# Combustion Modeling for Direct Fired Supercritical CO2 Power Cycles

SBIR Phase II Review Meeting
Award # DE-SC0017235
May 11th, 2021

Presented by

W. H. Calhoon, Jr., Senior Research Scientist (PI) and Stephen Mattick
7501 Memorial Pkwy South, Suite 219, Huntsville, AL 35802, (256) 883-1905
calhoon@craft-tech.com
Brian Connolly, SwRI, 6220 Culebra Rd, San Antonio, TX 78238, (210)-522-3618
brian.connolly@swri.org

Acknowledgment: This material is based upon work supported by the Department of Energy Award Number DE-SC0017235.

# Project Description and Objectives

## Project Purpose:

- Develop a tractable and accurate turbulent combustion modeling approach that may be applied to design trade studies of direct fired supercritical $CO_2$ power cycle combustors
- Supports DOE objective of improving the efficiency of large scale fossil energy based power generation systems
- Enhanced accuracy of a validated combustion model will enable design optimization for efficiency
- Current combustion modeling approaches not validated for supercritical flows

## Approach:

- Develop “direct quadrature method of moments” (DQMOM) combustion model for low-speed, supercritical flows
- Validate the model with new experimental data

# Turbulent Combustion Model Technology Comparison

| | predicted PDF | regime independent | mixture fract. NOT required | generalized b.c.s | tractable |
|---|---|---|---|---|---|
| **Stochastic Models:** | | | | | |
| PDF transport | ● | ● | ● | ● | ✖ |
| Linear-eddy model (LEM) | ● | ● | ● | ● | ✖ |
| One dimensional turbulent (ODT) | ● | ● | ● | ● | ✖ |
| **Moment Models:** | | | | | |
| DQMOM | ● | ● | ● | ● | ● |
| Flamelet progress variable (FPV) | ✖ | ✖ | ✖ | ✖ | ● |
| Conditional moment closure | ✖ | ✖ | ✖ | ✖ | ● |
| LEM – counter flow (LEM-CF) | ● | ● | ✖ | ✖ | ● |

CRAFT Tech SwRI

# Direct Quadrature Method of Moments (DQMOM)

## Foundation:

- Direct solution of the scalar PDF transport equation
- Eulerian solution procedure with discretized PDF
- Employs validated PDF mixing models

## Advantages:

- Applicable to low and high speed flows
- Generalize boundary condition treatment
- Comparable accuracy to velocity – scalar stochastic PDF model
- *Captures localized flame extinction*
- Tractable for routine design application

# Phase II Project Description

## Model Development Tasks:

Task 1.1: DQMOM Preconditioned (Low Speed) Formulation Extension

Task 1.2: Real Fluid Chemical Kinetic Effects Extension

Task 2.1: Detailed Chemical Model Development

Task 2.2: Reduced Chemical Model Development

## Model Validation Tasks:

Task 3.1: SwRI Bench-Top Combustor Validation

Task 3.2 – 3.4: SwRI 1 MW Combustor Validation

CRAFT Tech

SwRI

# Task 3.1: Bench-Top Combustor Validation

## Task 3.1 Objective:

- Validate the DQMOM combustion model for application to a laboratory scale $sCO_2$ combustor configuration
- Validation data generated by SwRI

## SwRI Bench-Top Combustor:

- SwRI has designed an new non-premixed laboratory scale combustor for this validation effort
- Co-axial jet configuration
- Will provide excellent validation data for combustion model development

# Task 3.1: Bench-Top Combustor Validation

## Test Objectives:

- Establish the ignition limits of the combustor
- Provide wall pressure and temperature measurements for a stable flame condition

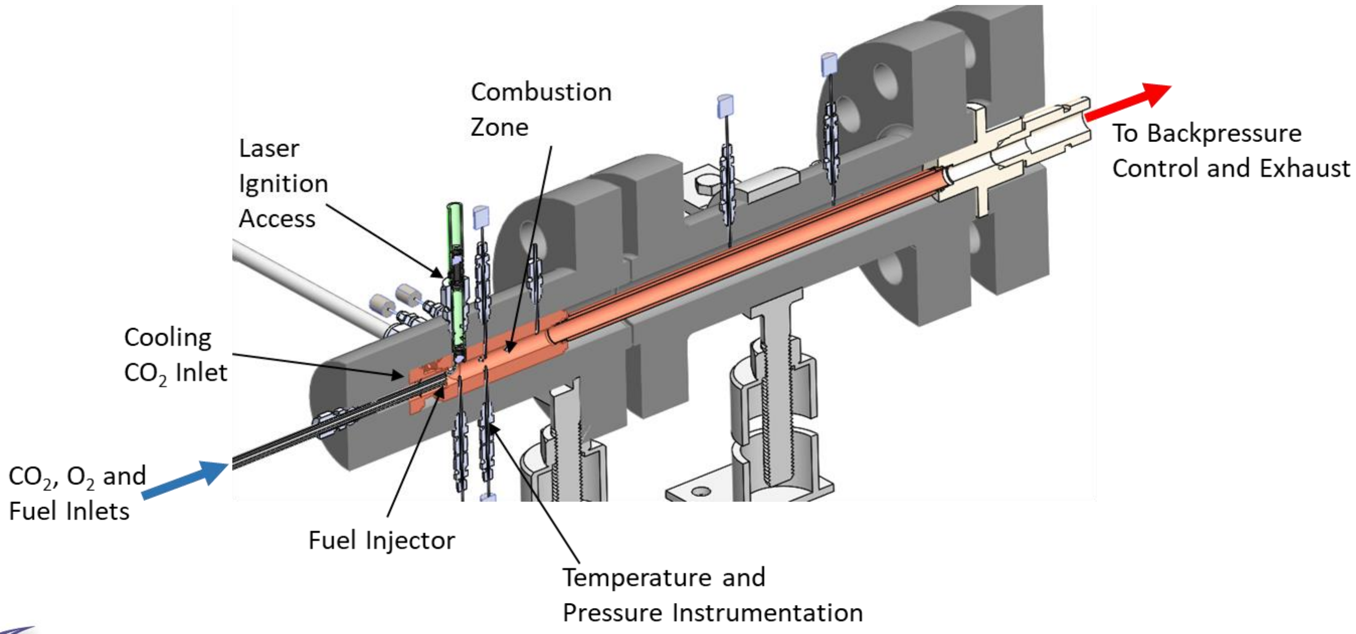
## Ignition Limit Determination:

