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

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UTSR Project: DE-FE0025174
PM: Seth Lawson

Backstory

Combustion Dynamics

Shock-tube, SCO_2 System

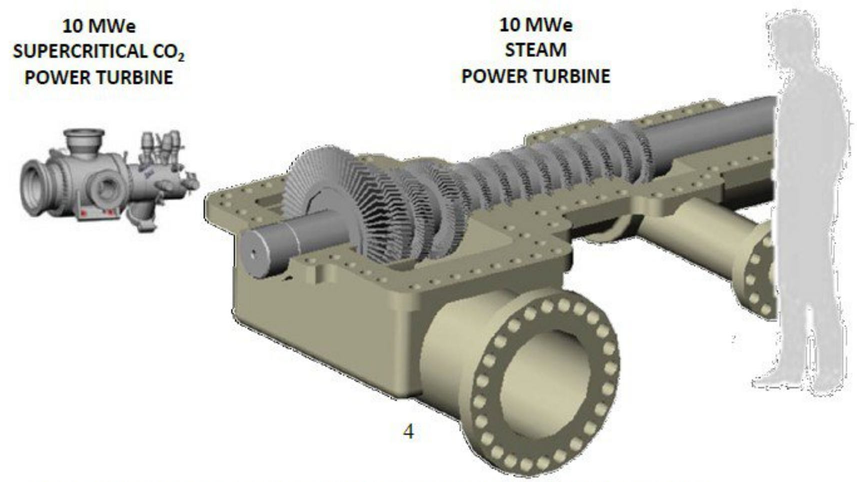
LES/DNS

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.

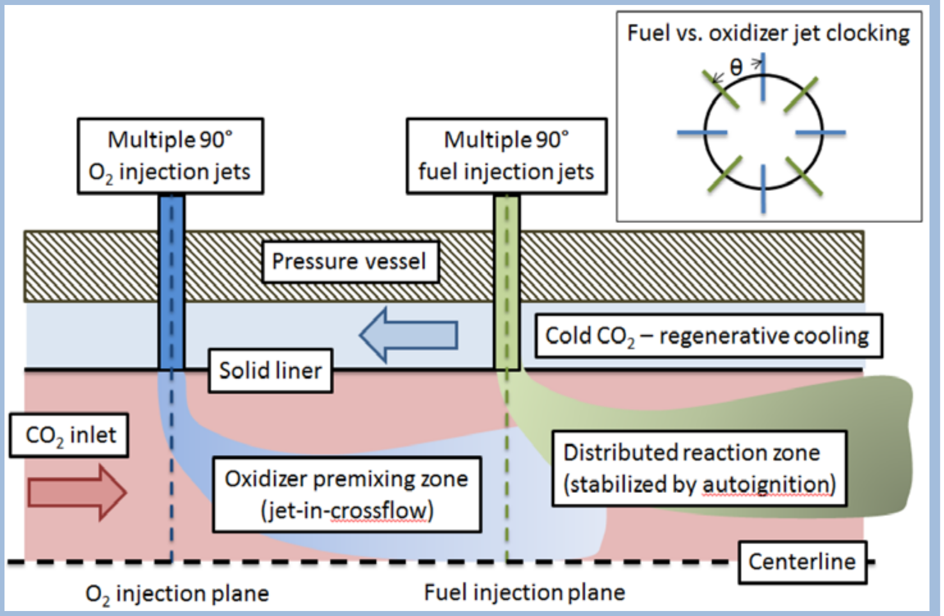
http://www.edwardtdodge.com/2014/11/20/sco2-power-cycles-offer-improved-efficiency-across-power-industry/

