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

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Backstory

Combustion Dynamics
Gas-Turbine Research

Shock-tube
Supercritical CO_2 System

LES/DNS
High Performance Computing

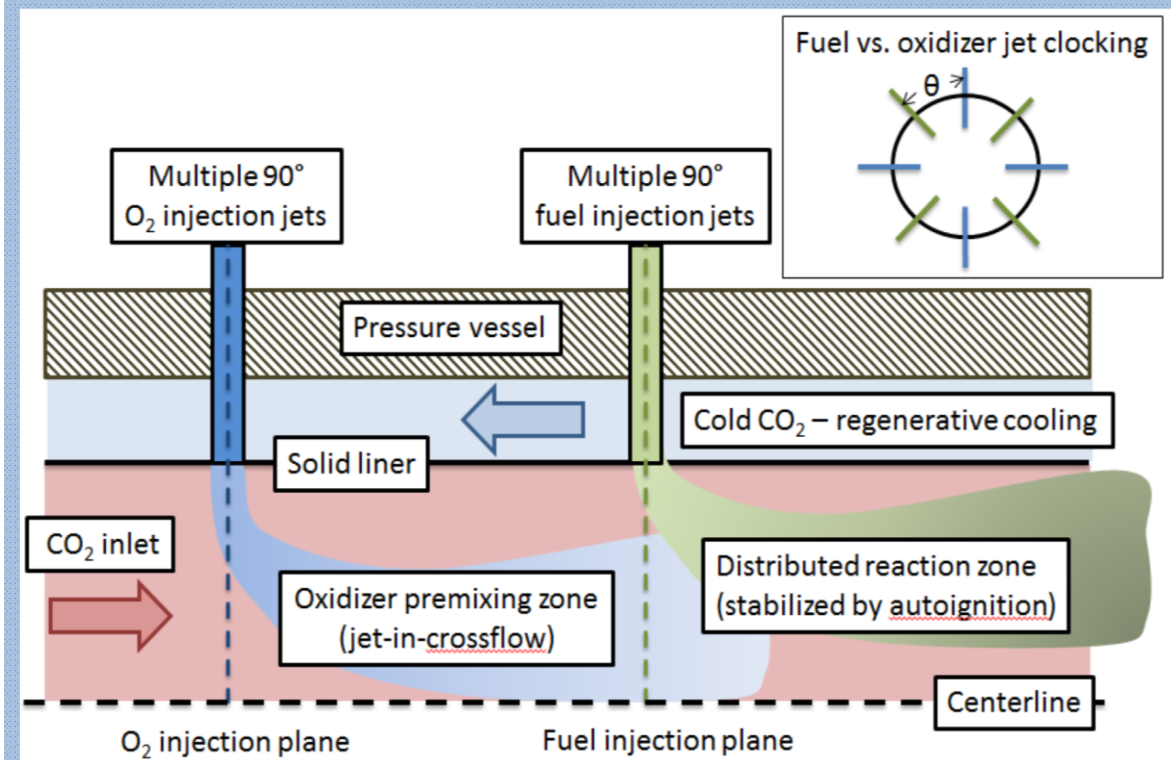
Combustion Chemical Kinetics

Supercritical CO_2 oxy-combustion system

Overview of the Scientific Problem

- What fundamental combustion properties/knowledge we need in order to design combustor for SCO_2 oxy-combustion?
  - Conventional gas turbine combustor won't work

Concept of autoignition stabilized combustor from SwRi



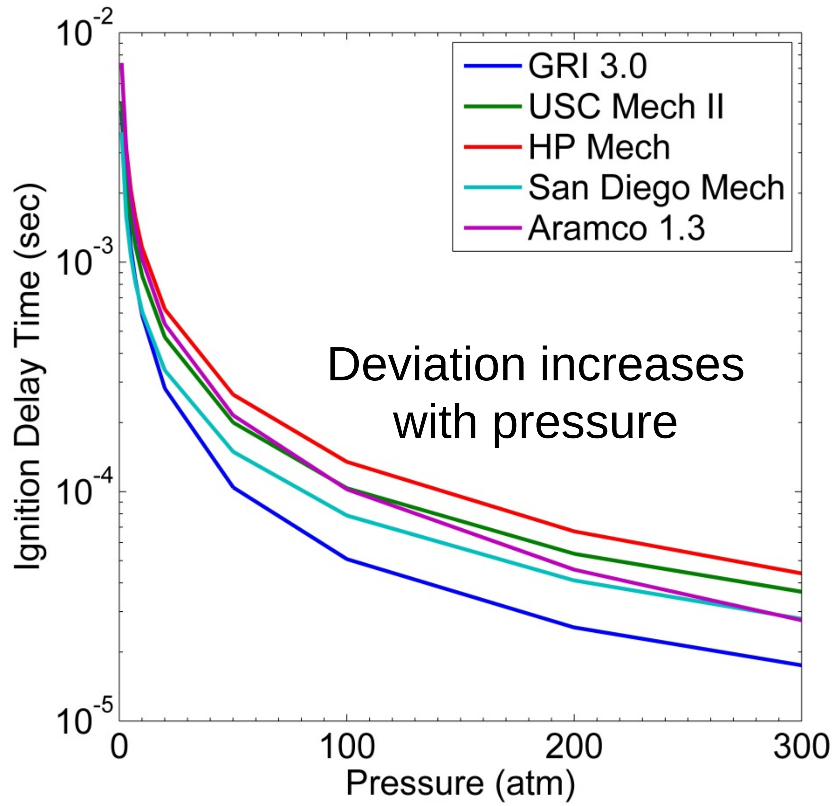
<u>Autoignition delays</u>
and
<u>combustion dynamics</u>
of jet in crossflow

Motivation

- The combustors in high efficiency supercritical CO_2 oxy-combustion power cycles work at conditions we have never reached before (up to 300 atm)

- Corresponding combustor design requires knowledge on combustion kinetics and dynamics at these operating conditions

- We have little understanding at those conditions. Knowledge cannot be extended to new operating conditions (see figure on right)



Predicted autoignition delays of stoichiometric methane/oxygen/carbon dioxide mixture at 1400 K from 1 atm to 300 atm from existing kinetic mechanisms

Overview of the Scientific Questions and Proposed Work

- What is the fundamental combustion properties?
  - 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)

Objectives and Approaches

Objectives:

