Combustion and Fluid Property Experimental Investigation for Improved Design of Supercritical CO_2 Power Cycle Components

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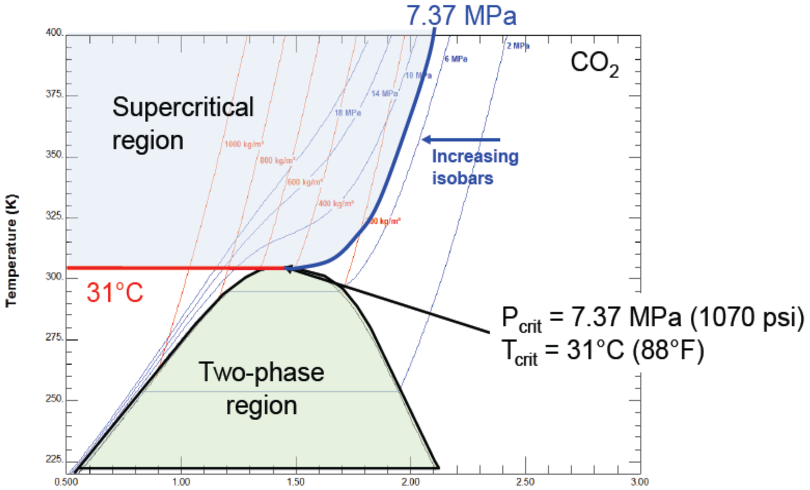
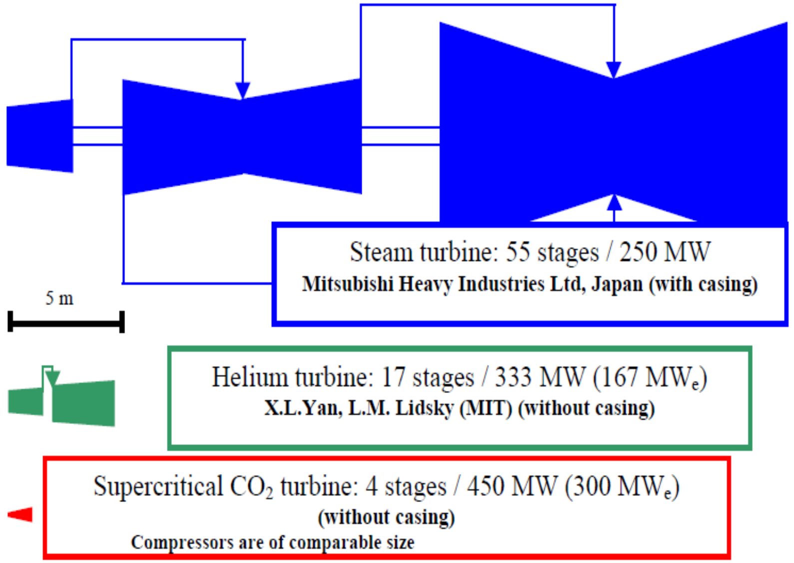
Supercritical CO_2 Cycles

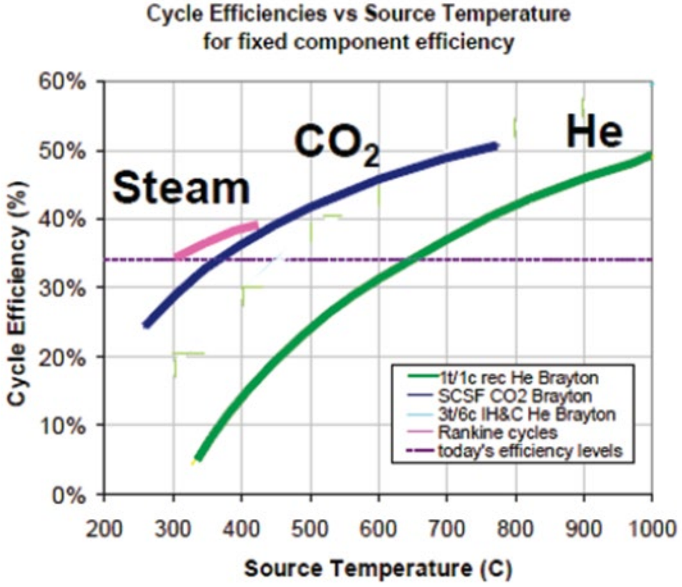


- High-pressure, closed or open Brayton Cycle
- CO_2 is used as the working fluid above the critical point
- High overall cycle efficiency

← Size comparison of various turbines (~ 20 time size reduction compared to steam cycles)

Significant reduction of compressor work due to high fluid density close to the critical point,





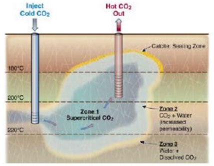
Vaclav Dostal, MIT thesis, 2004

Introduction to sCO_2 Power Cycles

- Possibility of wide application.

Concentrated Solar Power

Fossil Fuel



Geothermal

Nuclear

Ship-board Propulsion

What is challenging ?

