sCO2 oxy-combustion system.

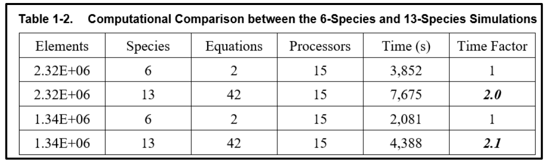
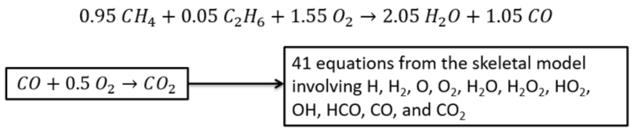


Table 1-2. Computational Comparison between the 6-Species and 13-Species Simulations

Elements	Species	Equations	Processors	Time (s)	Time Factor
2.32E+06	6	2	15	3,852	1
2.32E+06	13	42	15	7,675	***2.0***
1.34E+06	6	2	15	2,081	1
1.34E+06	13	42	15	4,388	***2.1***



$$0.95\ CH_4 + 0.05\ C_2H_6 + 1.55\ O_2 \rightarrow 2.05\ H_2O + 1.05\ CO$$

$$CO + 0.5\ O_2 \rightarrow CO_2$$

41 equations from the skeletal model involving H, H_2, O, O_2, H_2O, H_2O_2, HO_2, OH, HCO, CO, and CO_2

Figure 1-2. The Conversion of the 6-Species Kinetic Model to a 13-Species Kinetic Model

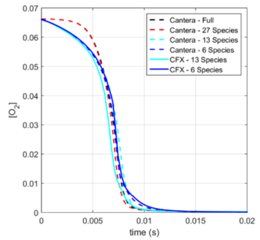


Figure 1-6. Predicted Mole Fraction O_2 Versus Time Results

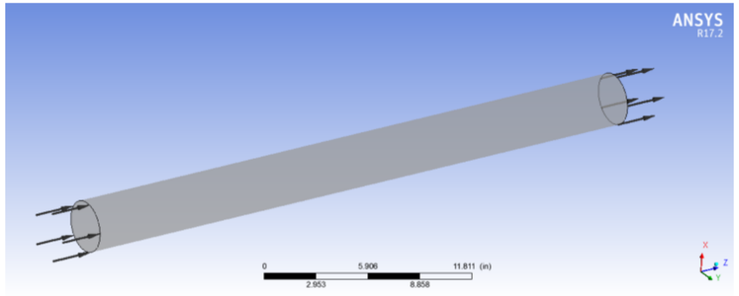
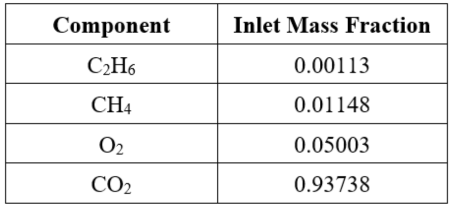


Figure 1-3. Simplified Premixed Reaction Chamber

Table 1-1. Premixed Chamber Inlet Species Mass Fractions



Component	Inlet Mass Fraction
C_2H_6	0.00113
CH_4	0.01148
O_2	0.05003
CO_2	0.93738

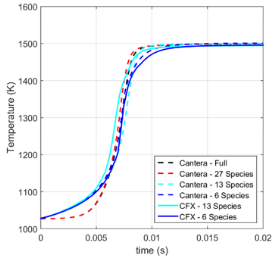


Figure 1-4. Predicted Temperature Versus Time Results

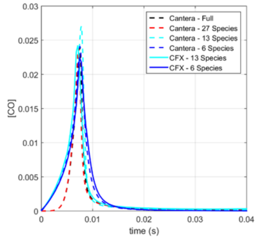


Figure 1-7. Predicted Mole Fraction CO Versus Time Results

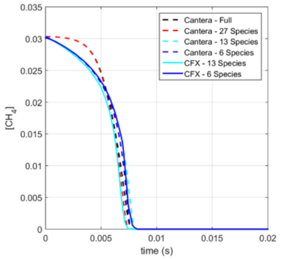


Figure 1-5. Predicted Mole Fraction CH_4 Versus Time Results

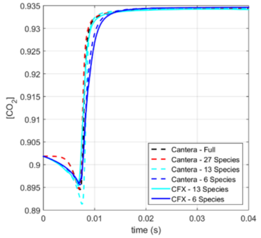
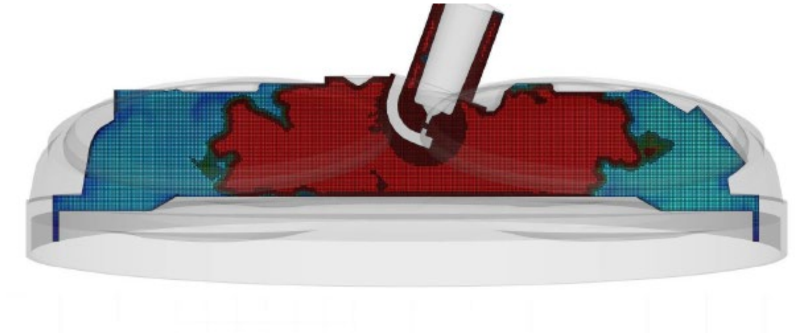


Figure 1-8. Predicted Mole Fraction CO_2 Versus Time Results

Turbulent Combustion

- Combustion is associated with **chemical reaction,** and **transport phenomena**
  Length scale varies
    - Smallest Kolmogorov length scale to integral turbulent length scale
    - Laminar flame thickness
- **Time scale varies**
    - Kolmogorov time scale to integral turbulent time scale
    - Laminar flame speed