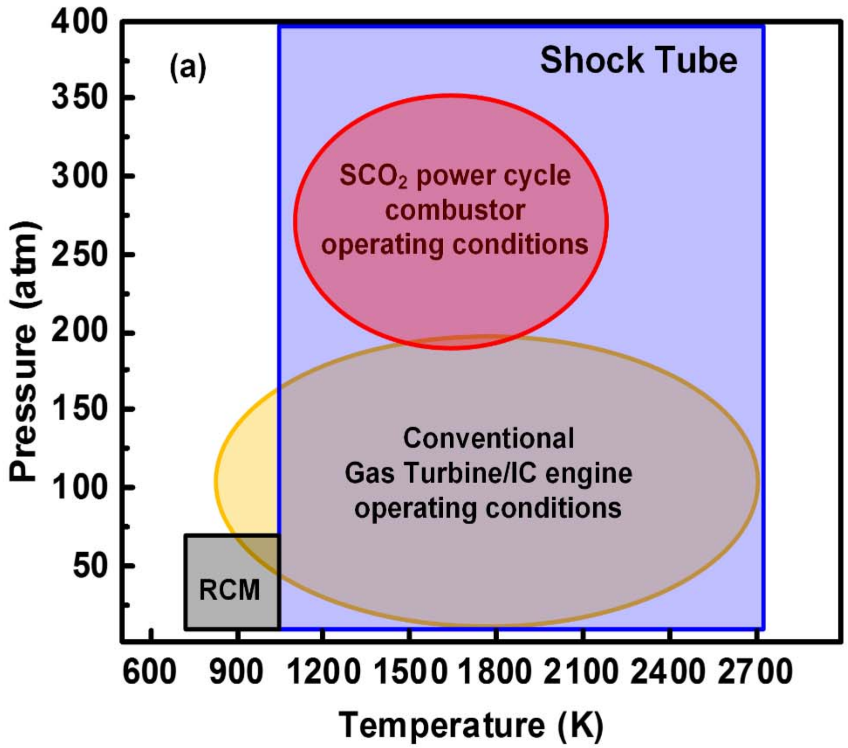
- Perform fundamental R&D on combustion kinetics and dynamics at supercritical CO_2 power cycle operating conditions for natural gas and syngas
- Focus on key knowledge gaps associated with supercritical CO_2 oxy-combustion including autoignition properties, development of predictive chemical kinetic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

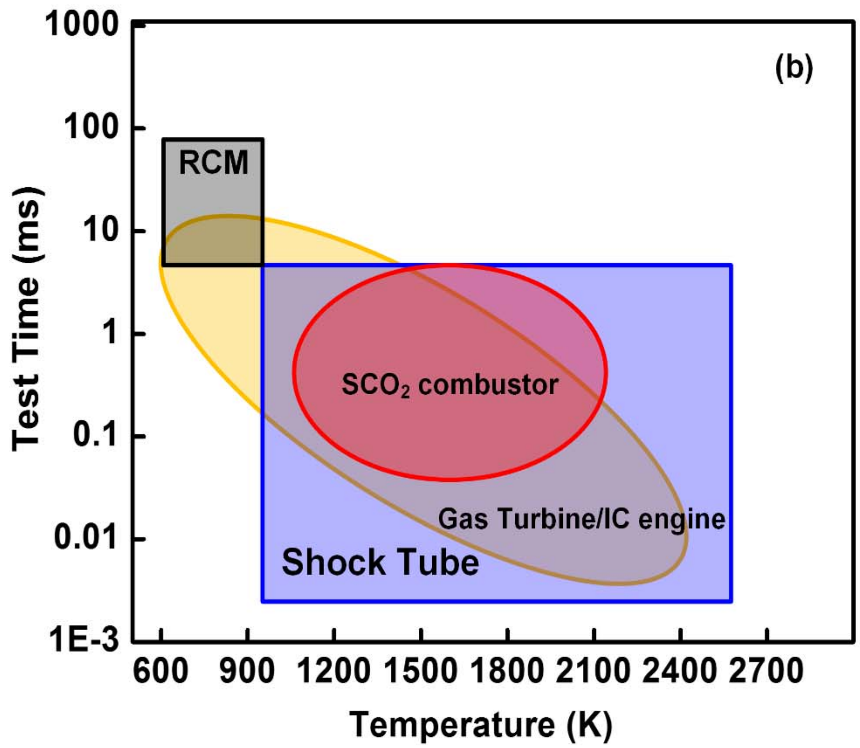
Approach:

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

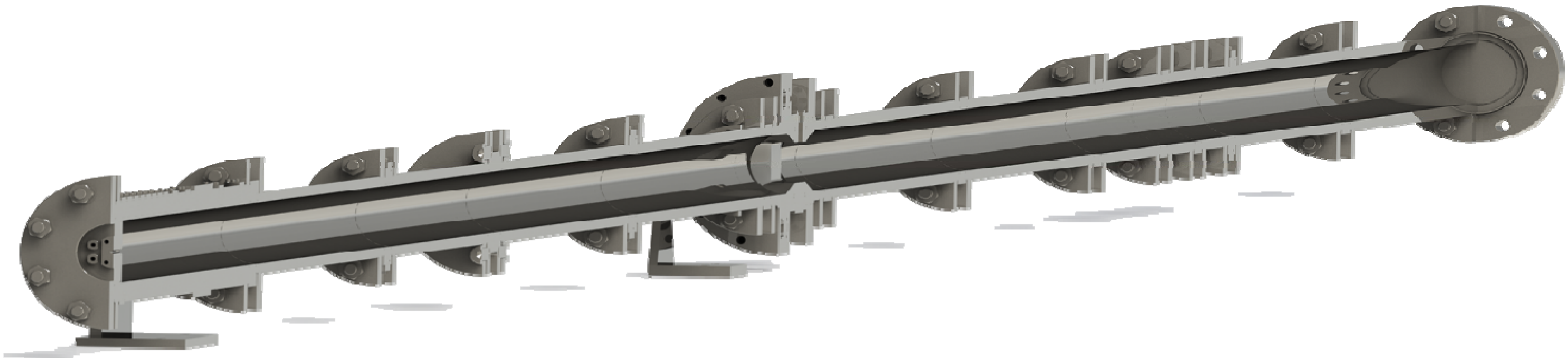
Task 1: Development of a High Pressure Shock Tube for Combustion Studies