"Typical" sCO2 Cycle Conditions

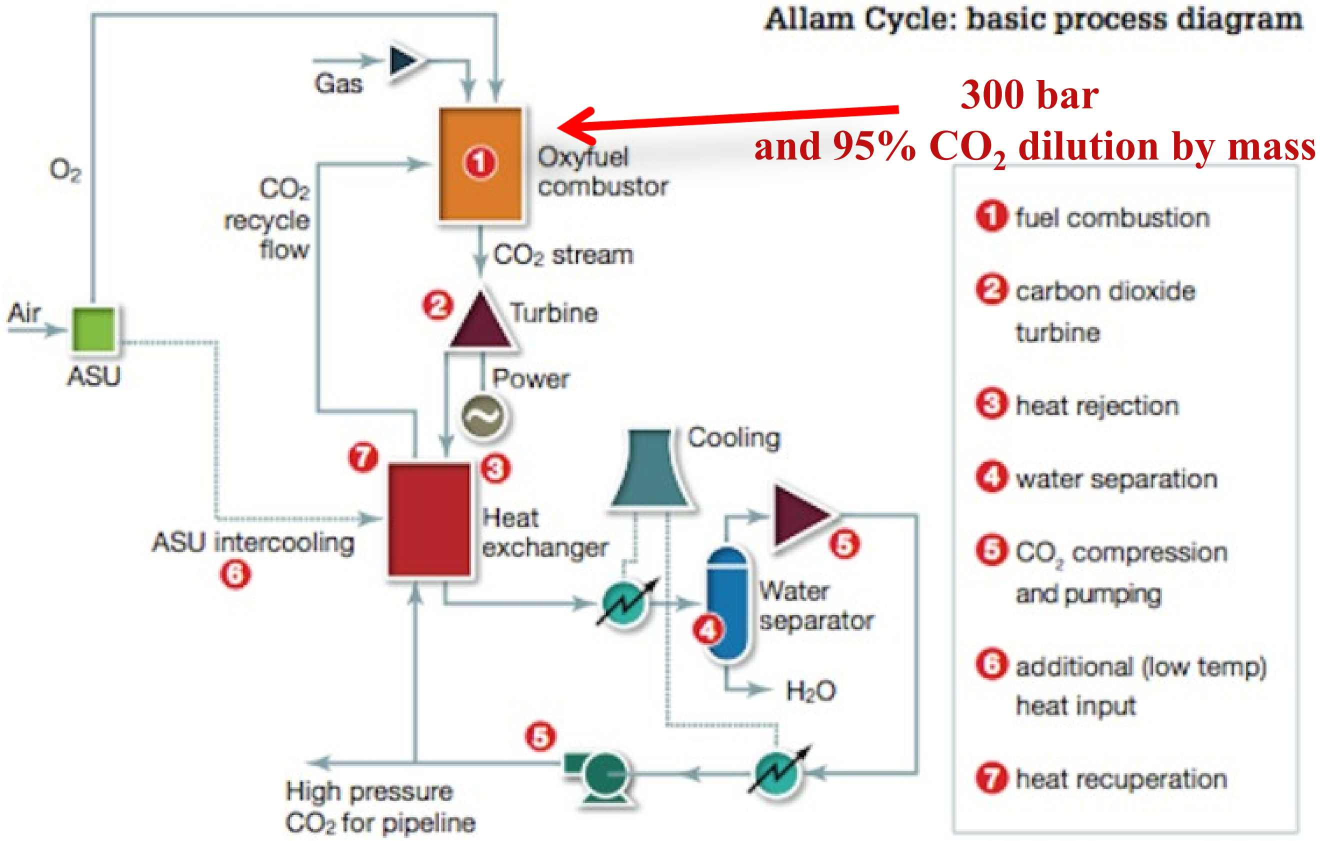
Application	Organization	Motivation	Size [MWe]	Temperature [C]	Pressure [bar]
Nuclear	DOE-NE	Efficiency, Size	300 - 1000	400 - 800	350
Fossil Fuel	DOE-FE	Efficiency, Water Reduction	500 - 1000	550 - 1200	150 - 350
Concentrated Solar Power	DOE-EE	Efficiency, Size, Water Reduction	10 - 100	500 - 800	350
Shipboard Propulsion	DOE-NNSA	Size, Efficiency	10, 100	400 - 800	350
Shipboard House Power	ONR	Size, Efficiency	< 1, 1, 10	230 - 650	150 - 350
Waste Heat Recovery	DOE-EE ONR	Size, Efficiency, Simple Cycles	1, 10, 100	< 230; 230-650	15 - 350
Geothermal	DOE-EERE	Efficiency, Working fluid	1, 10, 50	100 - 300	150

Source: Pictures are taken from SWRI tutorials

- At these high operating pressures, simulation tools are very important because the experiments at these operating conditions are expensive, time consuming and dangerous.

Direct-fired Cycle: The Allam Cycle

- It is the direct-fired sCO_2 cycle.



Source: https://www.modernpowersystems.com/features/featurebreaking-ground-for-a-groundbreaker-the-first-allam-cycle-power-plant-4893271/featurebreaking-ground-for-a-groundbreaker-the-first-allam-cycle-power-plant-4893271-477348.html

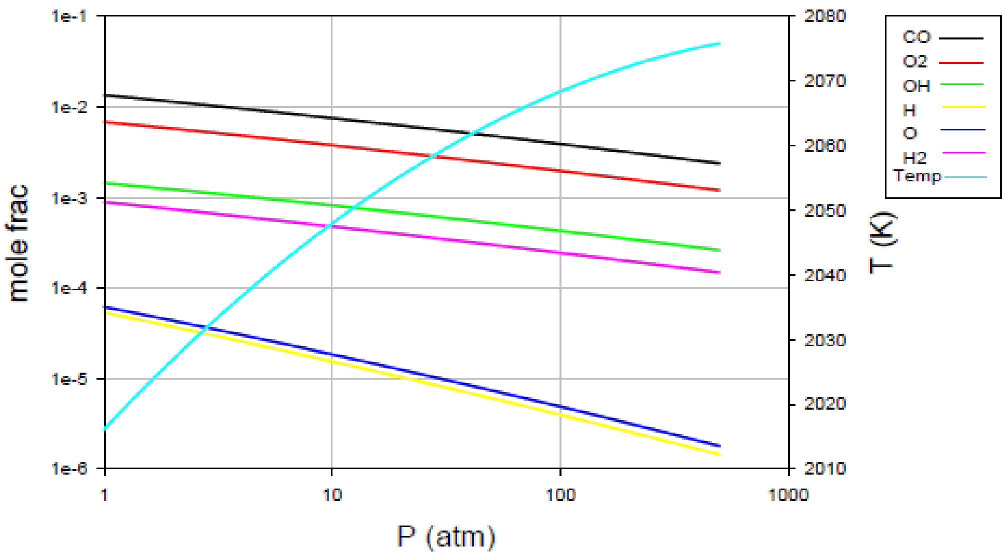
NET Power's Allam Cycle Demo Plant

Source: https://www.prnewswire.com/news-releases/net-power-achieves-major-milestone-for-carbon-capture-with-demonstration-plant-first-fire-300656175.html

- First successful test fire → May 2018
- Target for 300 MW commercial plant → 2021

Knowledge gaps before we started

- <u>Existing</u> state-of-the-art, such as GRI-3.0 Mechanism, has only been validated for pressures up to 10 atm
- Mechanisms have not been developed for CO_2 diluted mixtures
- Updated/new mechanism will allow for accurate combustor modeling with multi-step combustion using a validated mechanism
- CFD combustion models need to consider non-ideal effects
- Thermodynamics and kinetics are unknown!!
- Fundamental work can shed light into this challenge



Effects of Increasing Pressure. Equilibrium calculation for $CH_4/O_2/CO_2$ at ϕ = 1. Figure adapted from Strakey, 2014, sCO2 symposium

