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

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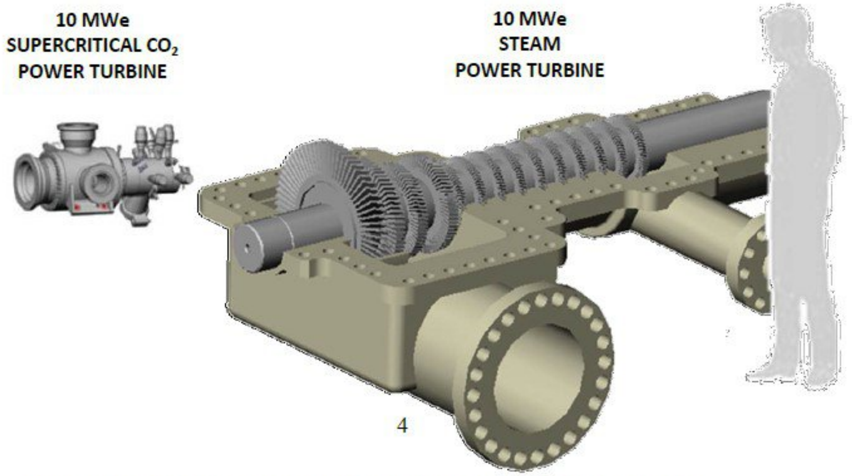
UTSR Project: DE-FE0025174 PM: Seth Lawson

2016 UTSR Project Review Meeting

Background of Directly Fired Supercritical CO_2 cycle

- High plant conversion efficiencies (~52% LHV) with ~100% carbon capture
- Lower electricity cost (by ~15%)
- Supercritical CO_2 (sCO_2) is a single-phase working fluid
  - No thermal fatigue or corrosion as in 2-phase flow (e.g., steam)

- Compact Systems possible
- Many challenges on combustion to address to develop system
  - Kinetics
  - Dynamics



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/

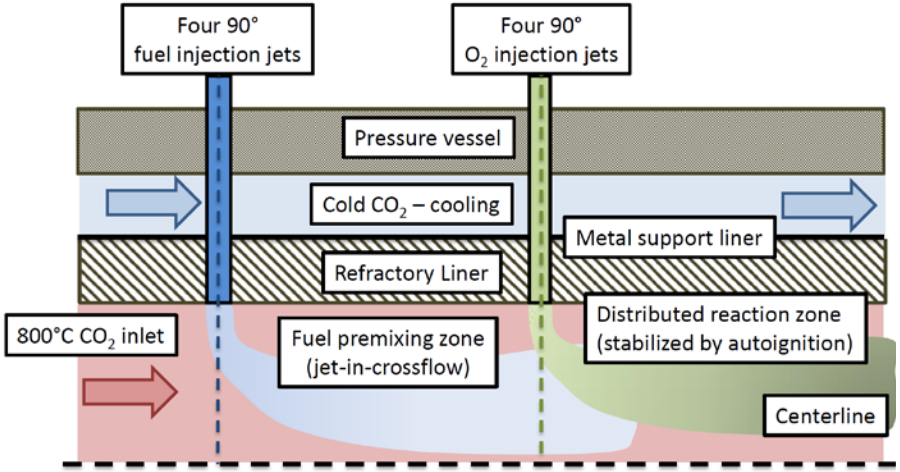
Overview of the Scientific Problem

- 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, severe thermal environment for fuel injector and flame holder
  - Mechanical strength (pressure)
  - Thermal strength (cold fuel, hot process)
  - Difficulty to meet 30,000 hours of operation
  - Nickel super alloys are limited to creep rupture strengths of 41 atm, less than 1,280 K

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

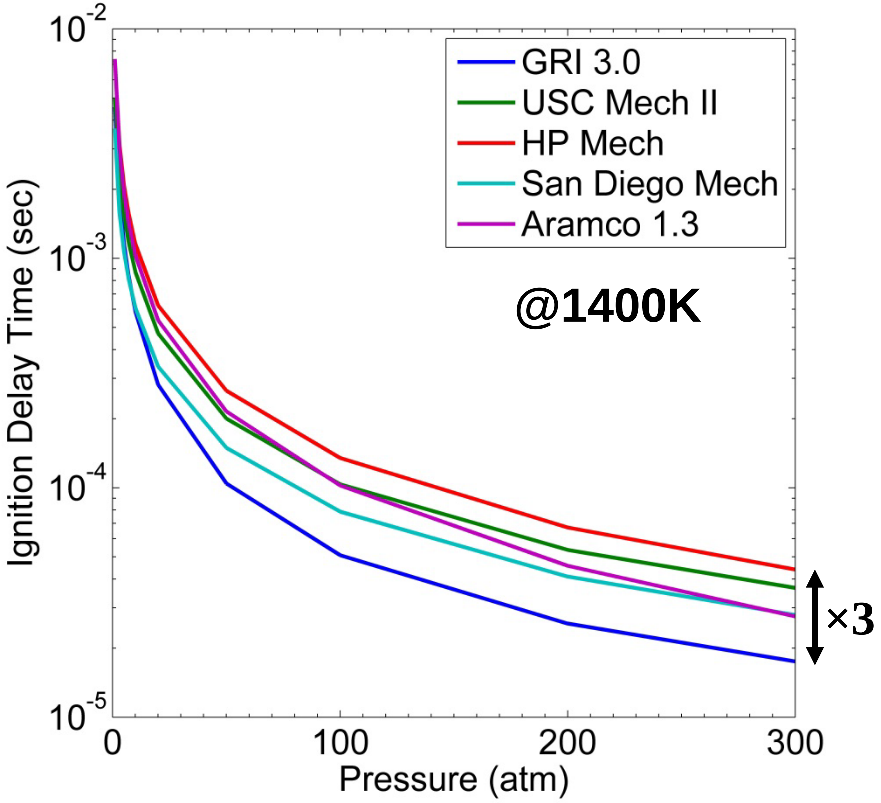
Concept of autoignition stabilized combustor*



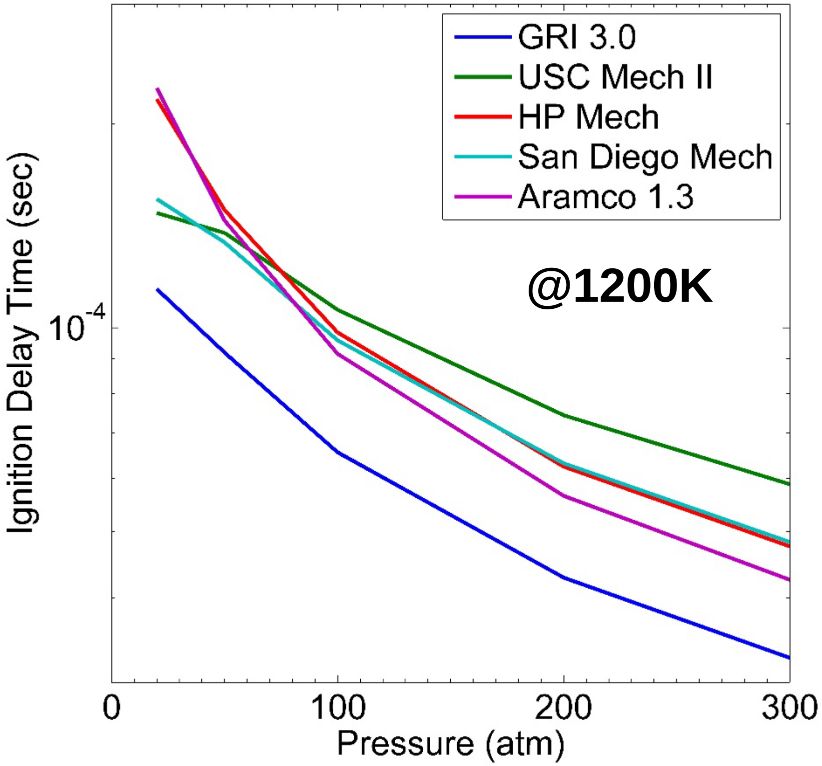
*J.Delimont, A. McClung, M. Portnoff, 2016 sCO2 symposium

Kinetic Challenges for sCO_2-fuel-O_2 Mixtures

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



$CH_4/O_2/CO_2$ (9.5%:19%:71.48%)



$H_2/CO/O_2/CO_2$ (14.8%:14.8%:14.8%:55.6%)

More intriguing results later !!

Overview of the Scientific Questions and Proposed Work

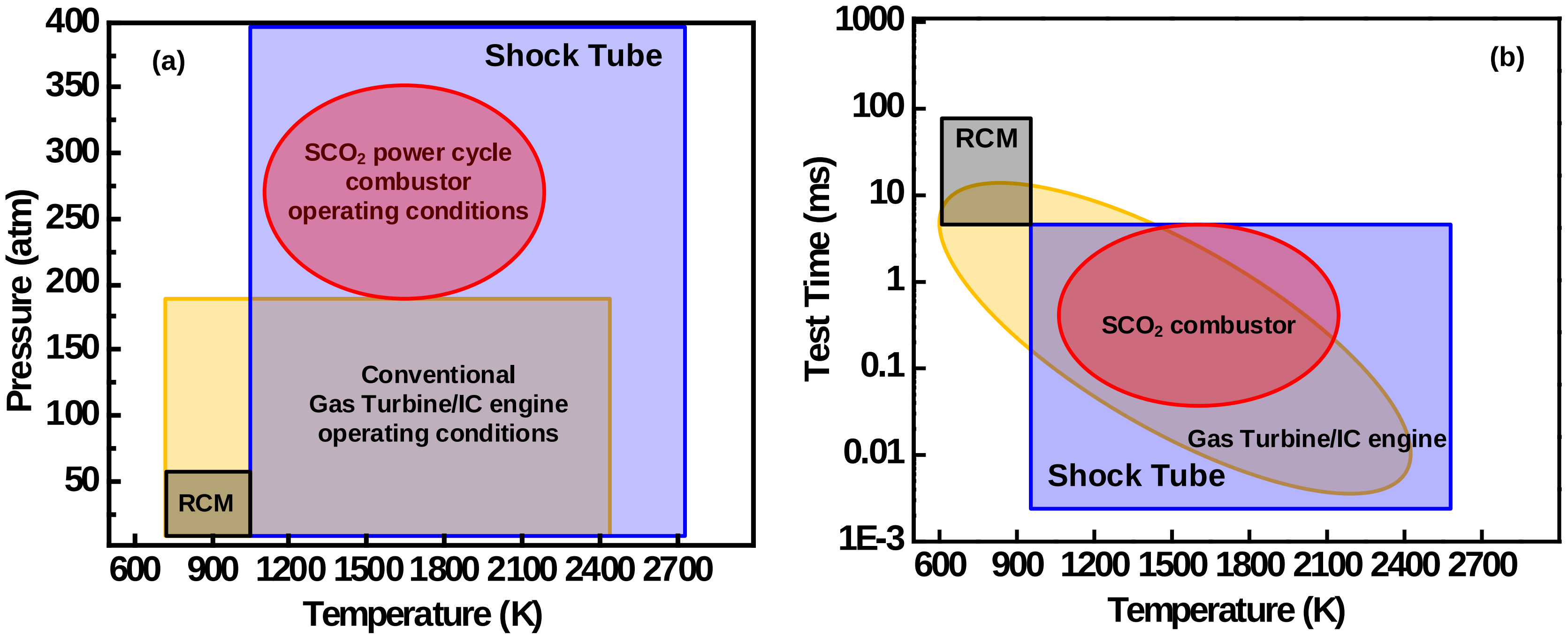
- What is the fundamental combustion properties?
  - Experimental investigation of chemical kinetic mechanisms for sCO_2 Oxy-combustion (Task 1&2: Ranjan & Sun)

- How can we use the kinetic model 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?

