Challenges, Fundamentals, and Recent Progress in Oxy-Combustion Allam Cycles

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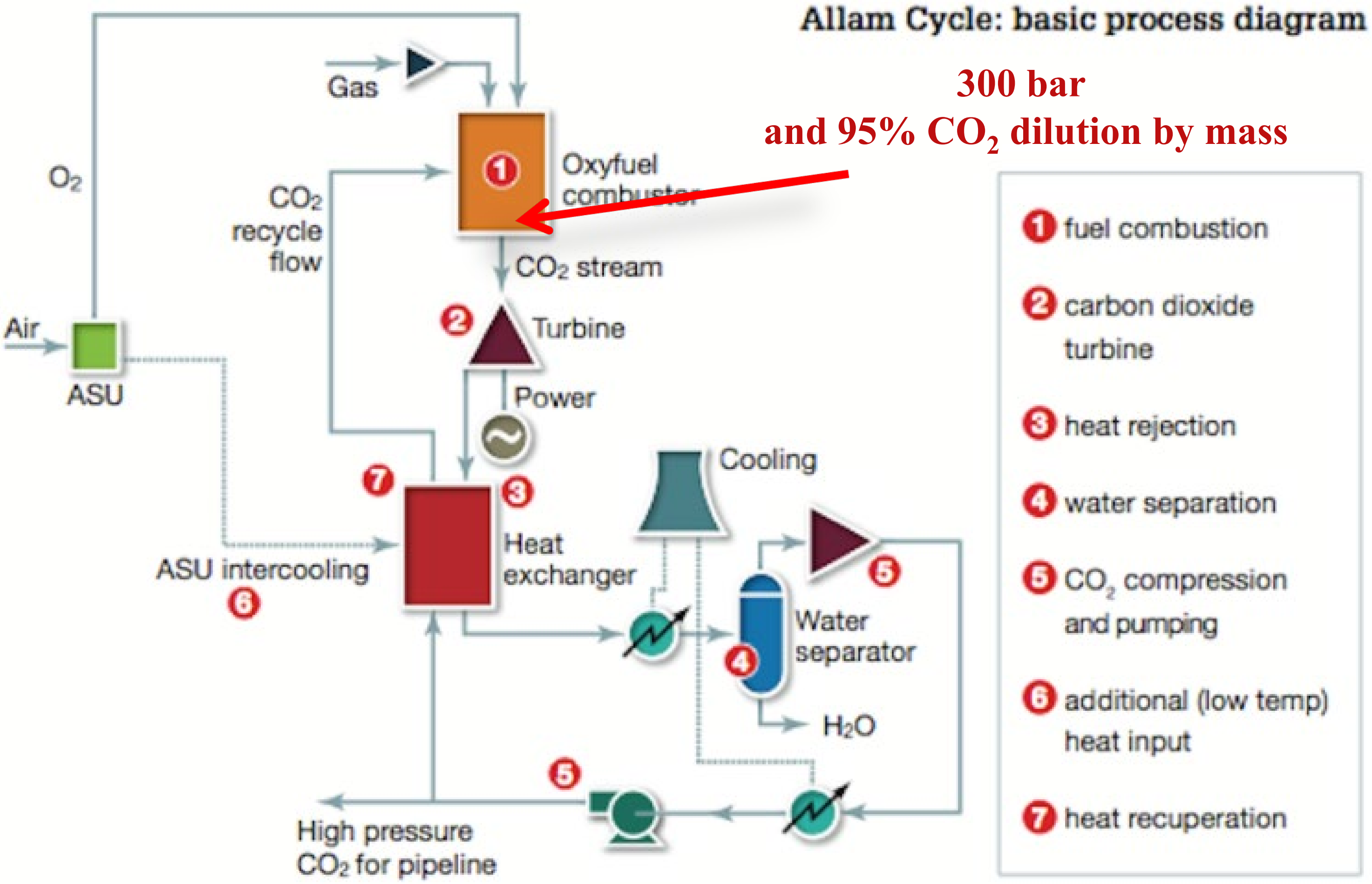
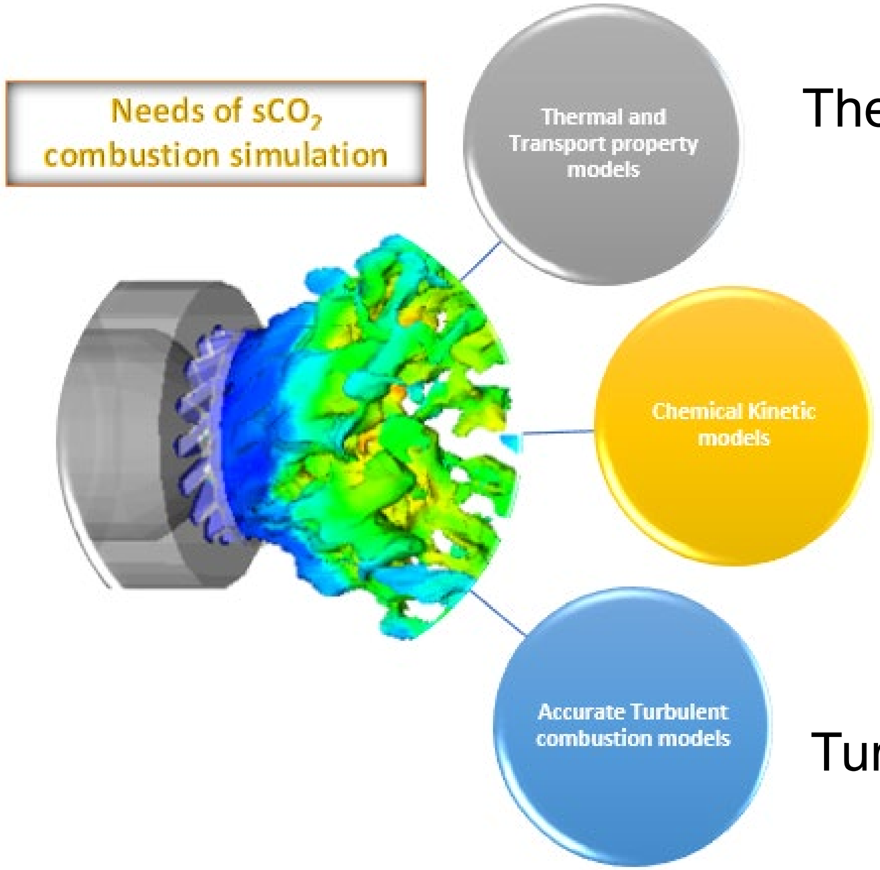
Direct-fired natural gas Cycle: The Allam Cycle