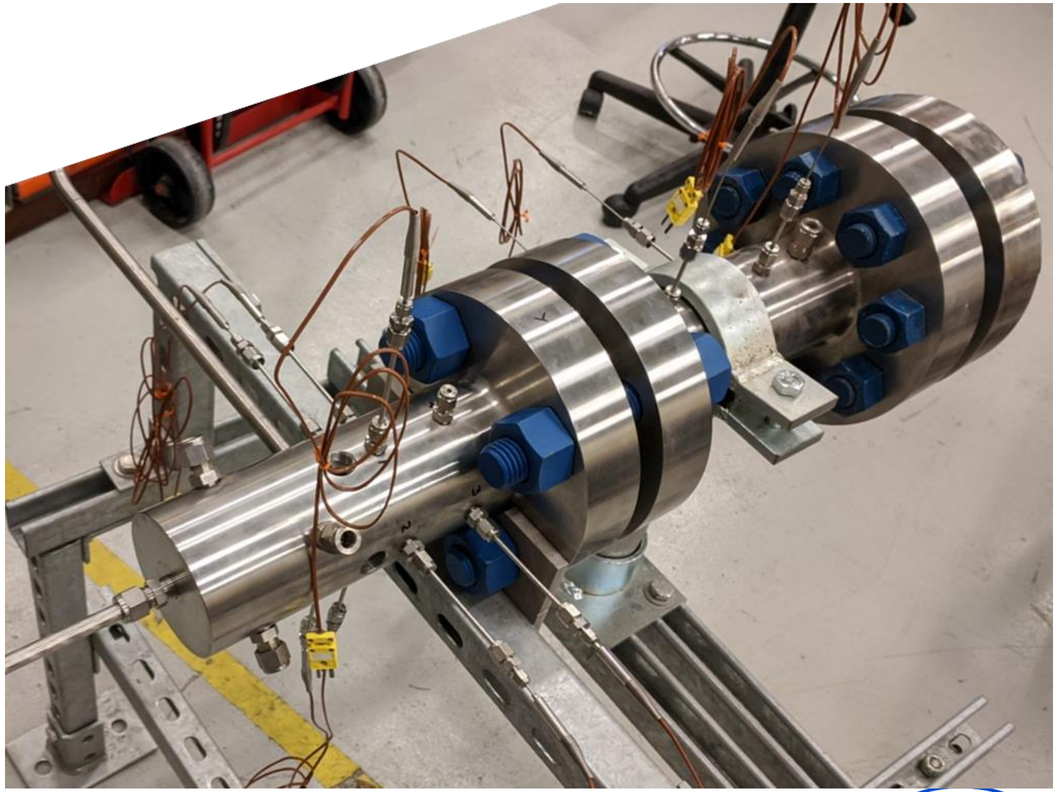
- Laser ignition of the flow occurs in the downstream jet shear layer
- Establishment of a stable flame will require the upstream propagation of the ignition front in the partially premixed shear layer up to the jet lip recirculation zone
- A series of cases varying the global O/F ratio used to established the ignition limits
- Ignition visualized through optical ports
- Possible lifted flames over a narrow O/F ratio range

# Task 3.1: Bench-Top Combustor Validation

## Rig Overview:

- Small, ~0.5 in diameter direct fired combustor
- Non-premixed, coaxial jet, fuel injector