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*

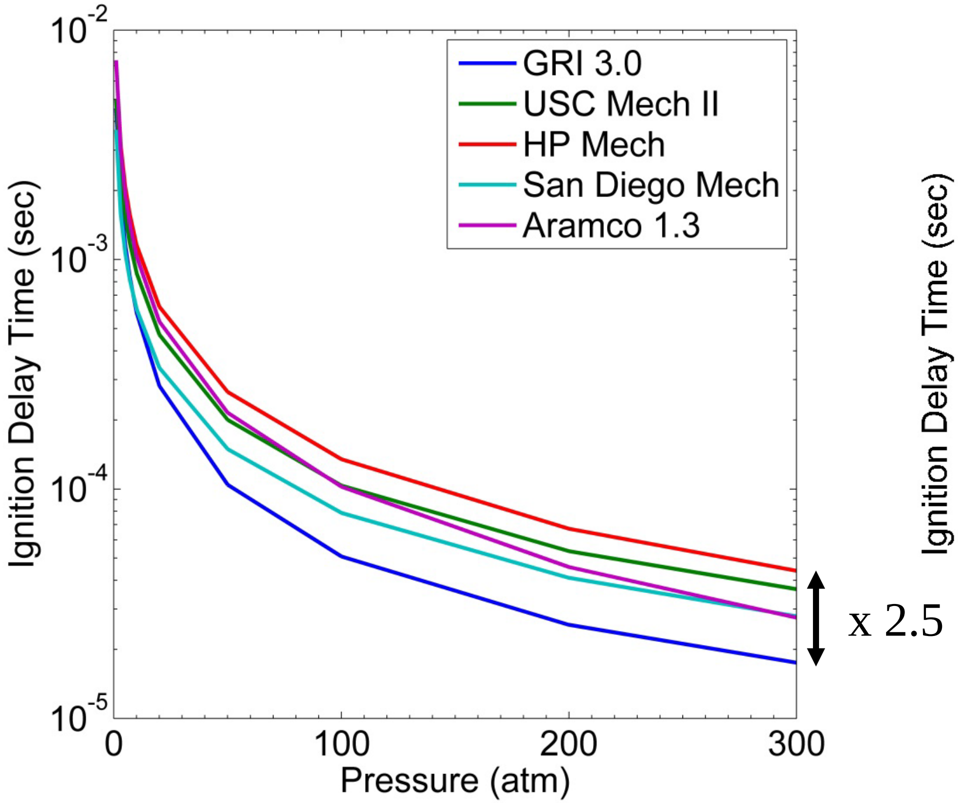


*A. McClung, DE-FE0024041 Q1FY15 Research Performance Progress Report, SwRI

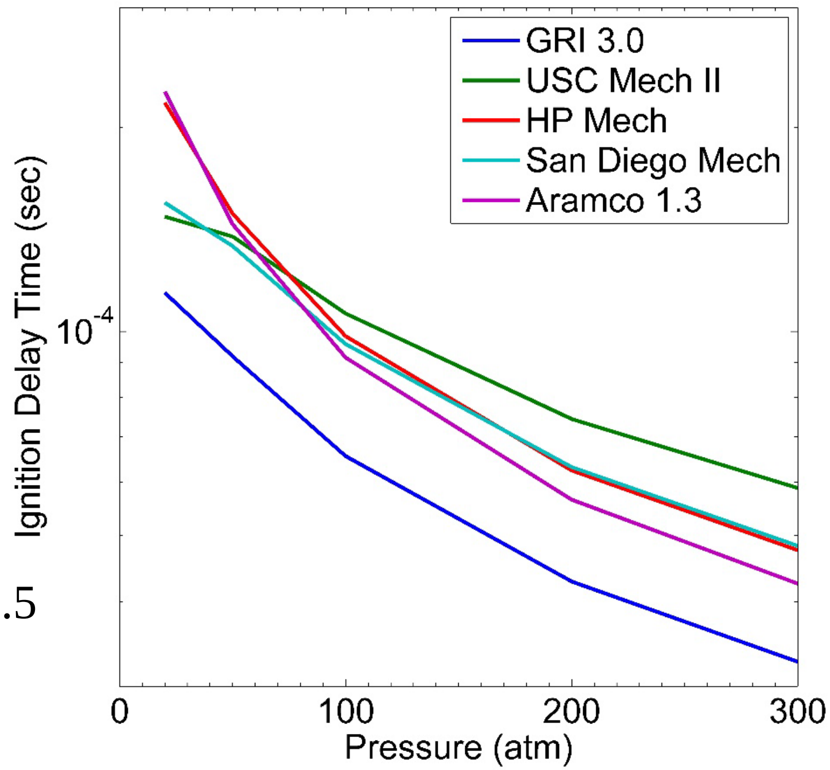
Motivation

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

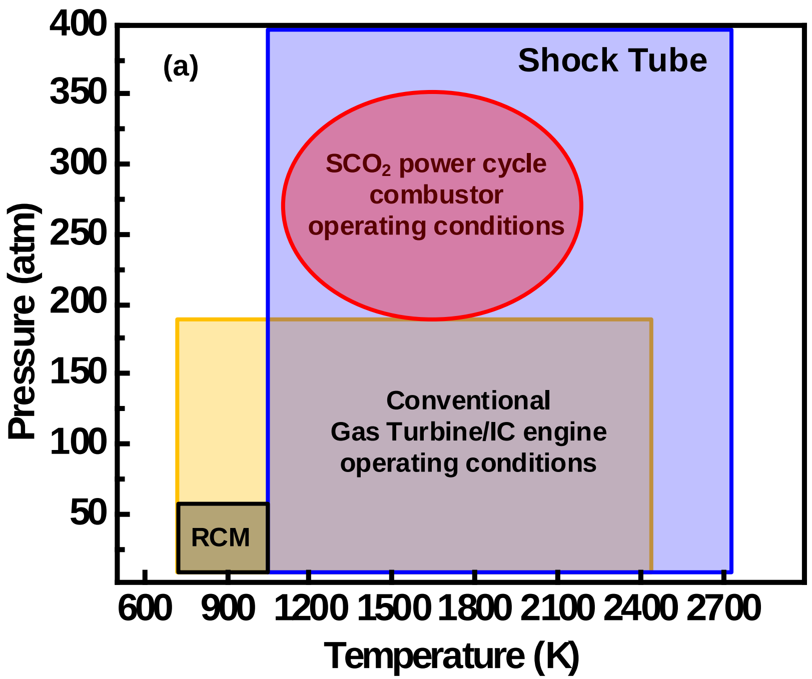
- What is the fundamental combustion properties?
  - Experimental investigation of chemical kinetic mechanisms for SCO_2 Oxy-combustion (Task 1&2: Ranjan & Sun)

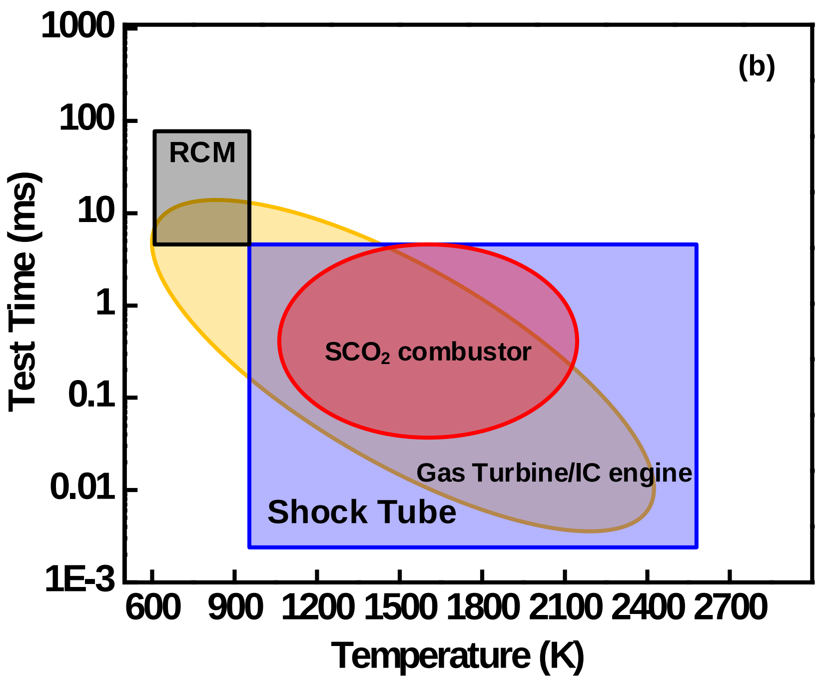
- How can we use the mechanism to design combustors?
  - Development of a compact and optimized chemical kinetic mechanism for SCO_2 Oxy-combustion (Task 3: Sun)

- 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)

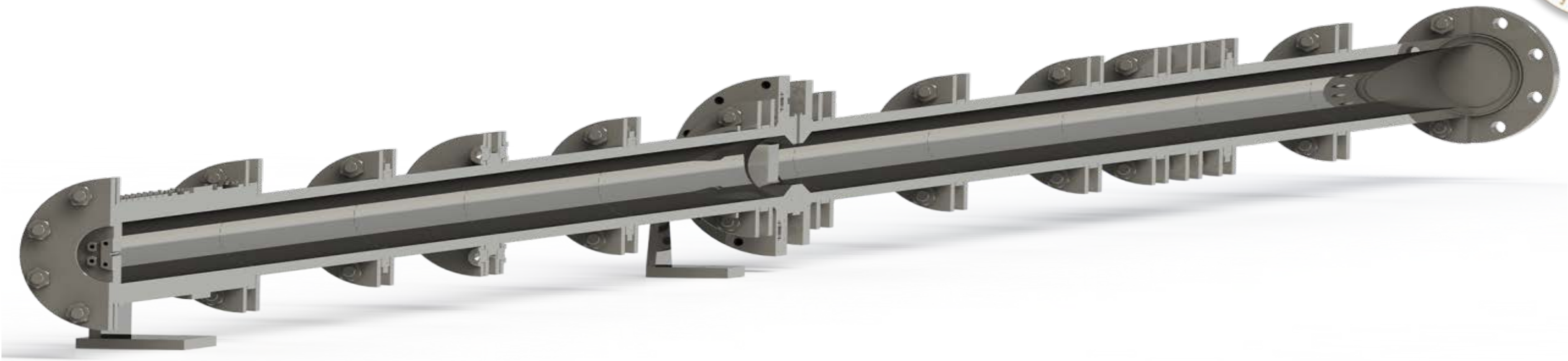
Task 1: Development of a High Pressure Shock Tube for Combustion Studies

