Investigation of Autoignition and Combustion Stability of High Pressure Supercritical Carbon Dioxide Oxy-combustion

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UTSR Project: DE-FE0025174
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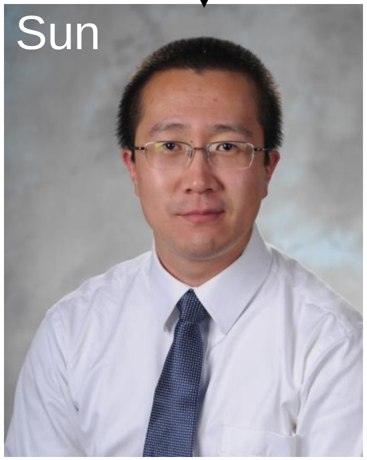
Backstory

Combustion Dynamics

Shock-tube, SCO_2 System

LES/DNS

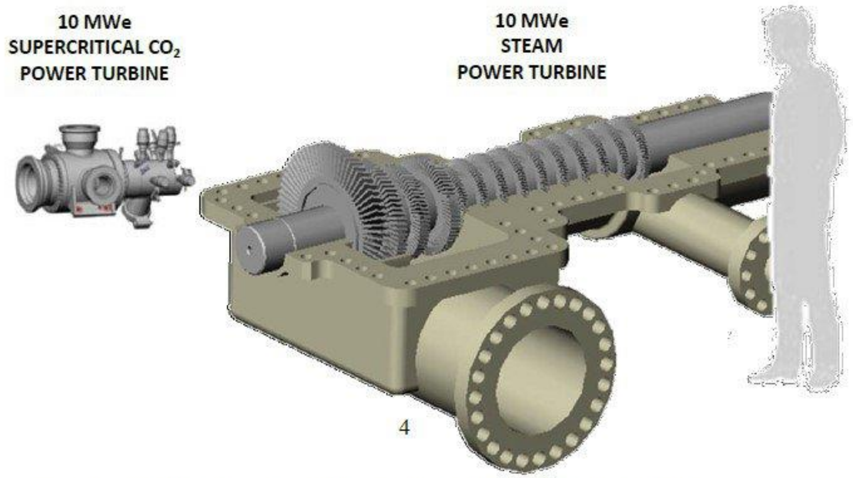


Combustion Chemical Kinetics

Supercritical CO_2 oxy-combustion system

Background of Directly Fired Supercritical CO_2 cycle

- High plant conversion efficiencies exceeding 52% (LHV) with ~100% carbon capture
- Lower electricity cost (by ~15%)
- SCO_2 is a single-phase working fluid, and does not create the associated thermal fatigue or corrosion associated with two-phase flow (e.g., steam)
- SCO_2 undergoes drastic density change over small ranges of temperature and pressure → large amount of energy can be extracted → small equipment size



Echogen's 10 MWe sCO_2 power turbine compared to a 10 MWe steam turbine.

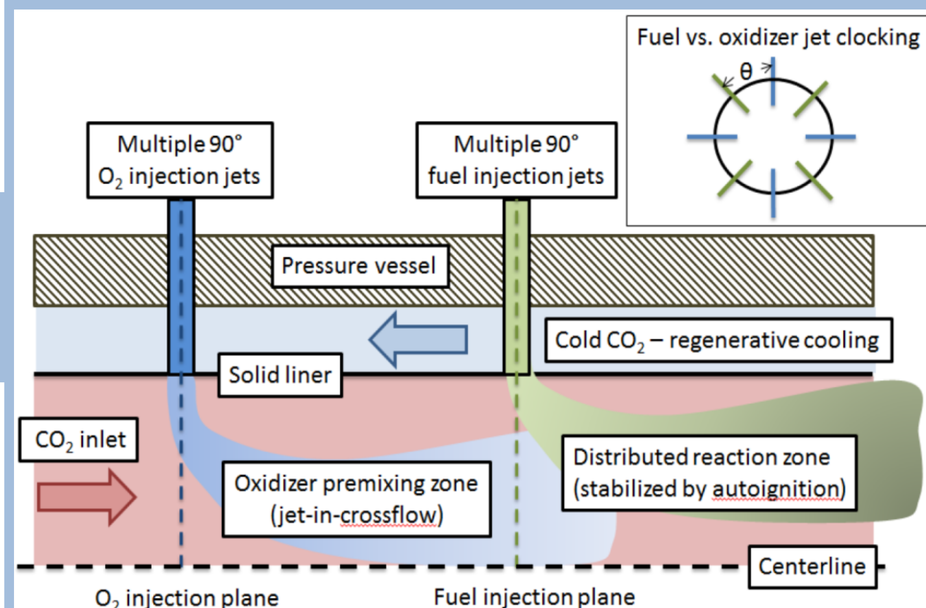
http://www.edwardtdodge.com/2014/11/20/sco2-power-cycles-offer-improved-efficiency-across-power-industry/

Overview of the Scientific Problem

- What fundamental combustion properties/knowledge we need in order to design combustor for SCO_2 oxy-combustion?
- High temperature (~1100 K) and high pressure (~200-300 atm) inlet condition
  - Conventional gas turbine combustor won't work owing to the failure of injector/flame holder at severe thermal environment