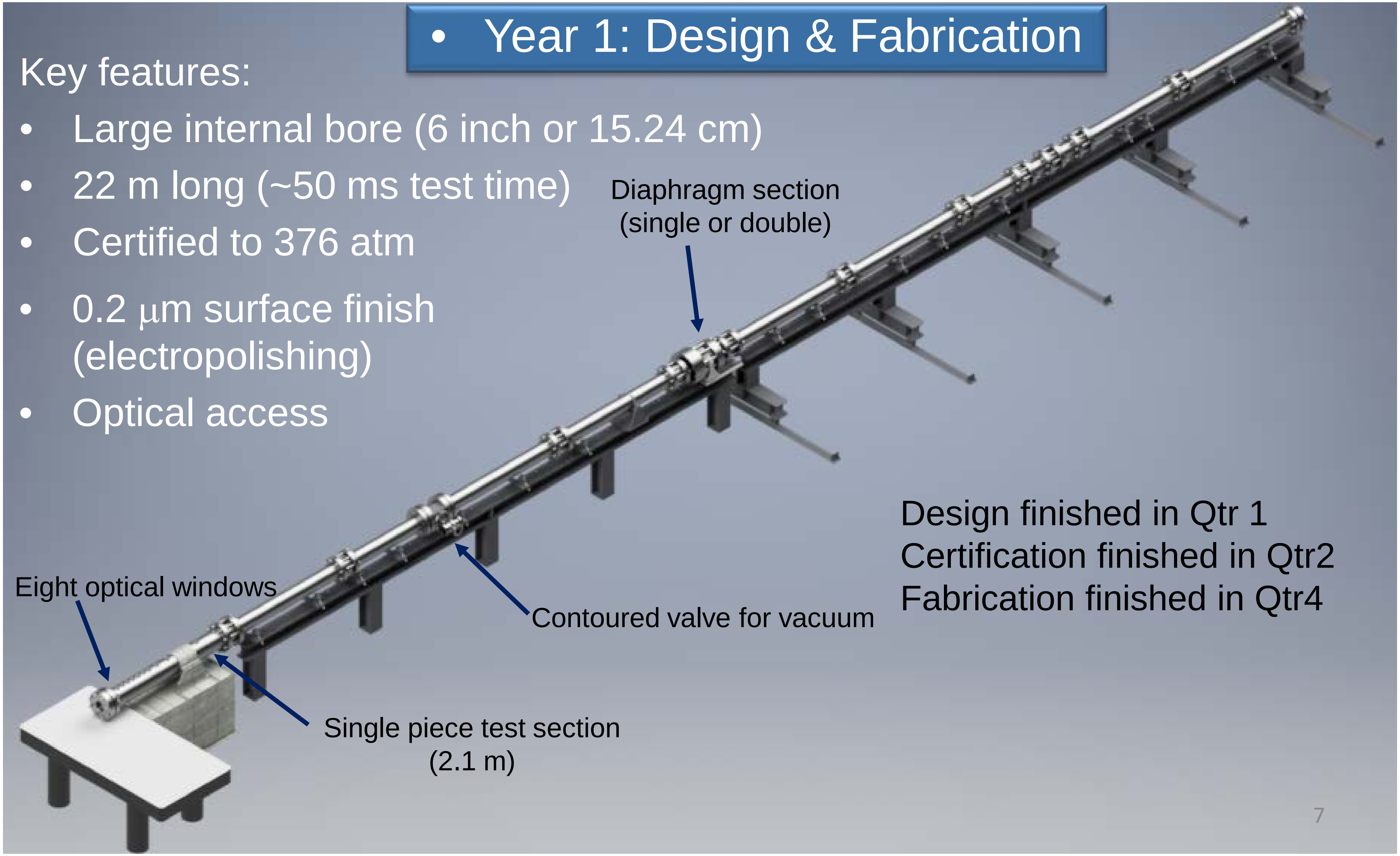


Task 1: Development of a High Pressure Shock Tube for Combustion Studies

- Year 1: Design & Fabrication

Key features:

- Large internal bore (6 inch or 15.24 cm)
- 22 m long (~50 ms test time)
- Certified to 376 atm
- 0.2 µm surface finish (electropolishing)
- Optical access



Diaphragm section (single or double)

Contoured valve for vacuum

Eight optical windows

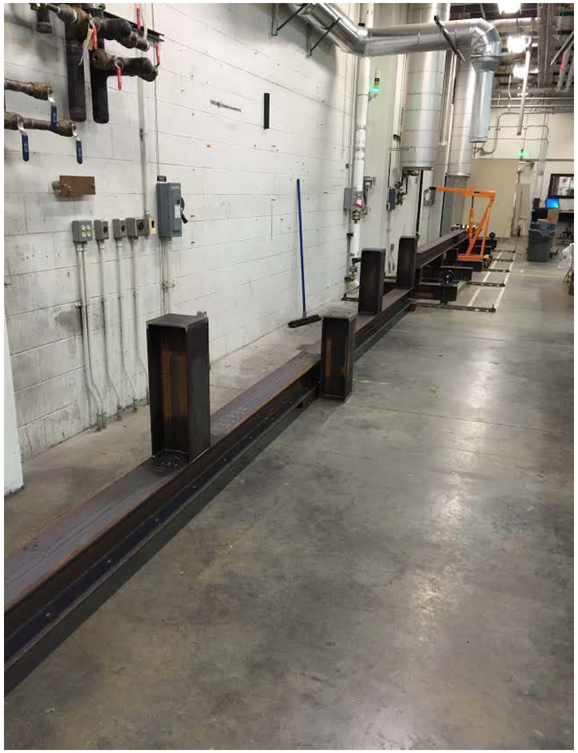
Single piece test section (2.1 m)

Design finished in Qtr 1
Certification finished in Qtr2
Fabrication finished in Qtr4

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

March 2016

April 2016



May 2016
Supporting frame installation

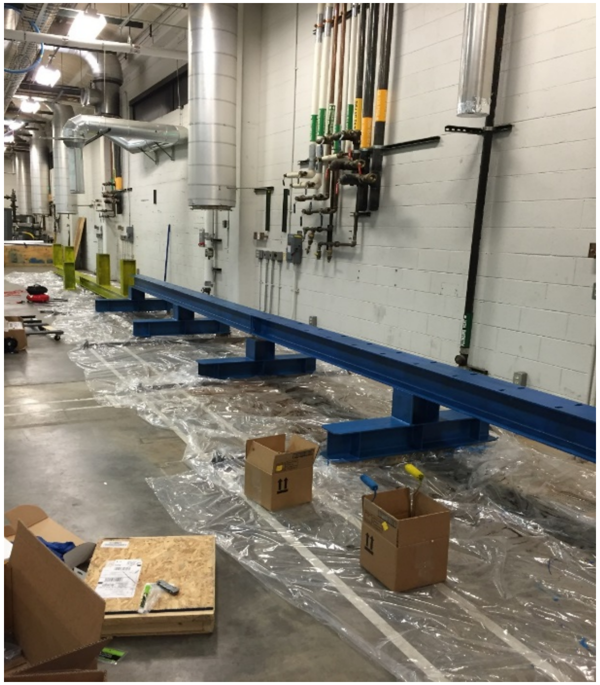
Task 1: Development of a High Pressure Shock Tube for Combustion Studies

Machining of test section

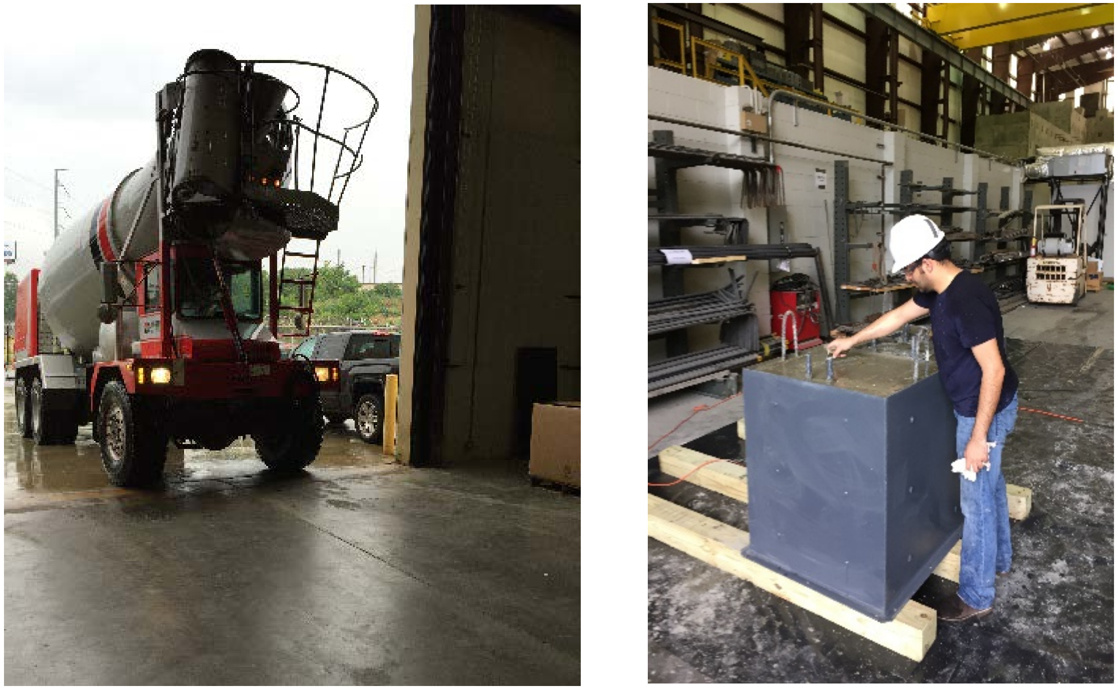
Dead mass metal casing delivering to GT

April 2016

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



Paintings supporting frame



Filling dead mass casing with reinforced concrete

May & June 2016

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

- Tube assembled for certification
- Hydraulic Tested at 376 atm
- Sent out for electropolishing

May & June 2016

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

- Anchoring supporting frame and dead mass
- Installing supporting wheels
- Waiting for the arrival of shock tube

July & Aug. 2016

Arrived!

- After tons of paper work and coordination

Sept. 2016

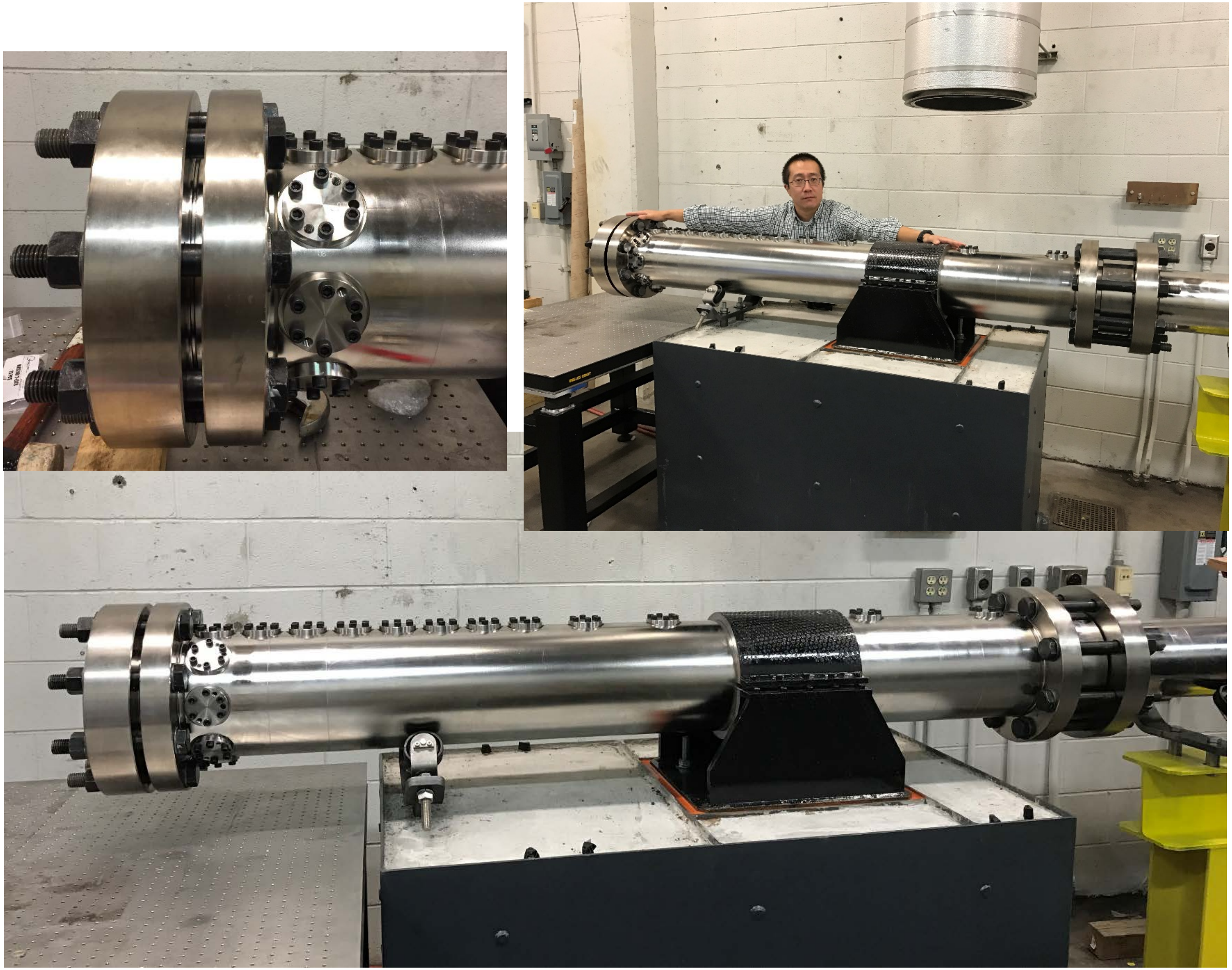
Here It Is!