300 bar and 95% CO_2 dilution by mass

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

Combustion Process



Thermal and transport models

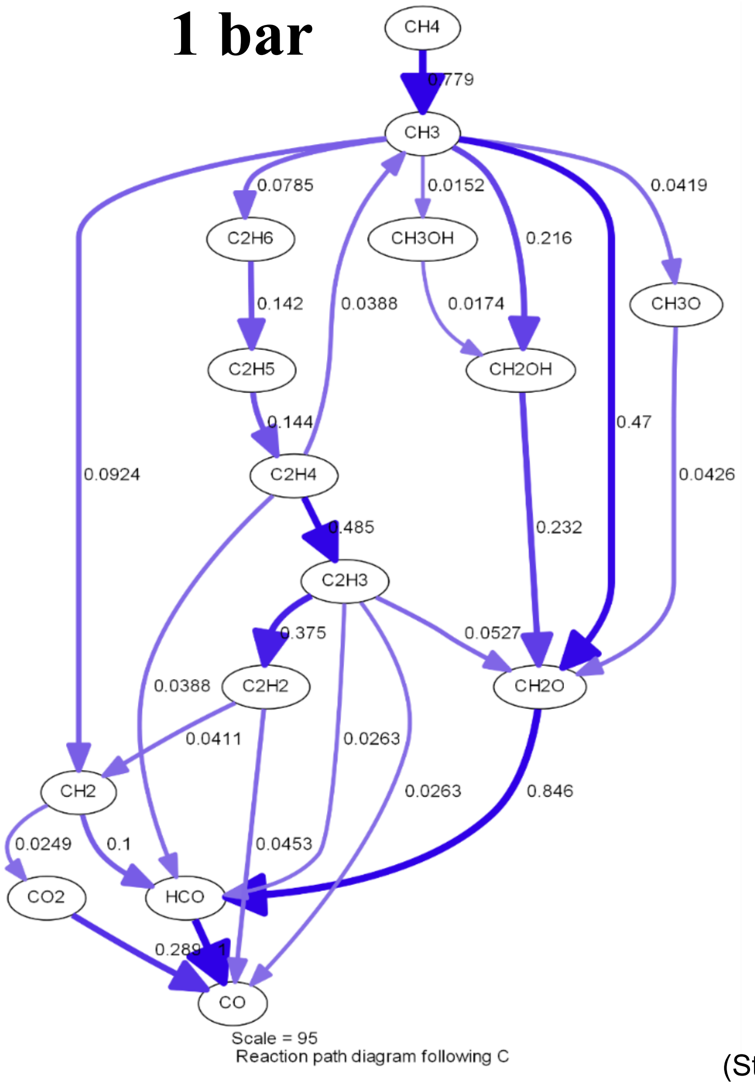
Chemical kinetic models

Turbulent combustion models

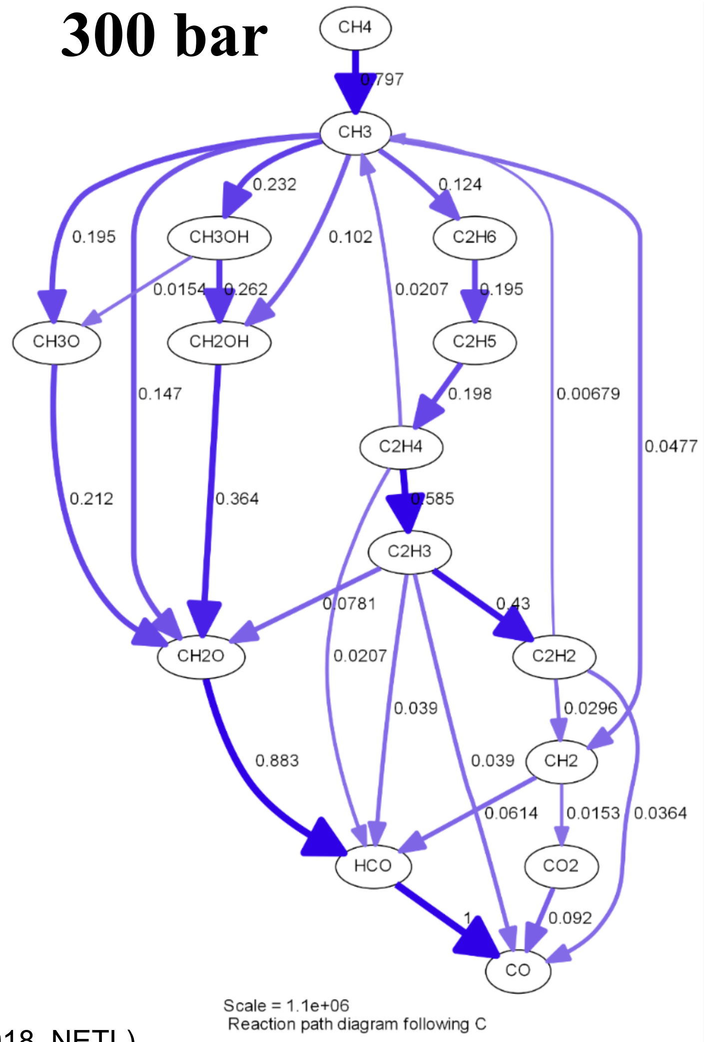
- List can extend to heat loss, soot, acoustic models etc. as this technology advances.