<u>Autoignition delays</u>
and
<u>combustion dynamics</u>
of jet in crossflow

Concept of autoignition stabilized combustor*

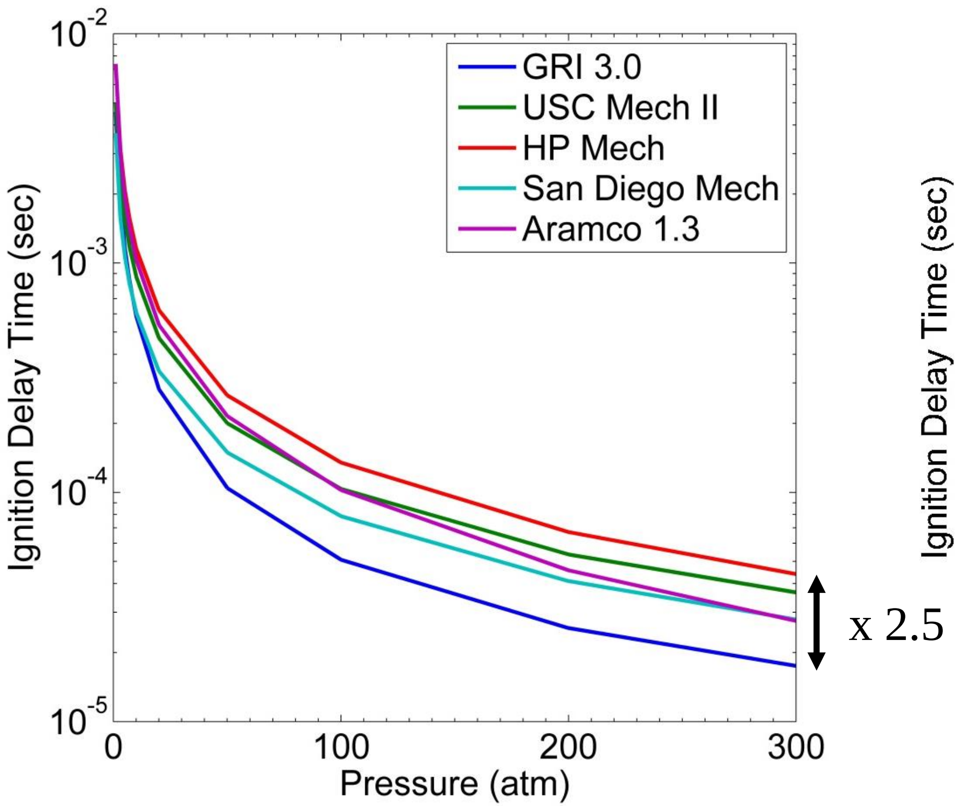


*A. McClung, DE-FE0024041 Q1FY15 Research Performance Progress Report, SwRI

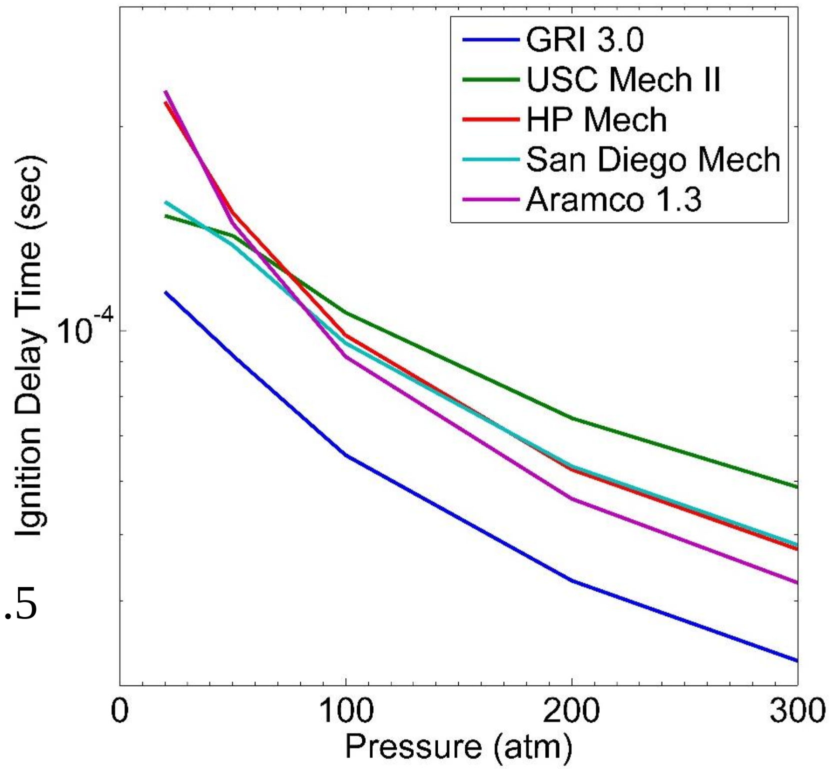
Motivation

Deviation increases with pressure: knowledge gap
Kinetic models must be validated at regime of interest !!