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





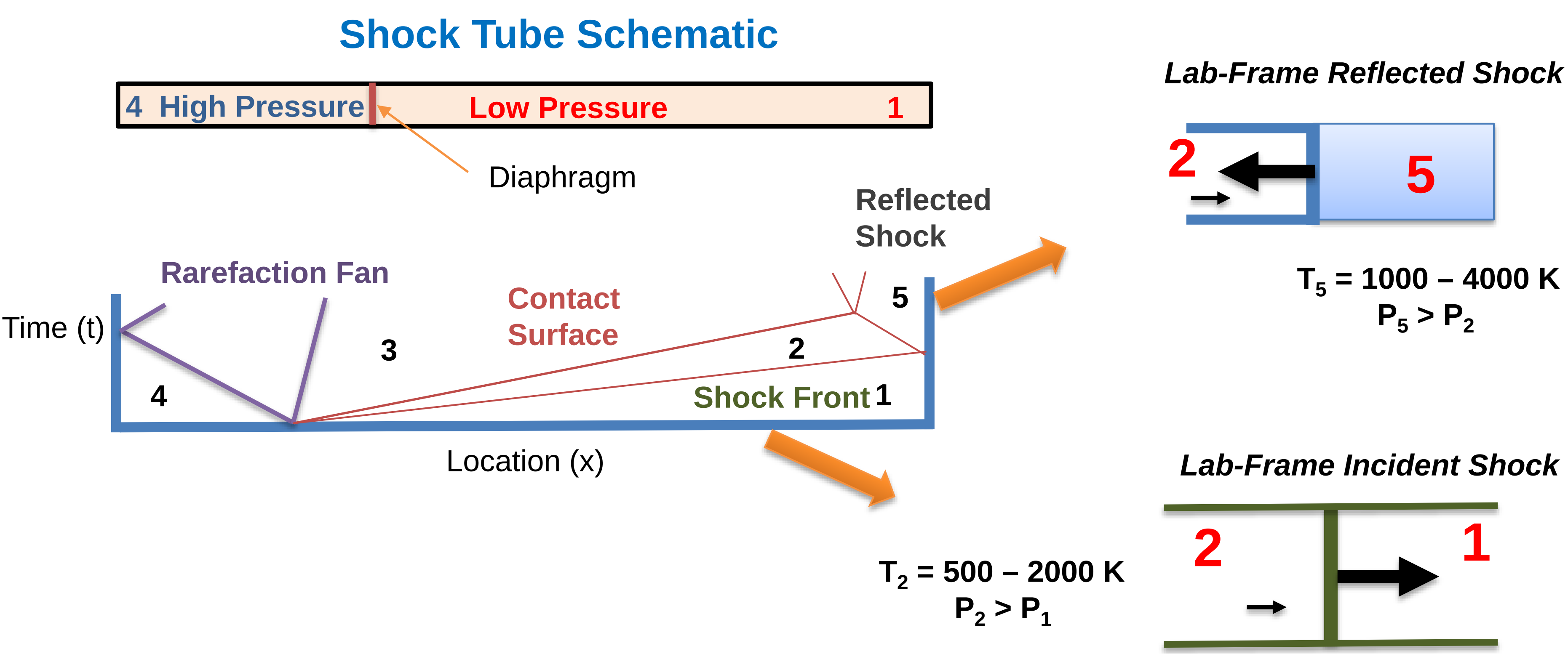
Task 1: Development of a High Pressure Shock Tube for Combustion Studies



- 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)

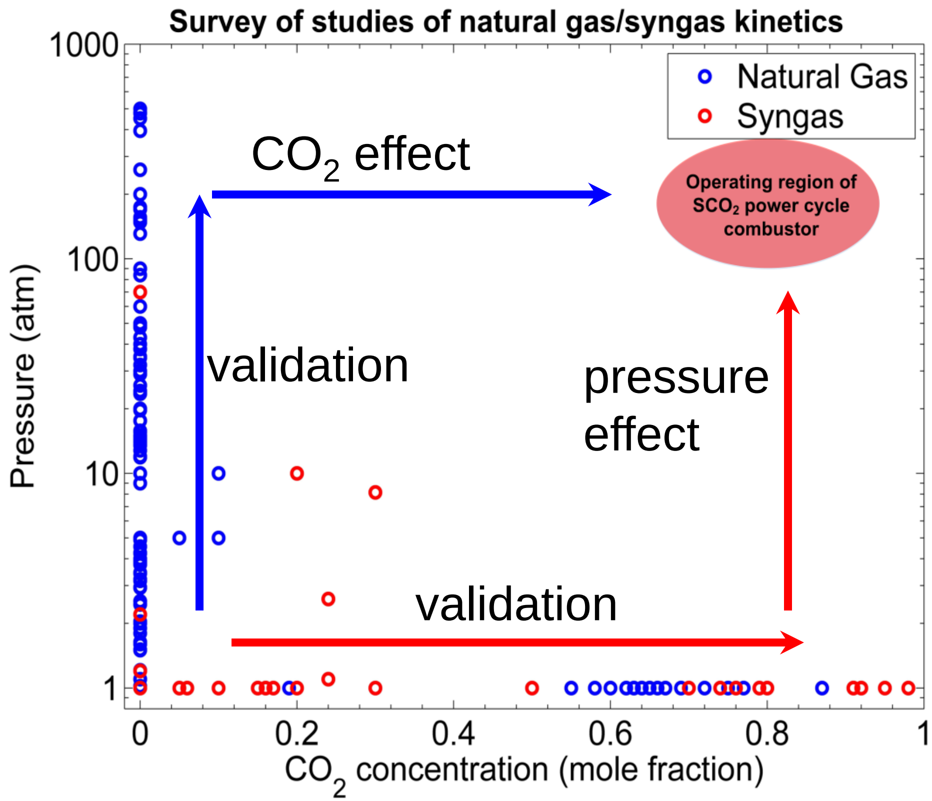
Task 1: Development of a High Pressure Shock Tube for Combustion Studies

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

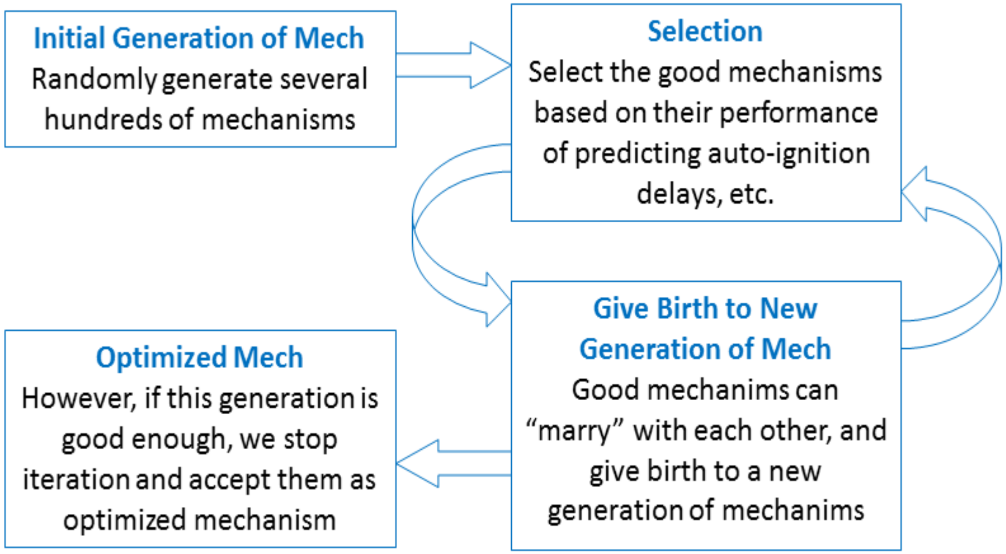
Task 3: Development of a Compact and Optimized Chemical Kinetic Mechanism for SCO_2 Oxy-combustion