Combustion pathways are different at high pressure

1 bar

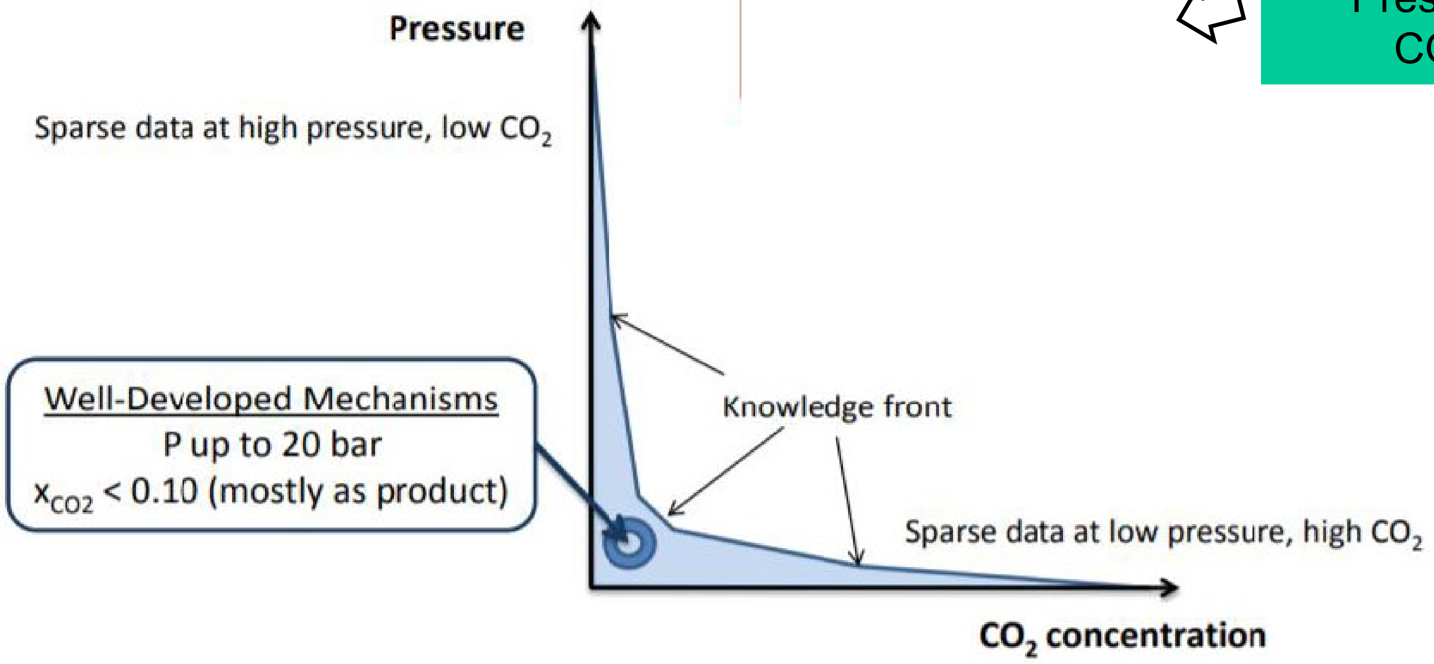


300 bar



(Strakey, SCO2 symposium 2018, NETL)

Knowledge Base of sCO_2 Combustion Properties

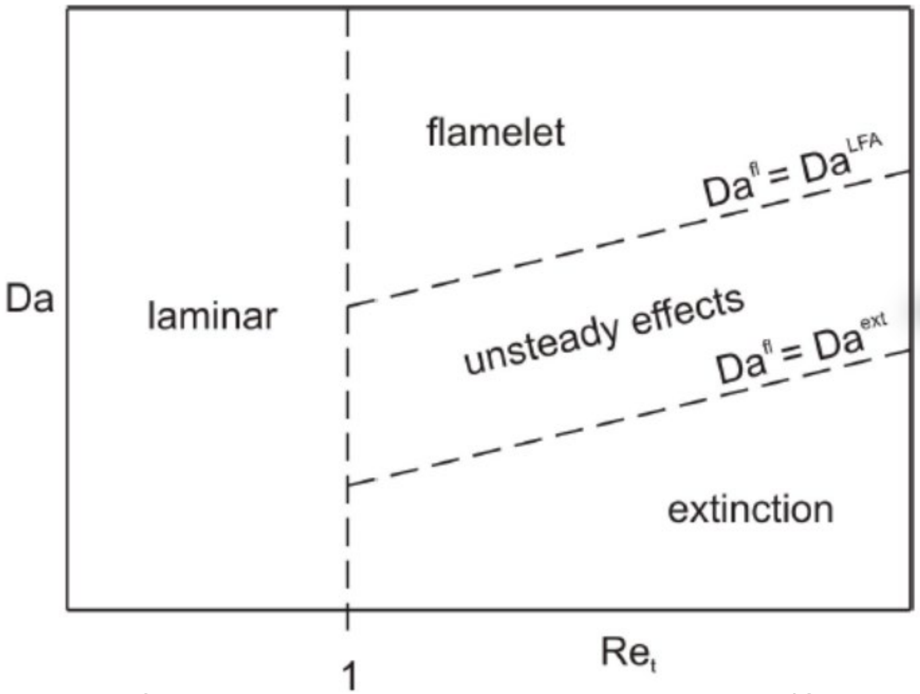


Source: Jacob Delimont et al. (2018)

Direct-fired Cycles Needs
Pressure up to 300bar
CO2 fraction 96%

- Lot of progress has been made in this area from last 5 years.

Knowledge Base of Turbulent Combustion Models



Regime diagram for non-premixed turbulent combustion (Source: Zhang et al. 2016)

Choosing an appropriate model is very crucial based on the sCO_2 combustion regime.

- Numerous models are available to simulate the combustion in each regime. However, the regime of sCO_2 combustion is unknown yet.