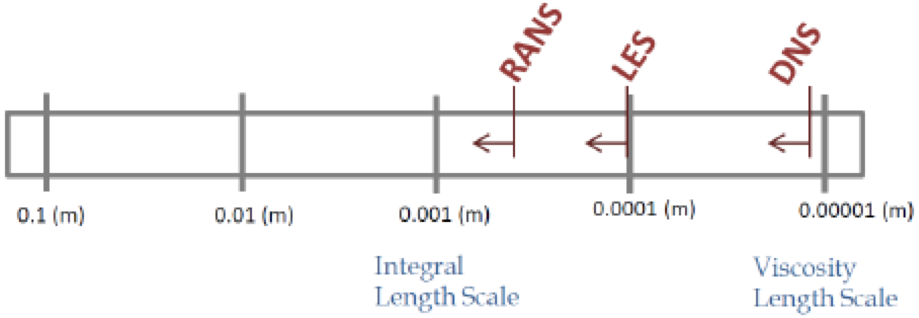


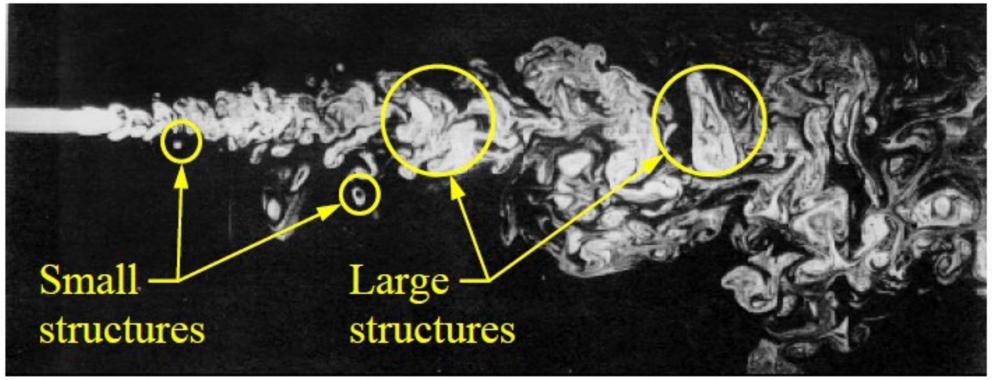
CONVERGE CFD

- To completely solve the combustion process , all **chemical species and reactions** need to be included and both time and length scale needs to be resolved
- To do that, **Direct Numerical Simulation (DNS)** needs to be performed which is computationally prohibitive
- To make it computationally feasible; combustion and turbulence modeling is required
- Careful selection of turbulence chemical kinetics models is needed! Flame speed measurements are very uncertain!

Turbulence Modeling

- Turbulent eddies in the flow enhances the rate of mixing of momentum, energy, and species
- These eddies are present at different length scales from small to large
  - **Reynolds-Averaged Navier-Stokes (RANS):** This model is used to account for mixing by introducing turbulent diffusion coefficients for momentum, energy, and species
  - **Large Eddy Simulations (LES) turbulence model:** Resolve the large length scale and model the small length scale
- Turbulence also affects flame speed, but that is worthy of its own presentation





CONVERGECFD

Grid Sensitivity

- The chemical kinetic simulations also explored grid dependence.
- 13 species mechanism were used, UCF and Georgia Tech have since published newer models.
- Results were a general understanding of the minimum resolution that supports adequate chemical resolution.
- Both reaction mechanisms adequately modeled species and temperature changes.
- Grid size requirements are dependent in part on turbulence models.

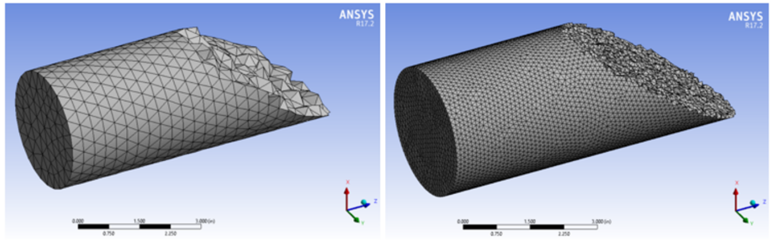


Figure 1-9. Examples of Coarse (left) and Fine (right) Meshing Results for Premixed Chamber

Table 1-3. Mesh Statistics for Premixed Chamber

Elements	Element Multiplication Factor
0.05E+06	1.0
0.40E+06	8.0
0.85E+06	17.0
1.30E+06	26.0
2.30E+06	46.0
1.34E+06	26.8
6.17E+06	122.0

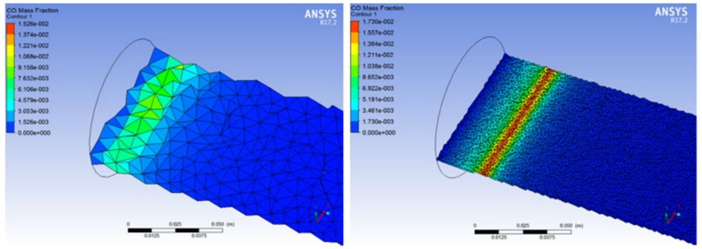


Figure 1-13. CO Mass Fractions Contoured to Show the Grid Resolution of the Combustion Reaction. Coarse Grid (left) and Fine Grid (right)

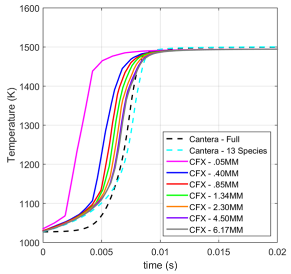


Figure 1-10. Predicted Temperature Versus Time Results for Various Resolutions

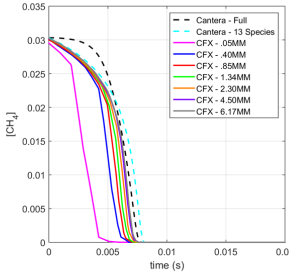


Figure 1-11. Predicted Mole Fraction of CH_4 Versus Time Results for Various Resolutions