Strategy successfully applied to Direct-fired Supercritical CO_2 Cycles: 300bar pressure CH_4/O_2, natural gas/O_2 mixtures

UTSR Project Impact:

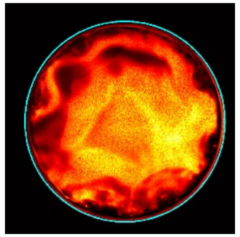
- **Understanding the reacting processes at 300bar require new facilities**
- **Vasu Lab published 26 journal papers**
- **> 40 conference papers** at ASME Turbo Expo, sCO2 symposium, AIAA Meetings, Combustion Institute Meetings
- **Prof. Vasu provided Tutorials at Turbo Expo, CelarWater Celan Energy Conference**

Burn Fuels in CO_2 Environment

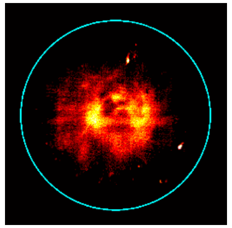
Fuel + O2 → CO_2 + H_2O

300 bar pressure
(similar to newer methane rocket engines SpaceX, Blue Origin)

Everything we have done so far is the first in the world! Thanks to the UTSR program

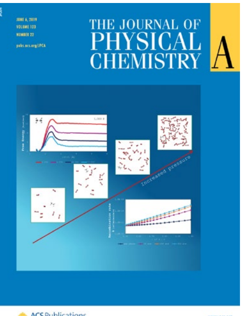


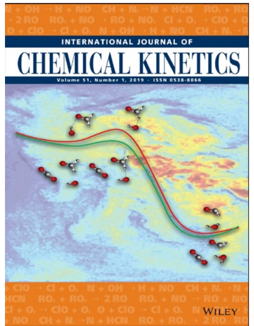
CH_4 without CO_2



CH_4 With CO_2

2 Cover Page Journal Articles





Vasu Lab helped NET Power's Allam Cycle Demo Plant

Industry/Government Sponsors and Collaborators

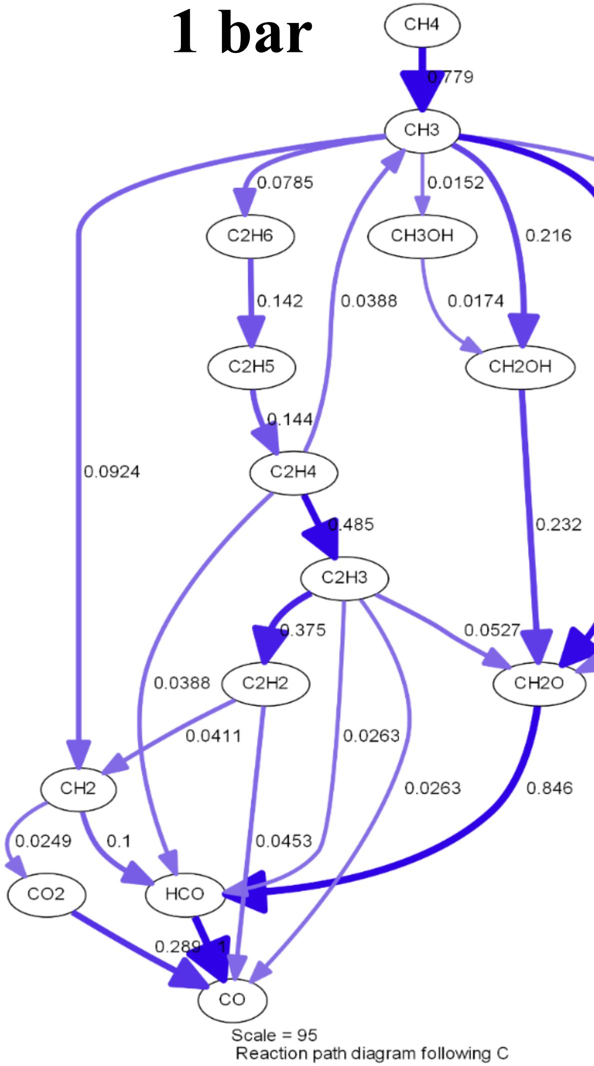
gti, GE, Hanwha, Office of Naval Research Science & Technology, KEPCO KEPRI, NETPOWER, United States Department of Energy, SwRI, 8 RIVERS