Predicted autoignition delays from different kinetic models



$CH_4/O_2/CO_2$ (9.5%:19%:71.48%) at 1400 K from 1 atm to 300 atm



$H_2/CO/O_2/CO_2$ (14.8%:14.8%:14.8%:55.6%) at 1200 K from 10 atm to 300 atm

Overview of the Scientific Questions and Proposed Work

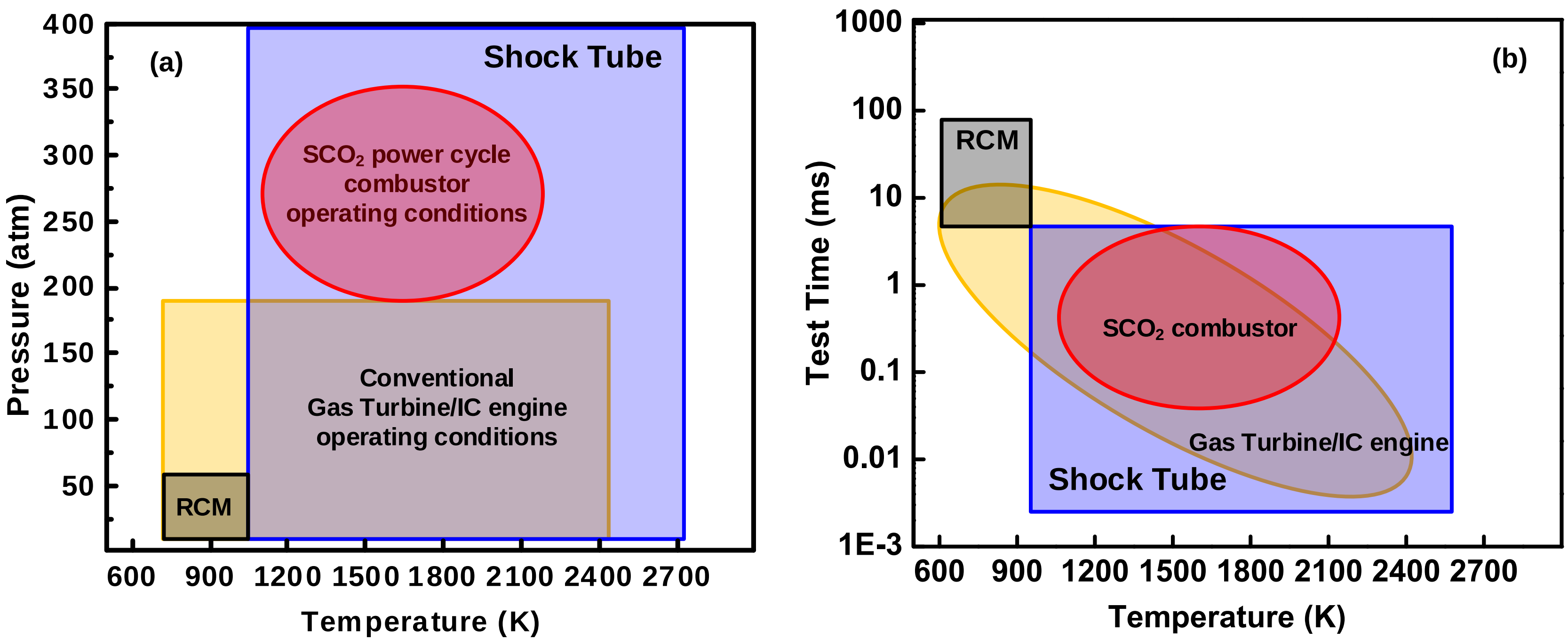
- What is the fundamental combustion properties?
  - Experimental investigation of chemical kinetic mechanisms for SCO_2 Oxy-combustion (Task 1&2: Ranjan & Sun)

- How can we use the mechanism to design combustors?
  - Development of a compact and optimized chemical kinetic mechanism for SCO_2 Oxy-combustion (Task 3: Sun)

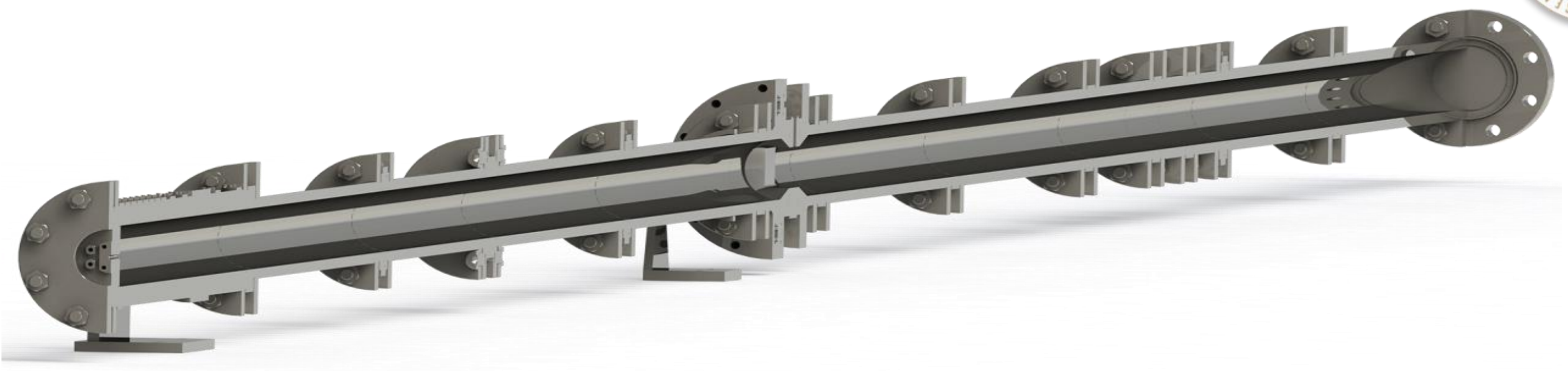
- What is the combustor dynamics at this new condition?
  - theoretical and numerical investigation of combustion instability for SCO_2 Oxy-combustion (Task 4&5: Lieuwen, Menon & Sun)

Task 1: Development of a High Pressure Shock Tube for Combustion Studies

- How to study autoignition delays at SCO2 Oxy-combustion condition?
  - Why Shock-Tube?