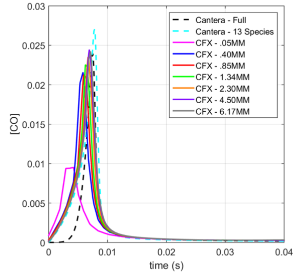
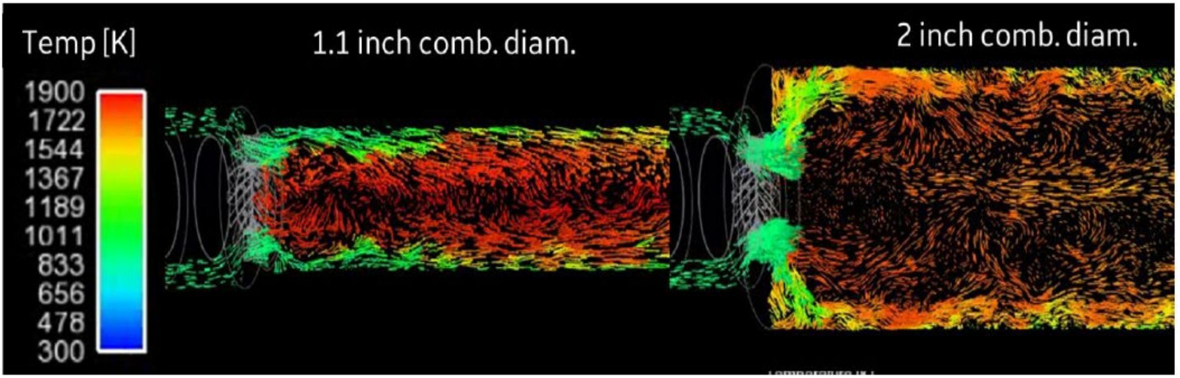
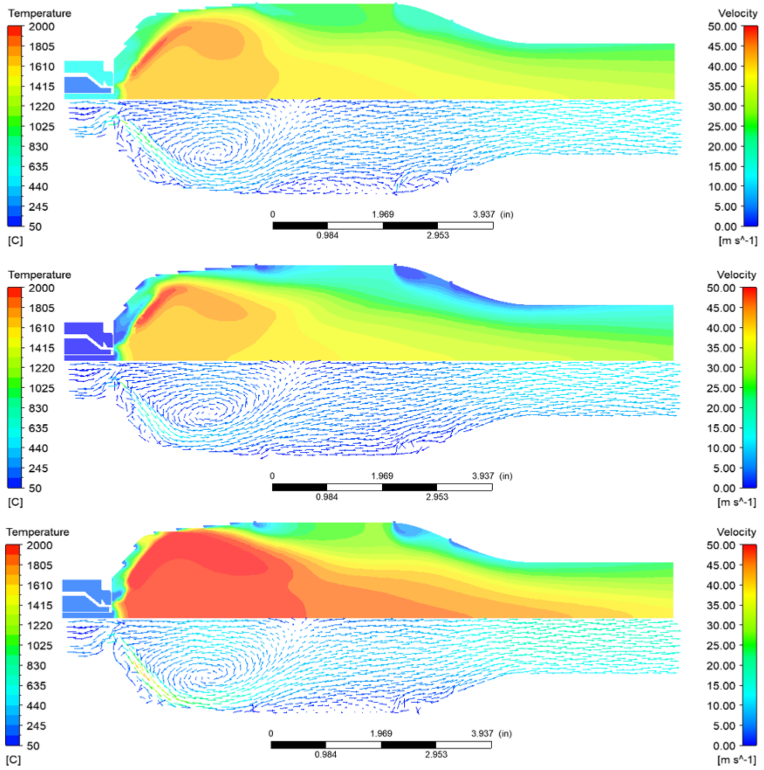


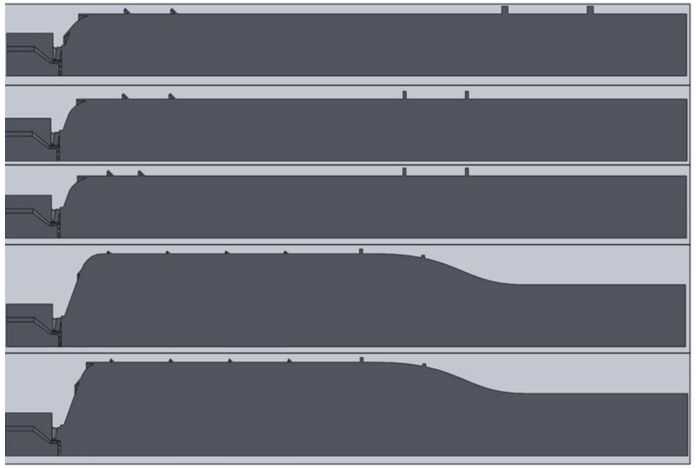
Figure 1-12. Predicted Mole Fraction of CO Versus Time Results for Various Resolutions