Selected Examples from Our Work→

UCF's 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)

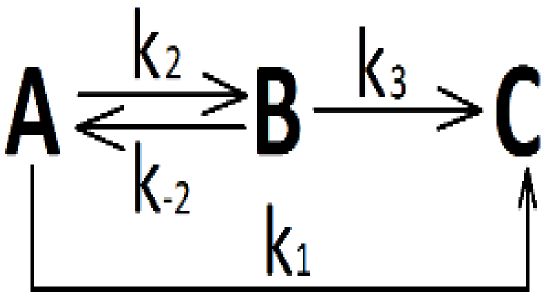
OVERALL REACTION: $\cdot OH + CO \rightarrow CO_2 + H\cdot$ (R1, k_1)

Actually goes through these 3 reactions including HOCO intermediate

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

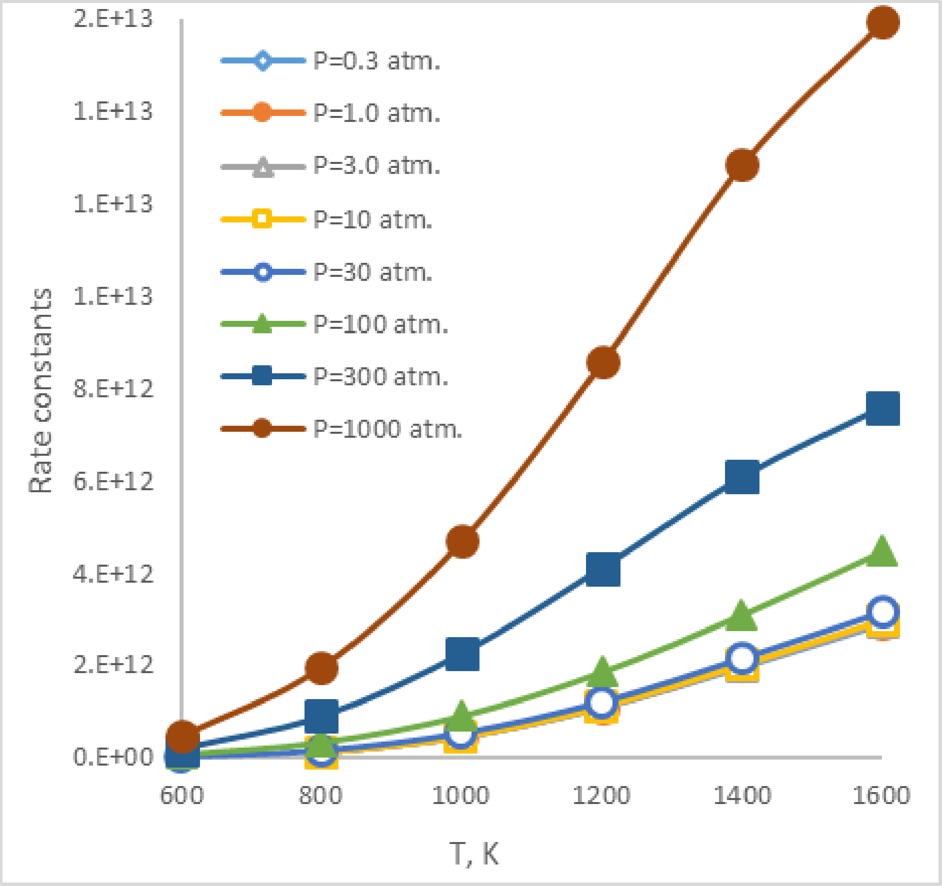
$HOCO\cdot \rightarrow \cdot OH + CO$ (R2r, k_{-2})

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



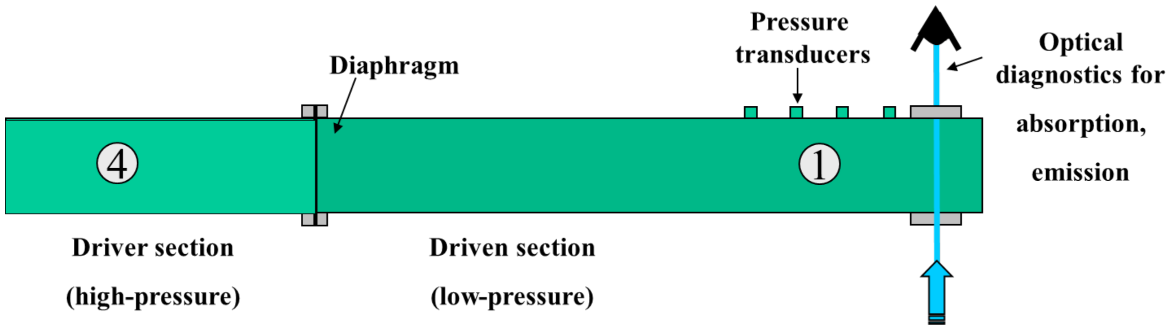
$$k_1 = \frac{k_2 k_3}{k_{-2} + k_3}$$

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



- 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

Shock Tubes for SCO_2 Combustion Experiments



- Shock tubes are ideal for studying combustion, ignition, injection, and flames
- Step change in T, P and well-defined time zero
- Simple fuel loading
- Accurate mixtures and pre-shock conditions
- Wide ranges of pressure (0.01-1000 atm) and temperature (600-4000K)