UCF

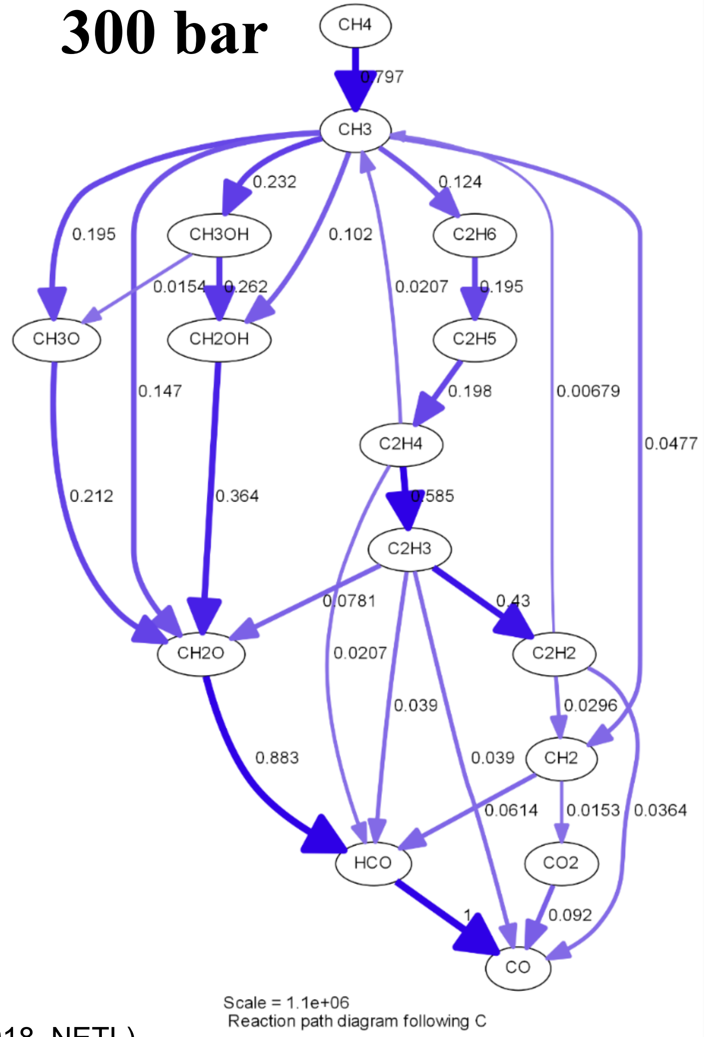
Selected Examples from Our Work→

Combustion chemistry/kinetics are different at high pressure

1 bar

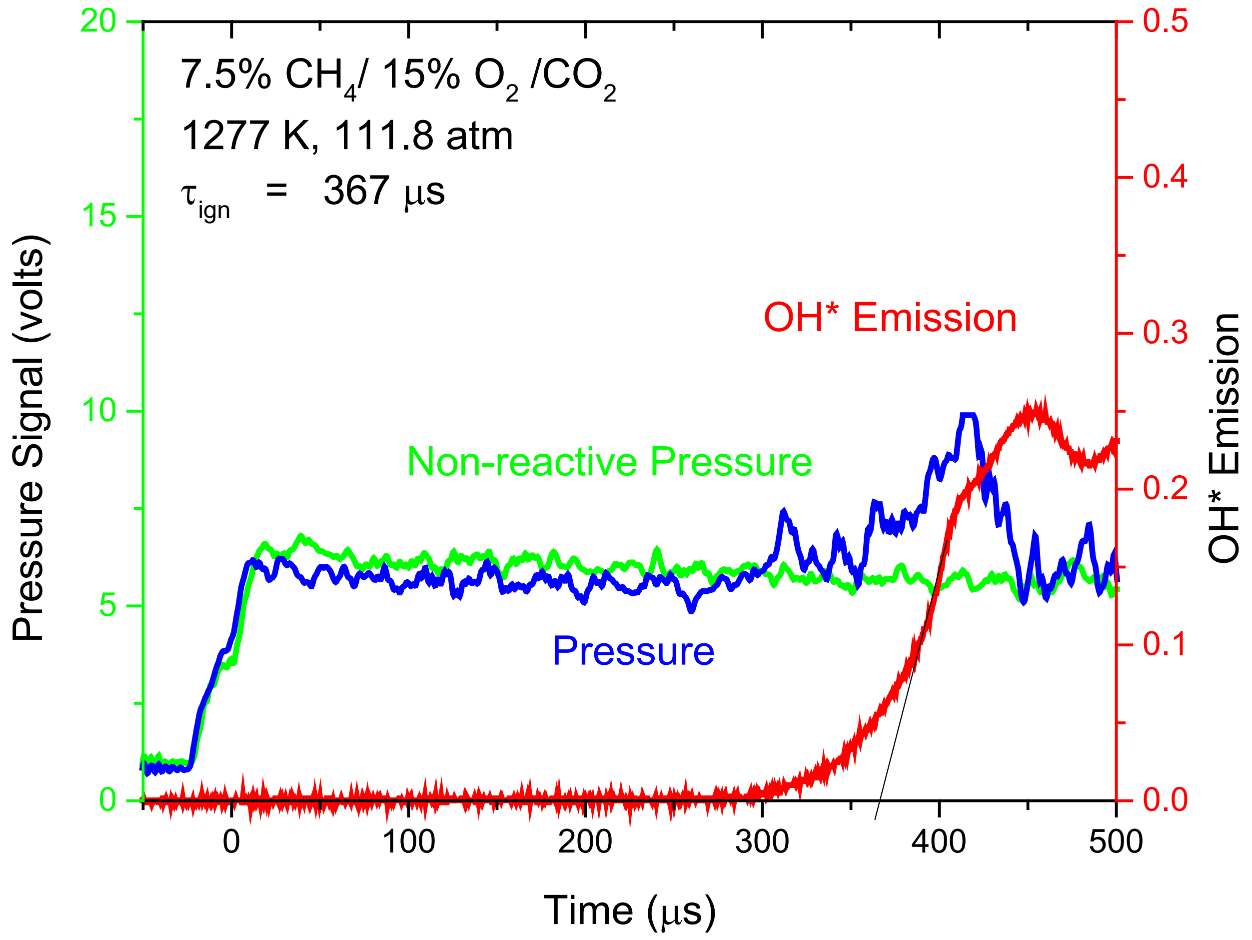


300 bar



(Strakey, SCO2 symposium 2018, NETL)

Ignition Results in CH_4 Under SCO_2 Conditions: 77.5% CO_2 addition



With CO_2 addition there is some pressure rise (7.5% fuel) after ignition→ but not as bad as the ones without CO_2

Chemical Mechanism Development Summary

- Combustion kinetics model refinement/development
- Existing kinetic models are only valid at low pressures < 50 atm
- We used multi-scale simulations to extend their validity to mixtures up to 300 bar by:

1. Quantum Mechanic simulations of the activation enthalpies in gas vs. CO_2 environment
2. Molecular Dynamic simulations of reaction processes

Molecular Dynamic Study: $CO+OH \rightarrow CO_2+H$ (results)

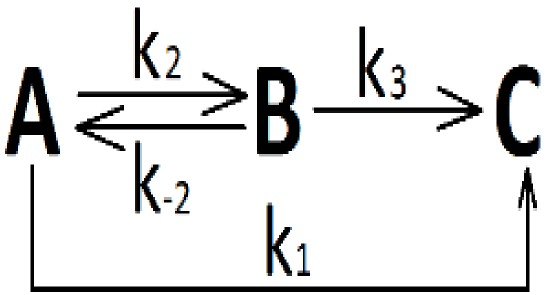
OVERALL REACTION: $\cdot OH + CO \rightarrow CO_2 + H\cdot$ (R1, k_1)

Actually goes through these 3 reactions including HOCO intermediate

$\cdot OH + CO \rightarrow HOCO\cdot$ (R2, k_2)

$HOCO\cdot \rightarrow \cdot OH + CO$ (R2r, k_{-2})

$HOCO\cdot \rightarrow CO_2 + H\cdot$ (R3, k_3)