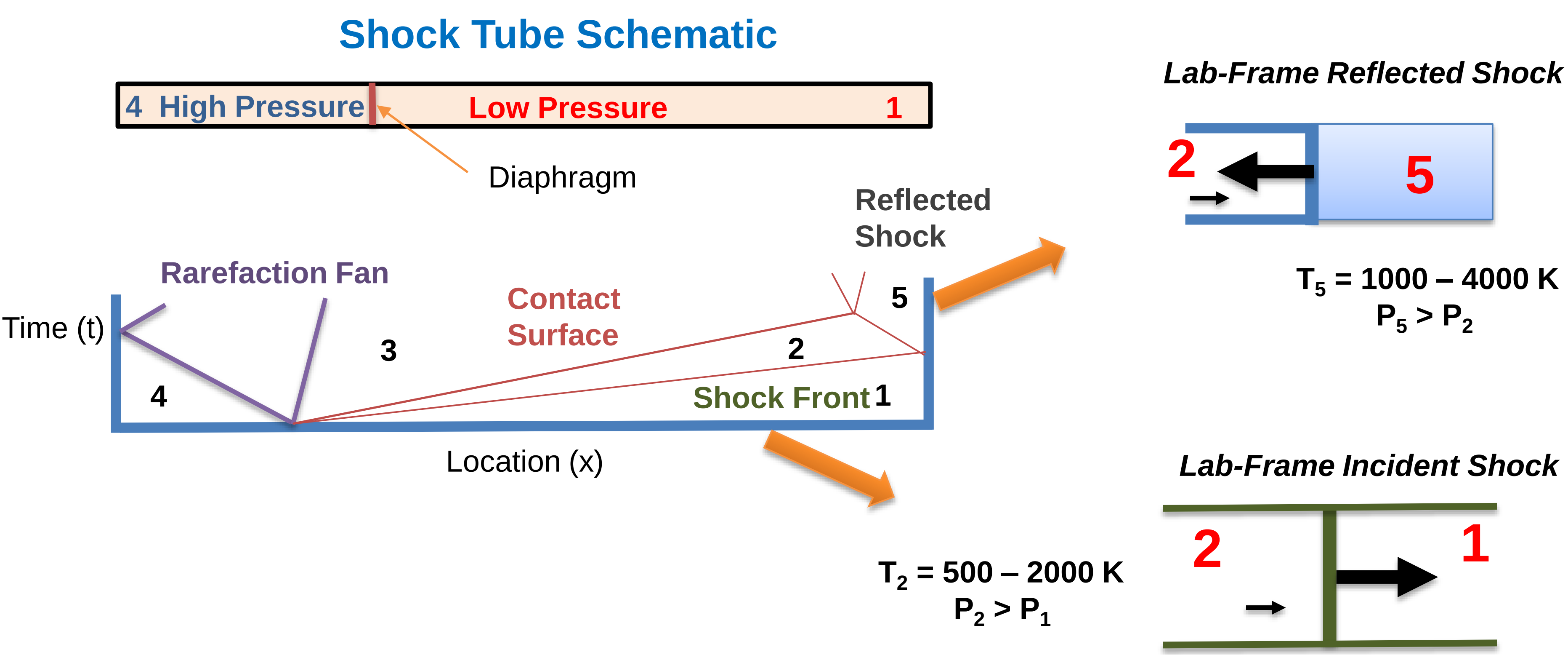
Task 1: Development of a High Pressure Shock Tube for Combustion Studies



- Georgia Tech shock tube for fundamental autoignition study is under construction
- Wide pressure range (P up to 300 atm)
- Large ID (152.4 mm) to minimize non-ideal effect at very high pressure condition

Task 1: Development of a High Pressure Shock Tube for Combustion Studies

Basics regarding the shock-tube:



Diagnostics: pressure and chemiluminescence

Remind: currently no absorption spectroscopy can work at this condition (above 50 atm)

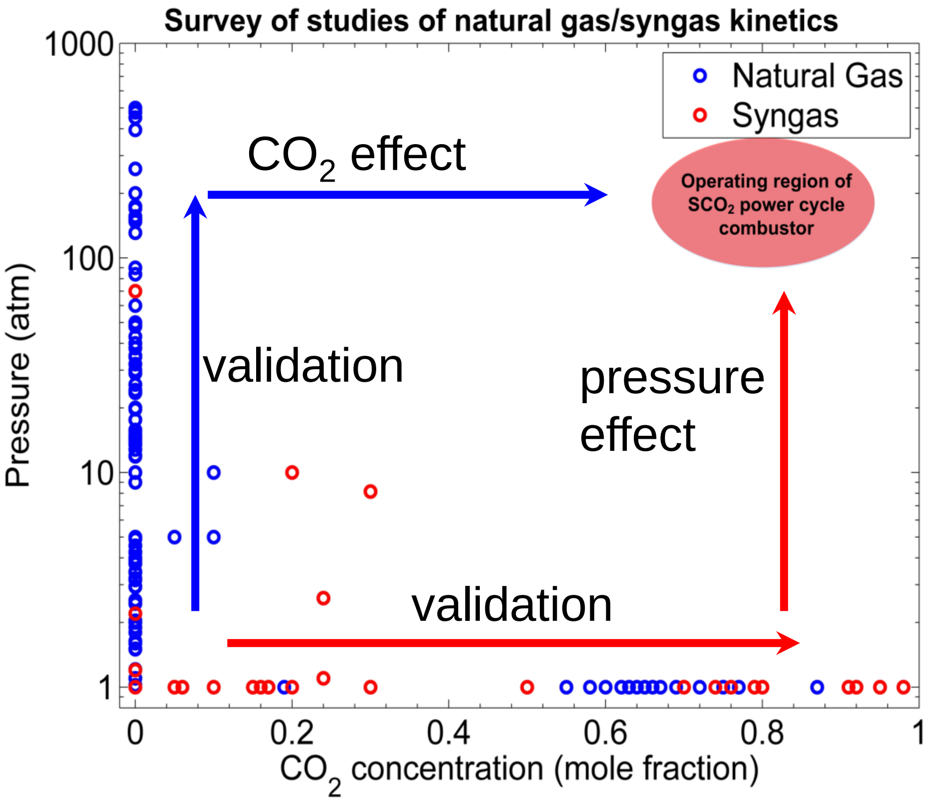
Task 1: Development of a High Pressure Shock Tube for Combustion Studies

Key Capability of the GT Shock-tube

- Large internal bore (15.24 cm)—to minimize the boundary layer effect (very critical at high pressure conditions)
- It will be long (20 m total)
- Test time 50 ms (can achieve high value with modification of driver gas mixture)
- Diaphragm section replicate the current design in the operational shock-tube for turbulent mixing study
- Test pressure ~300 bar
- Preheating capability
- 0.2 μm or better surface finish
- Optical access from end wall and side-wall
- Several locations for pressure transducers at the end wall and on side wall
- Diagnostic capability to understand the non-ideal effects in the shock-tube

Task 2: Investigation of Natural Gas and Syngas Autoignition in SCO_2 Environment

- Autoignition properties have never been investigated before in region of interest
- This task will investigate critical autoignition properties of natural gas and syngas diluted by CO_2 in region of interest
- Approach for high quality data:
  - Repeat existing experiments for validation
  - Ramp up pressure to study pressure effect
  - Ramp up CO_2 dilute concentration to study CO_2 dilution effect