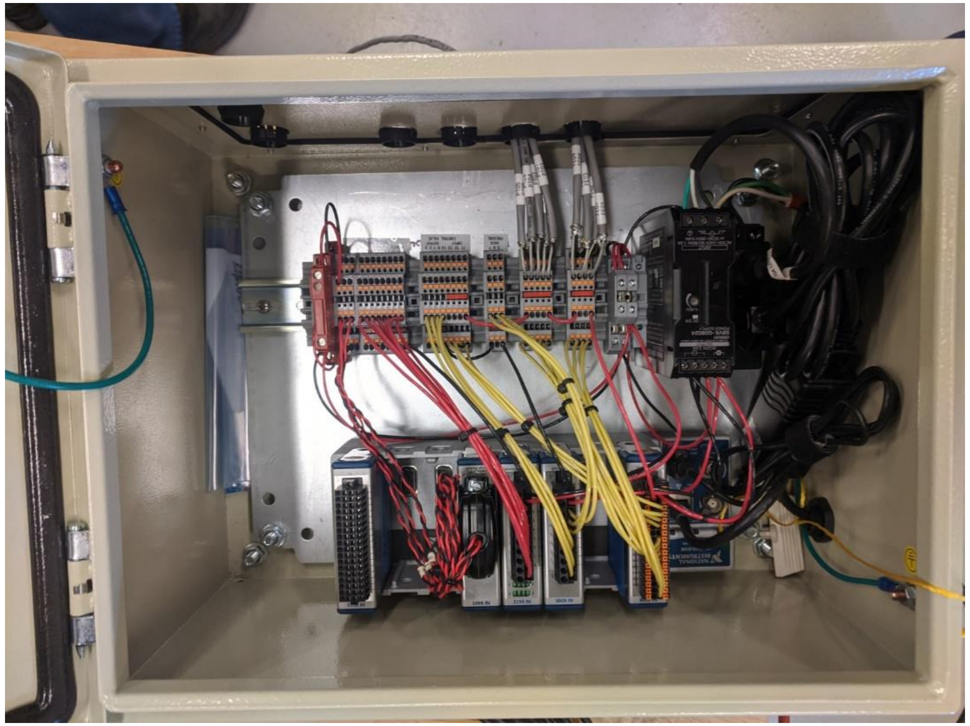
CRAFT Tech

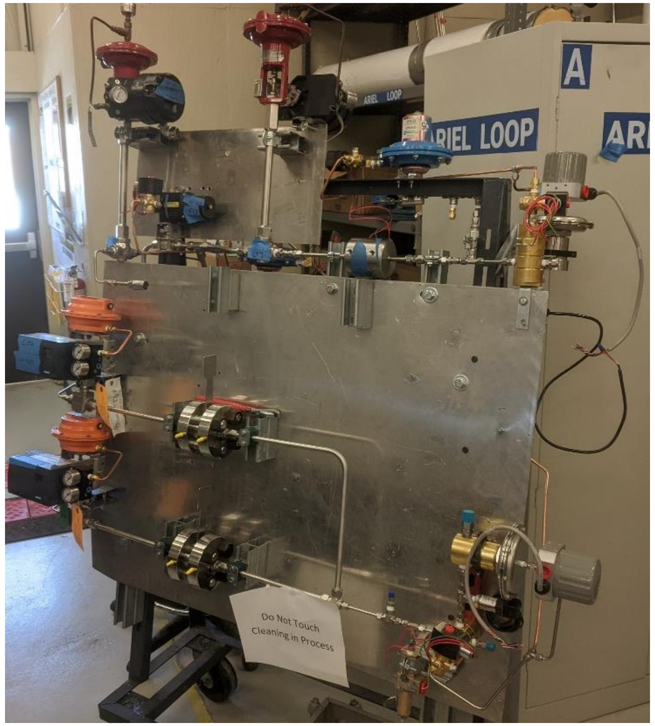
SwRI

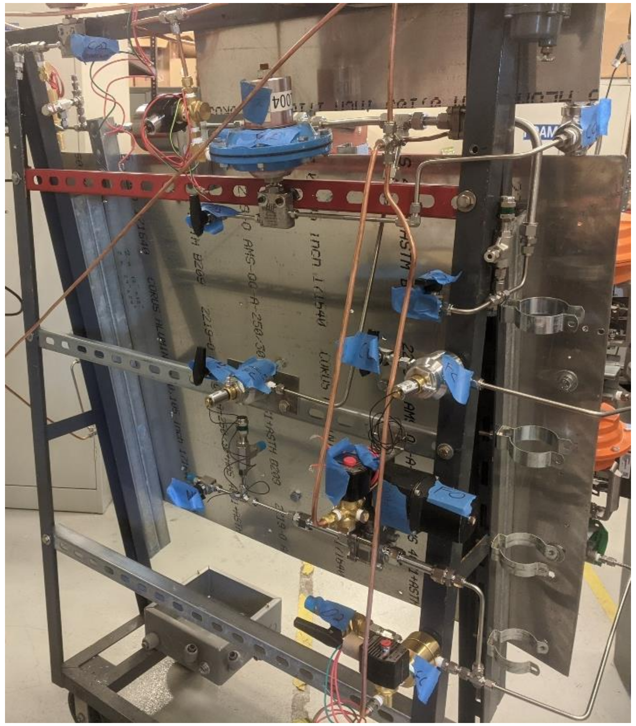
# Task 3.1: Bench-Top Combustor Validation

Instrumentation and controls:

- Instrumentation and DAQ installed, fuel cart assembled





# Task 3.1: Bench-Top Combustor Validation

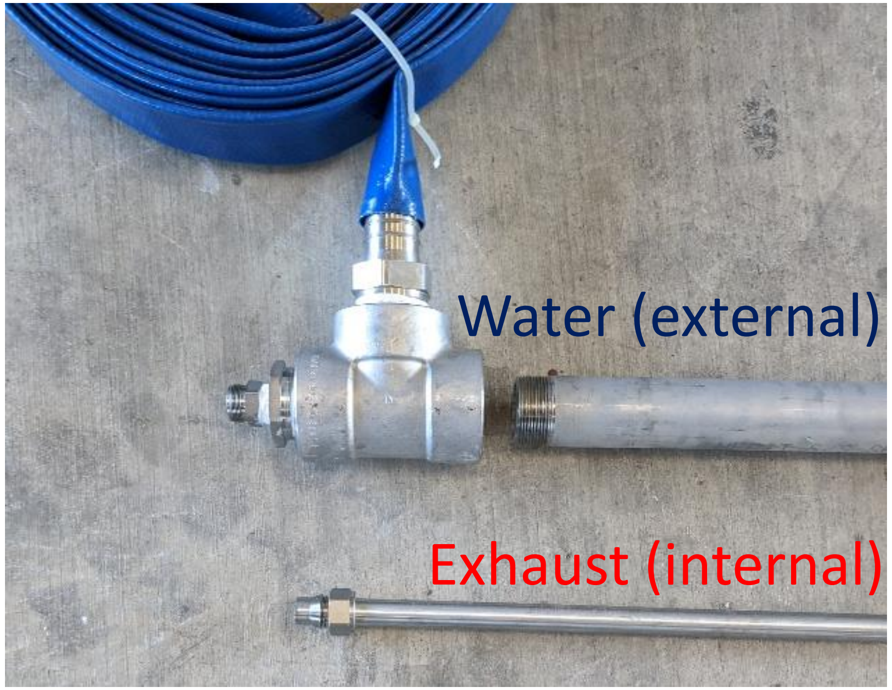
<u>Laser Ignition and Optical Probes:</u>

- Quantel Q-smart Twins 2W laser with water-cooled probe for ignition
- Water-cooled optical probes


# Task 3.1: Bench-Top Combustor Validation

Exhaust:

- Backpressure valve to maintain desired combustor pressures
- 13’ parallel flow water-cooled heat exchanger