Driven side view

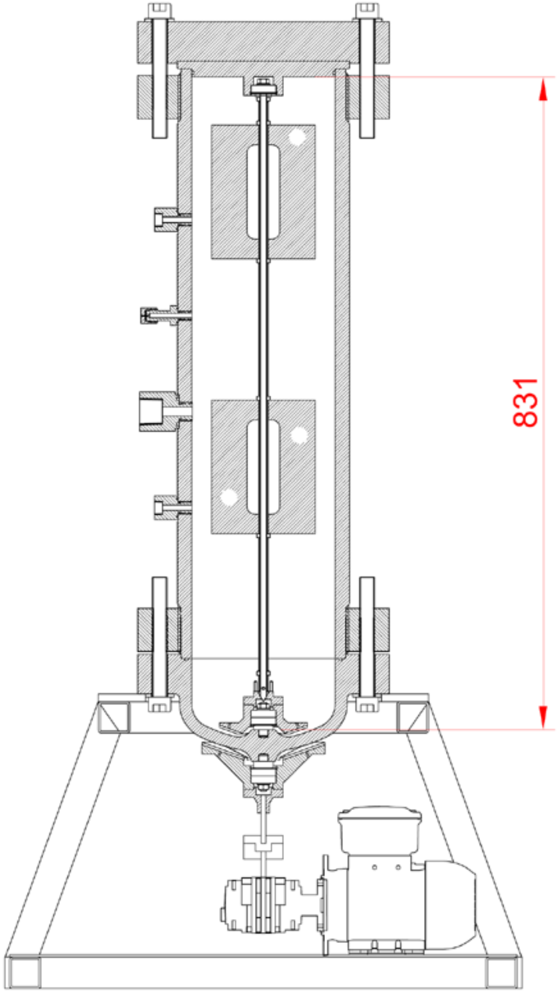
Driver side view

Oct. 2016

Test Section



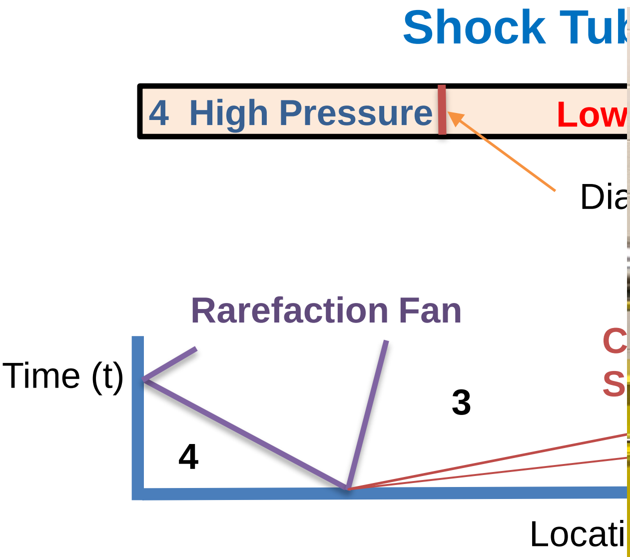
Mixture Preparation Tank

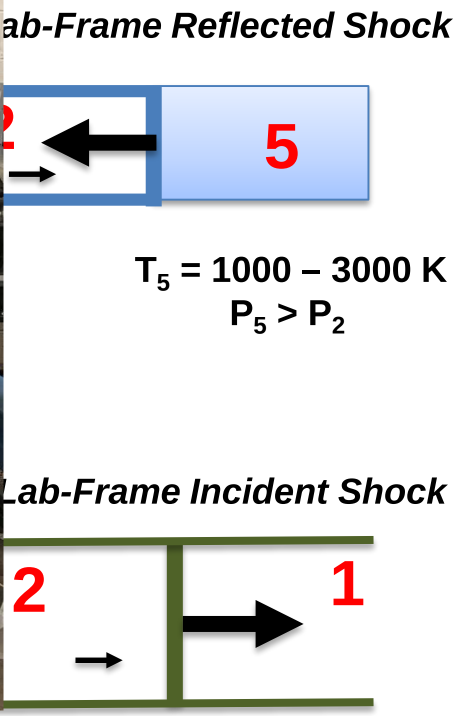


- Magnetic stir to promote mixing
- High accuracy Baratrons (0.05% accuracy) to measure partial pressure for mixture preparation

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

Basics regarding the shock-tube:





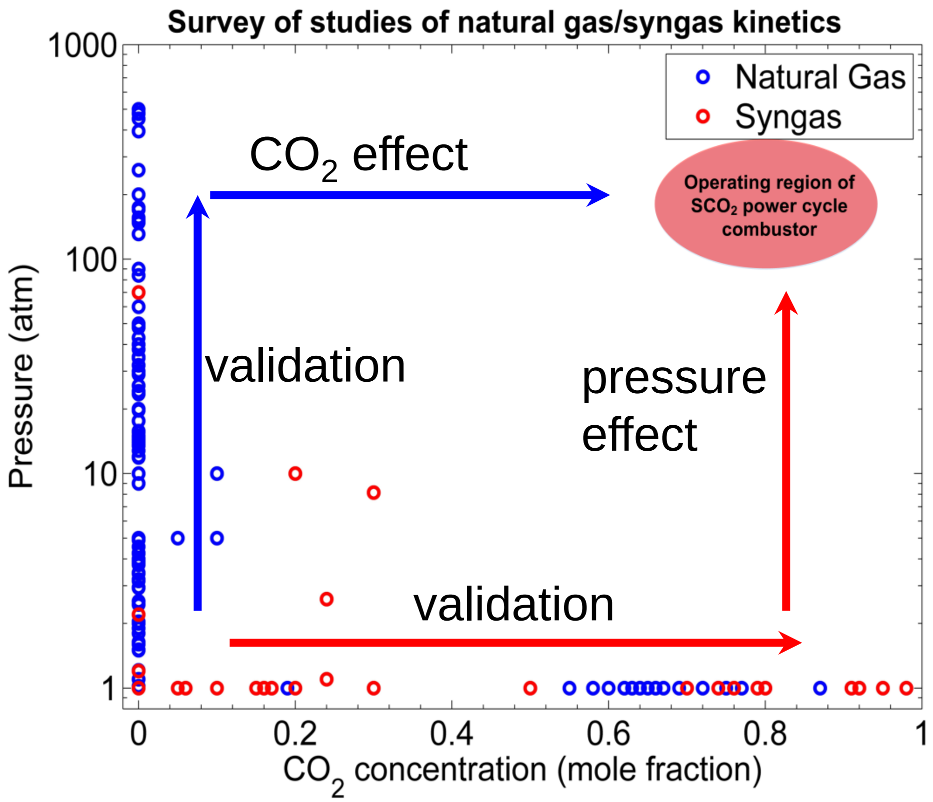
T_5 = 1000 – 3000 K
$P_5 > P_2$

Shock tube is ready and experiments on the way

Task 1 accomplished in year 1

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

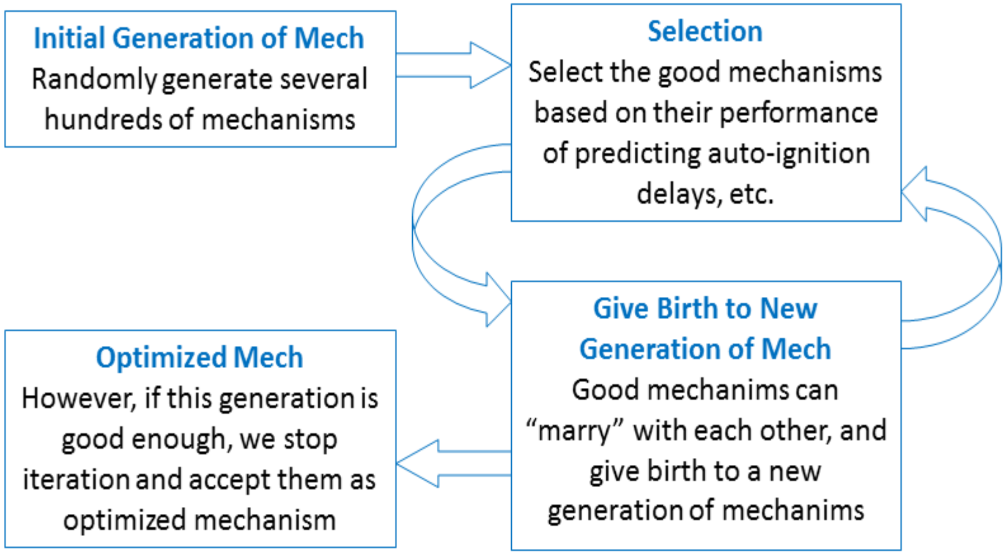


A new regime to explore!

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 Model 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



Initial Generation of Mech
Randomly generate several hundreds of mechanisms

Selection
Select the good mechanisms based on their performance of predicting auto-ignition delays, etc.

Give Birth to New Generation of Mech
Good mechanims can "marry" with each other, and give birth to a new generation of mechanims

Optimized Mech
However, if this generation is good enough, we stop iteration and accept them as optimized mechanism

Flow chart of using Genetic Algorithm to optimize chemical kinetic mechanisms

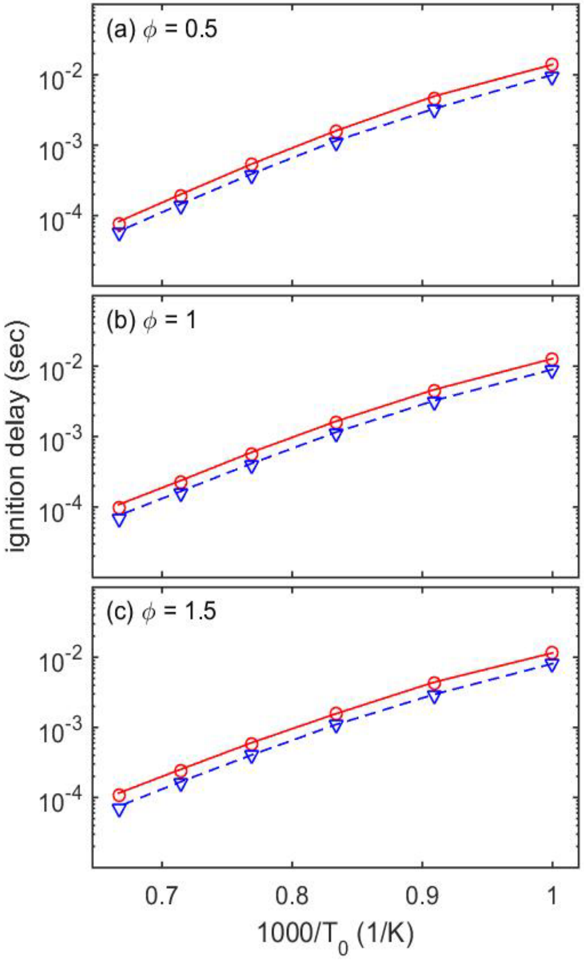
Task 3: Development of a Compact and Optimized Chemical Kinetic Model for sCO_2 Oxy-combustion

- 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

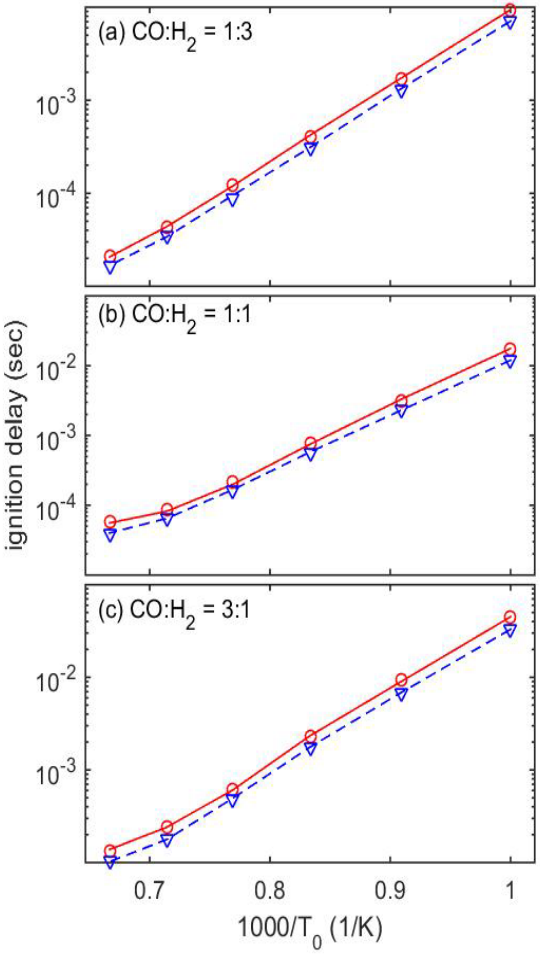
- A 27 species reduced mechanism[2] for natural gas (CH_4/C_2H_6) and syngas (CO/H_2) is developed

- Comparison of the results from reduced (marker) and detailed mech (line). Solid lines (p = 200atm), dashed line (p = 300atm)