Flow Field



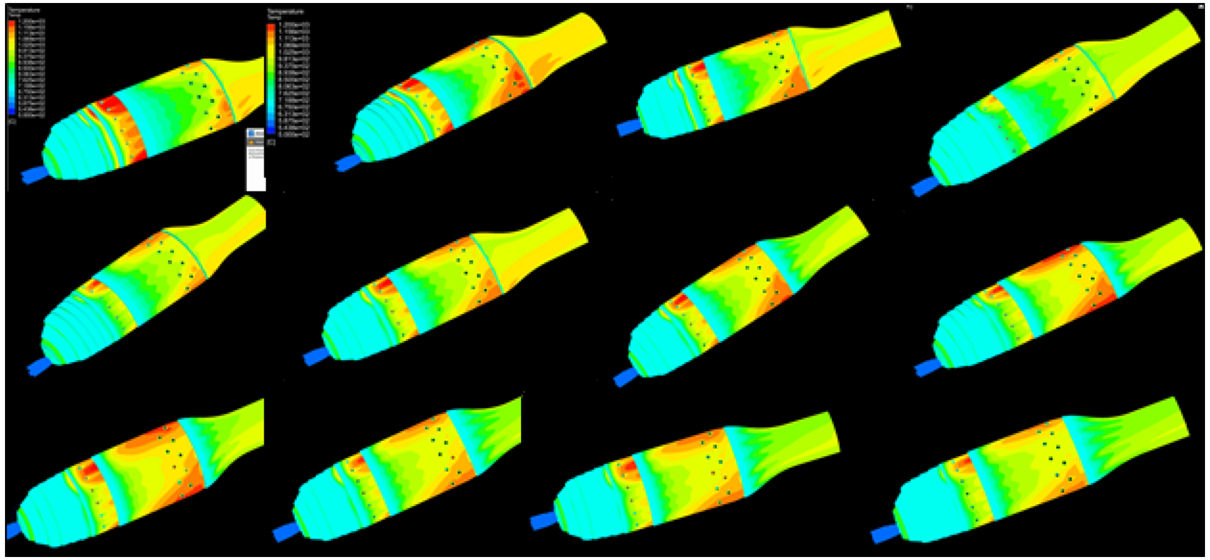
- Swirler design, combustor shape, fuel injection, and cooling flow allocation control the flow field inside the combustor
- Light-off should be conducted at **low temperatures and pressures**. But what about real gas effects? Operation near the critical point is poorly understood
- Fuel injection and flow must accommodate all operating conditions, including startup.
- Relevant fluid physics need to be modeled with increasing fidelity as design process proceeds.