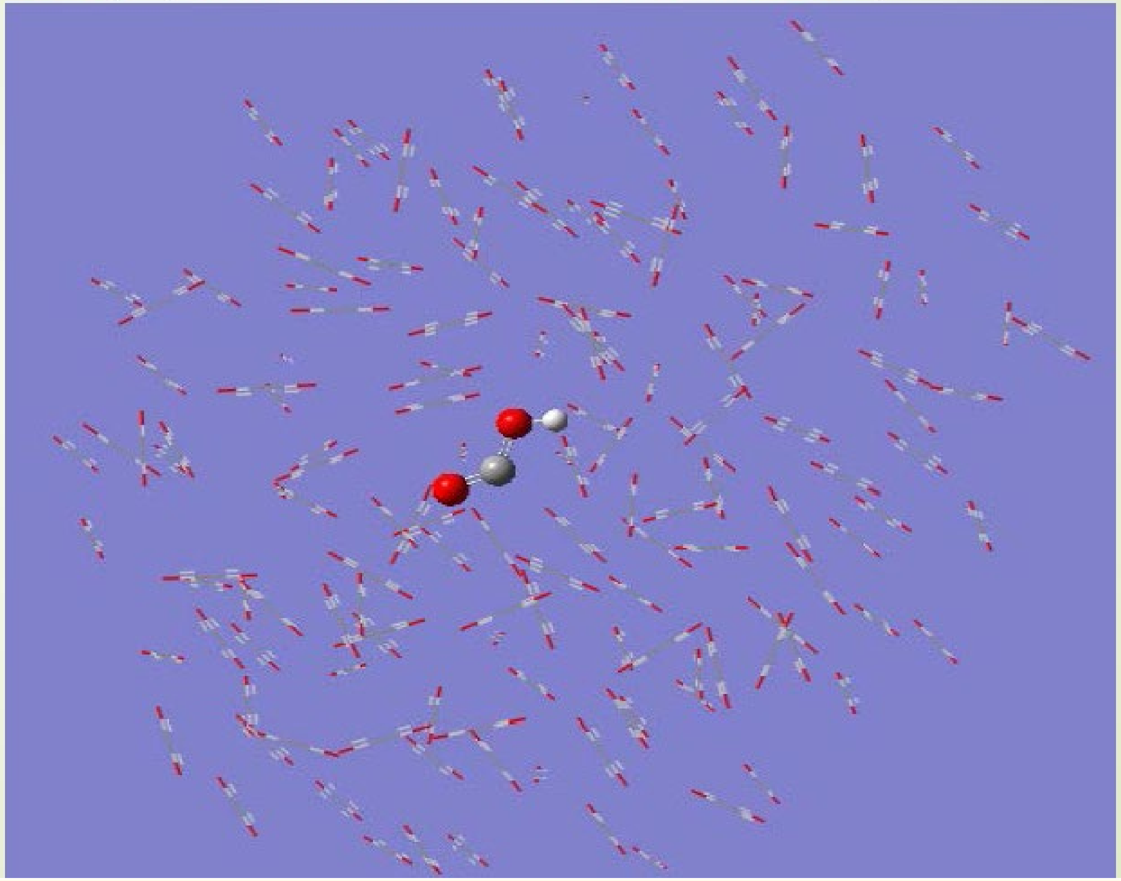
$$k_1 = \frac{k_2 k_3}{k_{-2} + k_3}$$

Molecular Dynamic Study: $CO+OH \rightarrow CO_2+H$ (results)

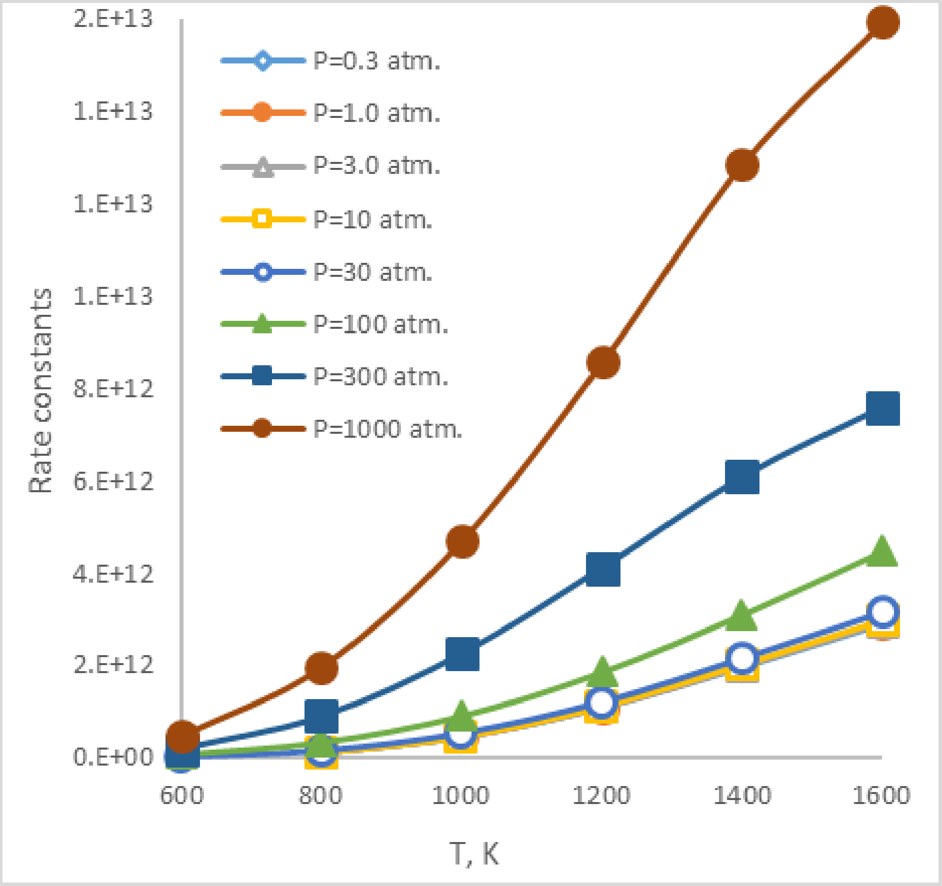
QM / MM model was used.