- 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

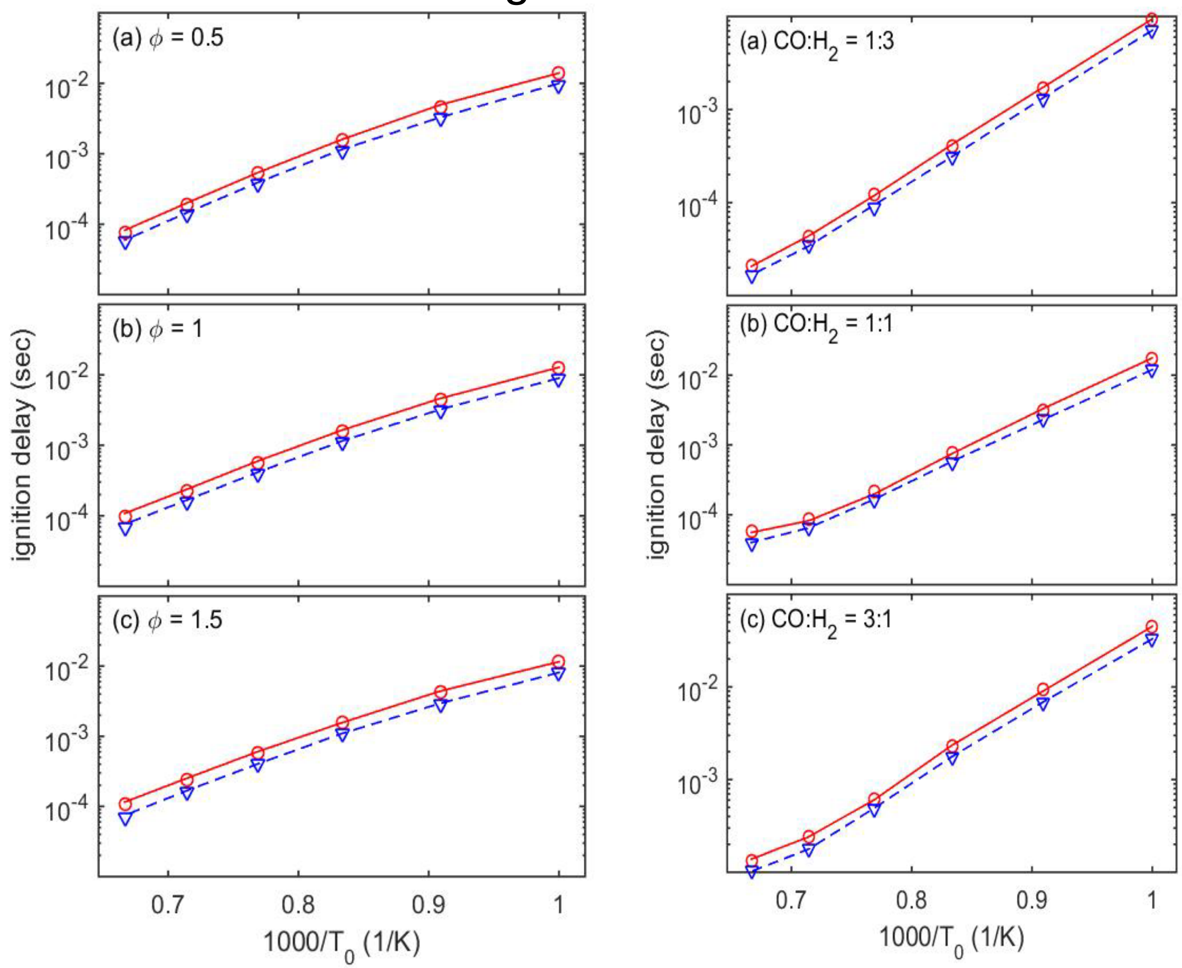
- A 27 species reduced mechanism[2] for natural gas (CH_4/C_2H_6) and syngas (CO/H_2) is developed

- 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

Autoignition



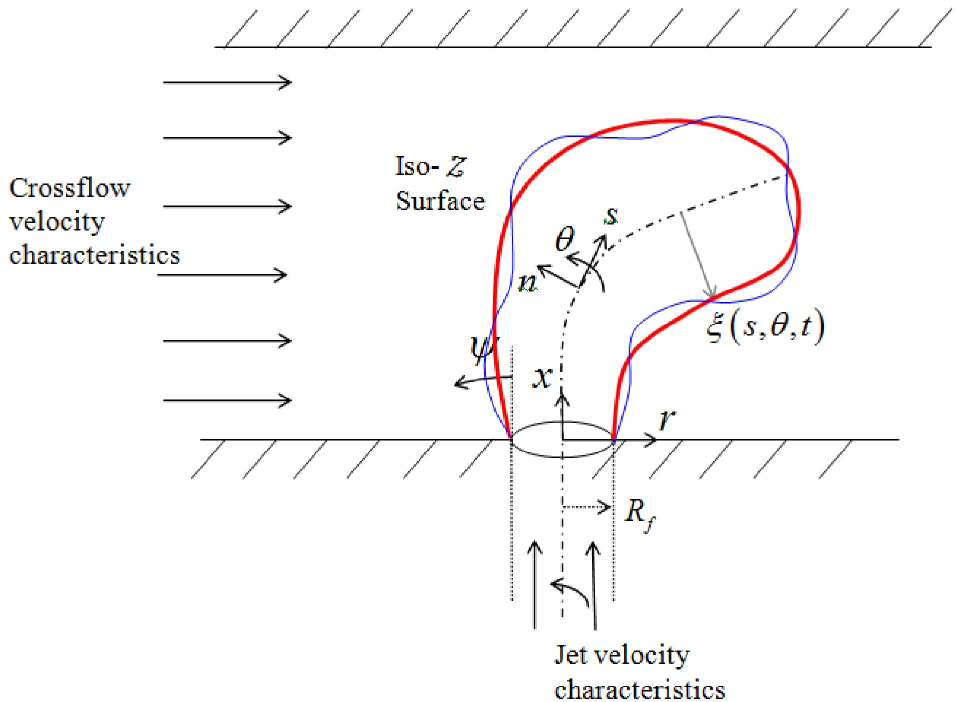
92.5% CO_2 diluted natural gas/O_2 (CH_4:C_2H_6=95:5)

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

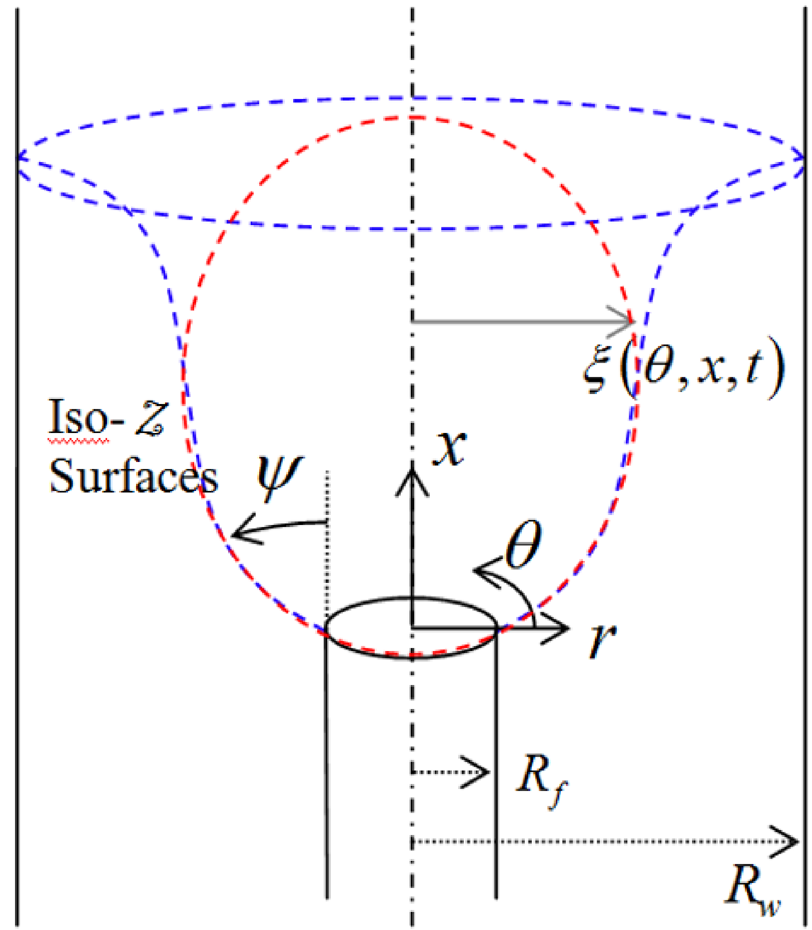
- Established model: Mixture fraction formulation