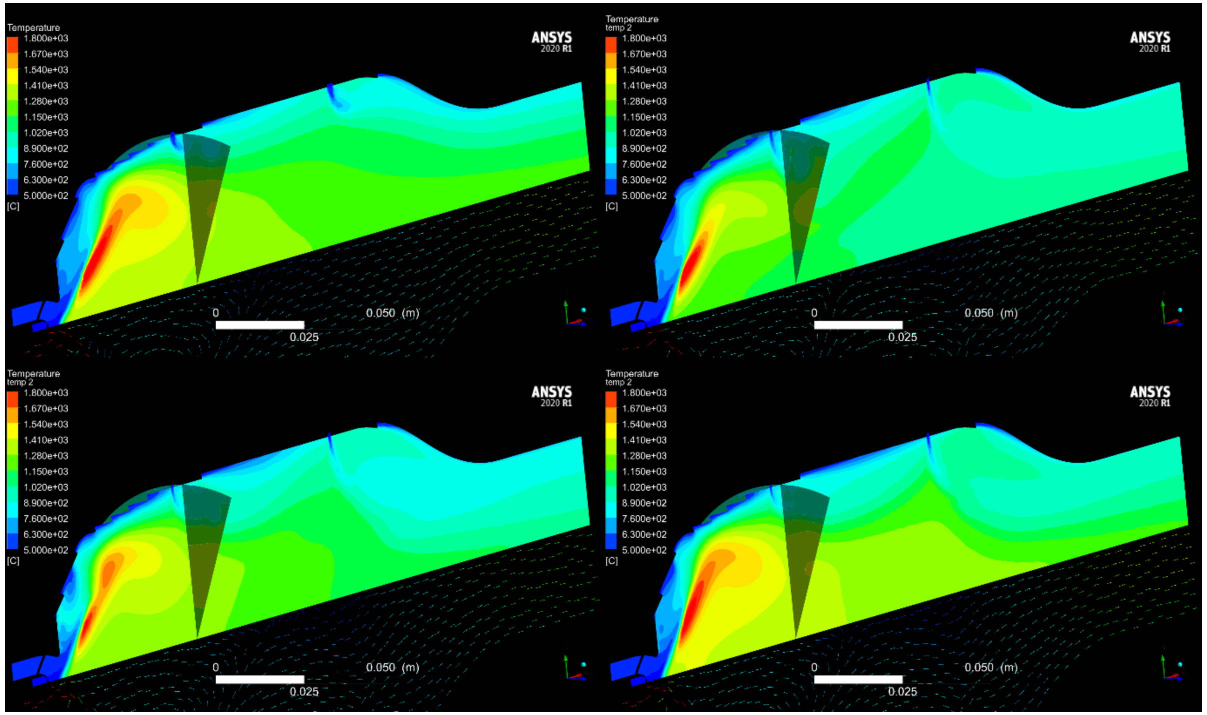


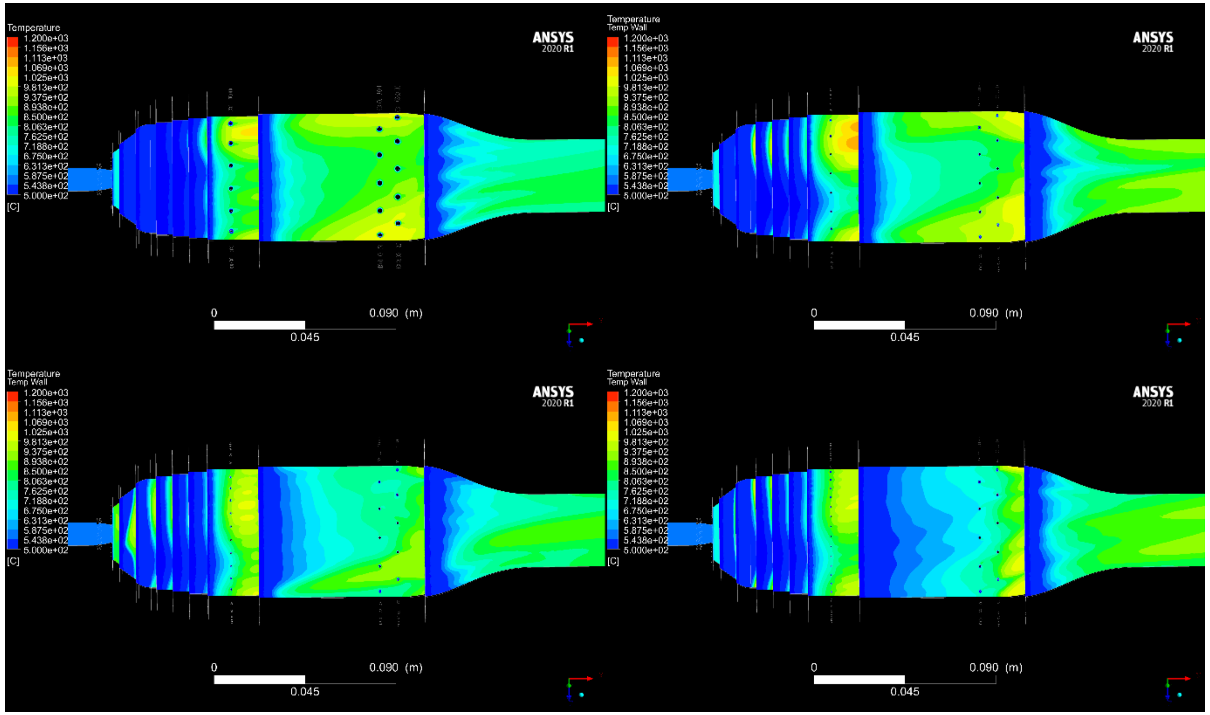


Design and Optimization

Preliminary approaches can explore the design space using low-cost, low-fidelity steady RANS simulations.