Autoignition



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

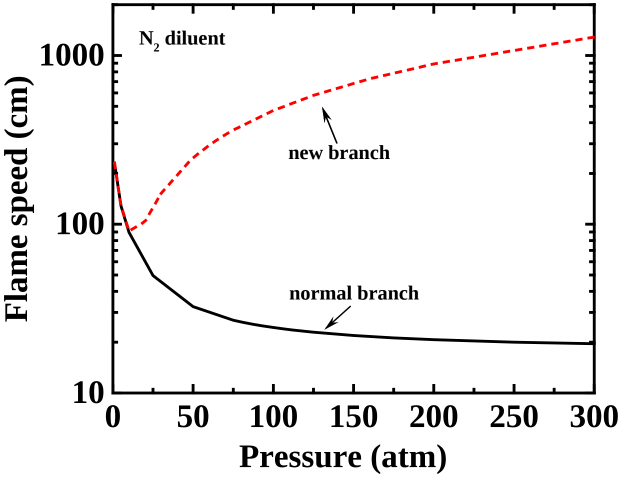


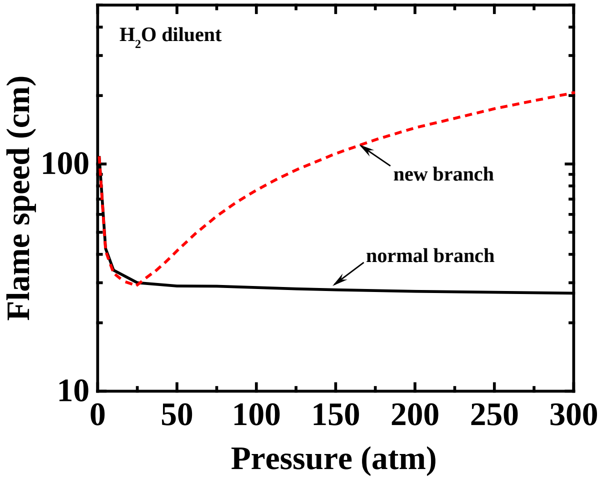
92.5% CO_2 diluted syngas gas/O_2 (ϕ=1)

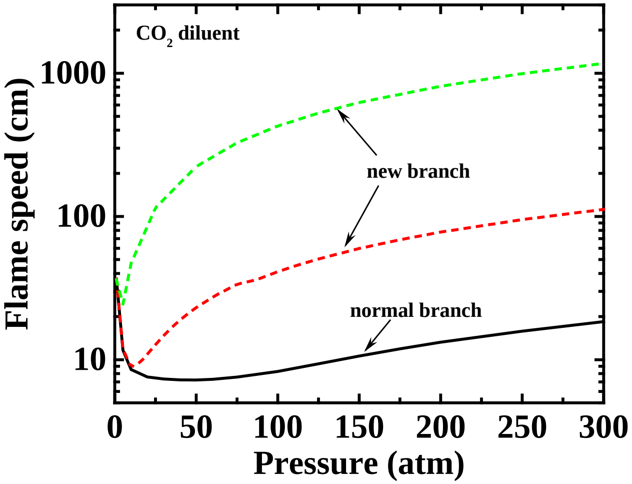
1. A. McClung, DE-FE0024041 Q1FY15 Research Performance Progress Report, SwRI
2. S. Coogan, X. Gao, W. Sun, Evaluation of Kinetic Mechanisms for Direct Fired Supercritical Oxy-Combustion of Natural Gas, TurboExpo 2016

Task 3: Development of a Compact and Optimized Chemical Kinetic Model for sCO_2 Oxy-combustion

- 1D Chemkin calculation with reduced model (only USC II converges)
- flame speeds at different pressure conditions of stoichiometric CH_4/O_2 with 80% diluent at 1000 K initial temperature





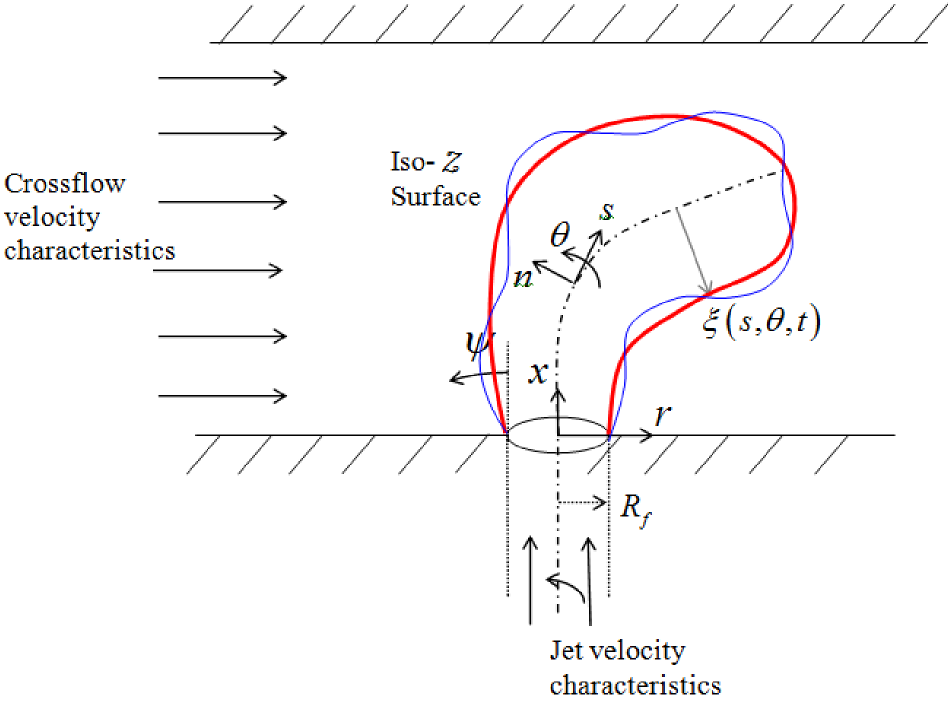


- Multiple solutions when P>25 atm
- At 300 atm, how fast flame propagates? What will be observed in experiments and LES?
- Large flame speed: pulsating flame? Small flame speed: blow out?

Critical for combustor design

Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

- Physics based models of reacting jet in crossflow (JICF)
  - Connect flow dynamics to flame dynamics
  - Modeling explicit flame position dynamics
- Understanding flow dynamics of a jet in crossflow



Analytic model of jet in crossflow

Challenges of Task 4

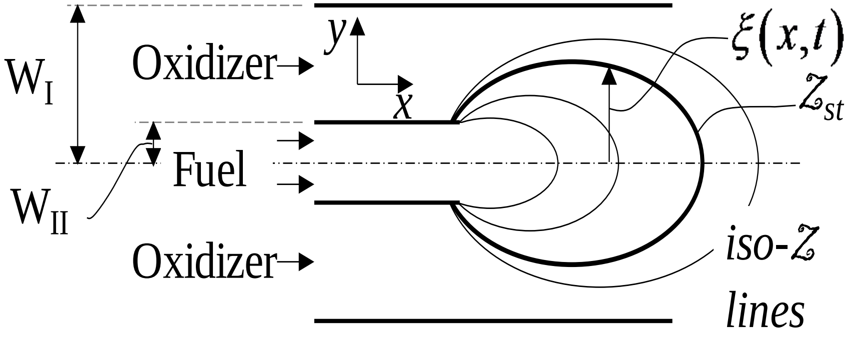
- Flame response modeling
  - Majority of past work has addressed models for premixed flames
    - Explicit governing equations describing dynamic flame surface evolution (e.g., G equation)
  - Non-premixed flames not well studied
    - mixture fraction framework, implicit representation of the flame
    - No explicit governing equations for flame position
- Challenges
  - Using governing equation for a full-field quantity (mixture fraction) to develop a governing equation for a given iso-contour of the mixture fraction solution
    - Boundary conditions are important => affect flame
    - Results in complicated non-linear governing equations, that require physics based simplifications
  - Flow dynamics for a jet in cross-flow are not easily understood or modeled
    - Requires detailed understanding of flow from experiments and LES
    - Developing an analytical representation of flow for use in analytical models

Modeling Flame Surface Dynamics

- The non-premixed flame is modeled using the Burke-Schumann framework
  - Governing equation based on the mixture fraction formulation
  - assuming fast chemistry but equal diffusivities

$$\frac{\partial \mathcal{Z}}{\partial t} + \vec{u} \cdot \nabla \mathcal{Z} = \nabla \cdot \left(\mathcal{D} \nabla \mathcal{Z} \right) \qquad \mathcal{Z} \equiv Y_{\mathrm{Fuel}} + \left(\frac{1}{\varphi_{ox} + 1} \right) Y_{\mathrm{Prod}}$$

- Flame location is based on the stoichiometric mixing of fuel and oxidizer
  - Stoichiometric iso-contour of mixture fraction field ($\mathcal{Z} = \mathcal{Z}_{st}$)
  - Example: simple ducted non-premixed flame with co-flowing fuel/oxidizer



Analytical Modeling Strategy

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

- The mixture fraction and flow-field can be decomposed into steady mean (subscript 0) and unsteady perturbations (subscript 1)
  - $u_i = u_{i,0} + u_{i,1}$; $\mathcal{Z} = \mathcal{Z}_0 + \mathcal{Z}_1$
  - Decomposes governing equations into separate equations for steady state and dynamics (unsteady state)

$$\left(\vec{u}_0 \cdot \nabla \right) \mathcal{Z}_0 = \mathcal{D} \left(\nabla^2 \mathcal{Z}_0 \right)$$

$$\frac{\partial \mathcal{Z}_1}{\partial t} + \left(\vec{u}_0 \cdot \nabla \right) \mathcal{Z}_1 - \mathcal{D} \left(\nabla^2 \mathcal{Z}_1 \right) = -\left(\vec{u}_1 \cdot \nabla \right) \mathcal{Z}_0$$

- Solutions provide description of complete mixture fraction field

Iso-surface dynamics

- In a frame of reference (Lagrangian representation) fixed to the iso-surface, the material derivative vanishes

$$\left.\frac{D\mathcal{Z}}{Dt}\right|_{\mathcal{Z}=\mathcal{Z}_{st}}=0$$

- In the observer fixed frame of reference, the equation translates to:

$$\left.\frac{\partial\mathcal{Z}}{\partial t}\right|_{\mathcal{Z}=\mathcal{Z}_{st}}+\left.\left(\vec{u}_f\cdot\nabla\mathcal{Z}\right)\right|_{\mathcal{Z}=\mathcal{Z}_{st}}=0$$

- The front velocity (u_f) is a combination of the ambient flow and the inherent front propagation velocity:

$$\left.\frac{\partial\mathcal{Z}}{\partial t}\right|_{\mathcal{Z}=\mathcal{Z}_{st}}+\left.\left(\vec{u}\cdot\nabla\mathcal{Z}\right)\right|_{\mathcal{Z}=\mathcal{Z}_{st}}=s_f\left(\mathcal{Z}_{st}\right)\left.\left|\nabla\mathcal{Z}\right|\right|_{\mathcal{Z}=\mathcal{Z}_{st}} \qquad s_f\left(\mathcal{Z}_{st}\right)=\frac{\left.\nabla\cdot\left(\mathscr{D}\nabla\mathcal{Z}\right)\right|_{\mathcal{Z}=\mathcal{Z}_{st}}}{\left.\left|\nabla\mathcal{Z}\right|\right|_{\mathcal{Z}=\mathcal{Z}_{st}}}$$

  - The equation is valid only at the stoichiometric iso-surface and the front speed is a function of the stoichiometric mixture fraction.

Front Propagation Velocity

- Since governing equation at iso-surface is not valid anywhere else, the following transformation applies

$$\mathscr{Z}-\mathscr{Z}_{st}=\xi(x,t)-y \qquad \frac{\partial\xi}{\partial t}+u\frac{\partial\xi}{\partial x}-v=s_f\left(\mathscr{Z}_{st}\right)\sqrt{1+\left(\frac{\partial\xi}{\partial x}\right)^2}$$

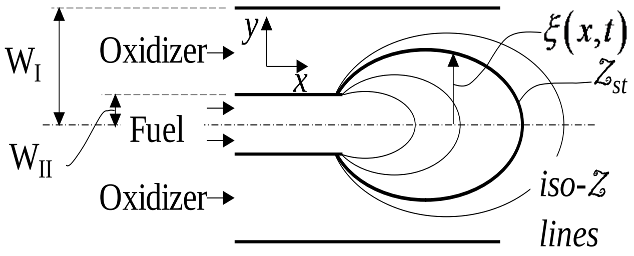
  - Transformation does not apply to front-speed (relationship derived from a full-field mixture fraction governing equation)

- Front-speed obtained from iso-surface solution ($\mathscr{Z}=\mathscr{Z}_{st}=g(x,\xi,t)$)

$$s_f\sqrt{1+\left(\frac{\partial\xi}{\partial x}\right)^2}=\left(\underbrace{\mathscr{D}\frac{\left(\partial_{\xi x}g\right)}{\left(\partial_{\xi}g\right)}}_{u_D(x,\xi)}\right)\frac{\partial\xi}{\partial x}+\mathscr{D}\frac{\partial^2\xi}{\partial x^2}-\underbrace{\mathscr{D}\frac{\left(\partial_{\xi\xi}g\right)}{\left(\partial_{\xi}g\right)}}_{s_D(x,\xi)}\left[1-\left(\frac{\partial\xi}{\partial x}\right)^2\right]$$

Properties of Position Dynamics PDE

$$\frac{\partial \xi}{\partial t}+\left(u-{\color{red}u_D(x,\xi)}\right)\frac{\partial \xi}{\partial x}-v={\color{magenta}\mathscr{D}\frac{\partial^2 \xi}{\partial x^2}}-{\color{blue}s_D(x,\xi)}\left[1-\left(\frac{\partial \xi}{\partial x}\right)^2\right]$$