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





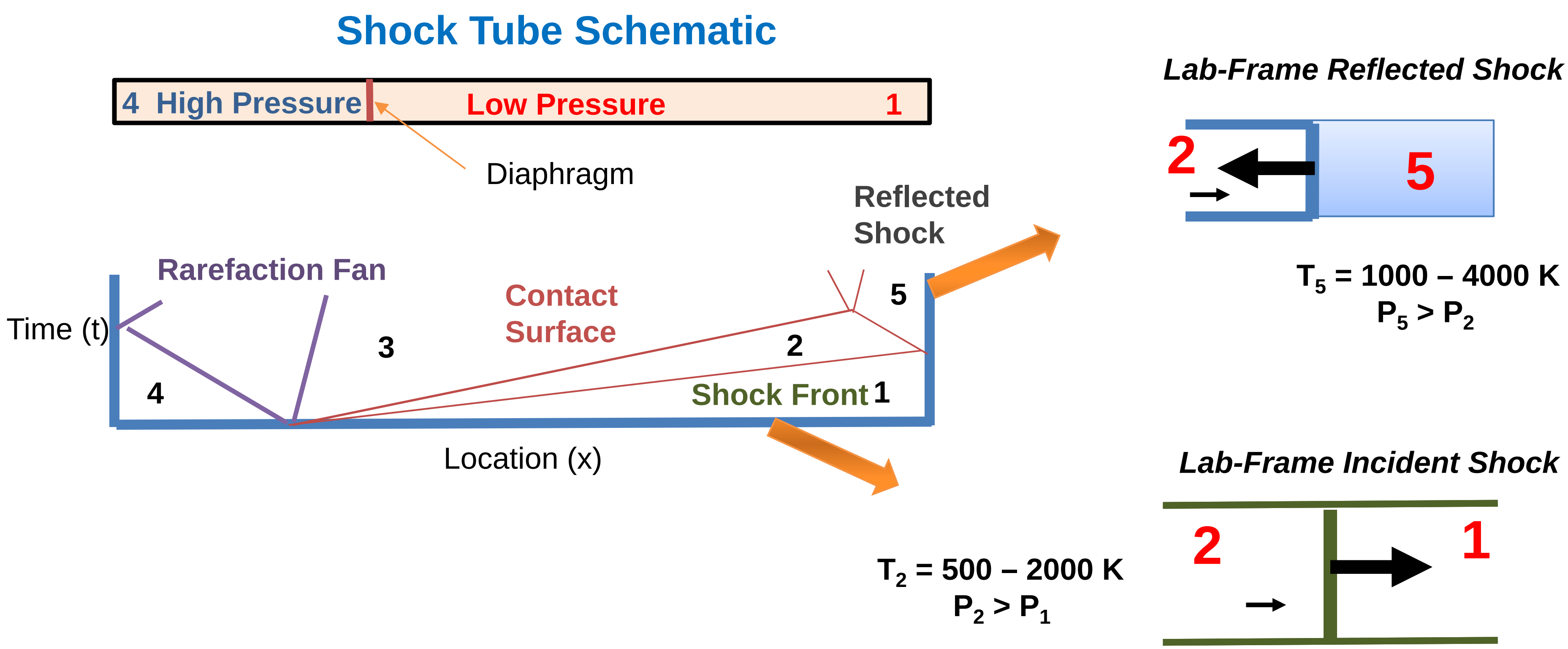
Task 1: Development of a High Pressure Shock Tube for Combustion Studies



- Georgia Tech shock tube for fundamental autoignition study is under construction
- Wide pressure range (P up to 300 atm)
- It will be <u>the longest one in US</u> (150 mm ID, 20 m long) for combustion research

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

Basics regarding the shock-tube:



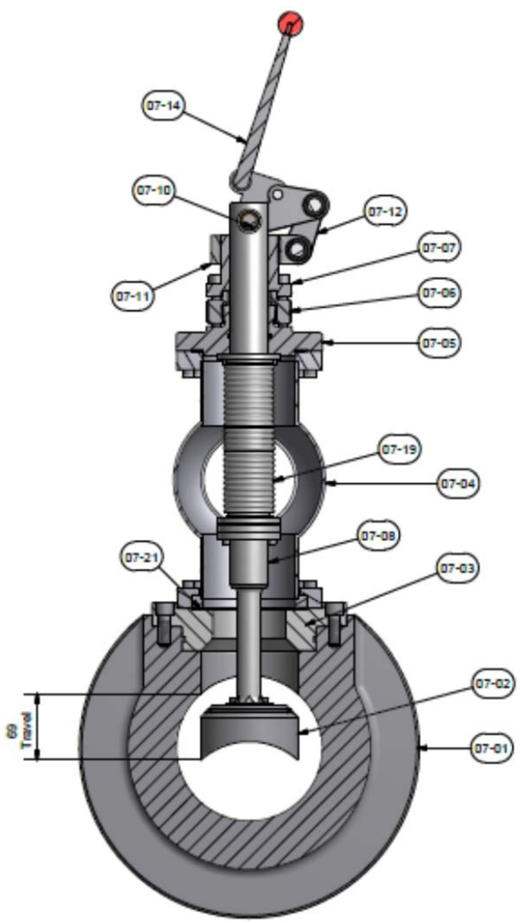
Task 1: Development of a High Pressure Shock Tube for Combustion Studies

Key Capability of the GT Shock-tube

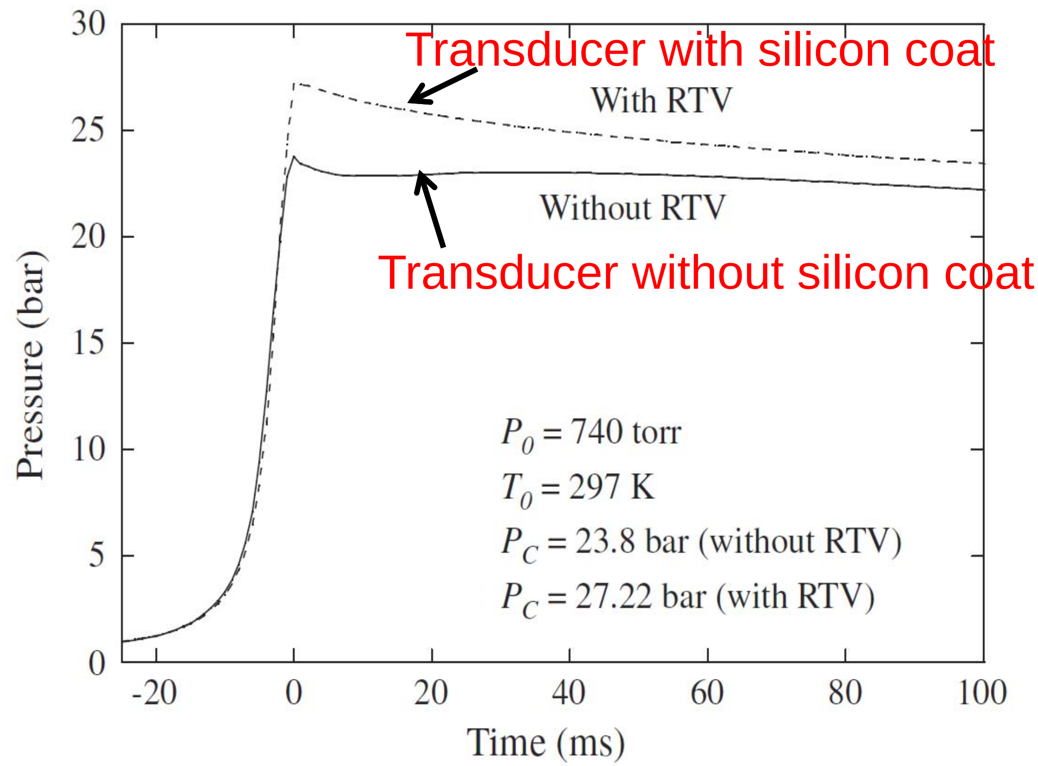
- Large internal bore (15.24 cm)—to minimize the boundary layer effect (very critical at high pressure conditions)
- It will be <u>the longest one in US</u> (10 m driver and driven section) for combustion research
- Test time 50 ms (can achieve high value with modification of driver gas mixture)
- Diaphragm section replicate the current design in the operational shock-tube for turbulent mixing study
- Test pressure 355 bar
- 473 K 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
- Emission and pressure can be measured from end wall as well as from side wall
- Diagnostic capability to understand the non-ideal effects in the shock-tube