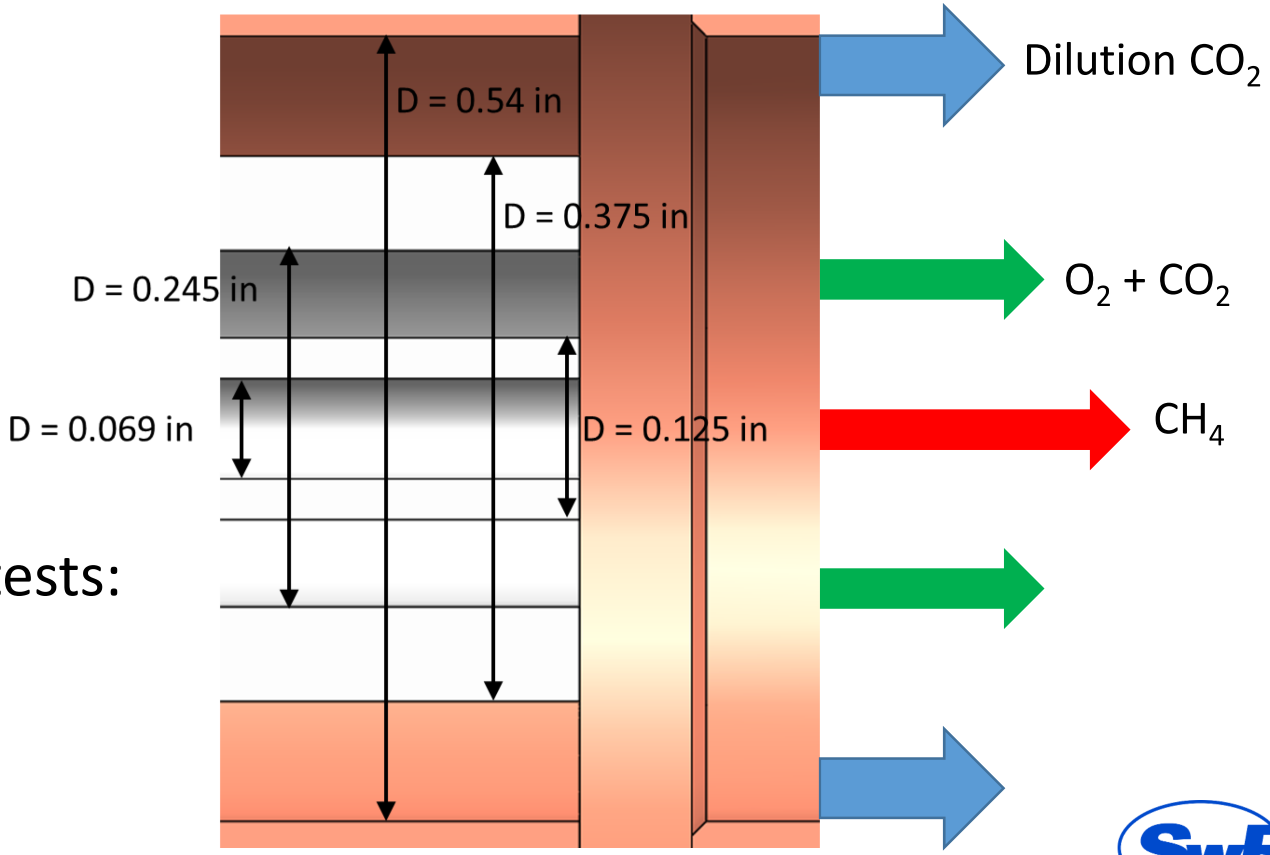



# Task 3.1: Bench-Top Combustor Validation

## Anticipated Test Conditions:

- Change in $sCO_2$ source necessitated new operating conditions
- Inlet $sCO_2$ pressure: 1600psi
- Inlet $sCO_2$ temperature: 200F
- ~45 tests to determine flammability
- Injector bevel removed
- Momentum flux ratio constant for all tests:

$$\sqrt{\frac{\rho_{\text{fuel}} U^2_{\text{bulk,fuel}}}{\rho_{\text{oxi}} U^2_{\text{bulk,oxi}}}} = 1.56$$