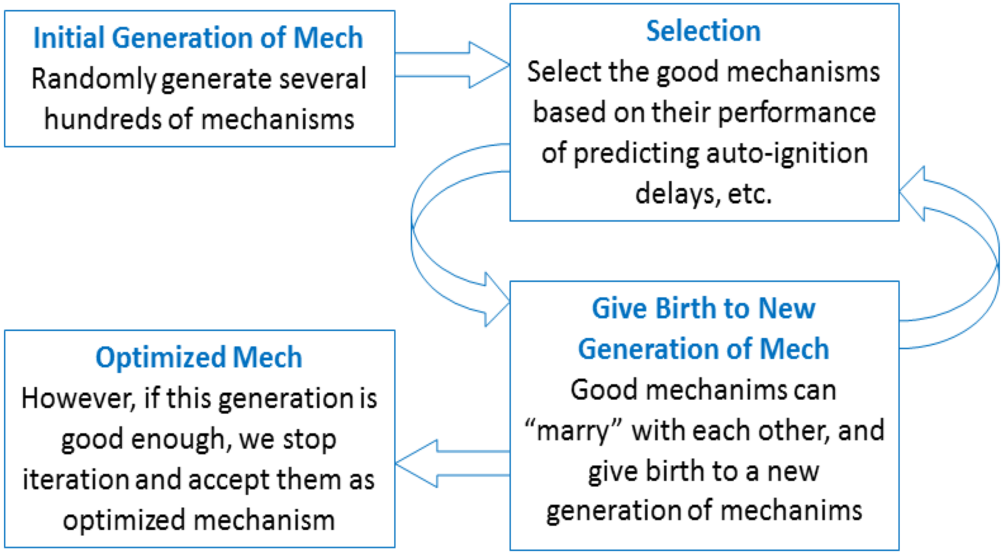


A new regime to explore!

e.g.:
E.L. Petersen, et al, Symp. Combust., 1996(26), 799-806
S. Vasu, et al, Energy Fuels, 2011(25), 990-997

Task 3: Development of a Compact and Optimized Chemical Kinetic Mechanism for SCO_2 Oxy-combustion

- Develop an optimized, validated and compact chemical kinetic mechanism
- Employ the optimized mechanism in LES to study combustion stability
- Approach: optimize chemical kinetic mechanism based on experimental data obtained in task 2.
- Explore other methodology: Bayesian optimization for better optimization

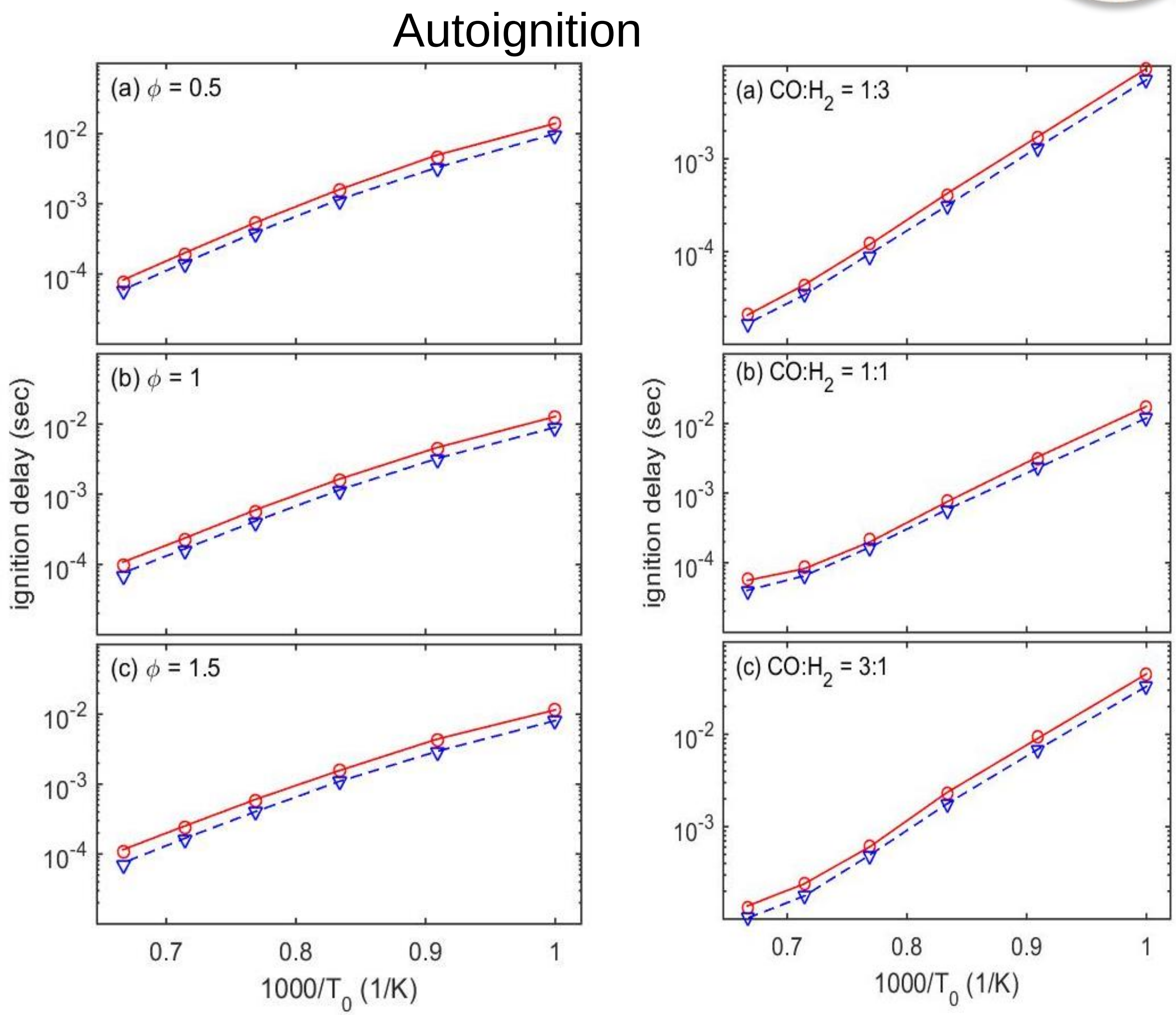


Flow chart of using Genetic Algorithm to optimize chemical kinetic mechanisms

Task 3: Development of a Compact and Optimized Chemical Kinetic Mechanism for SCO_2 Oxy-combustion