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

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

$\rightarrow \xi(x, \theta, t)$

$\rightarrow$ Heat release transfer function



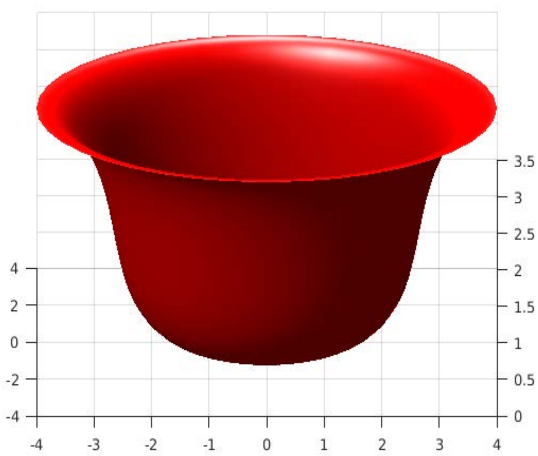
Magina, N., Lieuwen, T. “Three-dimensional and swirl effects on harmonically forced, non-premixed flames”. *9th US National Combustion Meeting* (2015).

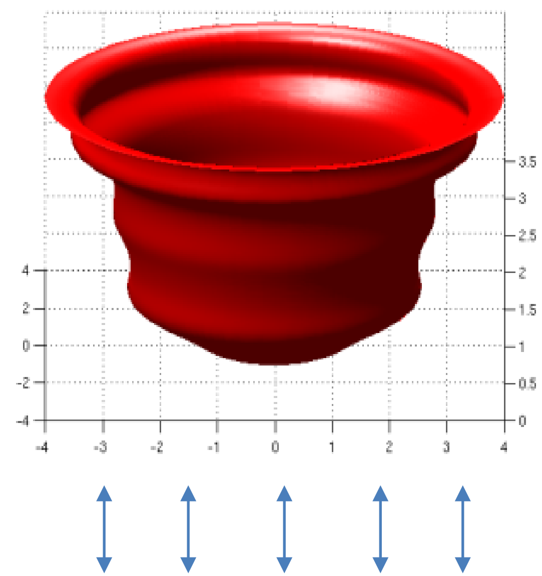
Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

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

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

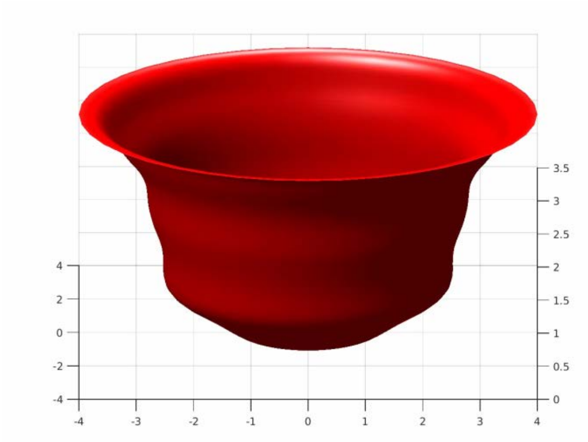
$Pe >> 1$ $$\frac{\xi_{1,n}(x,t)}{R_f} = \frac{i\varepsilon \exp[-i\omega t]}{2\pi St} \sin\psi_0(x)\left[1-\exp\left[2\pi i St\frac{x}{R_f}\right]\exp\left[-\frac{4\pi^2 St^2}{Pe}\frac{x}{R_f}\right]\right] + O\left(\frac{1}{Pe^2}\right)$$

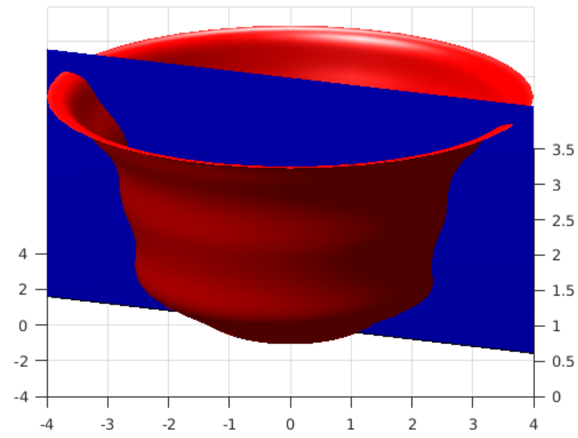


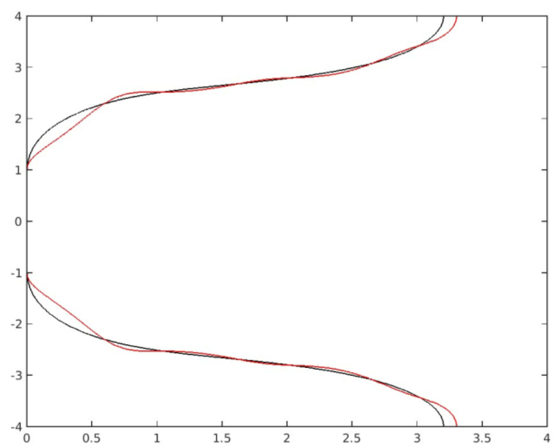


Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

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





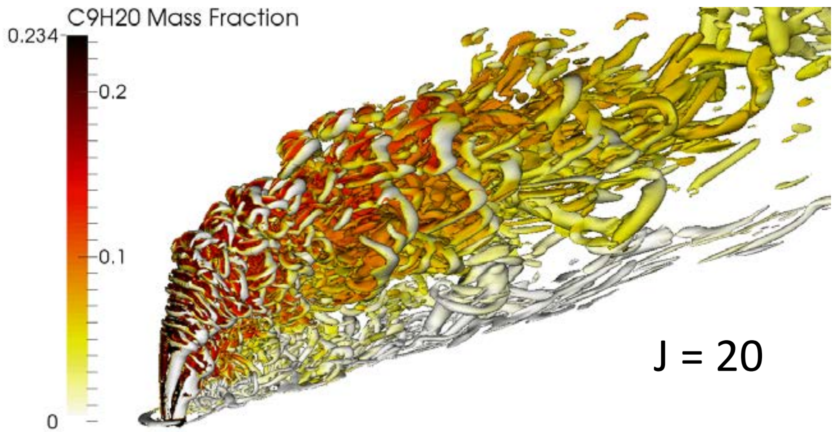


Key Goals of Task 4

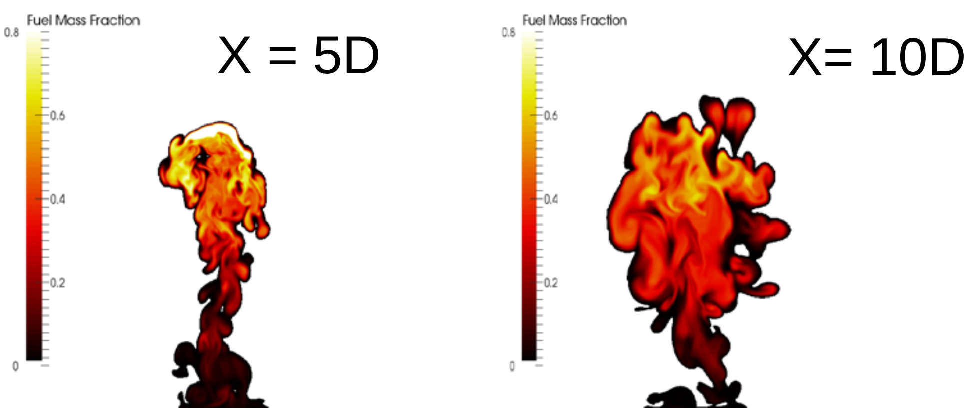
- Determine the gain-phase relationship between flow disturbances and heat release oscillations
- Compute time averaged flow and flame features
- Account for supercritical effects on diffusion coefficients, and radiation