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

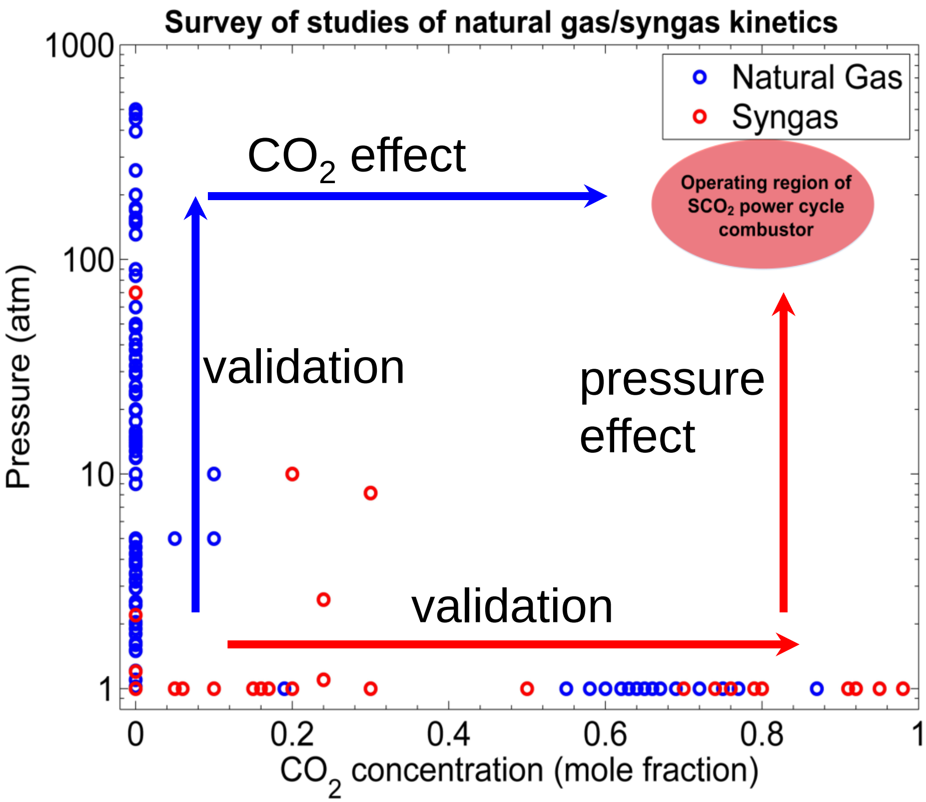


Kistler pressure sensors for measuring the ignition delay



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

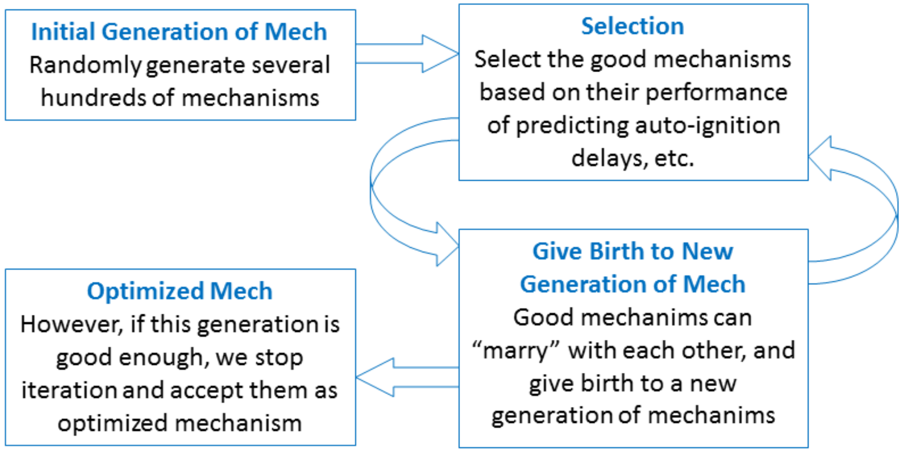
- Autoignition properties have never been investigated before in region of interest (see figure on right)
- This task will investigate critical autoignition properties of natural gas and syngas diluted by CO_2 in region of interest <u>for the first time</u>
- Approach for high quality data:
  - Repeat existing experiments for validation
  - Ramp up pressure to study pressure effect
  - Ramp up CO_2 dilute concentration to study CO_2 dilution effect