MM layer look like small tubes, QM layer – particle with balls

<u>QM: MNDO</u>; <u>MM: force field CHARMM27</u>



Molecular Dynamic Study: CO+OH→CO_2+H (results)

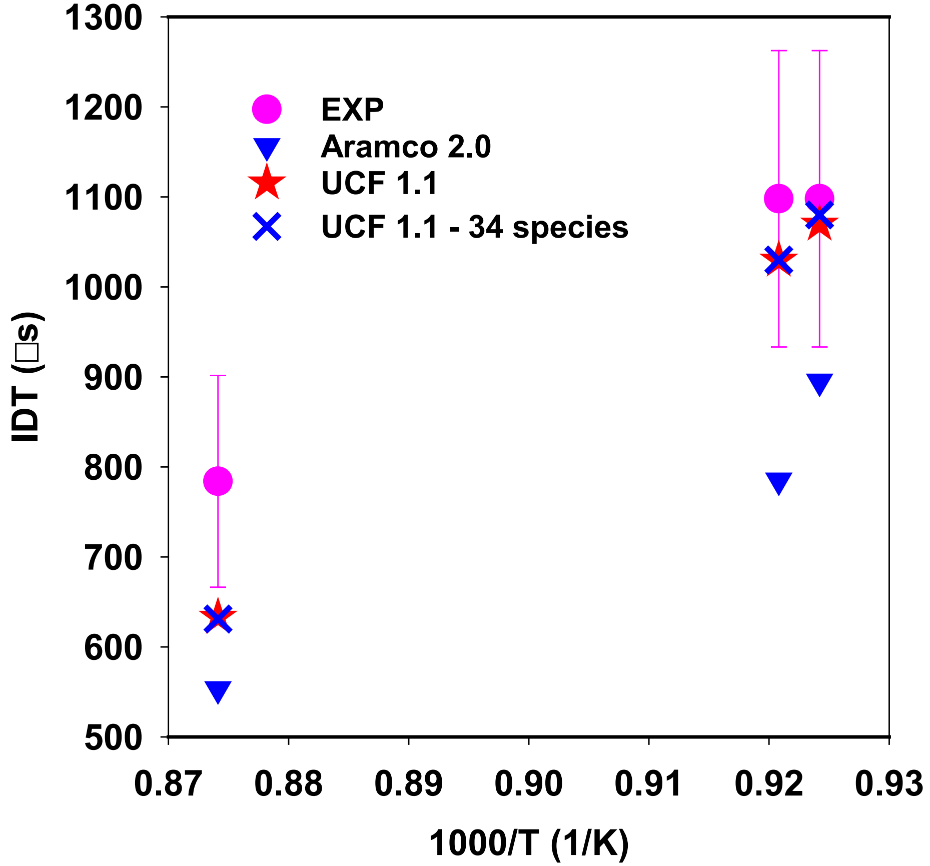


- CO_2 molecules are among the most efficient to accelerate heat release reaction with pressure
- mixed quantum mechanics/molecular mechanics (QM/MM) theory level and molecular dynamics (MD) approach

UCF's SCO_2 Combustion Mechanism Performance

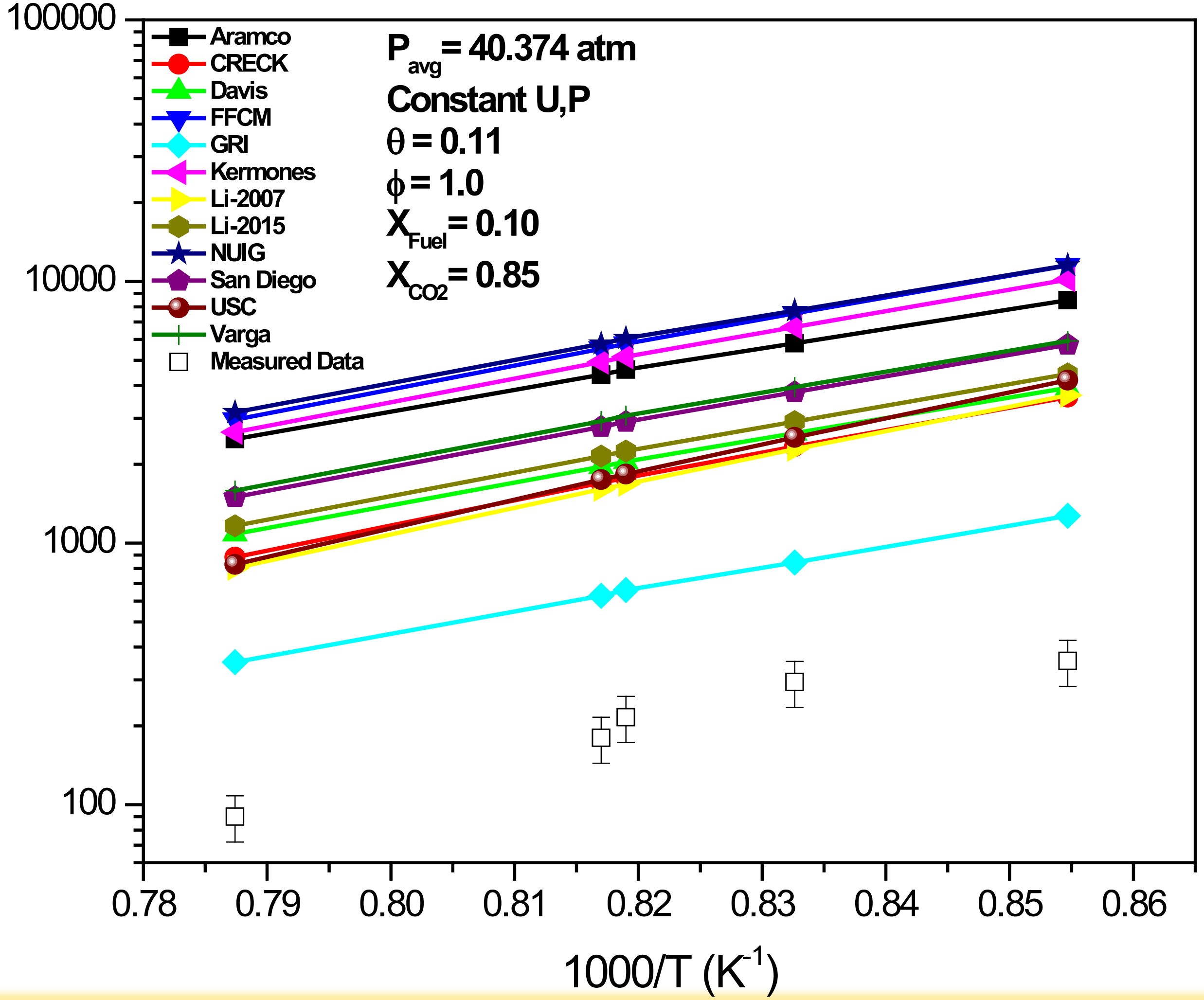
Mixture: 3.91% CH4, 9.92% O2, 86.77% CO2
Pressure: ~300 bar

- UCF 1.1 is performing better for this lean mixture compared to Aramco 2.0. Performance is significantly improved.
- Average deviation between UCF 1.1 detailed mechanism and 34-species mechanism is 0.25%.