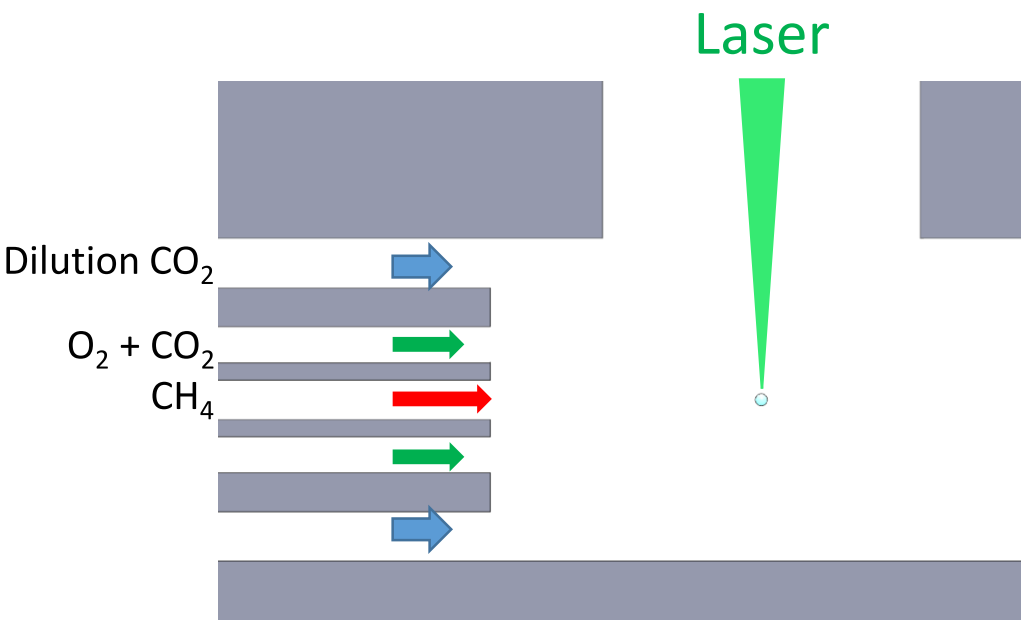



CRAFT Tech

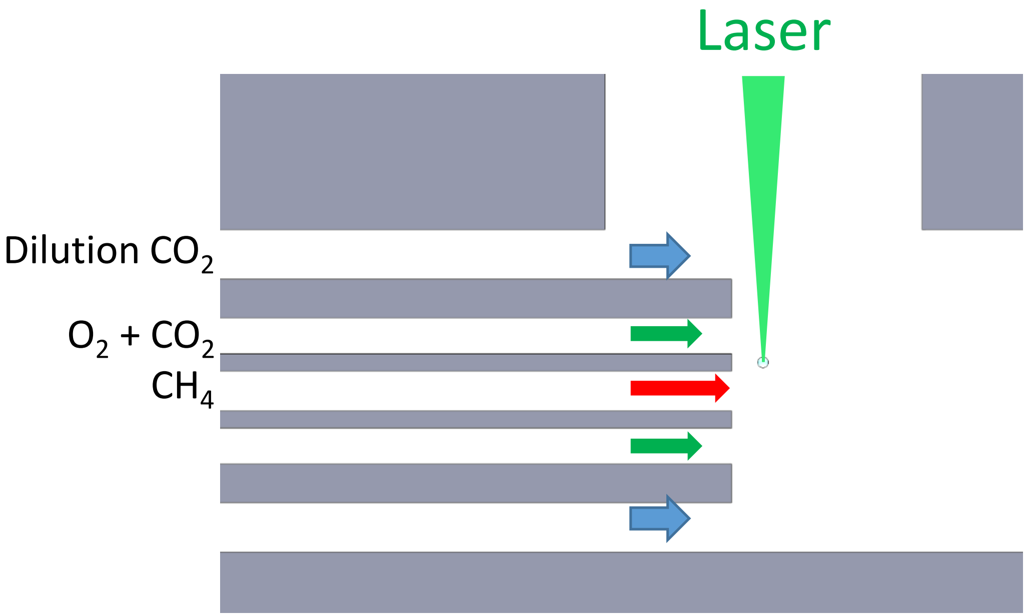
SwRI

# Task 3.1: Bench-Top Combustor Validation

Ignition locations:




Flame propagates upstream
(installed)




Ignition in recirculation region
(backup option)

# Task 3.1: Bench-Top Combustor Validation

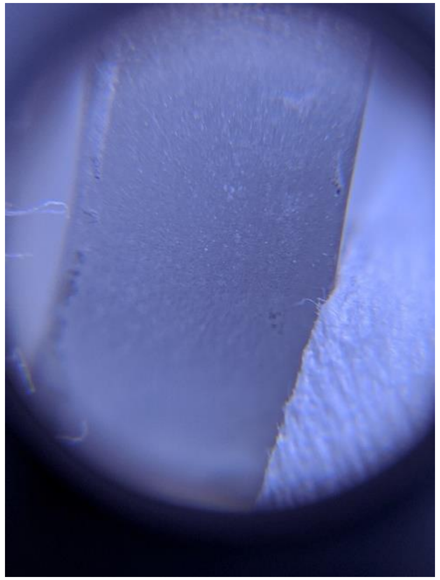
Testing Delays:

- $sCO_2$ sourcing difficulties: Delays of other SwRI projects tied up pumps and heaters, and denied access to test facilities during extended test campaign
- Staffing change: Dr. Jacob Delimont replaced by Dr. Brian Connolly
- COVID-19: SwRI personnel sick and/or quarantined for multiple weeks, as well as longer supplier lead times

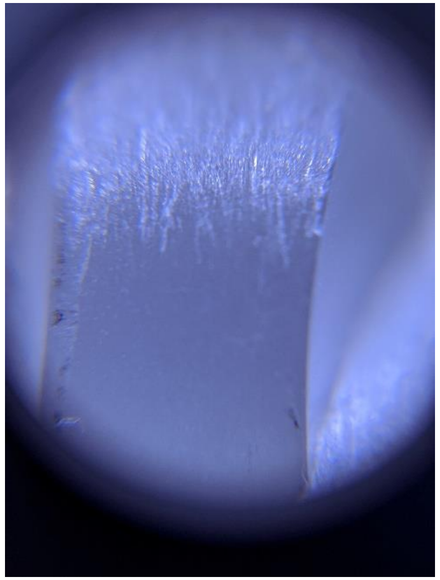
# Task 3.1: Bench-Top Combustor Validation

<u>Current Status:</u>

- Rig and fuel cart are assembled
- $sCO_2$ tank and heater reserved, control program written
- Plumbing and DAQ networking being completed
- Water-cooled laser probe assembled
- Abrading sapphire lenses for adhesive contact
- Final laser probe modifications ongoing
- Light-off imminent!