Survey of existing studies of natural gas and syngas combustion kinetics

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

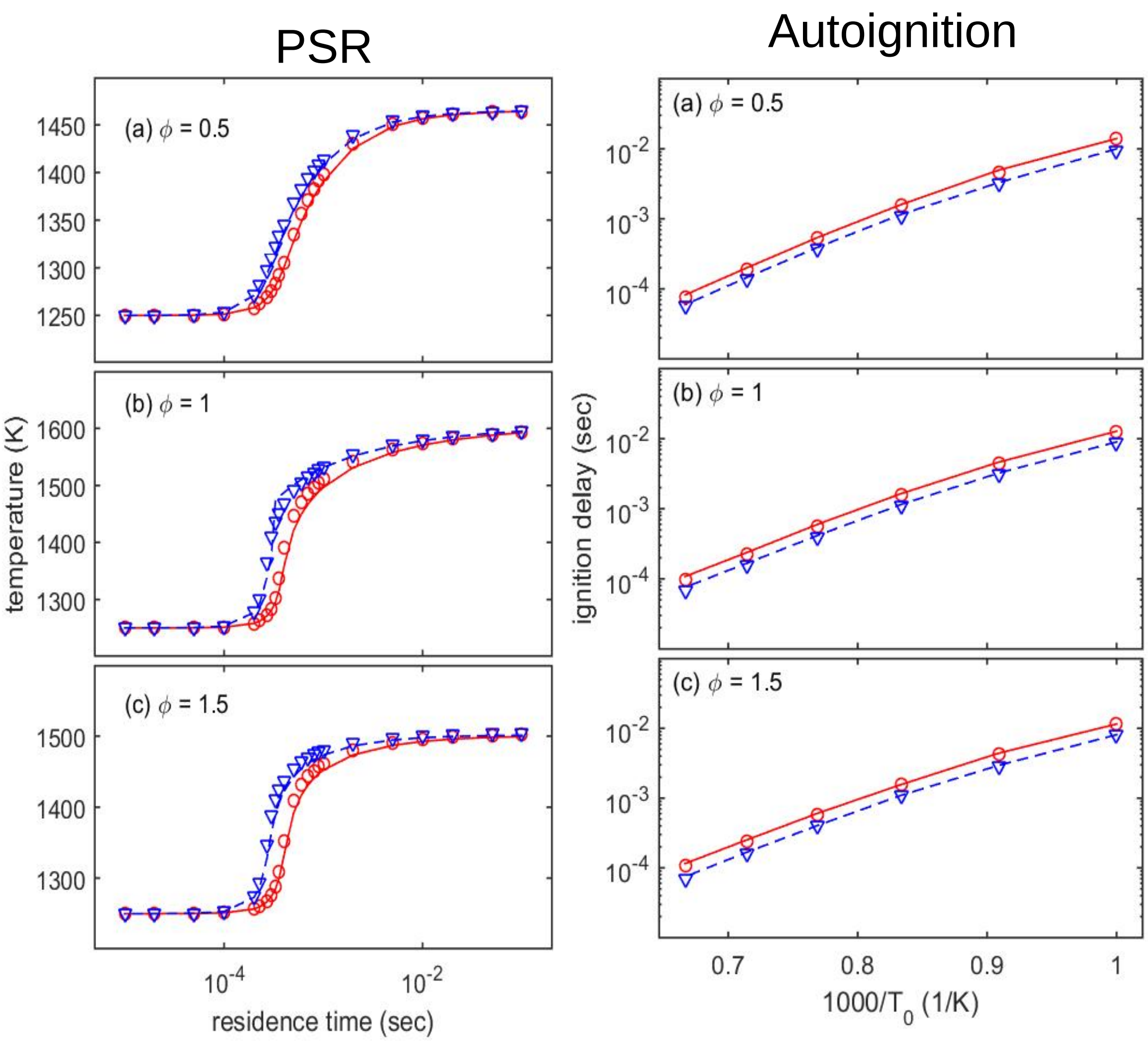
- In this task, an optimized, validated and compact chemical kinetic mechanism shall be developed
- This mechanism will then be used in CFD modeling to study combustion stability at relevant conditions
- Approach: optimize chemical kinetic mechanism based on experimental data obtained in task 2.



Flow chart of using Genetic Algorithm to optimize chemical kinetic mechanisms

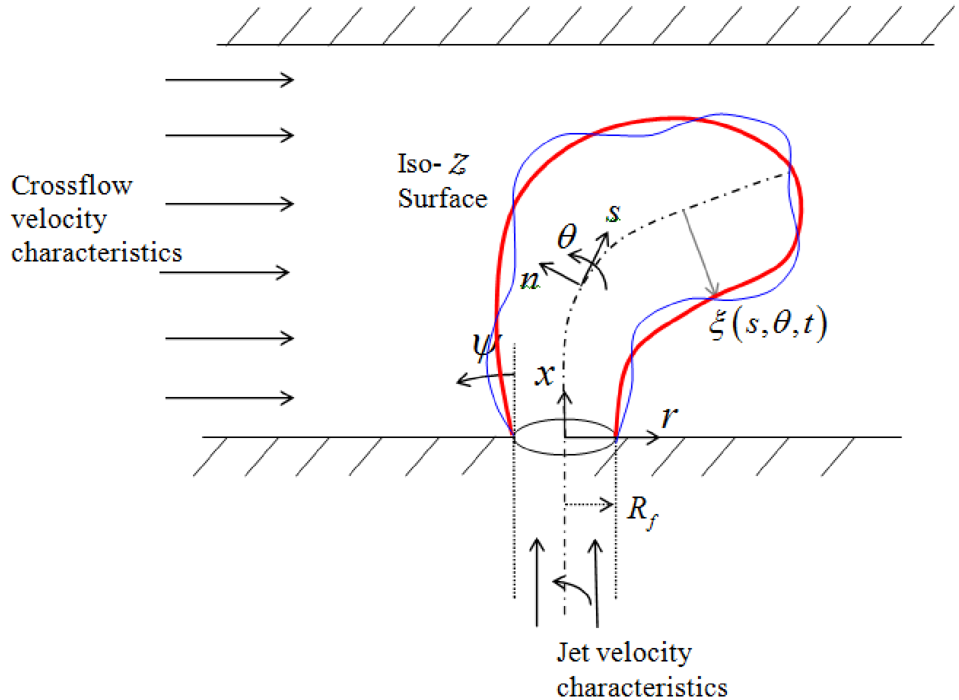
Task 3: Development of a Compact and Optimized Chemical Kinetic Mechanism for SCO_2 Oxy-combustion

- Comparing to existing high pressure autoignition delay data, USC Mech II has the best agreement. So it is used as a starting point for future optimized mechanism for SCO_2 oxy-combustion
- A 27 species reduced mechanism for natural gas (CH_4/C_2H_6) is developed
- Comparison of the results from reduced (marker) and detailed mech (line). Solid lines (p = 200atm), dashed line (p = 300atm)



Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

- The analytical work shall focus on physics based models of high pressure reacting jets 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