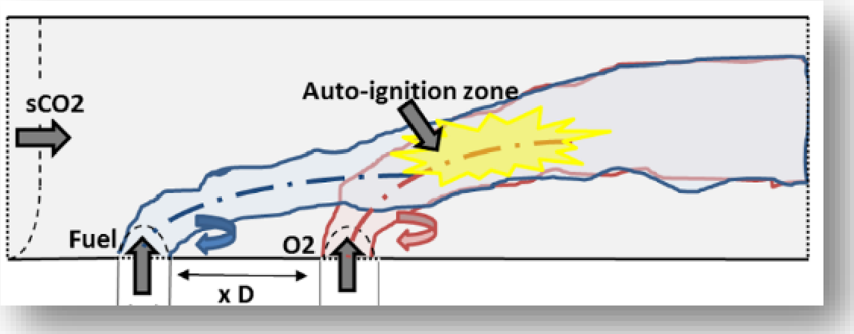


- Non-linear wrinkle convection
  - Flow based convection as well as position-coupled diffusion based convection
- Linear term from “Diffusion” of wrinkles
  - Similar to stretch effects in premixed flames (i.e. stretch correction to flame speed)
- Non-linear term from diffusion
- Boundary conditions
  - physics required input from full-field mixture fraction solutions (diffusion wave transport & non-linear diffusion term)
    - Stems from the fact that boundary conditions (at inlet, walls etc.) need to be accounted for in “reduced” governing equation for flame position

Future Directions for Task 4

- Linearization of position dynamics governing equation
  - Steady state governing equation
  - Flame wrinkle governing equation
- Application of position dynamics to reacting jet in crossflow configuration
- Identification of key control parameters
- Spatially integrated total heat release dynamics
- Comparisons with real reacting jets in crossflow

Task 5: LES Studies of Supercritical Mixing and Combustion



Baseline model
<u>NOT</u> actual design

- Systematic variation of design parameters
  - Momentum ratios for fuel and oxygen, number of sets
  - Size and spacing of injectors
  - Fuel upstream of oxidizer jet
  - Flow rates
- Computational modeling may be more cost effective but include its own challenges
  - Autoignition kinetics (large uncertainty, maybe wrong)
  - Turbulence-chemistry closure
  - Real gas effects

Task 5: LES Studies of Supercritical Mixing and Combustion

- Pressure: 300 bar
- ~90 % CO_2 concentration
- Inlet temperature: 1100K
- All incoming fluids are Supercritical
  - O_{2c} (50 bar, 155 K),
  - CO_{2c} (77 bar, 304 K),
  - CH_{4c} (46 bar, 190 K)
- Reduced Kinetics needed

Parameters	Value
P_{ref}	300 bar
T_{cross}	1100 K
U_{cross}	50 m/s
T_{jets}	300 K
J_{Ox}	20
J_F	18.4
D_F/D_{Ox}	0.6
Channel length	75 D_{ox}
Re_{JOx}, $Re_{JF,}$ Re_{CO2}	4.4×10^5, 7.8×10^5, 1.5×10^6

Mechanism	Species	Steps
USC II	111	784
Reduced[1]	27	150
Jones-Lindstedt[2]	7 (6*)	4

[1] Coogan et al., ASME Turbo Expo (2016)

[2] Jones & Lindstedt, Comb Fl. (1988)

* Does not include N_2

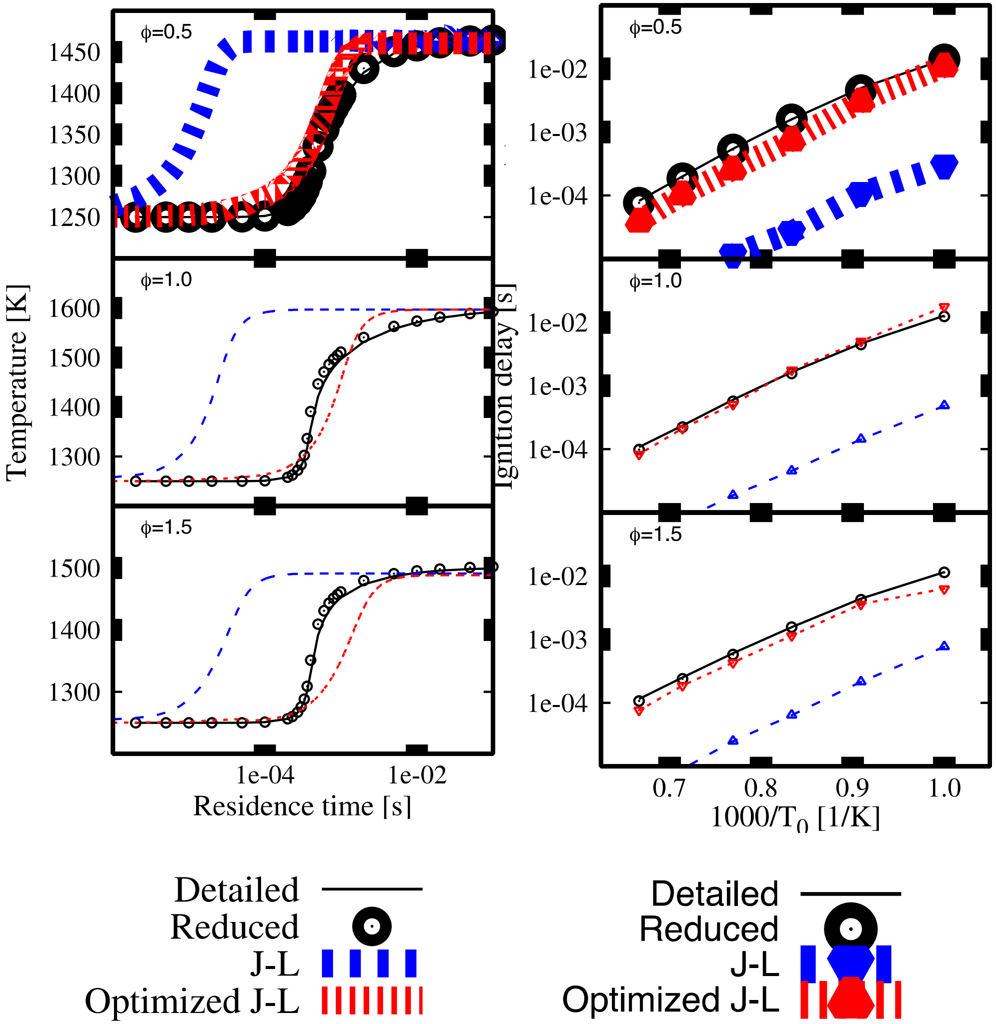
Modified Jones-Lindstedt (J-L) Mechanism

- Quick assessment
- Only CH_4, O_2, CO, H_2, H_2O, CO_2
- modified to predict T_{ad} and ignition

$$CH_4 + \frac{1}{2}\,O_2 \rightarrow CO + 2\,H_2$$
$$CH_4 + H_2O \rightarrow CO + 3\,H_2$$
$$CO + H_2O \leftrightarrow CO_2 + H_2$$
$$H_2 + \frac{1}{2}\,O_2 \leftrightarrow H_2O$$

Step Number	A (Original)	A (Modified)
1	4.4×10^{11}	1.1×10^{10}
2	3.0×10^{8}	7.21×10^{6}
3 (forward)	2.75×10^{9}	6.6×10^{7}
3 (backward)	8.0×10^{10}	1.91×10^{9}
4 (forward)	6.8×10^{15}	1.63×10^{14}
4 (backward)	7.1×10^{17}	1.70×10^{16}

[1] Jones & Lindstedt, Comb. Flame (1988)



P = 200 atm, T = 1250 K CO_2, molar concentration = 92.5%

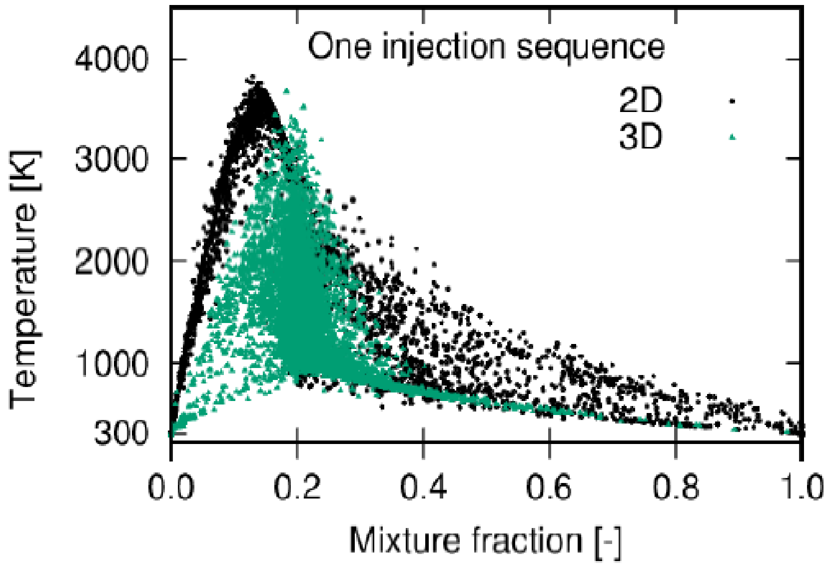
Numerical Methodology

- **LESLIE**; a multi-species compressible flow solver[1]:
  - 3D Adaptive Mesh Refinement finite-volume solver
    - Mesh adapted and then frozen once solution settles down
  - 2nd order Predictor-Corrector with artificial dissipation
  - Time integration: 2nd order explicit
  - Characteristics based boundary conditions
  - **Chung's transport** with **Peng Robinson Real Gas** EOS
  - Thermally perfect gas EOS used for comparison
- Subgrid-scale (SGS) closures:
  - Momentum, energy & scalar subgrid fluxes: One-equation model turbulent kinetic energy[2] model used for closure
  - Kinetics computed using filtered variables

[1] Genin & Menon, AIAA J., 48, 2010; [2] Kim & Menon, I. J. Numer. Meth. Fluids, 31, 1999

2D/3D Preliminary Investigations: Flame Structure

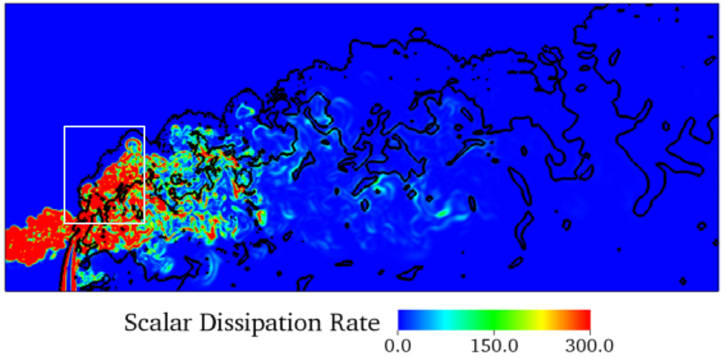
- Flame anchoring very different:
  - 2D: flame anchoring occurs on jets
  - 3D: Lifted flame anchored on oxidizer jet
  - engulfment and jet wake effects
- Differences in combustion regime:
  - 2D: reaction occurs in rich regime
  - 3D: **reaction occur close to stoichiometry and on lean side**
- 3D needed for accuracy:
  - CPU cost severe for multi-block grid
    - 32/65/90M for single/two/three
  - Use AMR as alternative approach
    - Cost effective and refined
    - Structured grid for high accuracy

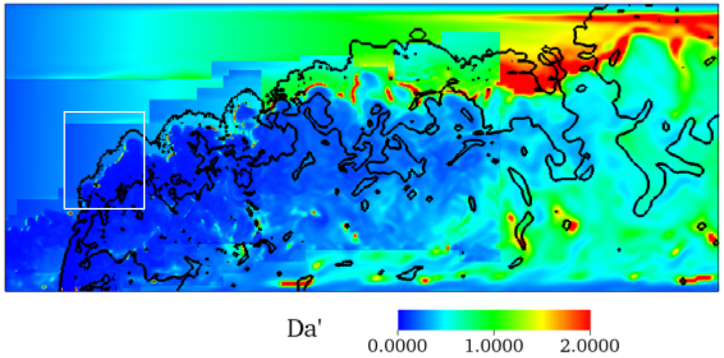


Combustion regime and flame structure

Non-Reacting: Analysis of Scalar Mixing

- Flow must have enough time for fuel and oxidizer to mix and then ignite (T is high enough)
- Da’: ranges from <<1 to O(1)
- Iso-lines represent the stoichiometric mixture fraction value
- The boxed regions:
  - Near stoichiometric with low S.D.R.
  - Possible auto-ignition region
  - Kinetics controlled