Unabraded



Abraded

# Task 3.1: Bench-Top Combustor Validation

Test Schedule:

- Commissioning to occur end of April or early May
- Data collection to begin in May
- This project has priority for all equipment and personnel

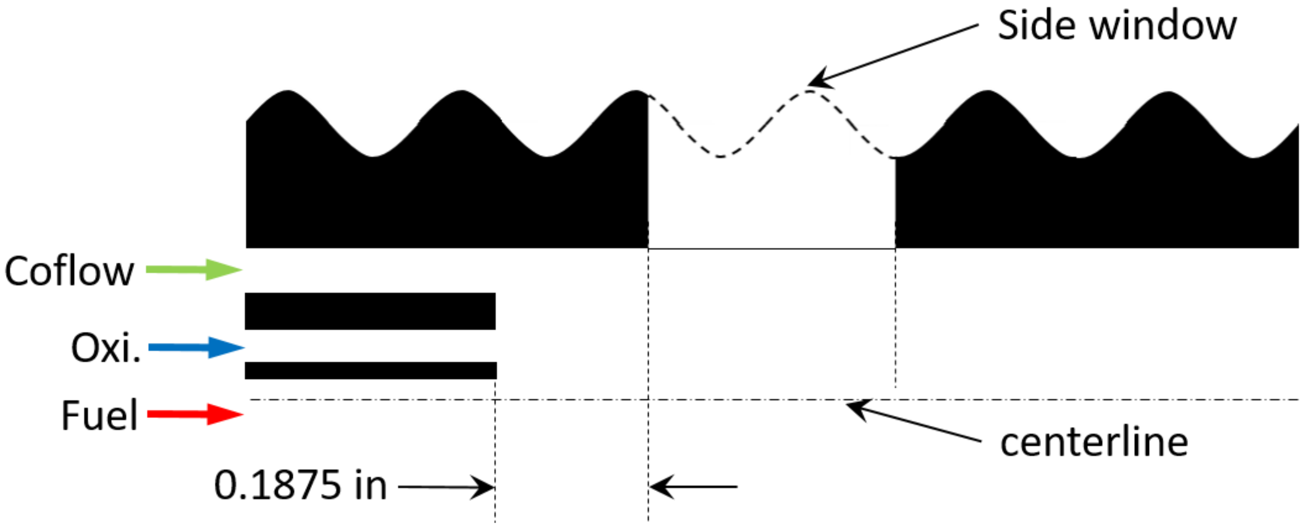
# Task 3.1: Bench-Top Combustor Validation

## Model Application Strategy for Validation:

- Apply unsteady, 2-D/axisymmetric RANS analysis to bracket ignition limit
- Refine ignition limit with 3-D LES analysis

## Combustor Analysis Schematic (to scale):

- Laser ignition in the center of the side window
- Flame must propagate upstream to the base recirculation zone



# Task 3.1: Bench-Top Combustor Validation

## Pretest Analysis:

- Unsteady, 2-D/axi RANS analysis of preliminary test conditions from Fall 2020
- Laser ignition modeled with 2 mm diameter energy source term to raise local temperature to ~ 3000 K
- Simulate unsteady combustor start-up, laser ignition transient, and flame development
- Test matrix generated for:
  - $P_0$ = *1.3e+7 Pa*
  - *Maintaining constant bulk fuel – oxidizer mass flux ratio*

| Feed Stream | Composition | Max. $\dot{m}$ (kg/sec) | Temperature (K) |
|---|---|---|---|
| Fuel | $CH_4$ | 0.004 | 473.15 |
| Oxidizer | $O_2+CO_2$ | $O_2$: 0.016, $CO_2$: 0.04 | 473.15 |
| Coflow | $CO_2$ | 0.2 | 473.15 |

# Task 3.1: Bench-Top Combustor Validation

## Pretest Analysis:

- Fuel and coflow/dilution stream conditions:

| Feed Stream | Composition | $\dot{m}$ (kg/sec) | $U_{bulk}$ (m/sec) | Temperature (K) |
|---|---|---|---|---|
| Fuel | $CH_4$ | 0.0025 | 15.0 | 473.15 |
| Coflow | $CO_2$ | 0.05 | 3.43 | 473.15 |

- Oxidizer stream conditions:

| | Mass fraction | | | | |
|---|---|---|---|---|---|
| Case no. | $O_2$ | $CO_2$ | $\dot{m}$ (kg/sec) | $U_{bulk}$ (m/sec) | Temperature (K) |
| 1 | 1.0 | 0.0 | 0.017915 | 6.926 | 473.15 |
| 2 | 0.75 | 0.25 | 0.01887 | 6.573 | 473.15 |
| 3 | 0.625 | 0.375 | 0.01941 | 6.389 | 473.15 |
| 4 | 0.5 | 0.5 | 0.02 | 6.200 | 473.15 |
| 5 | 0.4 | 0.6 | 0.02052 | 6.048 | 473.15 |
| 6 | 0.3 | 0.7 | 0.02107 | 5.887 | 473.15 |

# Task 3.1: Bench-Top Combustor Validation

<u>Simulation Procedure:</u>

- Simulation initialized with cold coflow fluid ($CO_2$) throughout the domain
- Fuel and oxidizer inflow transient simulated *nonreacting from* *t* = 0 to *t* = 0.01 sec:
  - Fuel – oxidizer shear layer sets up
  - Mixing region reaches past the laser ignition location
- *Reacting* flow simulation with laser ignition source *from* *t* = 0.01 to *t* = 0.014 sec:
  - Laser source a 2 mm diameter spot at the upstream edge of the viewing window
  - Energy source term raises the local minimum temperature to ~ 3000 K
  - Flame anchored to the laser ignition location
  - Flame may propagate upstream to the fuel – oxidizer base recirculation zone
- Laser source removed and *reacting* flow simulation continued from *t* = 0.014 to *t* ~ 0.032 sec:
  - Flames below the ignition limit blow out
  - Stable flames anchor to the base fuel – oxidizer base recirculation zone