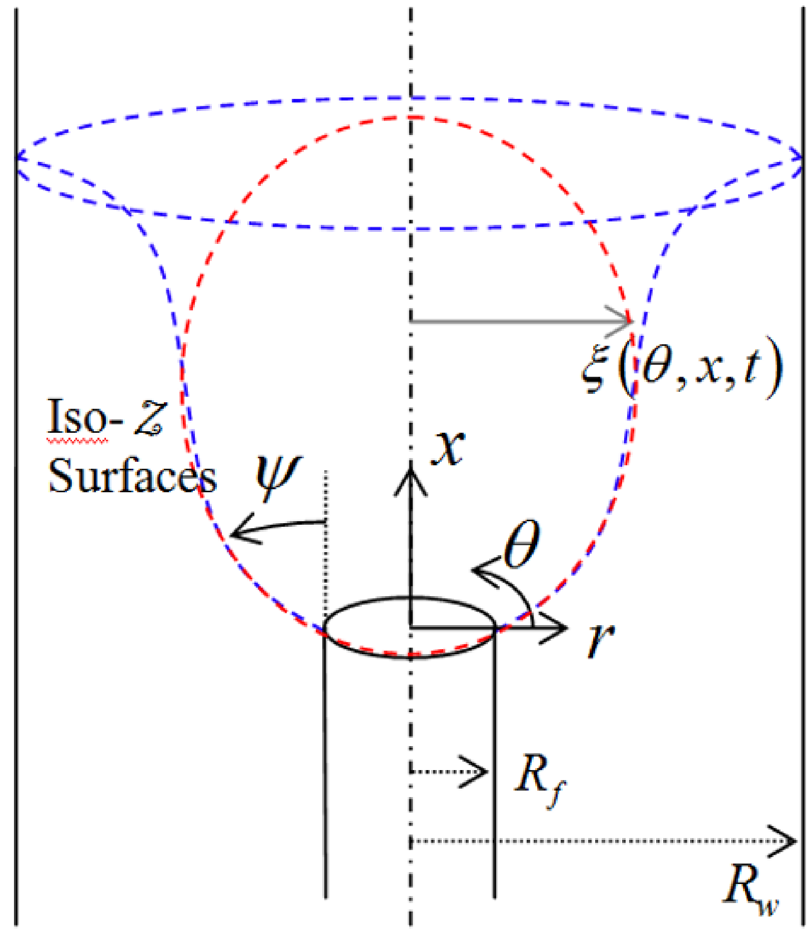
- Established model: Mixture fraction formulation

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

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

→ $\xi(x, \theta, t)$

→ 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).

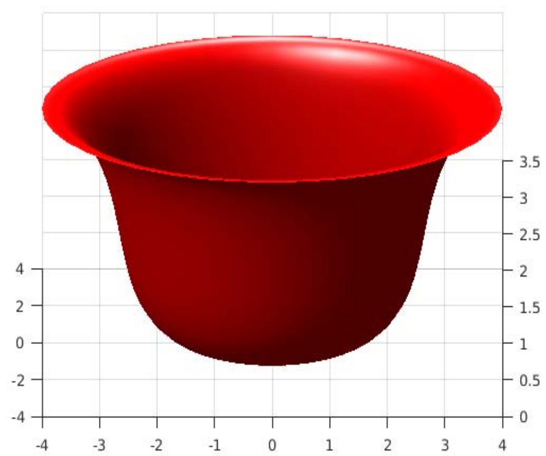
Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

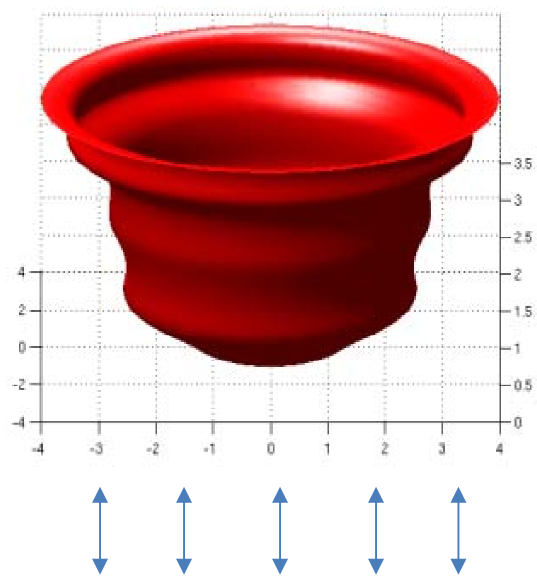
- **Solution: Space-Time Dynamics of $\mathcal{Z}_{st}$ Surface**

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

$Pe >> 1$

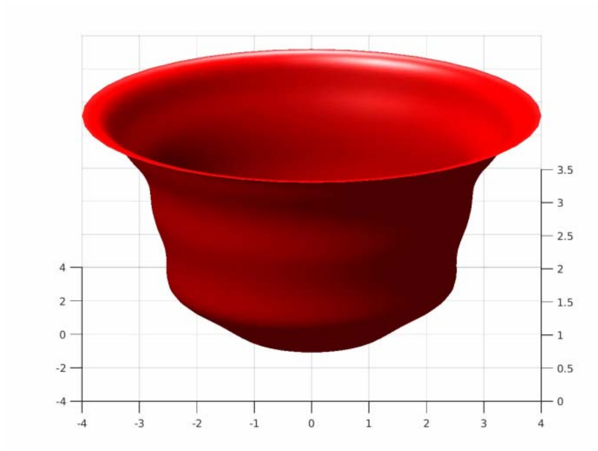
$$\frac{\xi_{1,n}(x,t)}{R_f} = \frac{i\varepsilon \exp[-i\omega t]}{2\pi St} \sin\psi_0(x)\left[1-\exp\left[2\pi i St \frac{x}{R_f}\right]\exp\left[-\frac{4\pi^2 St^2}{Pe}\frac{x}{R_f}\right]\right] + O\left(\frac{1}{Pe^2}\right)$$