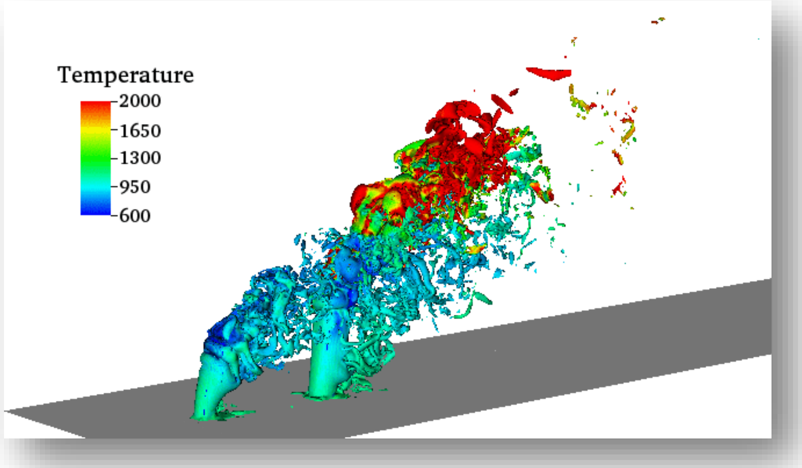


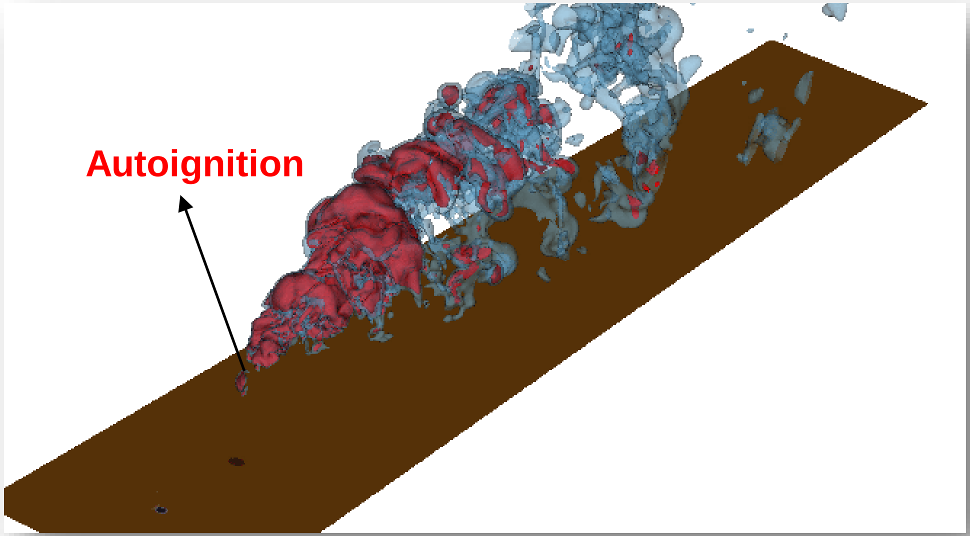


$$Da' = \frac{\tau_{mix}}{\tau_{ignition\ delay}}$$

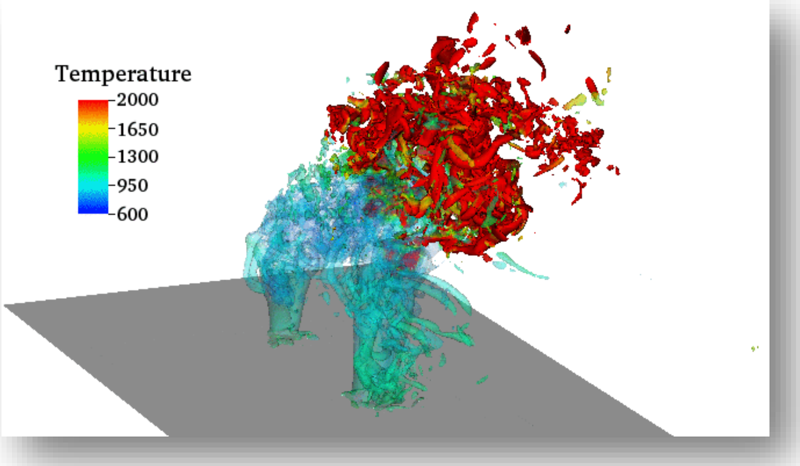
Instantaneous Reacting Flow Features

- Autoignition close to predicted location based on mixing
- Autoignition occurs slightly downstream of the oxidizer jet towards lean side
- Autoignition with lifted flame structure



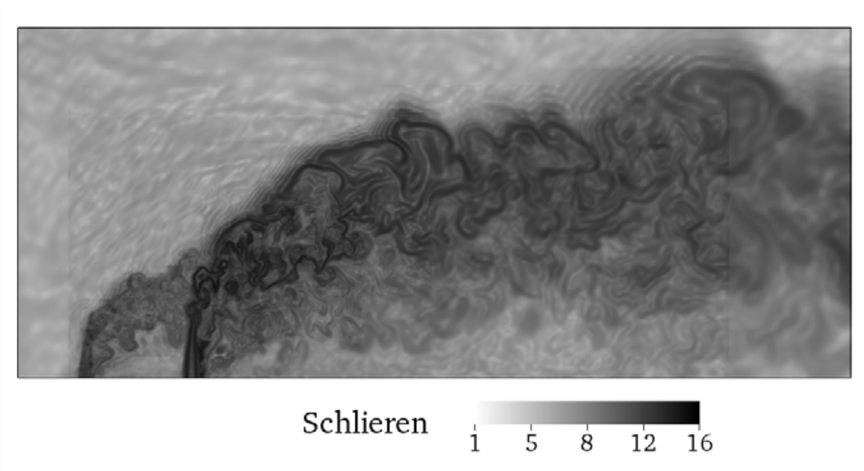


Temperature iso-surface (2100 K, 1500 K)

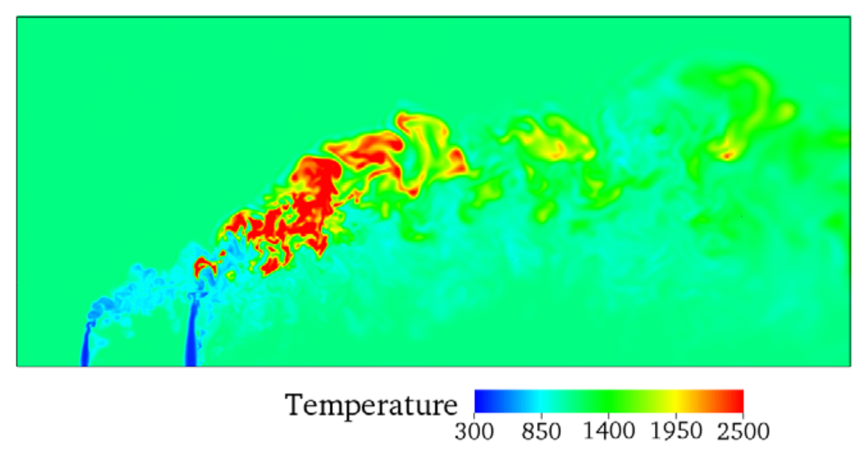


Vorticity magnitude colored by temperature

Instantaneous Reacting Flow Features



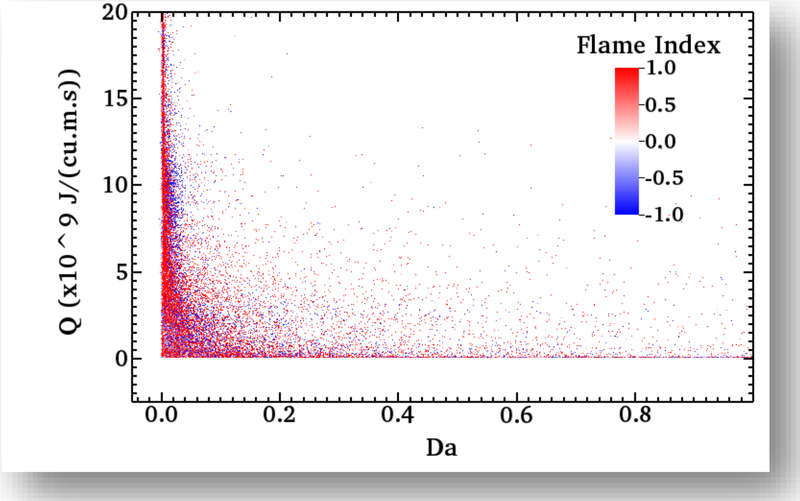
Schlieren



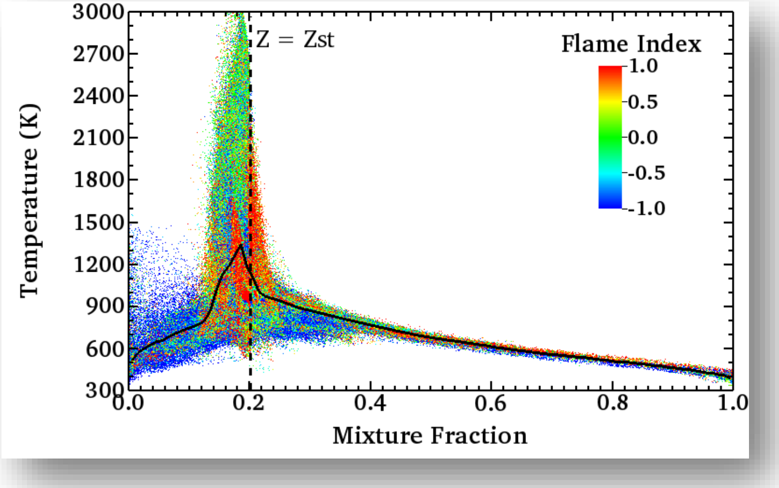
Temperature

- Large density gradient (Schlieren: log of density gradient)
- Mixing of fuel and oxidizer followed by ignition in lifted regions
- Autoignition in hot kernels where fuel mixes with oxidizer
  - Finite-size kernel but no continuous flame structure
- Autoignition sensitive to many parameters: mixing time, kinetics, local scalar dissipation rate, etc.

Instantaneous Flame Structure



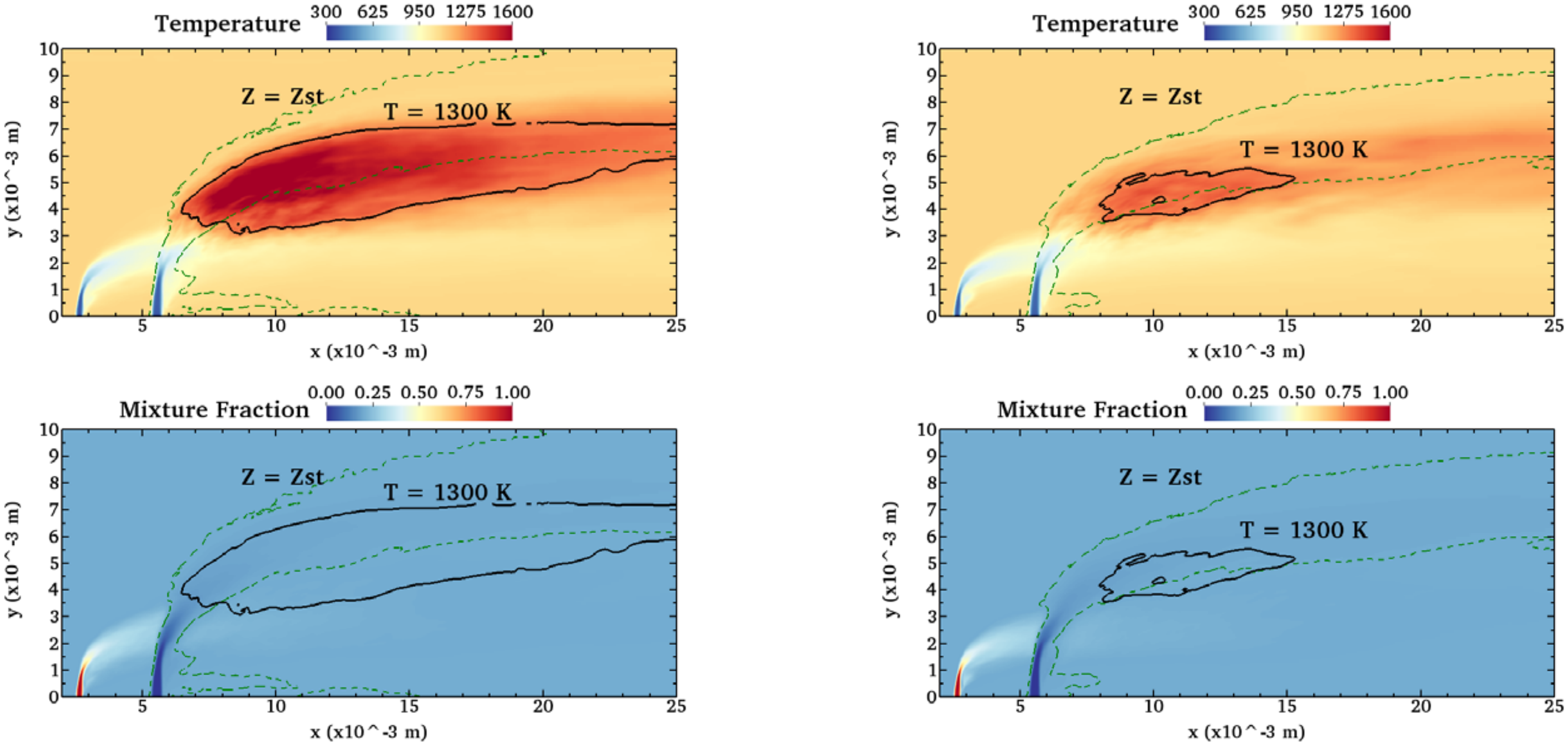
Heat release rate v/s Damkohler number



Temperature v/s mixture fraction

- Da <<1 (flow property resolved, slow chemistry)
- Multi-mode combustion after ignition
  - Flame Index is positive (premixed) & negative (non-premixed)
  - Most of burning occurs under lean conditions
- Compressibility factor shows marginal variations (is PG OK?)