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

High Pressure Extended Range Shock Tube for Advanced Research

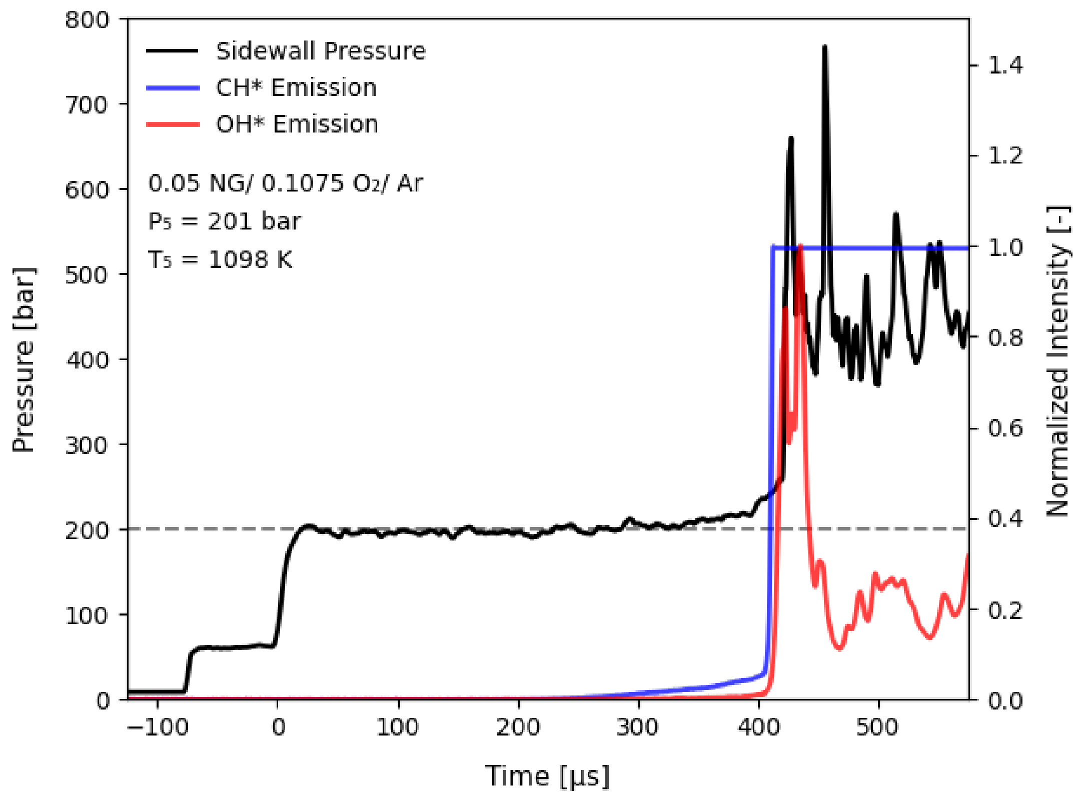
Capabilities

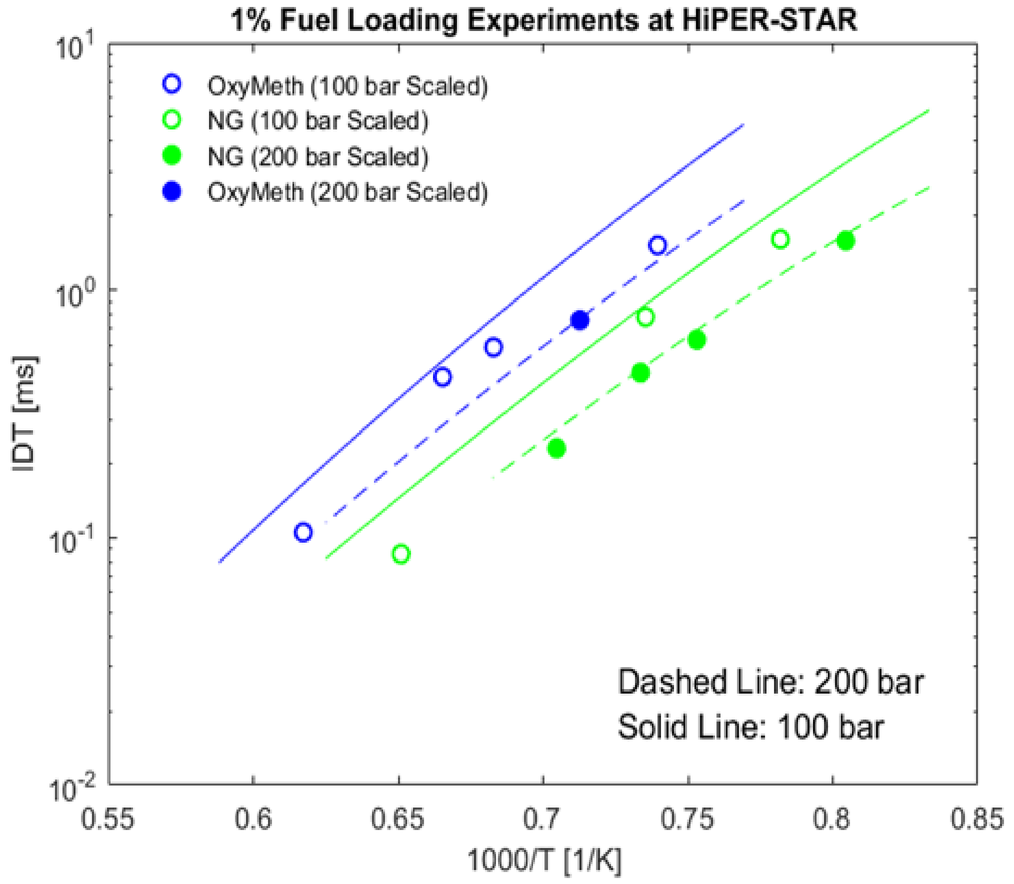
- High-Pressure Combustion and Autoignition Measurements of Fuels including SCO_2 conditions for Allam Cycle- Both syngas and natural gas.
- Toxic impurities NOx, SOx, H_2S,
- Hydrogen or ammonia combustion with impurities
- Coal-derived fuels