Task 5: LES Studies of Supercritical Mixing and Combustion

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



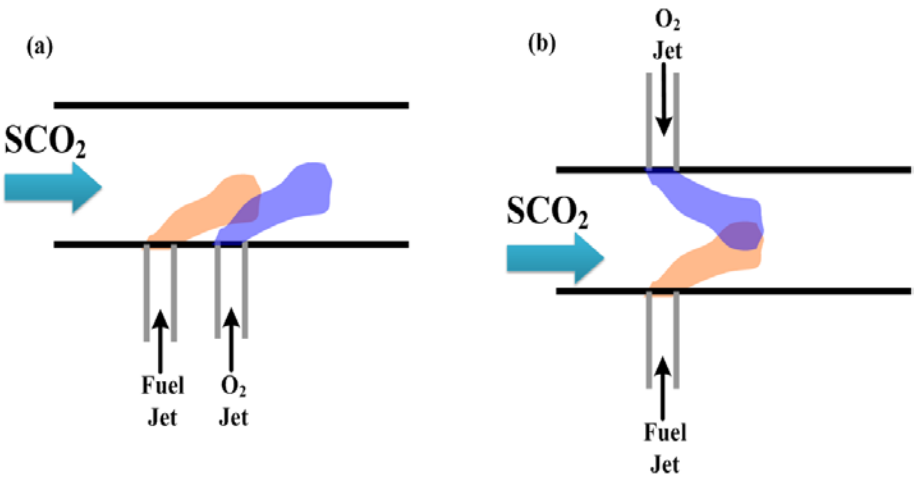
Vorticity Contours of supercritical Kerosene in air



- 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

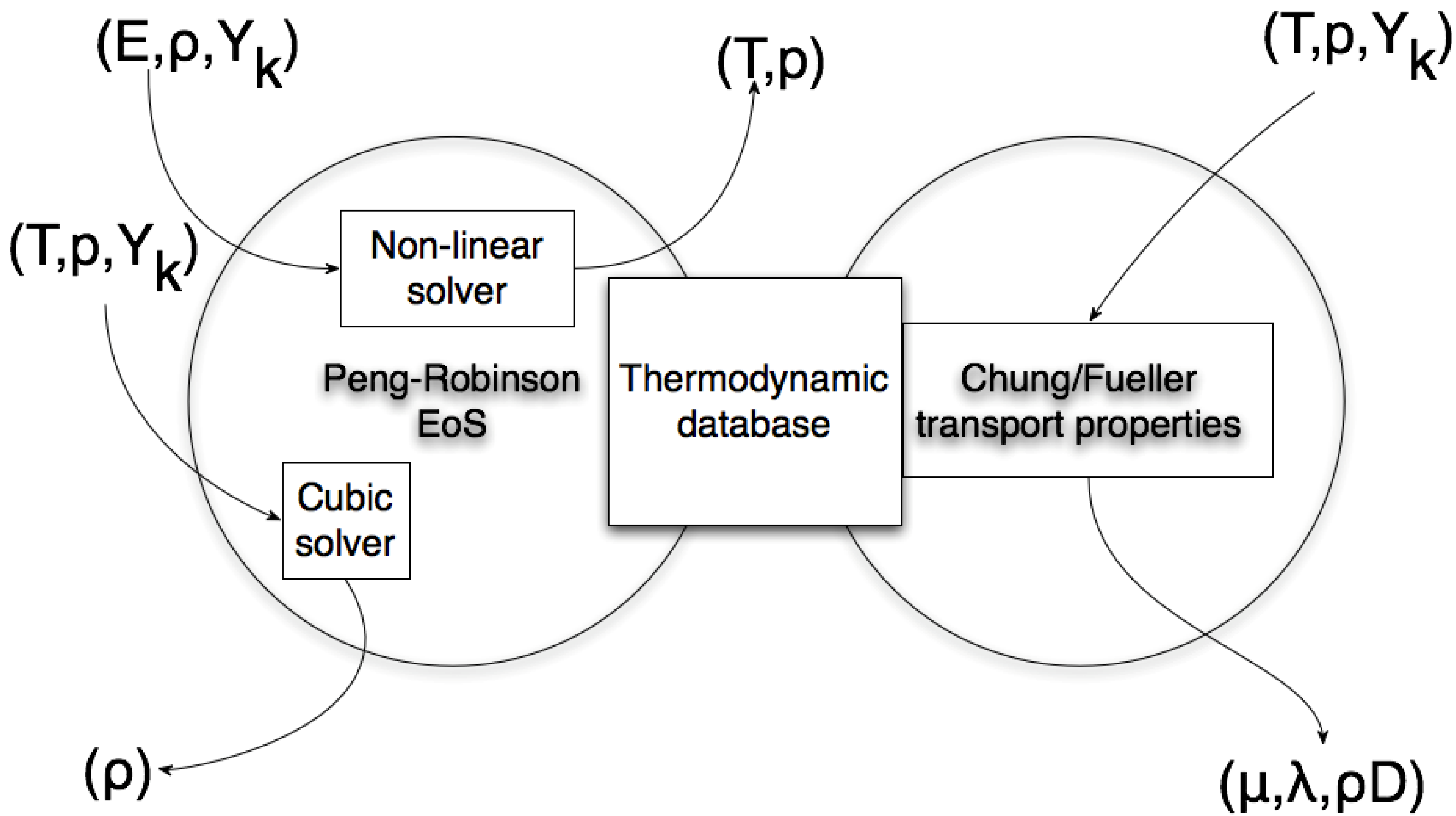
- New fundamental combustion data base for SCO_2 power cycles
- Optimized predictive kinetic mechanism for natural gas and syngas
- Analytic and numerical models of jet in cross flow at SCO_2 power cycle operating conditions

Thank you!
&
Questions?