- Comparing to existing high pressure autoignition delay data, USC Mech II (111 species) has the best agreement[1]. So it is used as a starting point for future optimized mechanism
- A 27 species reduced mechanism[2] for natural gas (CH_4/C_2H_6) and syngas (CO/H_2) is developed
- Comparison of the results from reduced (marker) and detailed mech (line). Solid lines (p = 200atm), dashed line (p = 300atm)

Warning: therm/trans data !!
e.g., CO_2, different trend



92.5% CO_2 diluted natural gas/O_2 (CH_4:C_2H_6=95:5)

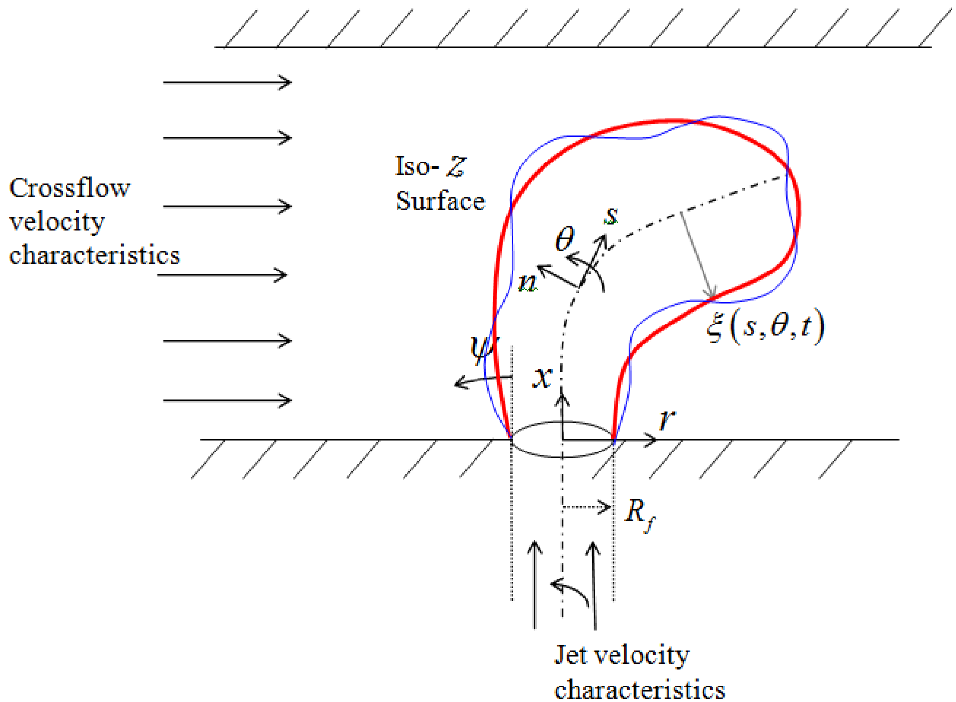
92.5% CO_2 diluted syngas gas/O_2 (ϕ=1)

1. A. McClung, DE-FE0024041 Q1FY15 Research Performance Progress Report, SwRI
2. S. Coogan, X. Gao, W. Sun, Evaluation of Kinetic Mechanisms for Direct Fired Supercritical Oxy-Combustion of Natural Gas, TurboExpo 2016

Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

- The analytical work shall focus on physics based models of high pressure reacting jet in crossflow (JICF)

- A key goal of this work shall be to determine the relationship between flow disturbances and heat release oscillations



Analytic model of jet in crossflow

Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

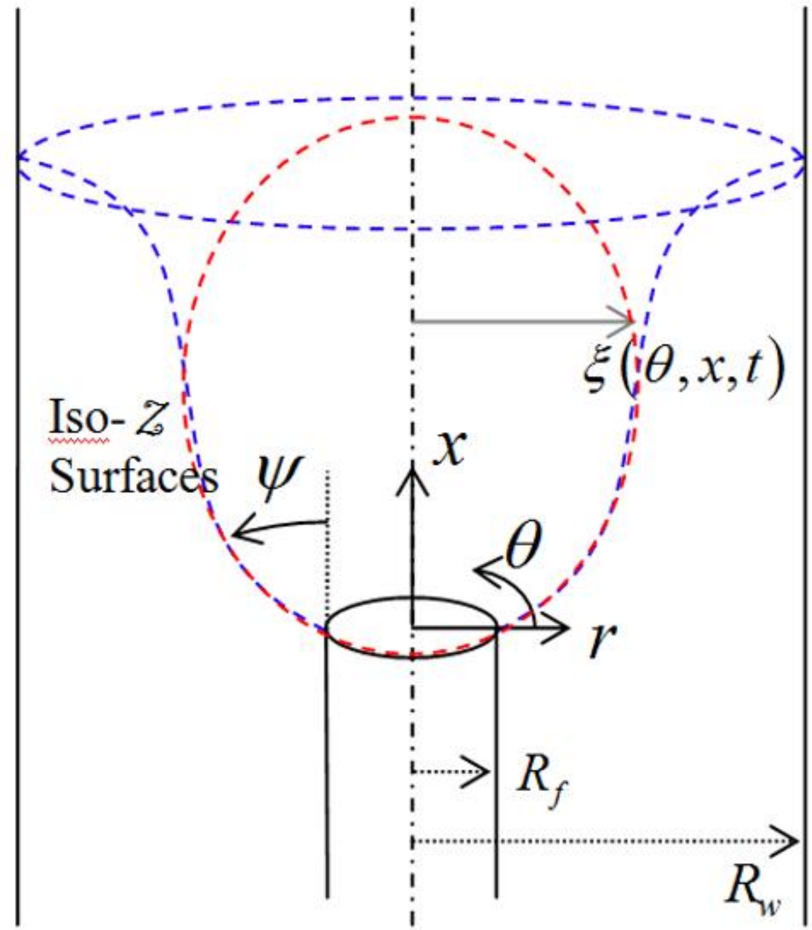
- Established model: Mixture fraction formulation

$$\frac{\partial Z}{\partial t} + \vec{u} \cdot \nabla Z = \nabla \cdot \left(\mathscr{D} \nabla Z \right)$$

$$Z\left(x, \theta, \xi(x,\theta,t), t\right) = Z_{st}$$

→ $\xi(x,\theta,t)$

→ Heat release transfer function



Magina, N., Lieuwen, T. "Three-dimensional and swirl effects on harmonically forced, non-premixed flames". *9th US National Combustion Meeting* (2015).