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

Auto-Ignition Delay Time Result: CH_4 and Natural Gas Under SCO_2 Conditions



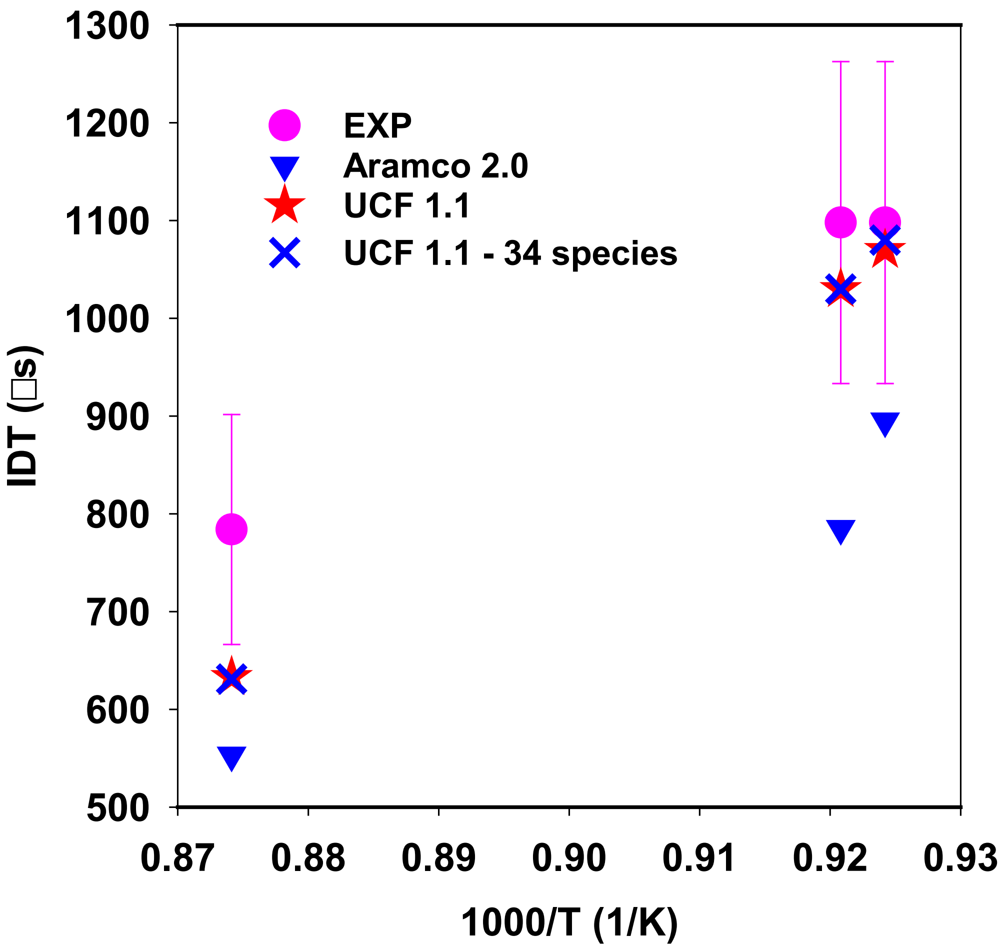


UCF's SCO_2 Combustion Mechanism Performance

- The UCF 1.1 mechanism

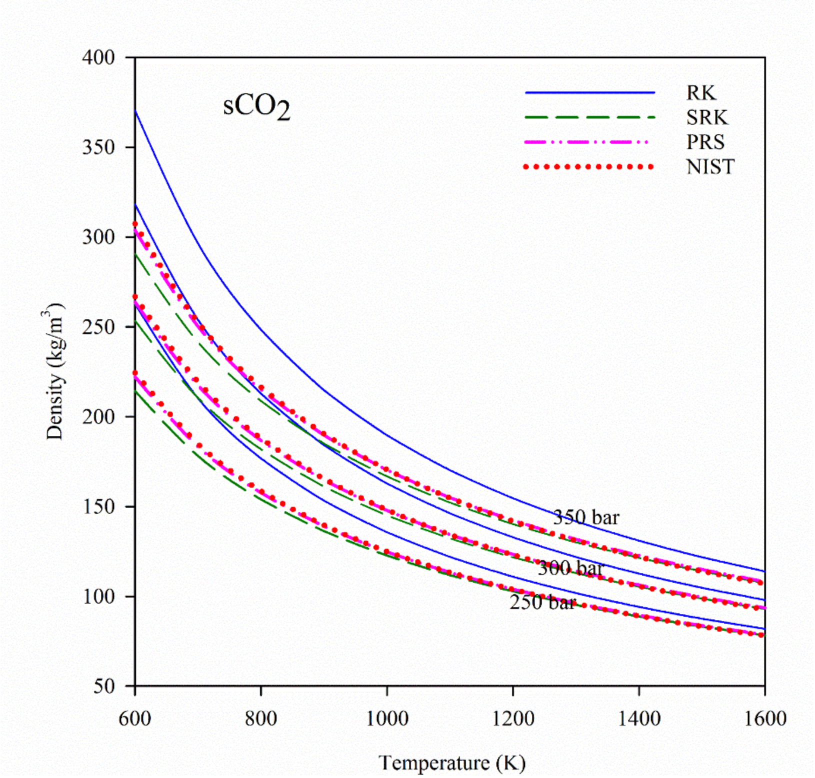
→ has important reaction rates calculated by **molecular level simulations**.

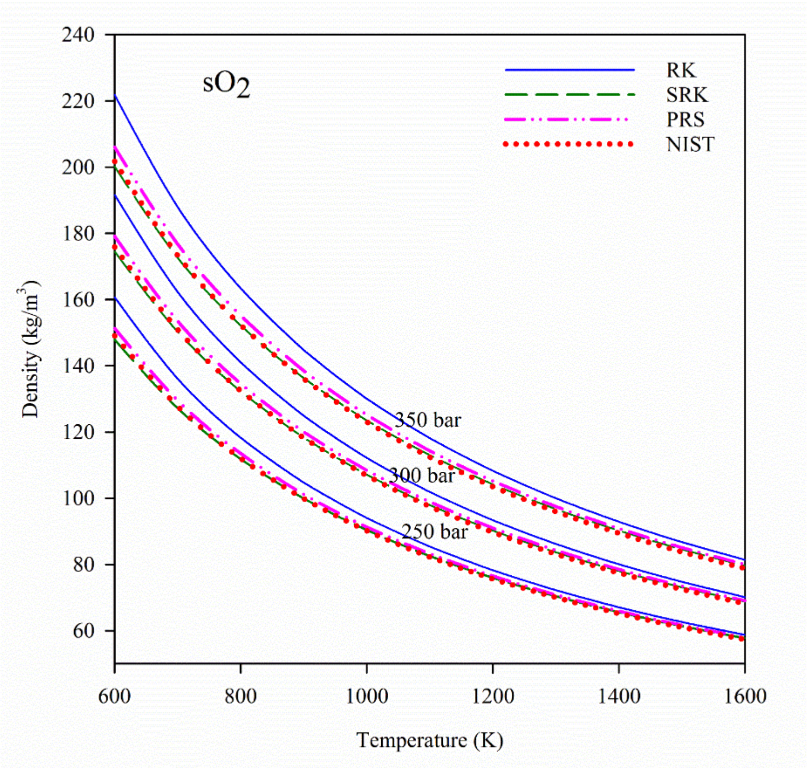
- UCF 1.1 is performing better for this lean mixture compared to Aramco Mechanism. Performance is significantly improved under SCO_2 conditions.