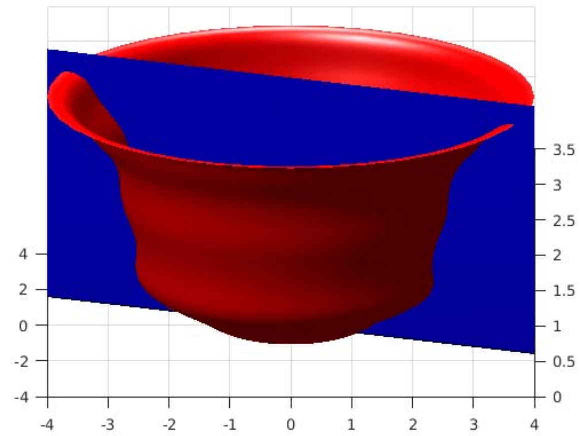


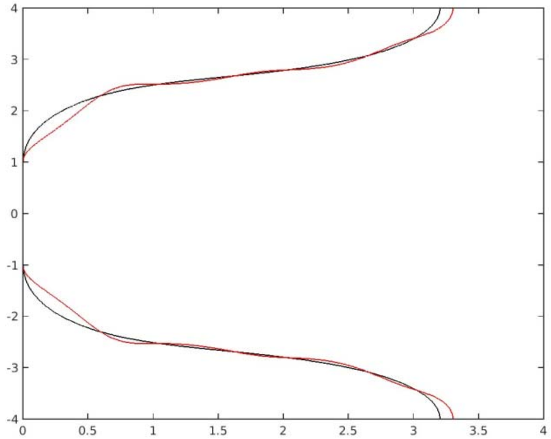


Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

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

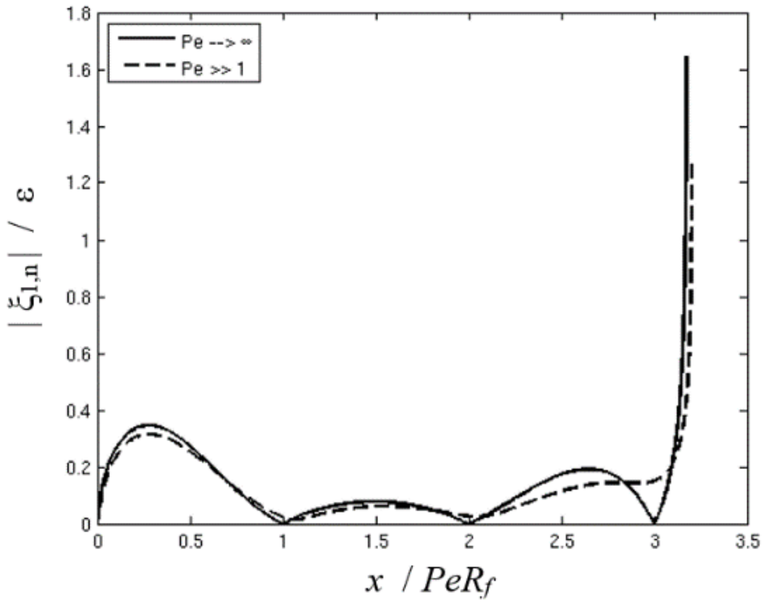


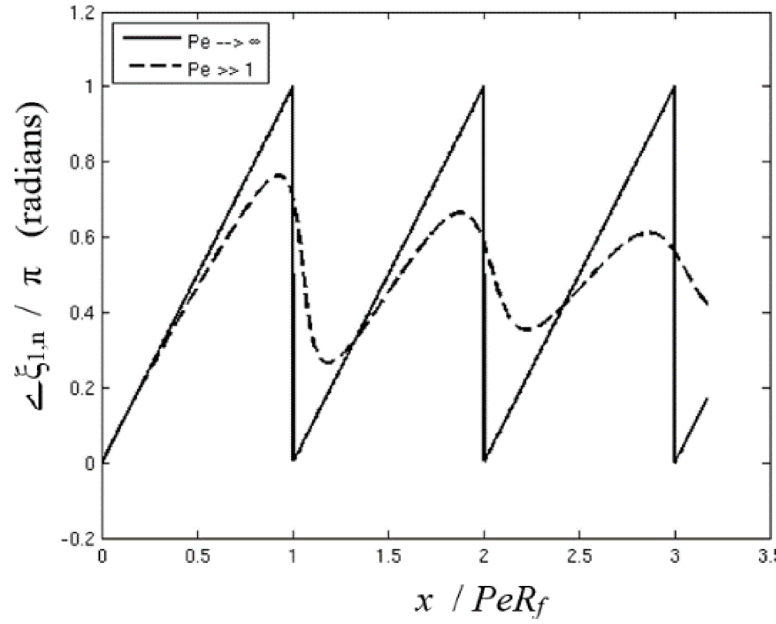




Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

- **Solution: Space-Time Dynamics of Z_{st} Surface**





$Pe >> 1$

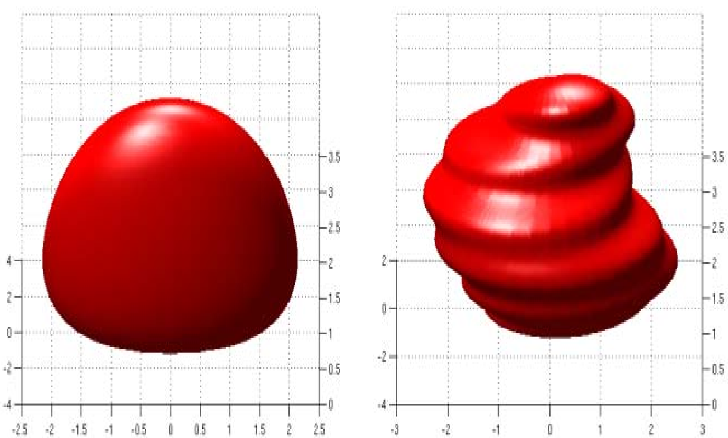
$$\frac{\xi_{1,n}(x,t)}{R_f} = \frac{i\varepsilon \exp[-i\omega t]}{2\pi St} \sin\psi_0(x) \left[1 - \exp\left[2\pi i St \frac{x}{R_f} \right] \exp\left[-\frac{4\pi^2 St^2}{Pe} \frac{x}{R_f} \right] \right] + O\left(\frac{1}{Pe^2} \right)$$