Syngas /O_2/CO_2 Ignition Delay Time Measurements: Comparisons with Modeling

CO_2=85%



12 Literature kinetic mechanisms tested

All mechanisms overpredict data at high pressure !

Performance of sCO_2 Mechanism Developed by UCF: Summary

High pressure Ignition Delay Times in Methane:

- The UCF 1.1 mechanism

→ better than **Aramco 2.0**

→ has important reaction rates calculated by **molecular level simulations**.

UCF's HiPER-STAR Facility (for Allam cycle)

High Pressure Extended Range Shock Tube for Advanced Research

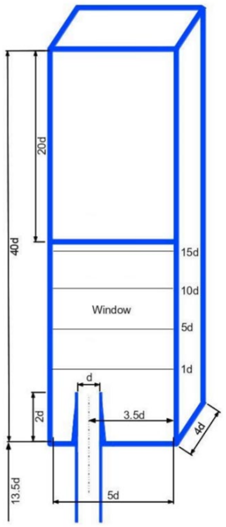
Capabilities

- High-Pressure Combustion and Autoignition Measurements of Fuels including SCO_2 conditions for Allam Cycle- Both syngas and natural gas.
- Toxic impurities NOx, SOx, H_2S,
- Hydrogen or ammonia combustion with impurities
- Coal-derived fuels

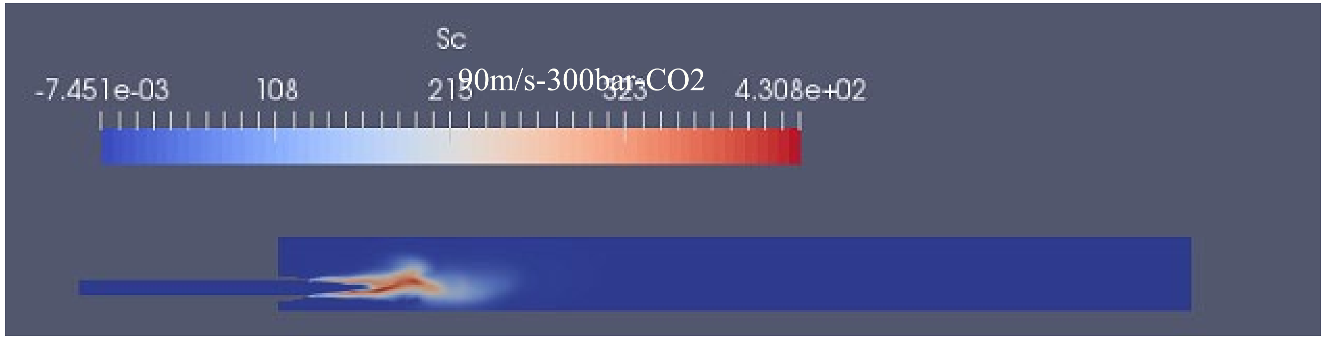
Up to 1000 bar sCO_2 shock tube with capabilities to include natural gas and real syngas and impurities (e.g., Nitrogen oxides)

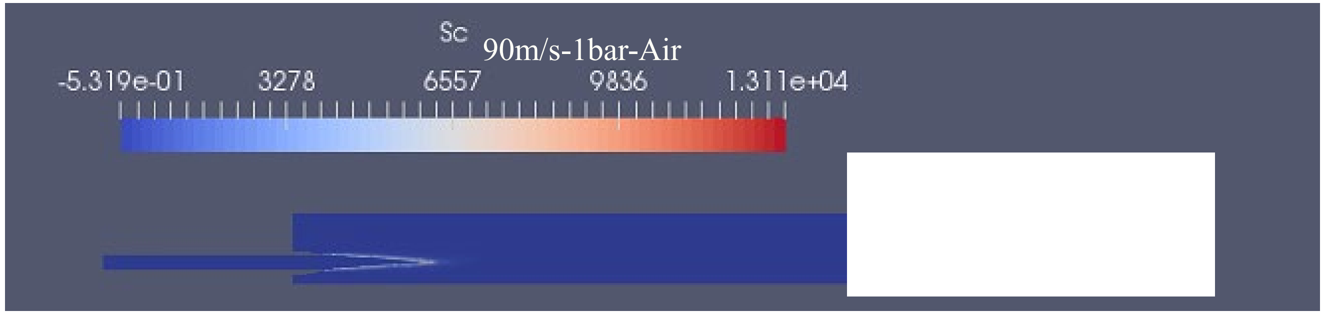
Unique facility in the world where all types of syngas mixtures can be tested for Allam cycle conditions

SCO_2 combustor CFD: also developed industry tools for design and analysis



Simulated DLR-Jet

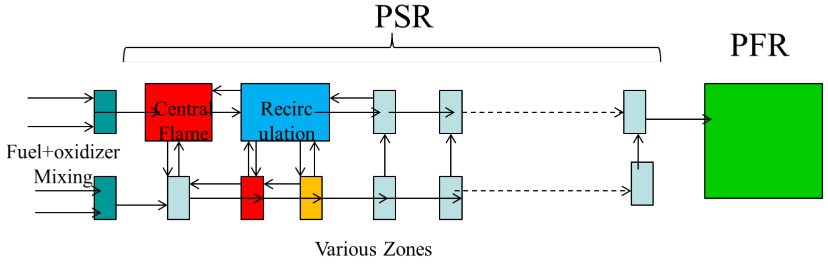




- CFD Simulation is performed with the premixed CMC in the OpenFOAM RANS CFD code.
- The current PCMC-OpenFOAM model is capable of using large mechanisms. The current simulation uses 493 species and 2,714 reactions.
- Stoichiometric CH4/O2 with 95% by mass CO2.