Mixture: CH4, O2, CO2
Pressure: ~300 bar

The comparison of EOS for sCO_2 and sO_2:

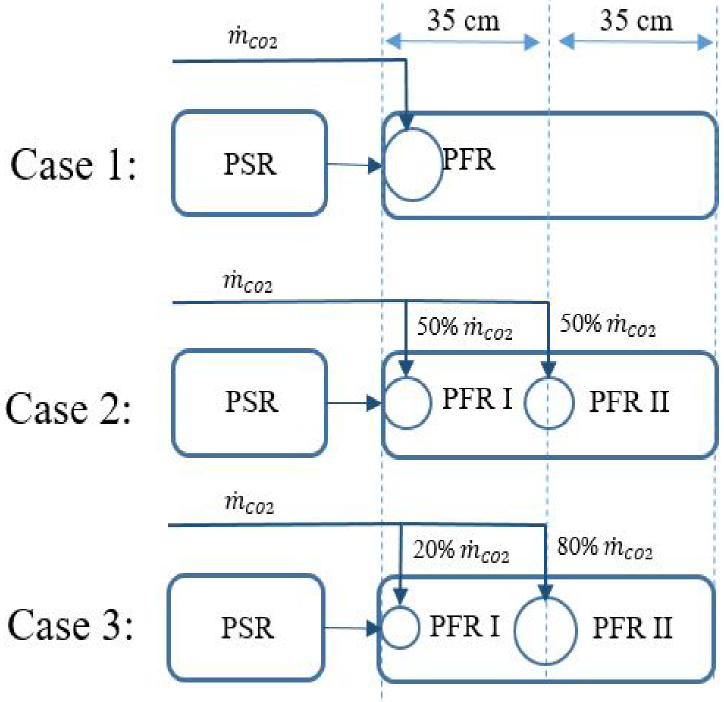




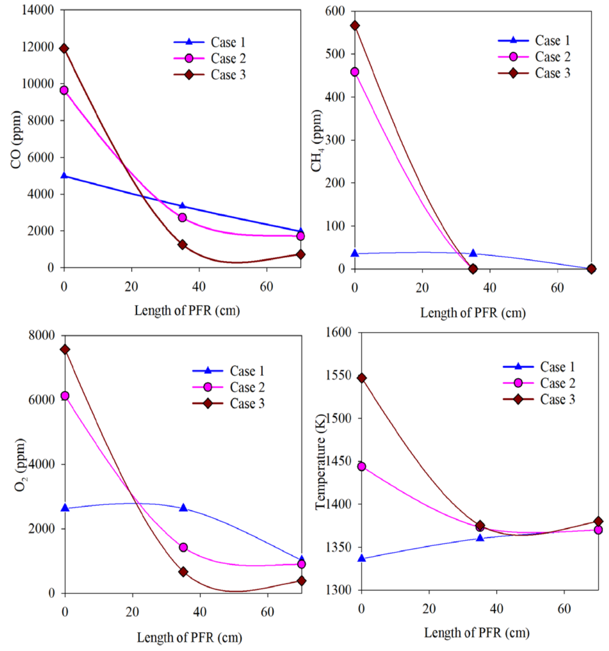
- PRS is accurate for sCO_2 and SRK is accurate for sO_2.
- The EOS has to be validated for mixtures of combustion.

Design strategy identified for future CFD simulation of dilution zone:

Mixing strategies in Dilution zone

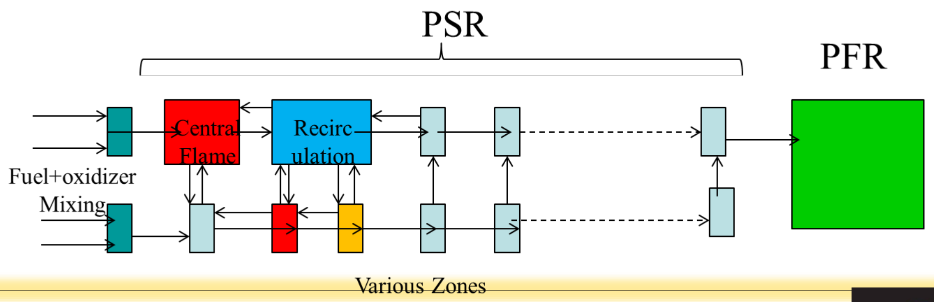


Effect of mixing strategy on PFR emissions



Reactor network modeling

- Extensively used by the gas turbine community



- Stoichiometric CH4/O2 with 95% CO2 by mass. Half of the CO2 injected in the PSR and the remainder added to the PFRs

- Real gas code with detailed Aramco mechanism

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

DOE UTSR Project Impact:

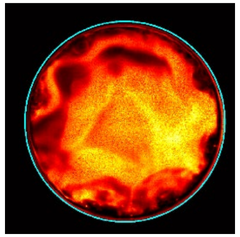
- **Understanding the reacting processes at 300bar require new facilities**
- **Vasu Lab published 27 journal papers**
- **> 45 conference papers** at ASME Turbo Expo, sCO2 symposium, AIAA Meetings, Combustion Institute Meetings
- **Prof. Vasu provided Tutorials at Turbo Expo, CelarWater Celan Energy Conference**

Burn Fuels in CO_2 Environment

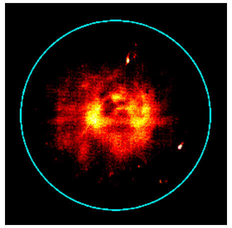
Fuel + O2 → CO_2 + H_2O

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

Everything we have done so far is the first in the world!