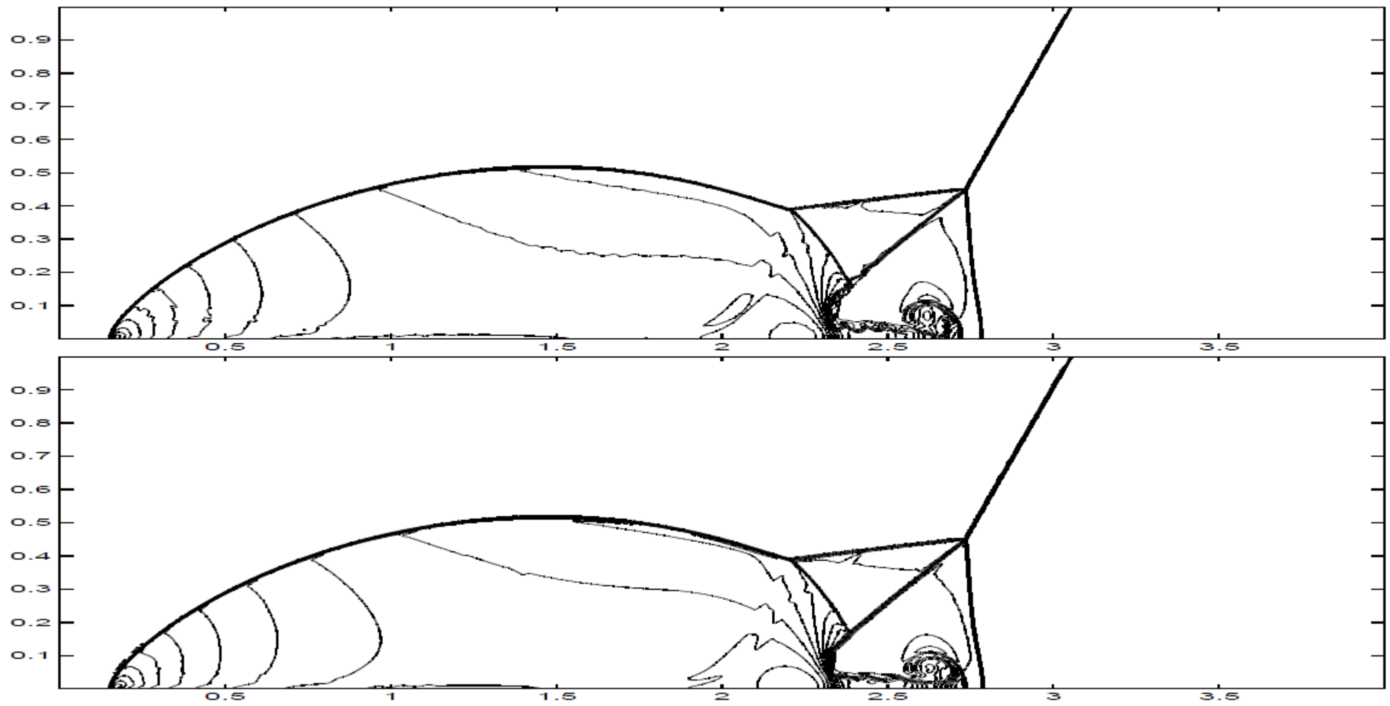
Acknowledgement:
UTSR Project: DE-FE0025174; PM: Seth Lawson

Task 5: LES Studies of Supercritical Mixing and Combustion

Real gas framework



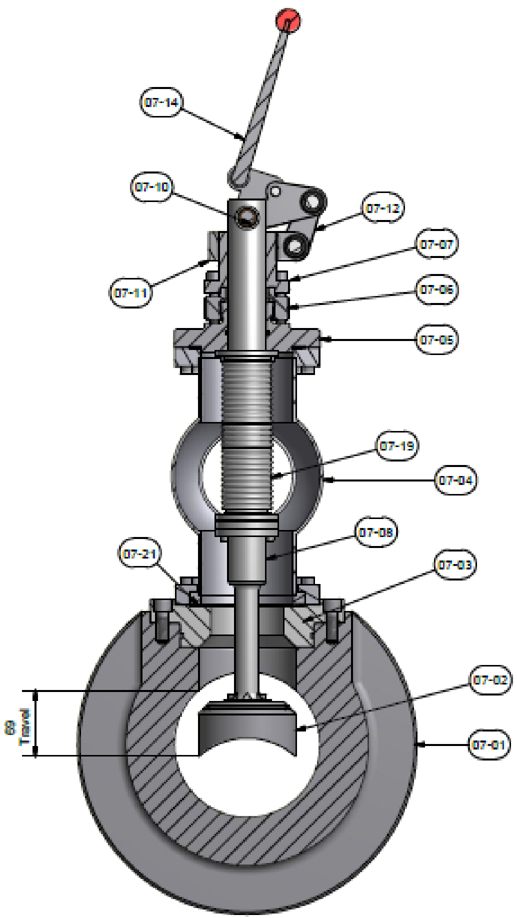
2D Effect in Shock Tube



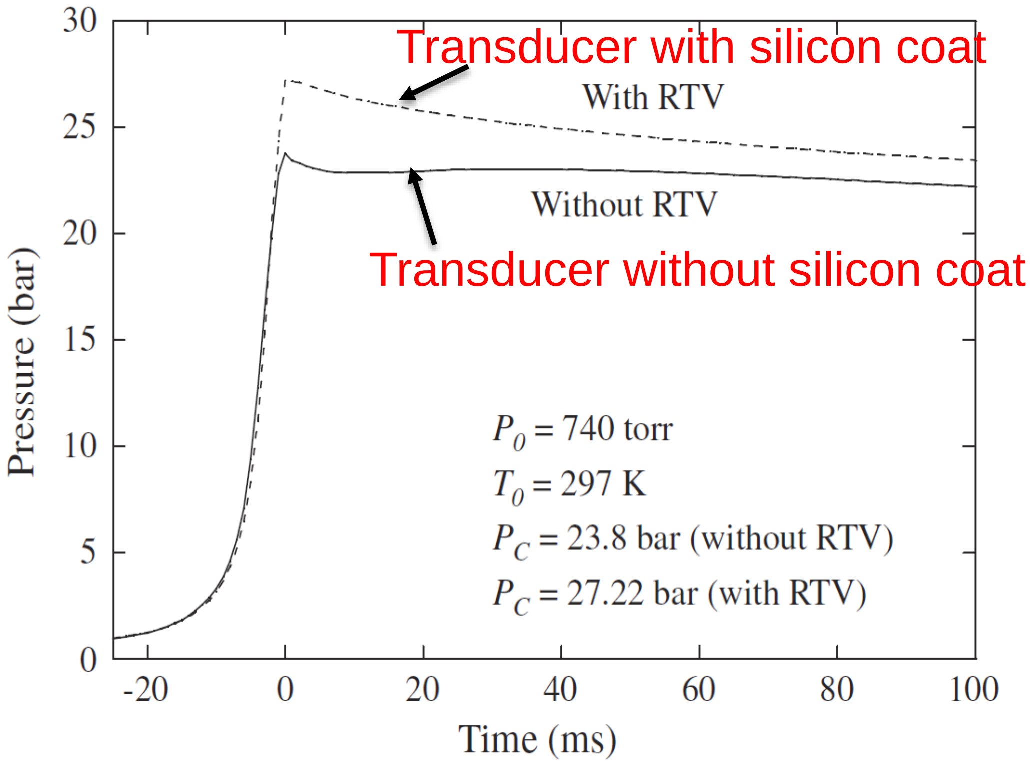
Density contour of Double Mach reflection

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

Plugs/valves have the same curvature with the inner surface of the tube to minimize the flow and shock obstruction