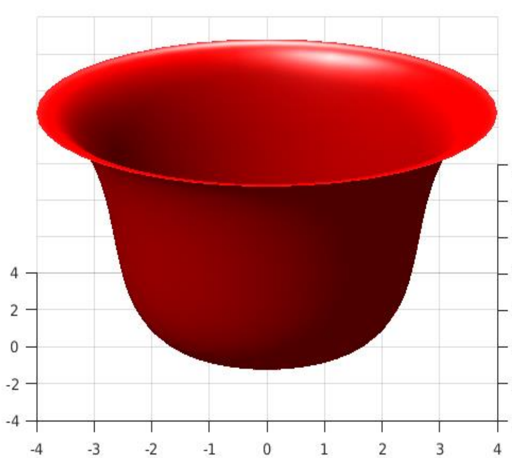
Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

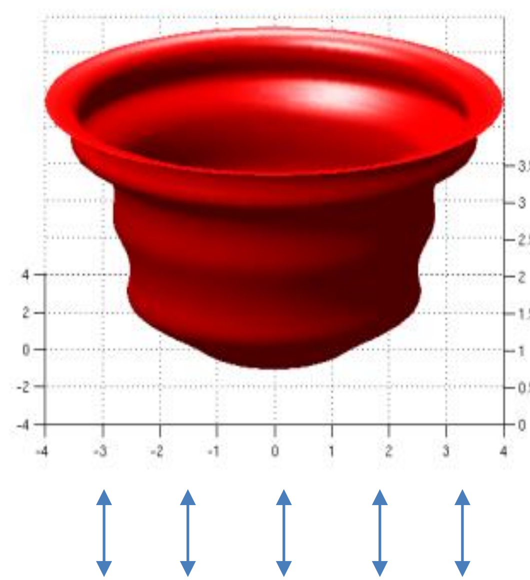
- **Solution: Space-Time Dynamics of $\mathcal{Z}_{st}$ Surface**

Bulk Axial Forcing $u_{x,1} = \varepsilon U_0 \exp[-i\omega t]$

$Pe >> 1$

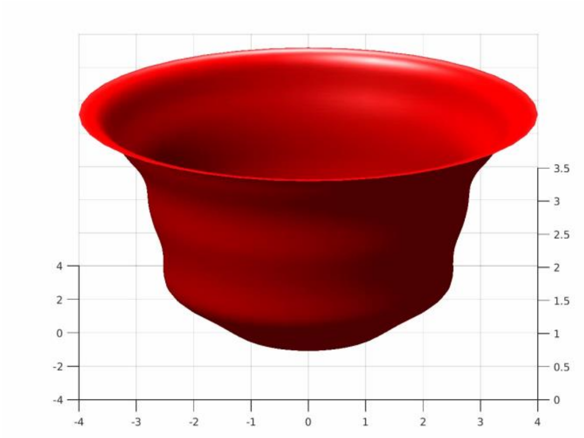
$$\frac{\xi_{1,n}(x,t)}{R_f} = \frac{i\varepsilon \exp[-i\omega t]}{2\pi St} \sin\psi_0(x)\left[1-\exp\left[2\pi i St \frac{x}{R_f}\right]\exp\left[-\frac{4\pi^2 St^2}{Pe}\frac{x}{R_f}\right]\right] + O\left(\frac{1}{Pe^2}\right)$$