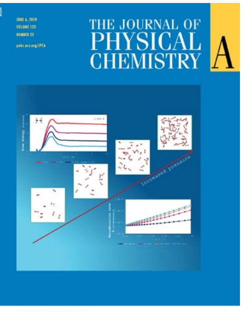


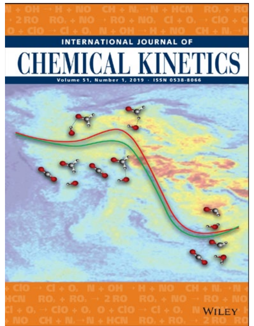
CH_4 without CO_2



CH_4 With CO_2

Cover Page Journal Articles





Industry/Government Sponsors and Collaborators

Argonne NATIONAL LABORATORY, gti, GE, Hanwha, ONR, KEPCO KEPRI, NET POWER, NASA, SwRI, U.S. Department of Energy, 8 RIVERS

Vasu Lab helped NET Power's Allam Cycle Demo Plant

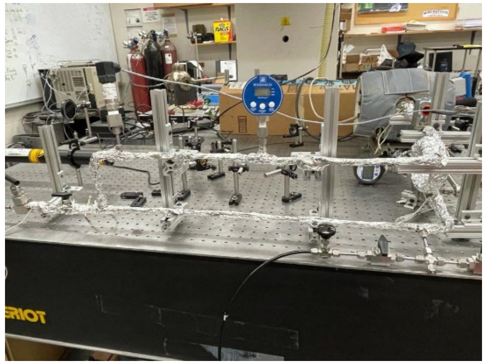
UCF

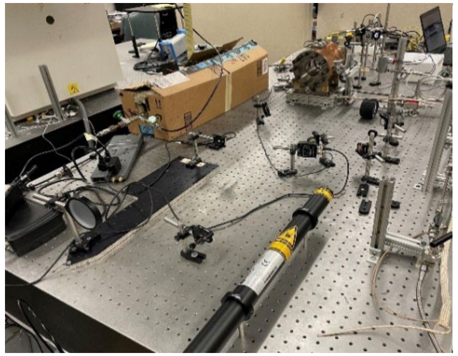
Schlieren visualization of methane injection into sCO_2:

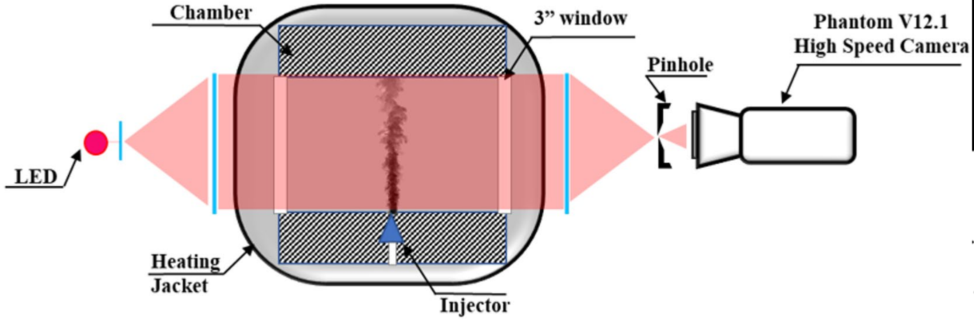
P_{CO2} =209.61 bar
P_{CH4} = 291.57 bar
P_{CH4}/P_{CO2} = 1.4
T = 90 C

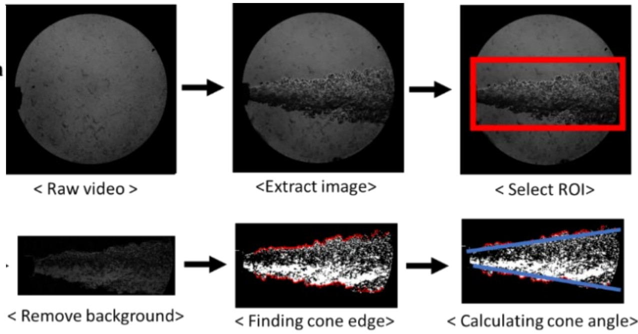
P_{CO2} =203.93 bar
P_{CH4} = 250.83 bar
P_{CH4}/P_{CO2} = 1.23
T = 91 C

P_{CO2} 205.85 bar
P_{CH4} = 228.3 bar
P_{CH4}/P_{CO2} = 1.1
T = 47 C







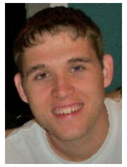


What else to be done at fundamental level to support sCO_2 combustor development?

Area	What has been done	In future?
Chemical kinetics	300 bar -90% CO_2-CH4 (also natural gas)	-300bar-90%CO_2-Natural Gas/H_2/Syngas/Biogas -CO and species time histories - Impact of impurities
Thermal properties	In another DOE project, UCF measured density up to 150 bar	-Must be extended to 300 bar
Transport properties	Diffusion coefficients investigated for CH_4/C_2H_6/CO_2 systems in this project	-MD data is still needed for all binary diffusion coefficients -Accurate mass diffusion models must be developed -Thermal conductivity and thermal diffusivity of sCO_2 mixtures must be experimentally measured
Other fundamental studies	Other fundamental experiments needs attention	Well-stirred-reactor, Counterflow flame, etc.
For CFD validation	Non-reacting jet flows experiments are conducted as a part of this project	Reacting jet flow experiments must be performed, test rig data

Students and postdocs trained

PhD Students



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

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

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

Post docs

1) Dr. Chun-Hung Wang,
now faculty in Arizona

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

Undergraduate Students

1) Elizabeth Wait
(now at Los Alamos)

5 journal papers as an
undergraduate

Thank You

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Mini Golf 2021

Vasu Lab

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Nature Hike 2022