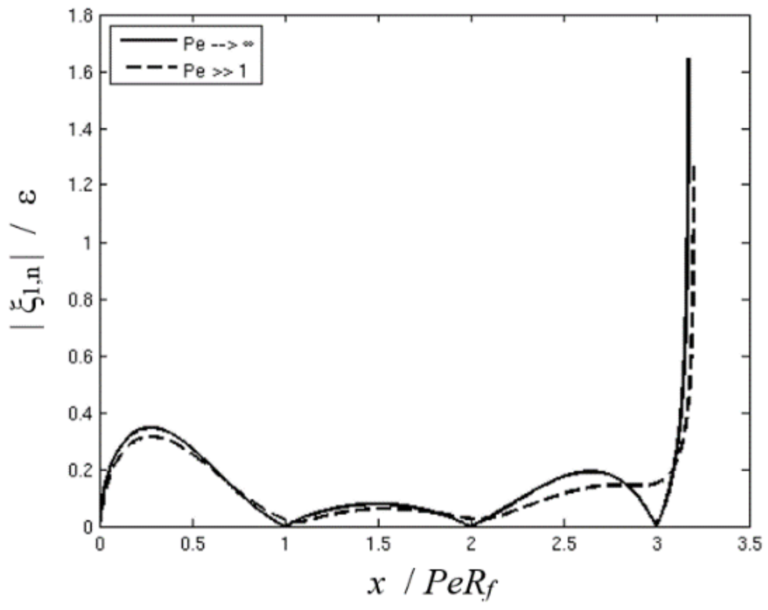
Pressure sensors for measuring the ignition delay

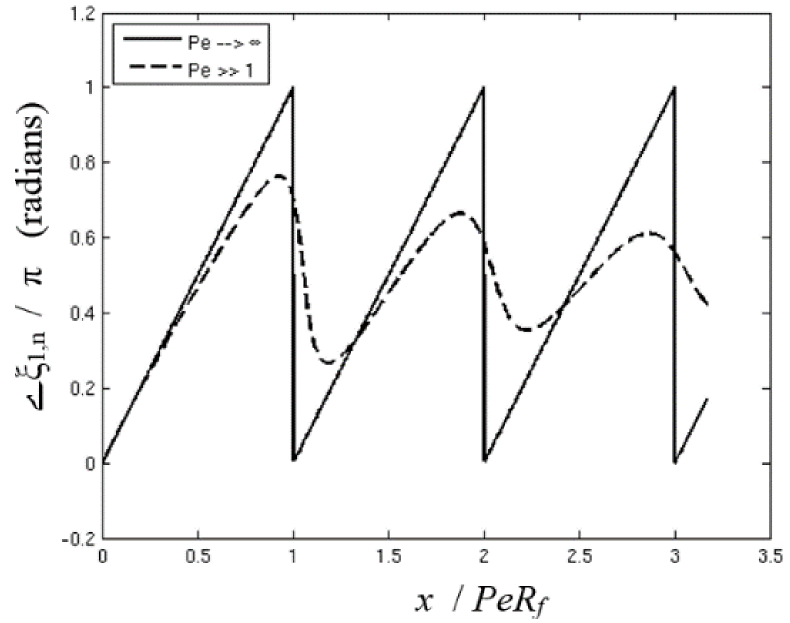


Mittal, Gaurav, and Anil Bhari. "A rapid compression machine with crevice containment." *Combustion and Flame* 160.12 (2013): 2975-2981.

Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

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





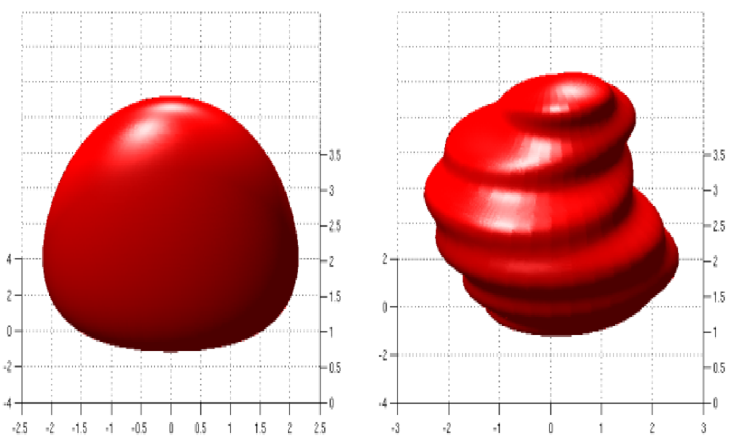
$Pe >> 1$

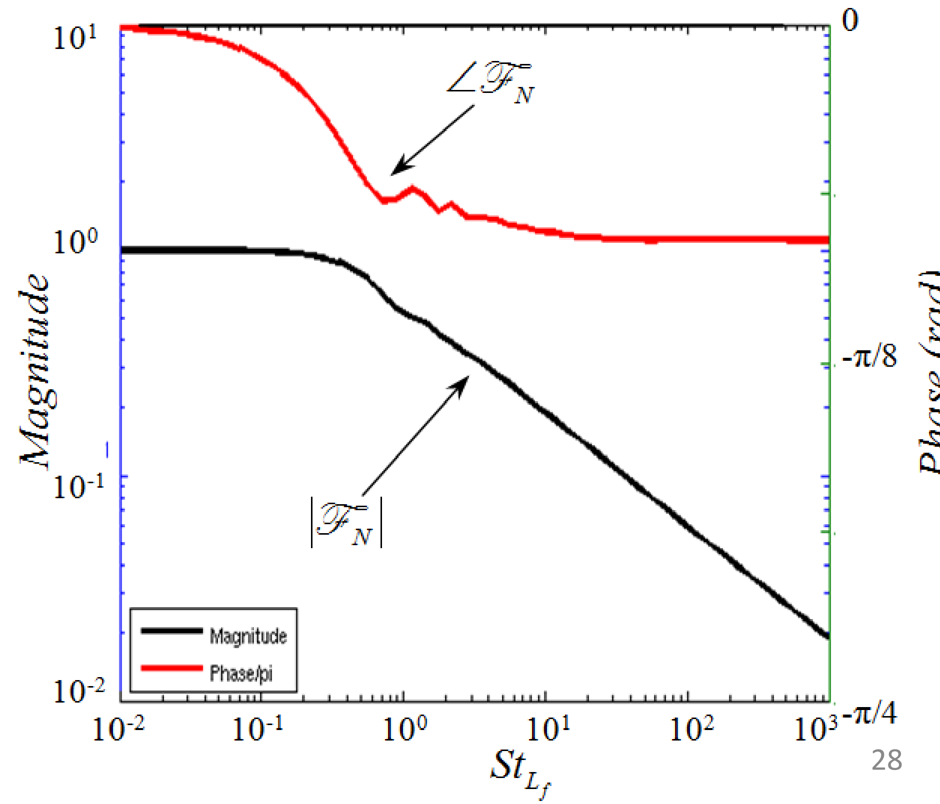
$$\frac{\xi_{1,n}(x,t)}{R_f} = \frac{i\varepsilon\exp[-i\omega t]}{2\pi St}\sin\psi_0(x)\left[1-\exp\left[2\pi iSt\frac{x}{R_f}\right]\exp\left[-\frac{4\pi^2 St^2}{Pe}\frac{x}{R_f}\right]\right]+O\left(\frac{1}{Pe^2}\right)$$

Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

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

$$Q(t) = \int_{flame} h_R \vec{m}_F''' \cdot dS \qquad \mathscr{F} = \frac{\dot{Q}_1 / \dot{Q}_0}{u_{x,1} / U_0}$$





Objectives and Approaches

Objectives:

- Perform fundamental R&D on combustion kinetics and dynamics at supercritical CO_2 power cycle operating conditions for natural gas and syngas
- Focus on key knowledge gaps associated with supercritical CO_2 oxy-combustion including autoignition properties, development of predictive chemical kinetic mechanism, and analyses of flow, mixing, and flame dynamics

Approaches:

- New experiments to generate fundamental data base
- Development of new predictive kinetic mechanism assisted by experiments
- Study of flame/flow stability based on newly developed kinetic mechanism
- Integration of experimental, numerical, and theoretical efforts