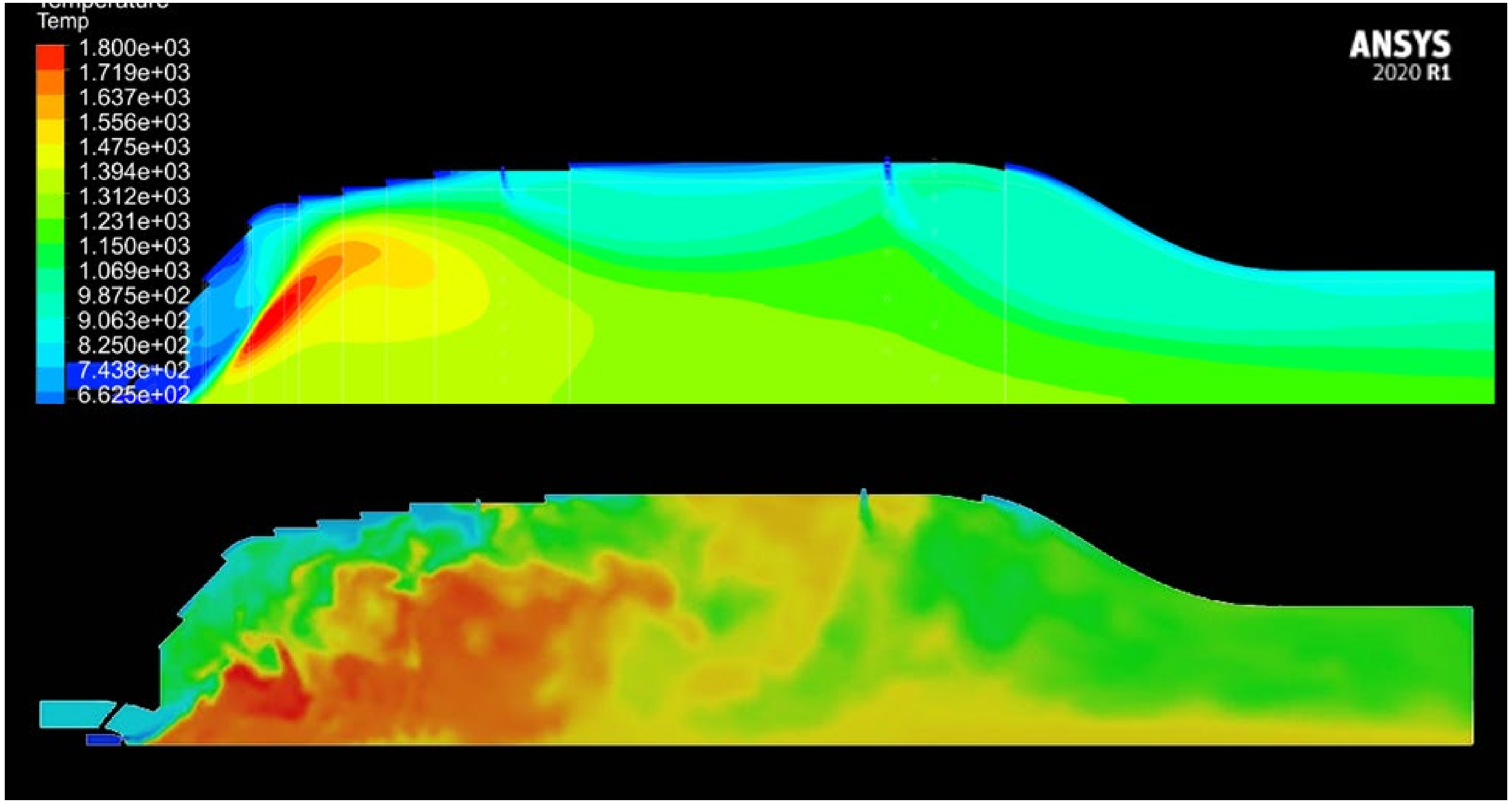




Steady vs. Unsteady Modeling

Steady RANS Simulation

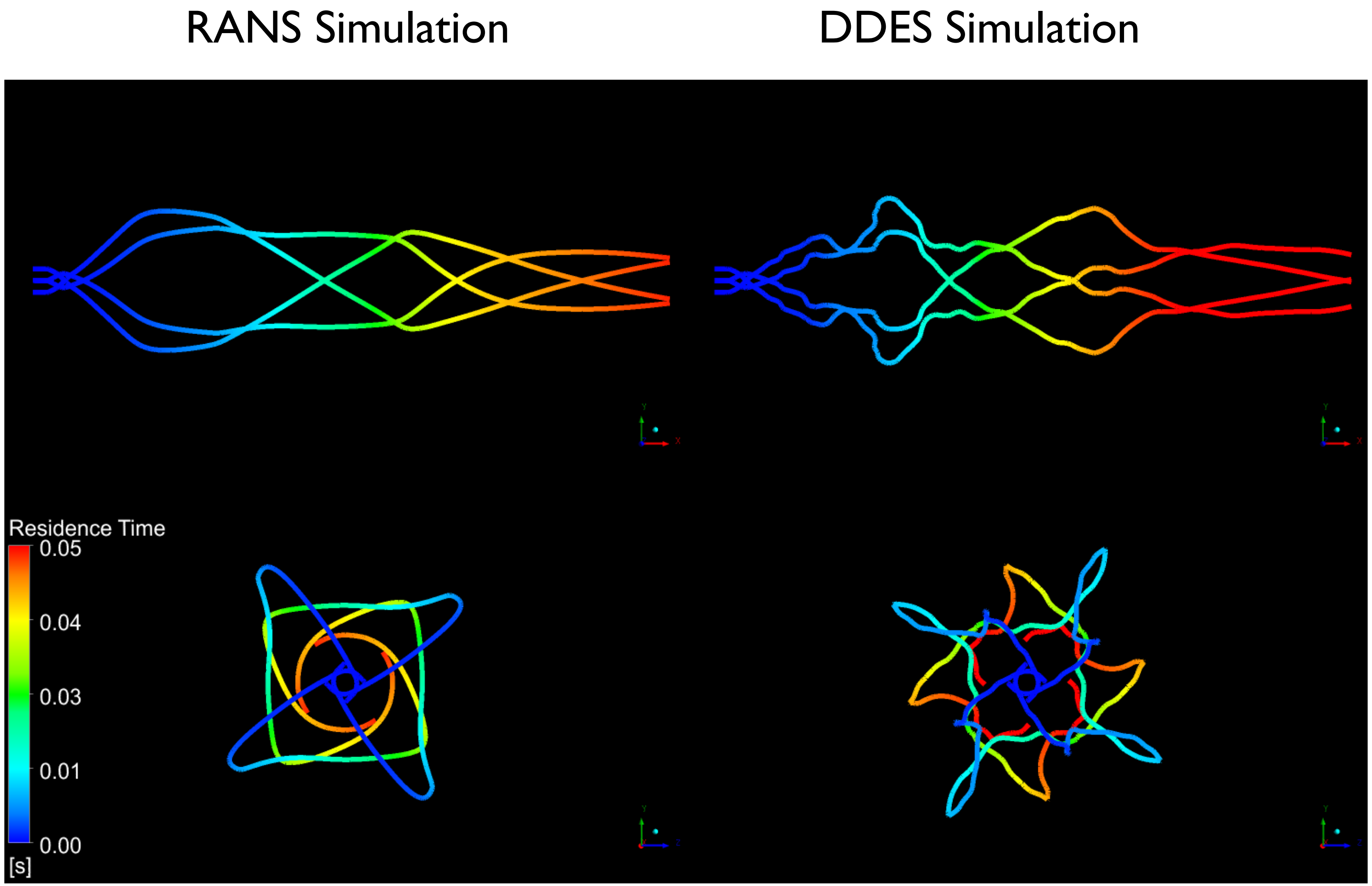
Unsteady DDES Simulation