Effect of Compressibility



Real gas EOS

Perfect gas EOS

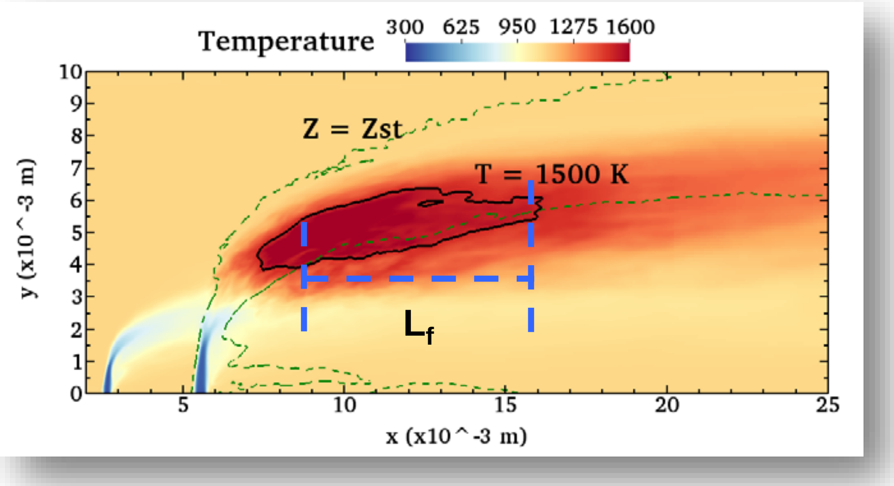
- Both cases simulated at same operating conditions
- Reduced jet penetration with perfect gas EOS in comparison to Peng Robinson EoS – clearly shows RG effects
- Heat release also decreased with perfect gas EOS

Flame Length and Combustion Efficiency

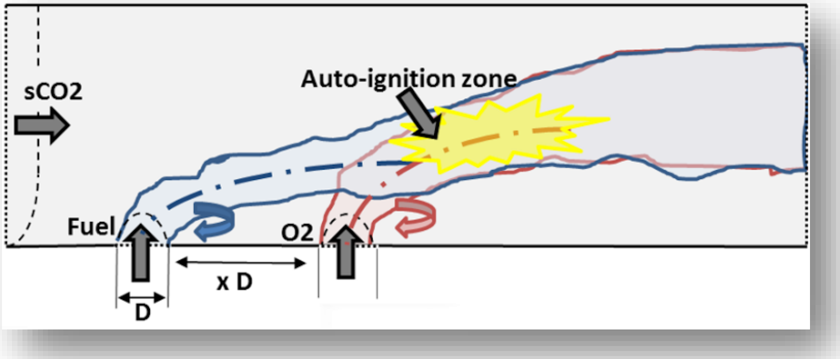
- Combustion is not efficient
- Combustion efficiency estimated as:

$$\eta = 100 \times \frac{\dot{m}_{f,in} - \dot{m}_{f,out}}{\dot{m}_{f,in}} \sim 49\%$$

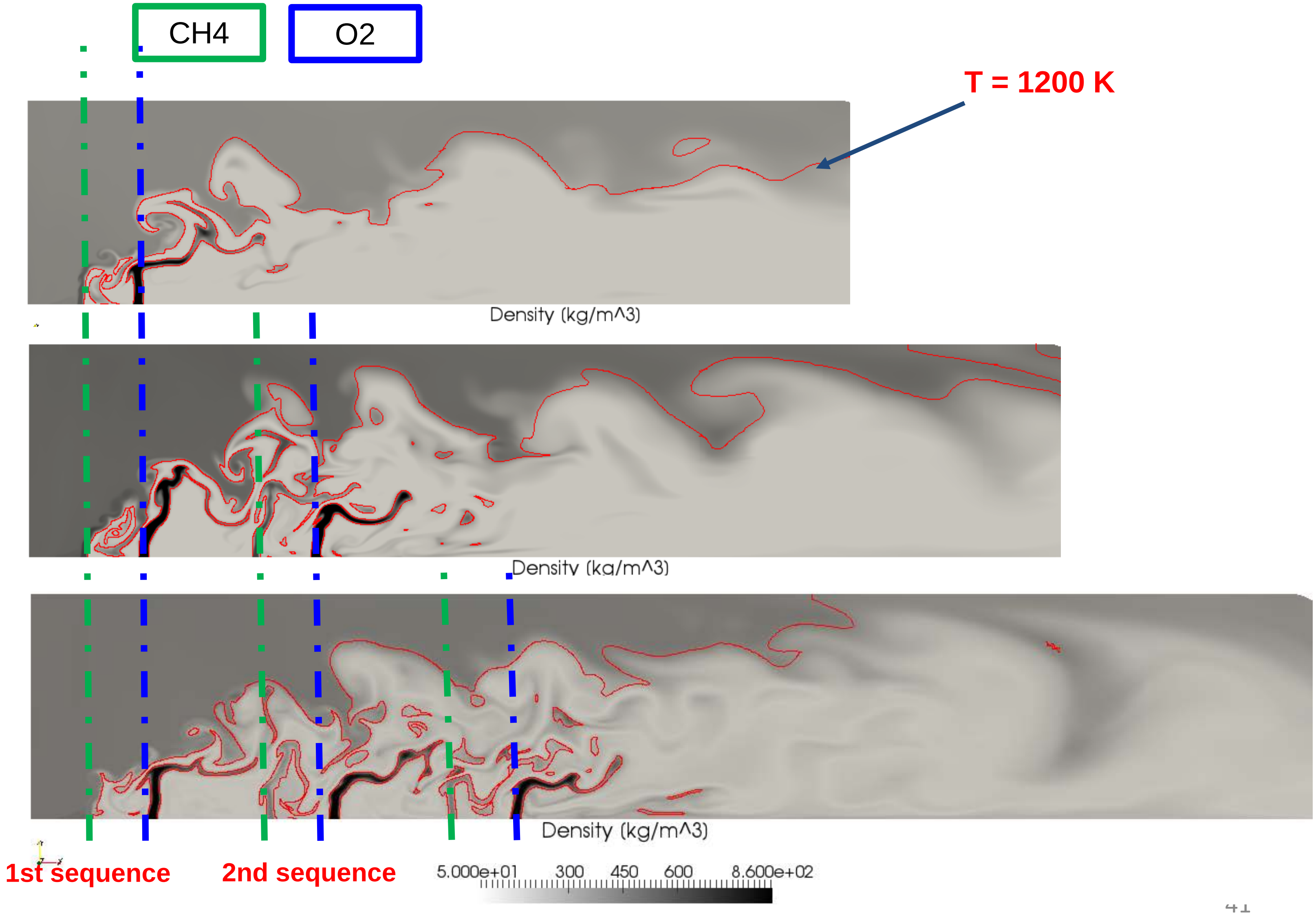
- Flame length, $L_f \sim 14.5\ D_{ox}$
  - estimated as intersection of $Z = Z_{st}$ and T = 1500 K
- η needs to be improved
  - Inflow realistic turbulence
  - Modify J and jet spacing
  - Mass flow rate changes
  - Jet-staging and distributed mixing
  - Inflow swirl
- More studies needed and underway