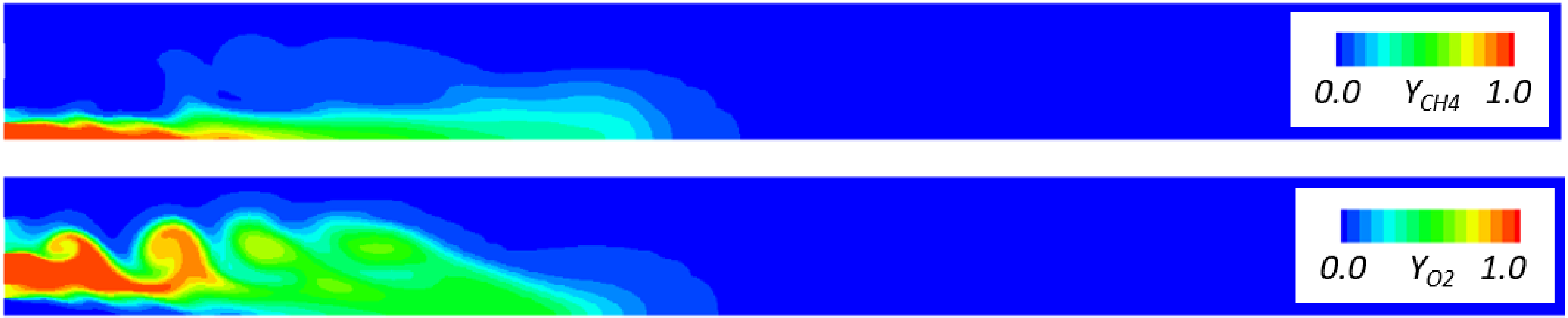
CRAFT Tech

SwRI

# Task 3.1: Bench-Top Combustor Validation

Case 1 Predictions (oxidizer flow – $Y_{O2}$ *= 1.0)*:

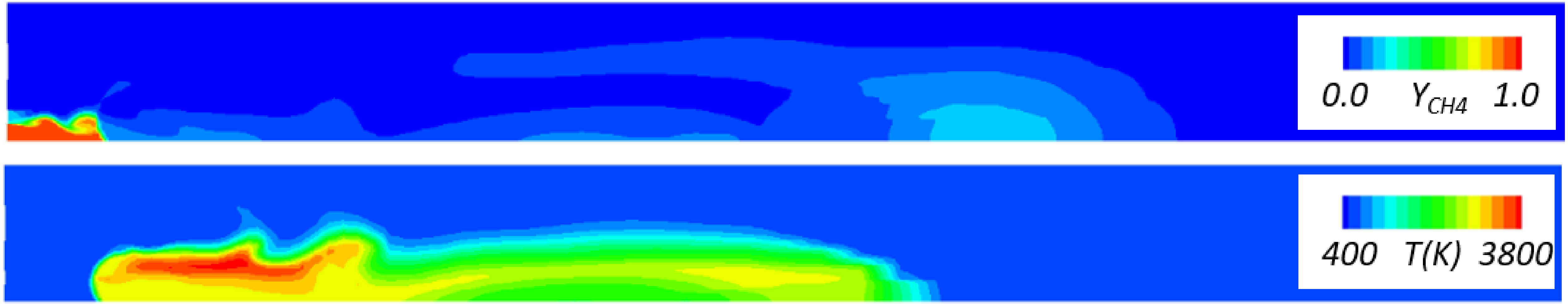
***t = 0.006 sec***



# Task 3.1: Bench-Top Combustor Validation

Case 1 Predictions (oxidizer flow – $Y_{O2}$ *= 1.0)*:

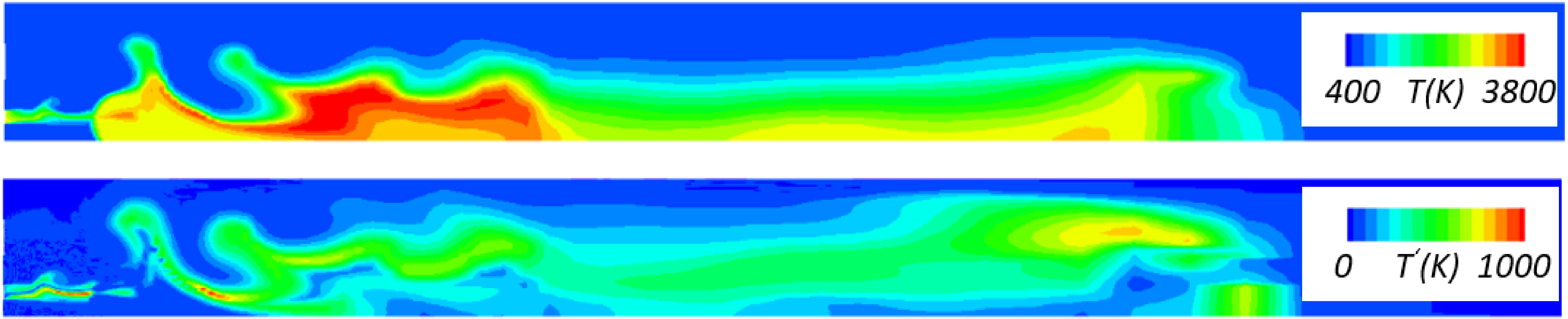
***t = 0.0114 sec***



# Task 3.1: Bench-Top Combustor Validation

Case 1 Predictions (oxidizer flow – $Y_{O2}$ = *1.0)*:

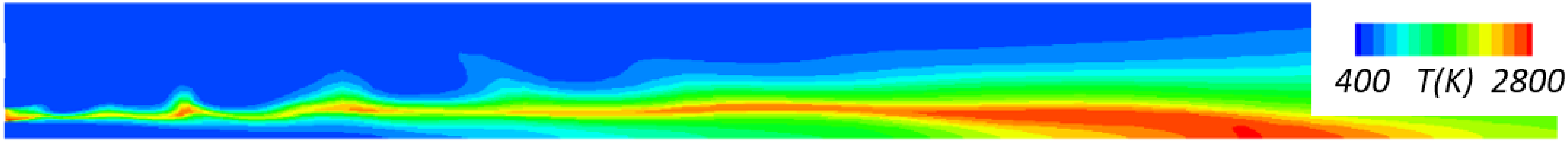
***t = 0.0114 sec***

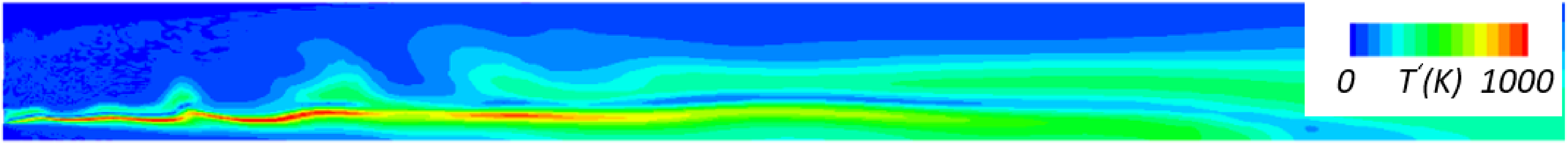


# Task 3.1: Bench-Top Combustor Validation

Case 1 Predictions (oxidizer flow – $Y_{O2}$ = *1.0)*:

***t = 0.031 sec***



# Task 3.1: Bench-Top Combustor Validation

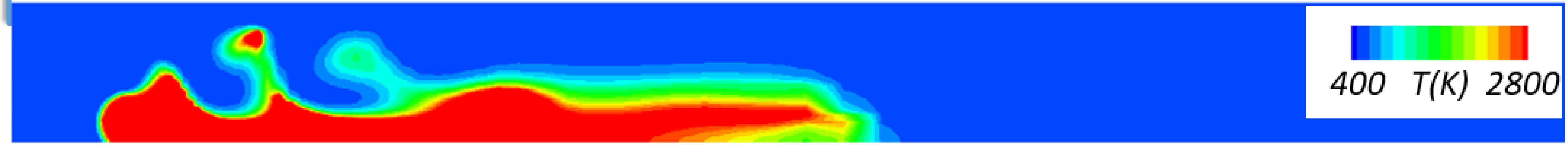
Preliminary Pretest Ignition Results:

| Case no. | $O_2$ Mass Fraction | Ignition/Stabilization Status |
|---|---|---|
| 1 | 1.0 | *anchored flame* |
| 2 | 0.75 | *anchored flame* |
| 3 | 0.625 | *anchored flame* |
| 4 | 0.5 | *flame blow-out* |
| 5 | 0.4 | *flame blow-out* |
| 6 | 0.3 | *flame blow-out* |

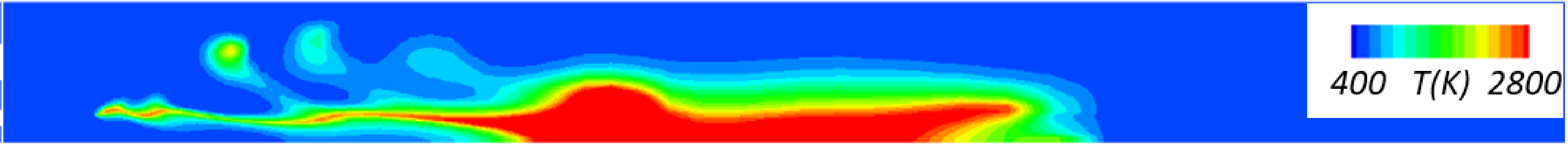
# Task 3.1: Bench-Top Combustor Validation

Case 4 Predictions (oxidizer flow – $Y_{O2}$ = *0.5)*:

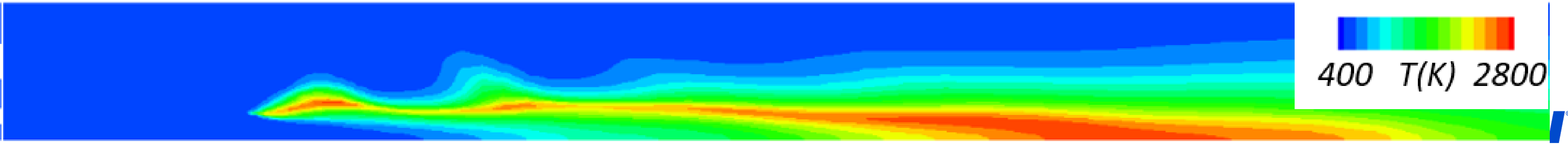
**t = 0.0147 sec**




**t = 0.01641 sec**




**t = 0.0431 sec**



# Current Status

<u>Task 3.1:</u>

- 3-D LES grid generated for the combustor ( ~ 2.3m points)
- Computational efficiency enhancements implemented:
  - Decoupled scalar solution procedure – ~ 50% cpu time reduction
  - Automated parallel ODE chemistry procedure – ~ 50% cpu time reduction
- Waiting on final test conditions from SwRI

<u>Task 3.2 – 3.4:</u>

- 3-D LES grid generated for January 2021 combustor geometry ( ~ 2.3m points)
- Initial testing for preliminary design operating condition
- Waiting on final geometry and test conditions for SwRI

CRAFT Tech

SwRI

# Preparing Project for Next Steps

## Project Market Benefits/Assessment:

- Validated and *tractable* simulation tool developed for $sCO_2$ direct fired combustor design parametric studies
- Ignition data generated for validation of other modeling approaches
- Applicable to rocket engine design and analysis

## Technology-to-Market Path:

- Project technology implemented with CRAFT Tech commercial software products:
  - — CRAFT CFD®, RPFM® and RNFM®
- Validation with data remains to be completed due to testing delays
- New research direction – parameterized chemistry for efficiency enhancement
- Continued collaboration with SwRI critical to the validation effort

# Concluding Remarks

- DQMOM turbulent combustion model provides a *tractable* avenue for accurate design and analysis prediction of $sCO_2$ direct fired applications
- DQMOM formulation:
  - — Provides for a *predicted* scalar PDF within the flow
  - — Applicable to generalized boundary conditions characteristic of real combustors
- Model development efforts "complete":
  - — Refinements may be required as validation effort continues
- Model validation effort slowed by testing delays:
  - — Bench-top combustor – data collection to begin in May
  - — 1 MW combustor – data collection to begin at the end of 2021

CRAFT Tech

SwRI®