Reactor network modeling

- Therefore, this work mainly focuses on reducing the domain of design considerations for sCO_2 combustor development with simple 0-D and 1-D modeling.
- Extensively used by the gas turbine community



Ongoing Work→ (Some of the materials are retracted as they are not yet publicly releasable)

Need for Transport Data Base

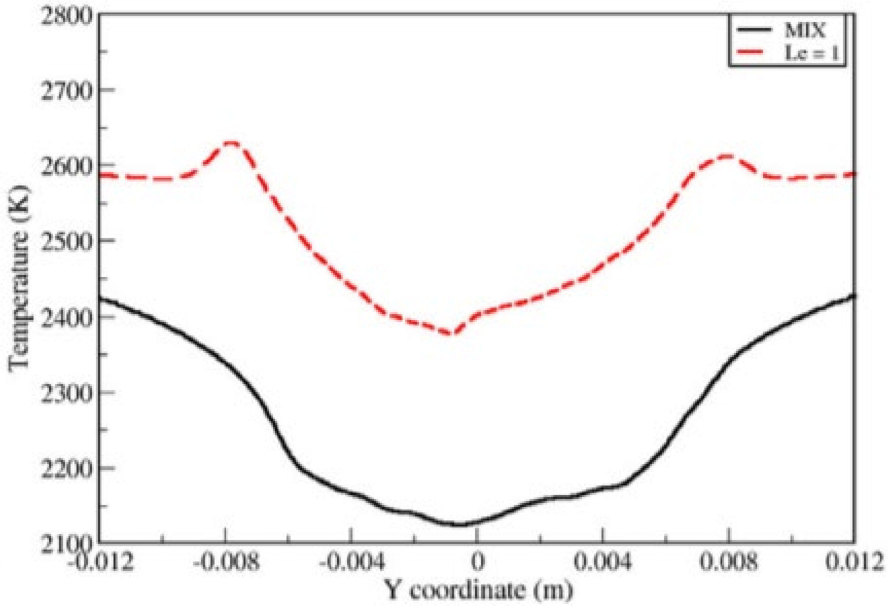


Figure 1: temperature profiles predicted by LESLIE with mixture-averaged diffusion and with constant Lewis number = 1 at different time instants (Masi et al., 2013)

Masi, E., Bellan, J., Harstad, K. G., and Okong'o, N. A., 2013, "Multi-species turbulent mixing under supercritical-pressure conditions: modelling, direct numerical simulation and analysis revealing species spinodal decomposition," Journal of Fluid Mechanics, 721, pp. 578-626.

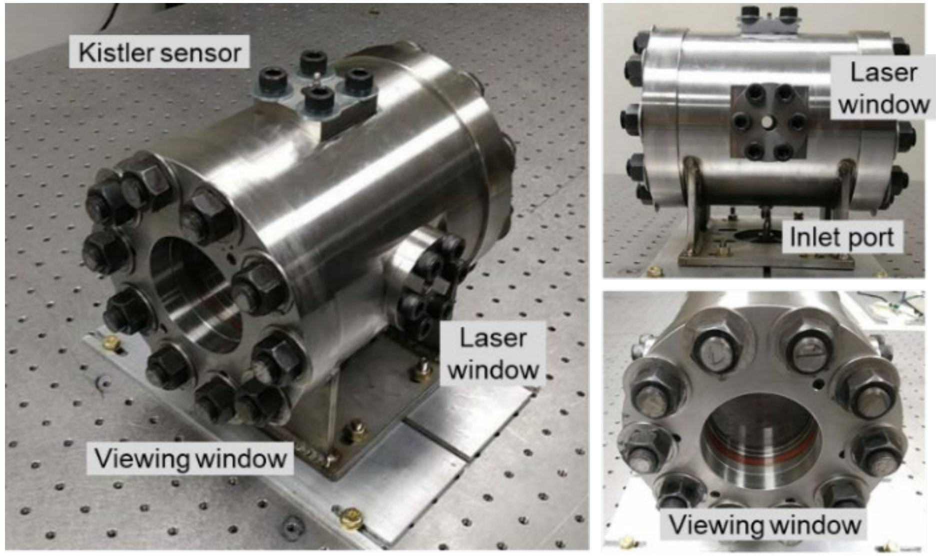
MD Simulations for Transport Properties

- Molecular dynamics simulations are performed by open-source LAMMPS (large-scale atomic/molecular massively parallel simulator) package.

- Some preliminary result for sCO_2 diffusion

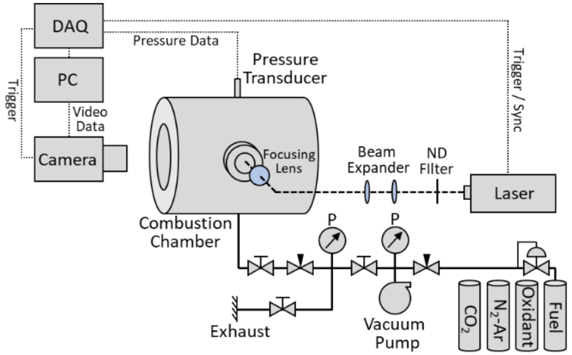
		32 CO_2			
NPT	<E>	<T>	<V>	<P>	D
5 ns	kcal	Kelvin	$Å^3$	atm	10^{-8} m^2/s
1,000 K	-1888.65	999.266	20145.8	99.7942	24.2
1,000 K	-1863.83	1001.17	14498.9	206.885	17.6
1,000 K	-1846.55	998.28	12044.1	298.9	14.3

sCO2 Flame Test Rig -670bar (ignition experiments, flame development, flame speed, flow visualization)

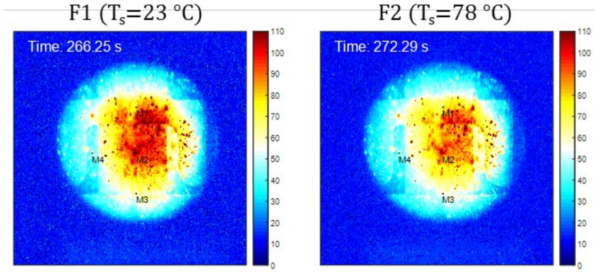


Combustion chamber without heating jacket and Schematic of combustion test rig

Techniques to be used are PLIF, Shadow Imaging



First measurements of Temperature Distribution using Laser-Induced Fluorescence (LIF) in SCO_2 flows conducted near 80bar, *Suhyeon Park, Subith Vasu, et al. Optics Letters*



Students and postdocs

Graduate Students

1) Owen Pryor
(Ph.D. 2018, now at Southwest Research Inst. -SwRI)

2) Raghu Kancherla
Ph.D. 2019, UCF postdoc

3) Samuel Barak
Ph.D. 2019, UCF, Siemens, Boeing

Post docs

1) Dr. Chun-Hung Wang, Northland

2) Dr. Sergey Panteleev
(Lead Engineer, Center of Metrology of Nizhny Novgorod, Russia))

3) Dr. Batikan Koroglu
(Research staff, LLNL)

Undergraduate Students

1) Elizabeth Wait
(now at Los Alamos)

5 journal papers as an undergraduate

- Acknowledgement: DE-FE0025260
- Dr. Matt Adams as program manager
- Dr. Seth Lawson (previous program manager
- Rich Dennis, Rin Burke

Vasu Lab