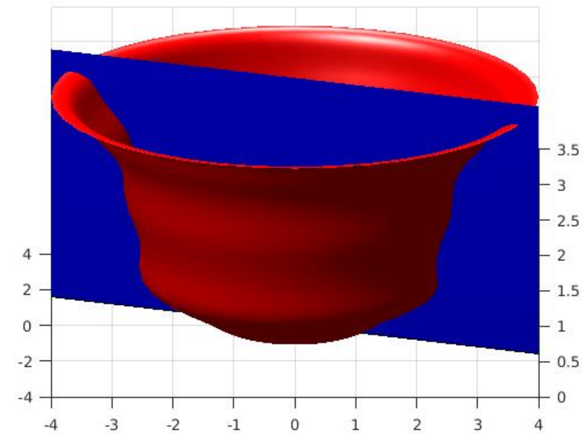


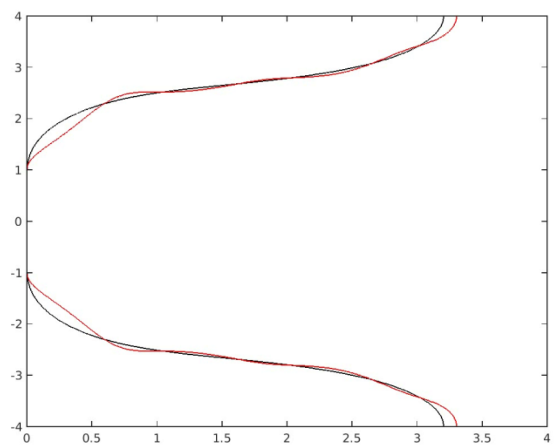


Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

- **Solution: Space-Time Dynamics of $\mathcal{Z}_{st}$ Surface**





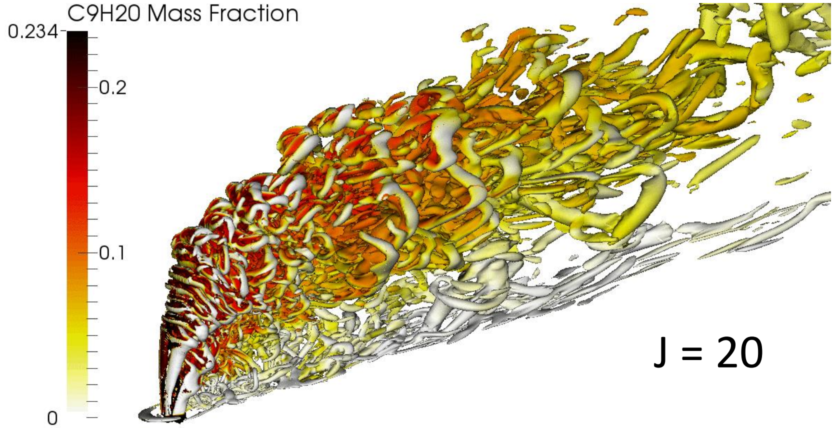


Key Goals of Task 4

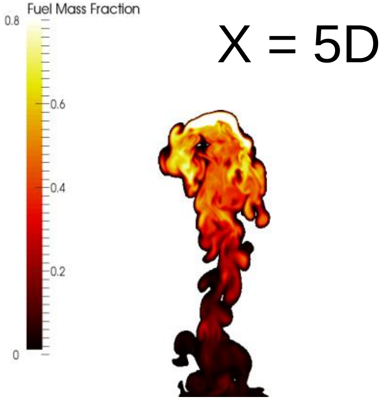
- Determine the gain-phase relationship between flow disturbances and heat release oscillations
- Compute time averaged flow and flame features
- Account for supercritical effects on diffusion coefficients, and radiation

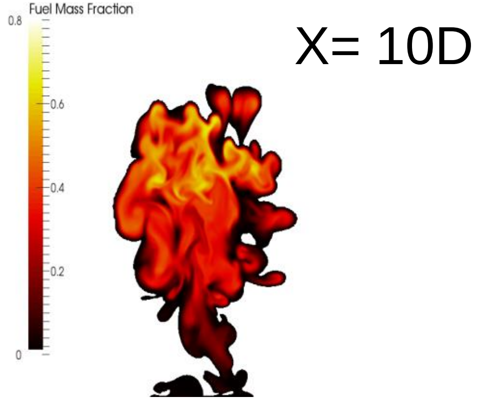
Task 5: LES Studies of Supercritical Mixing and Combustion

Supercritical Mixing in JICF (leveraged by our rocket engine work)



Vorticity Contours of supercritical Kerosene in air

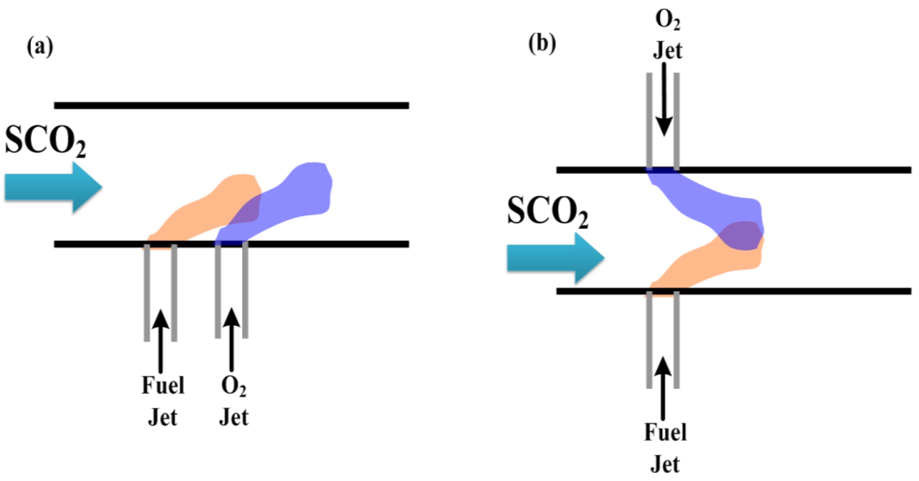




- LES capability exists to simulate supercritical mixing and reacting flows
- Uses Peng-Robinson EOS for real gas properties with finite-rate kinetics
- Simulations to be used to study mixing and combustion between SCO_2, fuel/oxidizer
- Effect of radiation

Task 5: LES Studies of Supercritical Mixing and Combustion

- Task 5a: Simulate supercritical mixing/combustion in JICF
- Task 5b: Implement optimized kinetics from Task 3 for reacting studies
- Task 5c: Simulate and analyze conditions resulting in combustion stability in possible combustor geometries
  - Vary inflow and combustor operating conditions
  - Vary injection conditions
- Task 5d: Feedback sensitive reactions to Task 3 to further refine the mechanism



Possible circular combustor design for SCO2 power cycle (will be modeled)

Task 5: LES Studies of Supercritical Mixing and Combustion

Regime of interest: P = 200-300 atm

fluid	Critical temperature (K)	Critical pressure (atm)
CO_2	304	72.9
H_2O	647	**217.8**
CH_4	190	45.4
C_2H_6	305	48.1
H_2	32.9	12.8
CO	125.9	34.5
O_2	154.6	49.7

Warning: Mixing rule !!

A mixture may have one, more than one, or no critical points

$P_{c,\ CO2}$ = 72.9 atm
$P_{c,\ C16H34}$ = 25 atm
$P_{c,mixture}$ = 238 atm
(CO_2:$C_{16}H_{34}$=0.94:0.06)

Transcritical regime exists and is very challenging to model

New physics and chemistry in gas turbine !!

Deliverables

- New fundamental combustion data base for SCO_2 power cycles
- Optimized predictive kinetic mechanism for natural gas and syngas
- Analytic and numerical models of jet in cross flow at SCO_2 power cycle operating conditions

Thank you!
&
Questions?

Acknowledgement:
UTSR Project: DE-FE0025174; PM: Seth Lawson