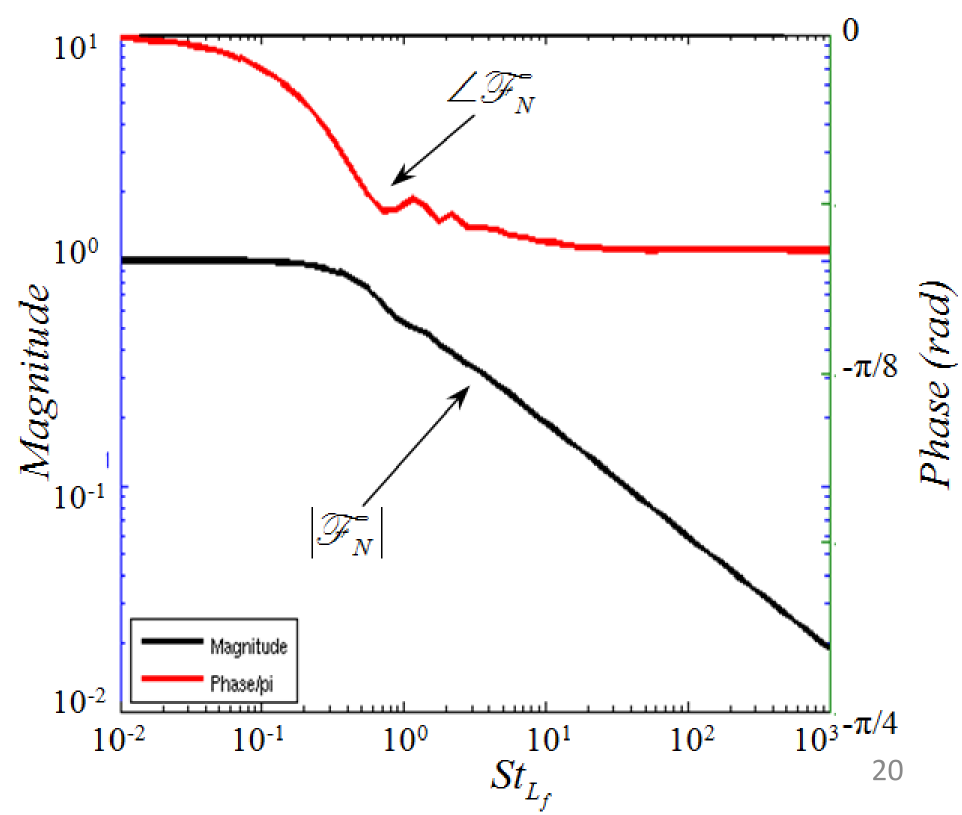
Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

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

$$Q(t) = \int_{flame} h_R \dot{\vec{m}}_F''' \cdot dS$$

$$\mathscr{F} = \frac{\dot{Q}_1 / \dot{Q}_0}{u_{x,1} / U_0}$$



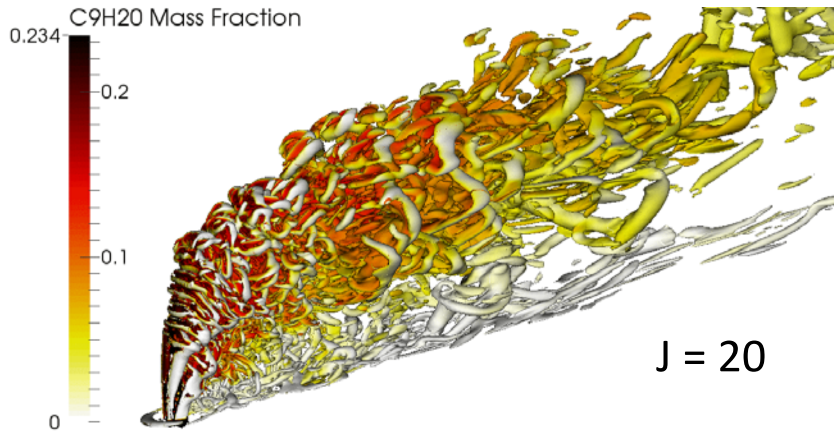


Key Goals of Task 4

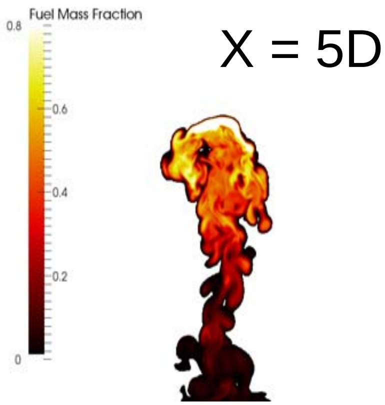
- Determine the gain-phase relationship between flow disturbances and heat release oscillations
- Use model profiles extracted from other jet in crossflow data
- Computed time averaged flow and flame features
- Account for supercritical effects on diffusion coefficients

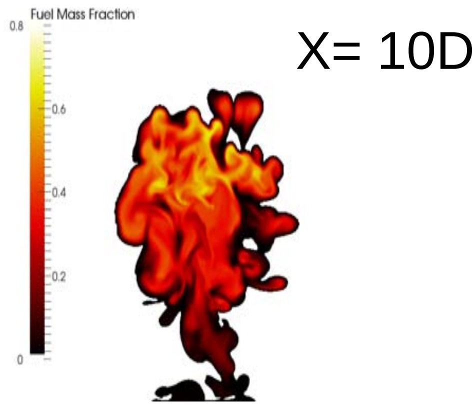
Task 5: LES Studies of Supercritical Mixing and Combustion

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



Vorticity Contours in supercritical Kerosene in air



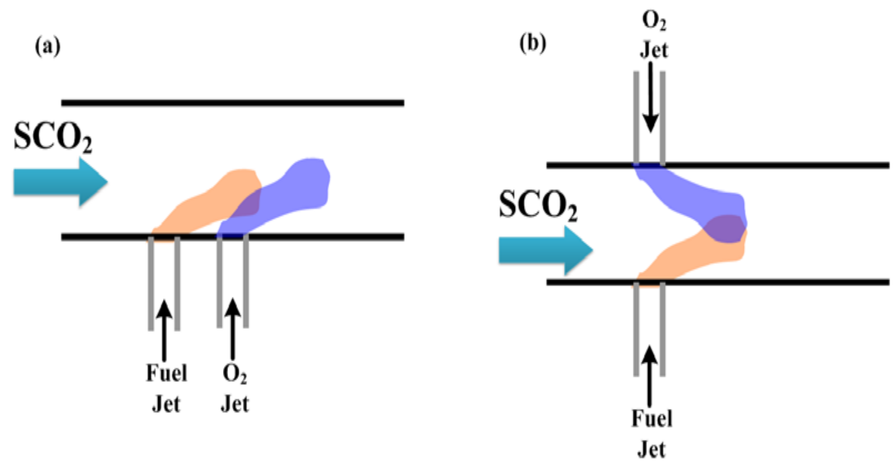


- LES capability exists to simulate supercritical mixing and reacting flows
- Uses Peng-Robinson EOS and real gas properties with finite-rate kinetics
- Simulations to be used to study mixing and combustion between sCO2, fuel/air

Vaporized fuel mass fraction at two axial locations

Task 5: LES Studies of Supercritical Mixing and Combustion

- Task 5a: Simulate supercritical mixing in JICF for experimental setup and conditions
- Task 5b: Implement optimized kinetics form 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)

Deliverables

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