(~5-10x cost per run)



Combustor Design

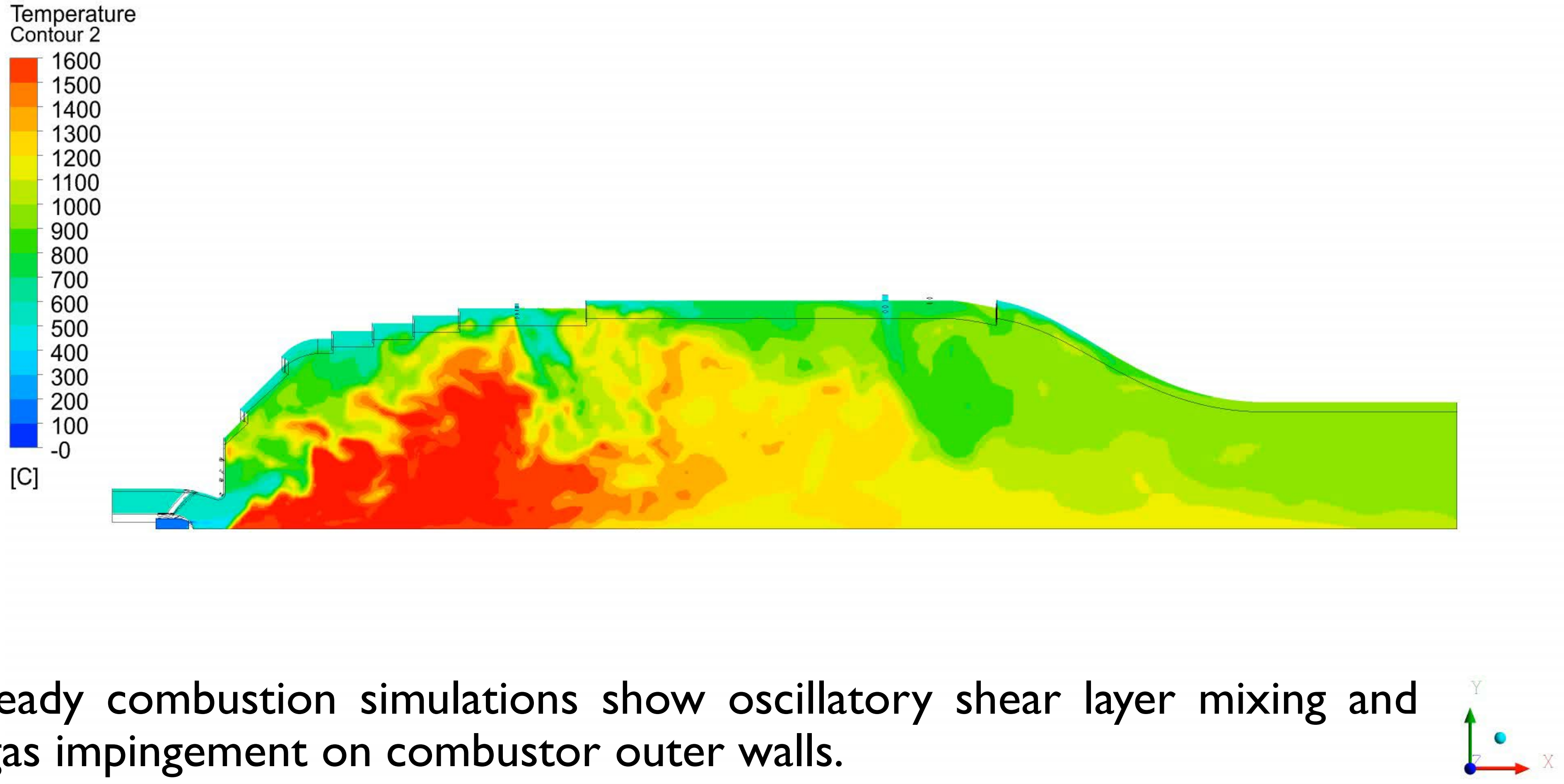
When switching from RANS to an unsteady simulation are the key flow features preserved? In our case:

- Swirl – Yes
- Mixing – No



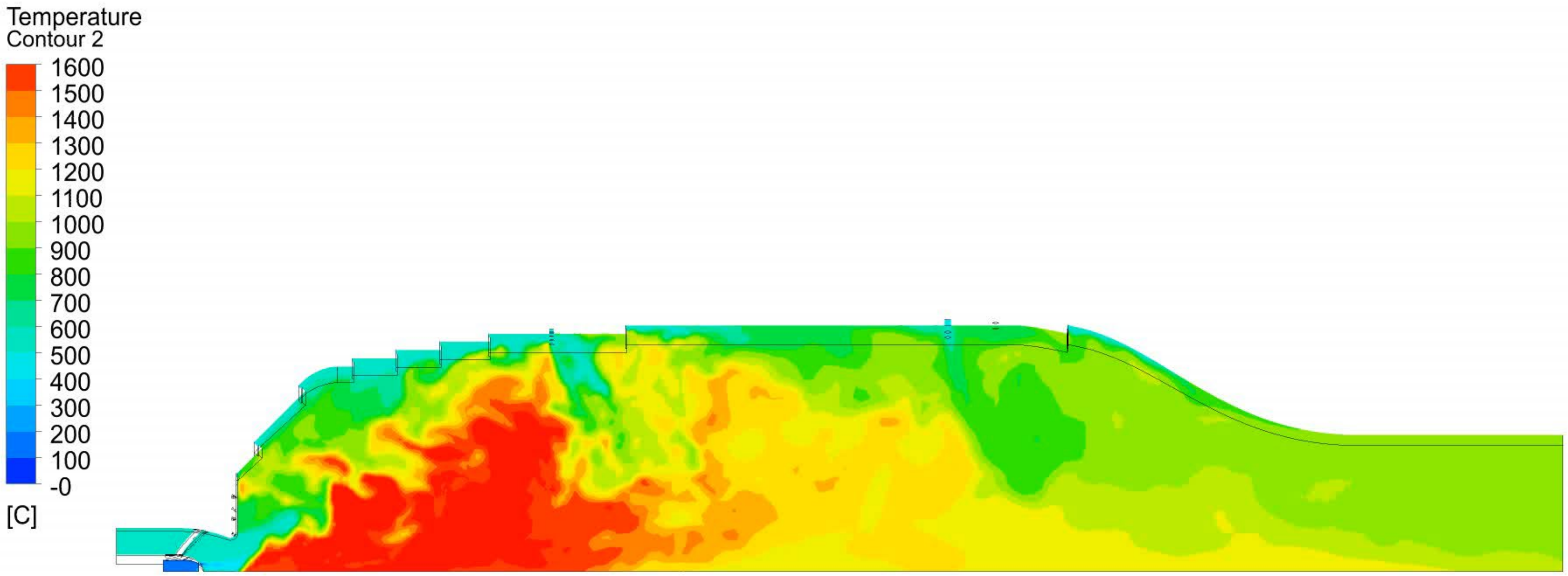
Streamlines Comparison

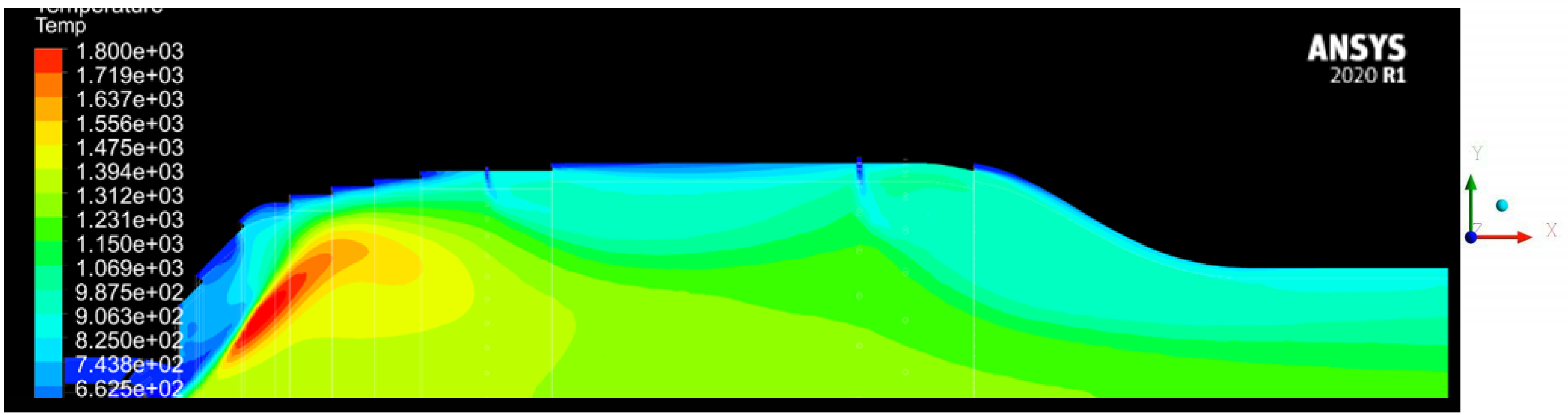
Unsteady Combustion Simulations



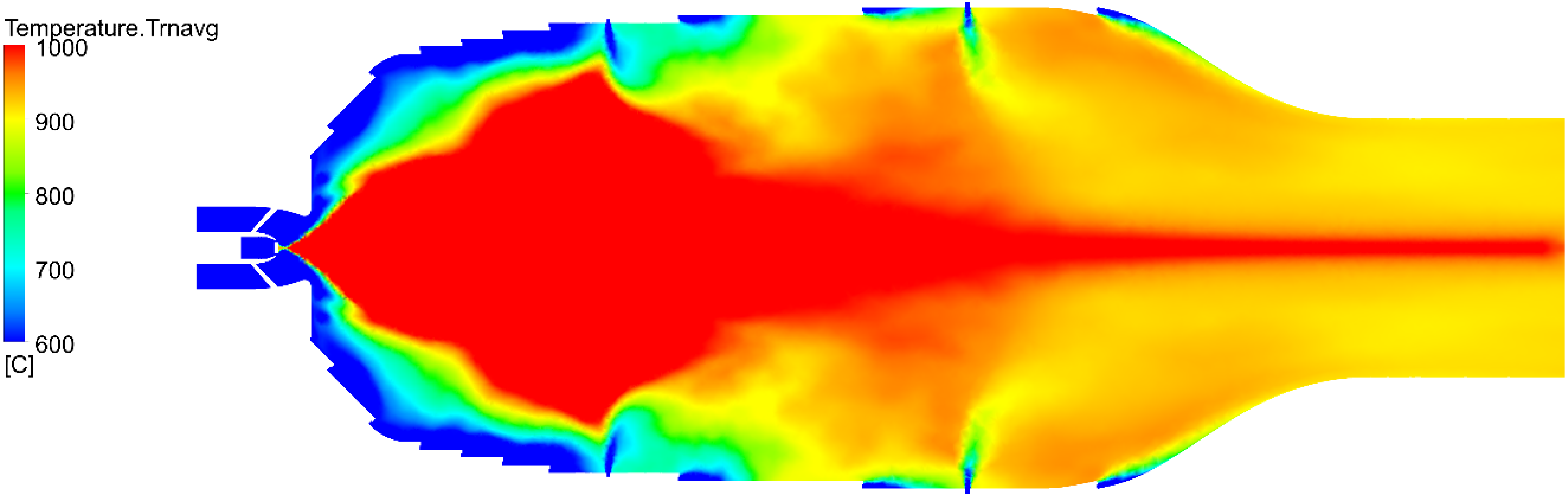
Unsteady combustion simulations show oscillatory shear layer mixing and hot gas impingement on combustor outer walls.

Unsteady Combustion Simulations

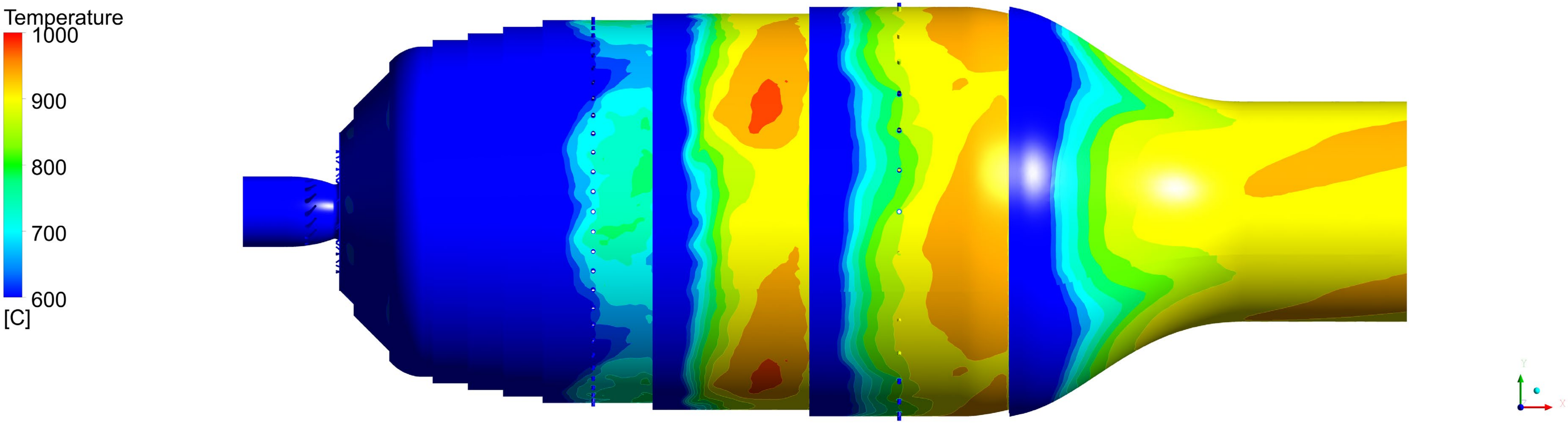




Time-averaged DES results



Notional Wall Temperatures



Conservative adiabatic simulations suggest peak combustor wall temperatures near 1000 C, which will be decreased further with exterior cooling flows.

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