Temperature overlaid with stoichiometry line



2D Preliminary Investigation: Density



Injection sequences

One

Two

Three

CH4

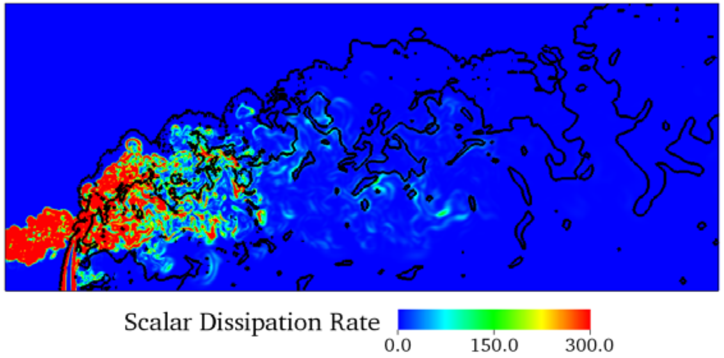
O2

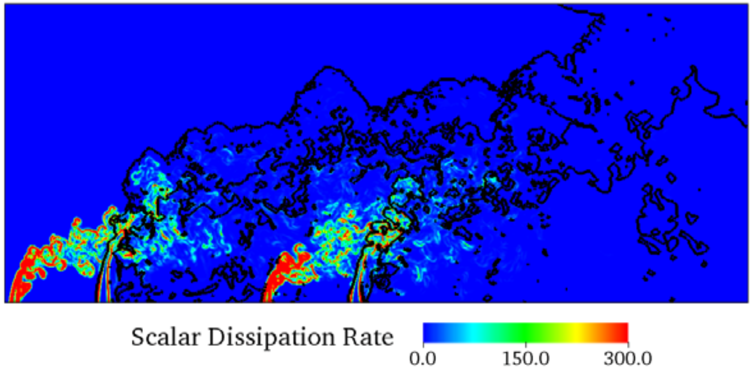
T = 1200 K

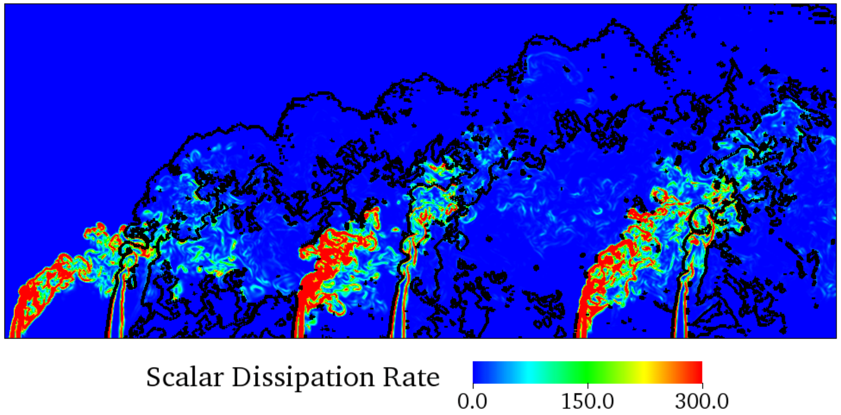
1st sequence

2nd sequence

Multi-Jet Mixing with Real Gas

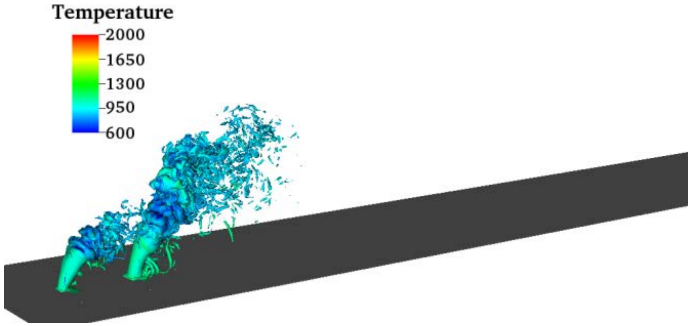


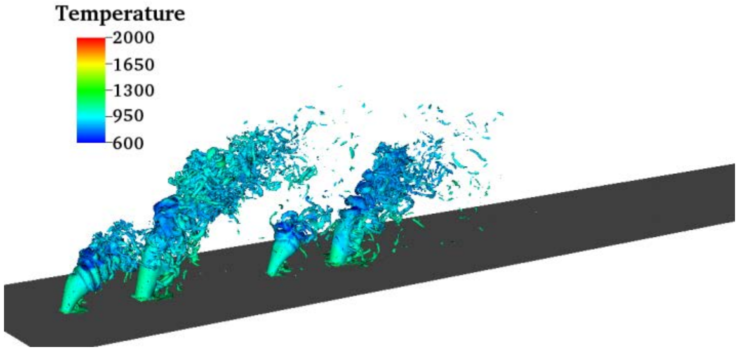


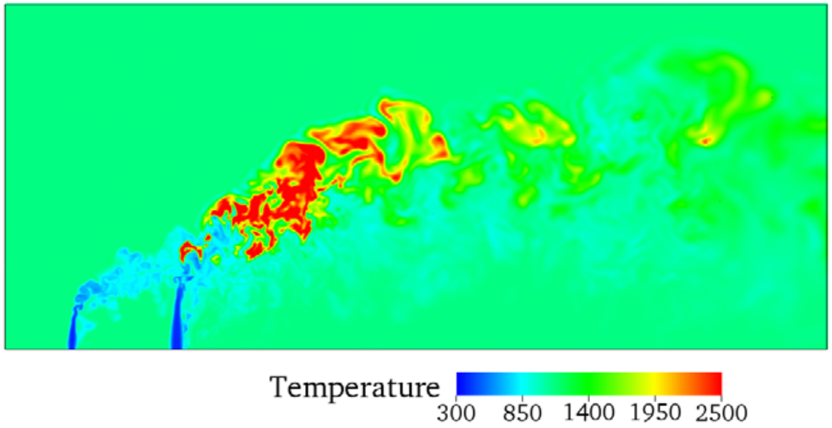


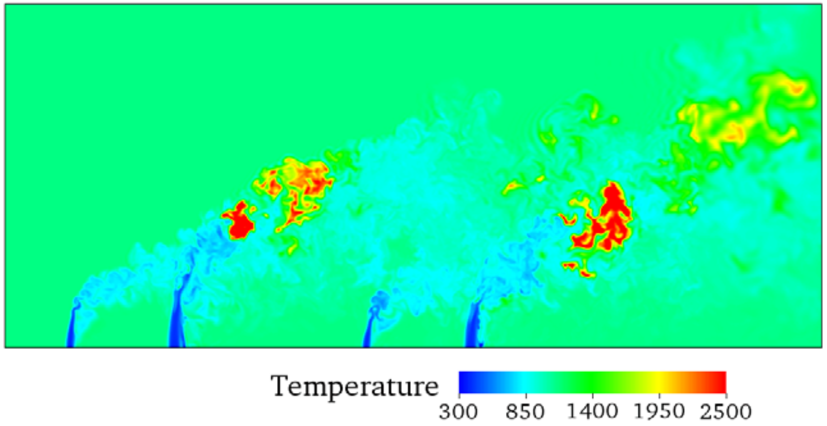
- 1-set, 2-set and 3-set show differences in mixing and locations of low SDR
- Possible interactions due to acoustic waves in subsonic
- Multiple JICF configurations may all be unique

AutoIgnition and Blow out









- Limitations of kinetics
- Influence of upstream acoustic waves

Future Directions for Task 5

- Future studies to focus on
  - Effect of chemical kinetics – employ more detailed kinetics
  - Locations and injection strategies for fuel and oxygen non-reacting mixing studies with different injector locations to determine how to increase the low SDR regions (autoignition)
  - 1D LEM to handle all flame regimes
- Challenges
  - reliable mixing rules and kinetics
  - SGS closure for high Re multi-mode combustion (how to dynamically switch between different combustion regimes)

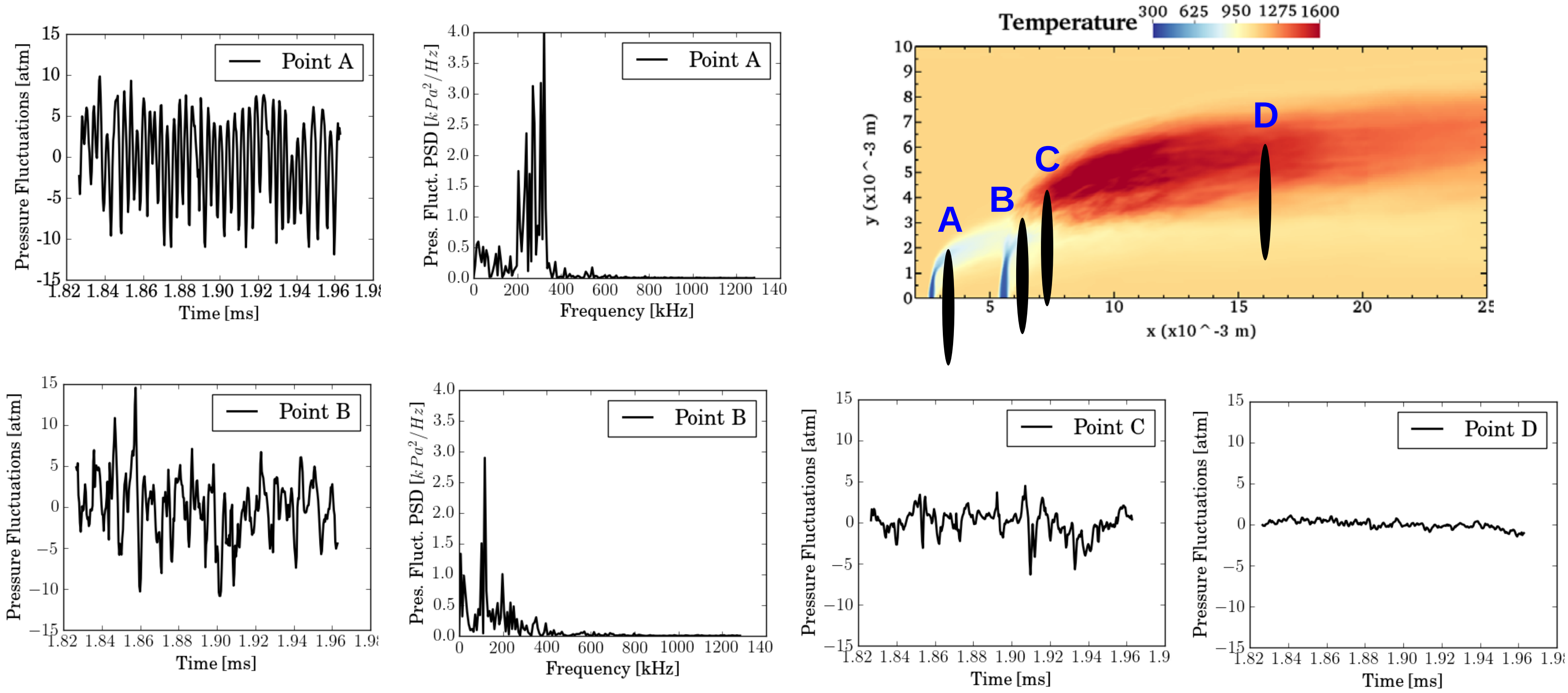
Summary of Year 1 Achievement

- High pressure shock tube developed
- Reduced kinetic model with 27 species for natural gas and syngas
- Governing equation developed for theoretical frame work
- LES investigation of JICF
  - Real gas effect
  - 3D effect
  - Deficiency of kinetics, insight to combustor design

Thank you!
&
Questions?

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

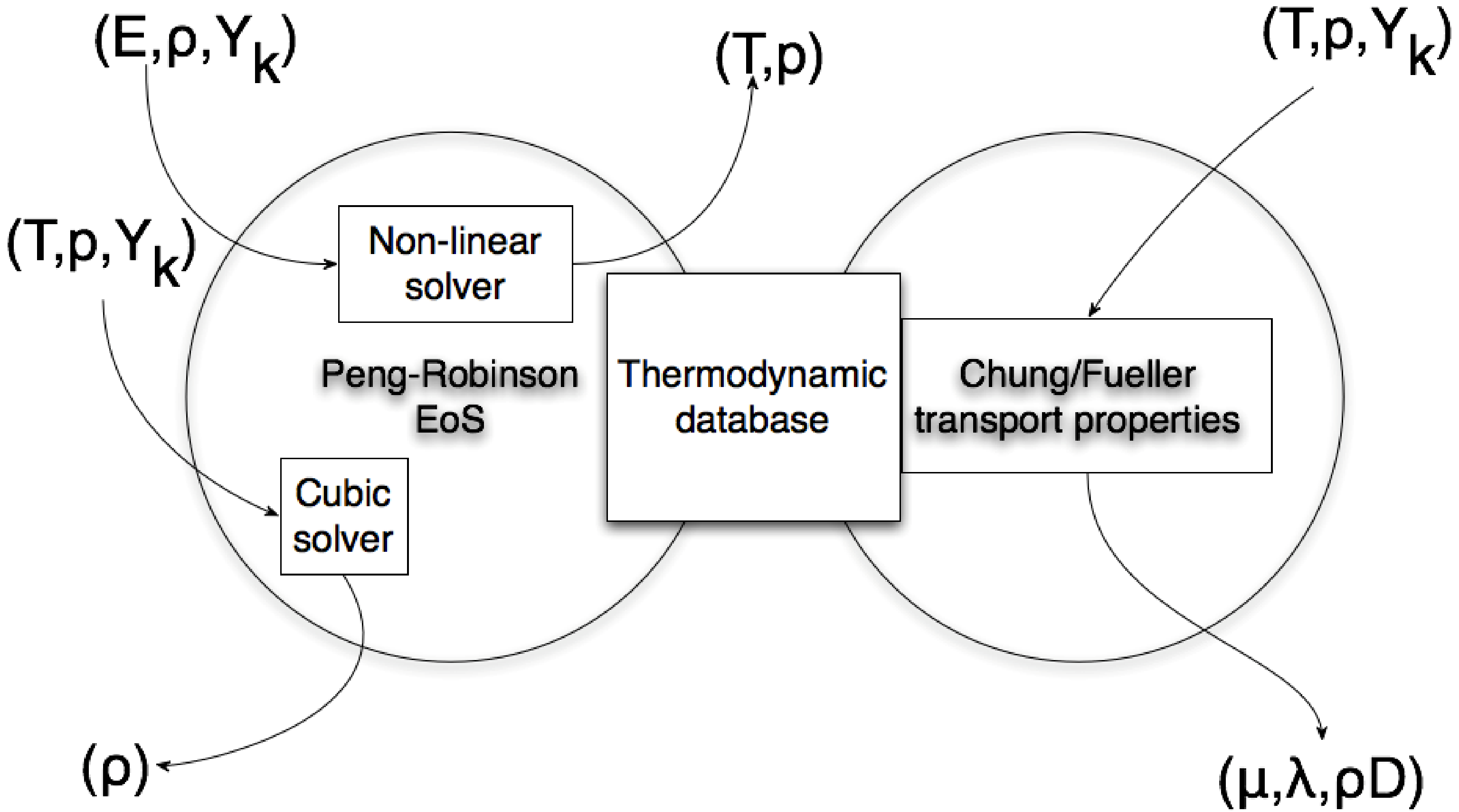
Analysis of Pressure Fluctuation



- Pressure at various locations (Autoignition location C)
- At A and B ~ 3-5% fluctuations due jet interacting with cross flow
  - St of peak frequencies range from 0.1 – 1.1 (~ jet preferred modes)
- At C and D, the fluctuations are purely indicative of turbulent fluctuations

Task 5: LES Studies of Supercritical Mixing and Combustion

Real gas framework



(E,ρ,Y_k)

(T,p)

(T,p,Y_k)

(T,p,Y_k)

Non-linear solver

Peng-Robinson EoS

Cubic solver

Thermodynamic database

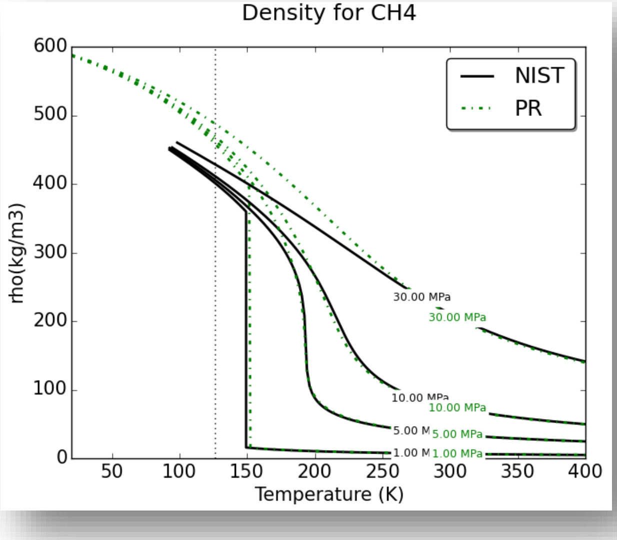
Chung/Fueller transport properties

(ρ)

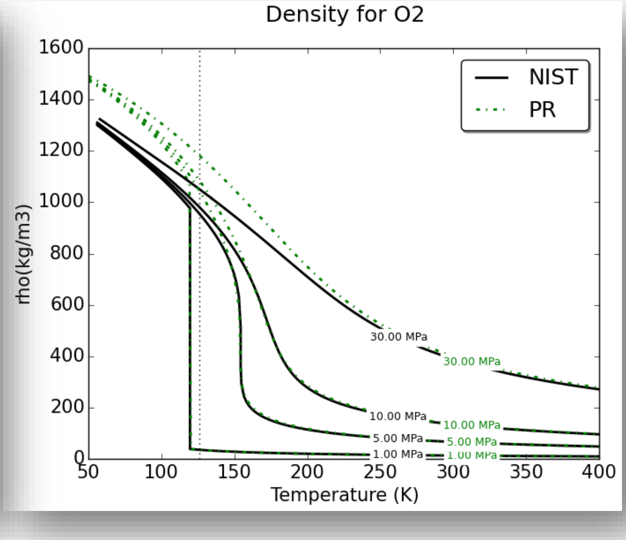
$(\mu,\lambda,\rho D)$

Modeling Under Supercritical Conditions

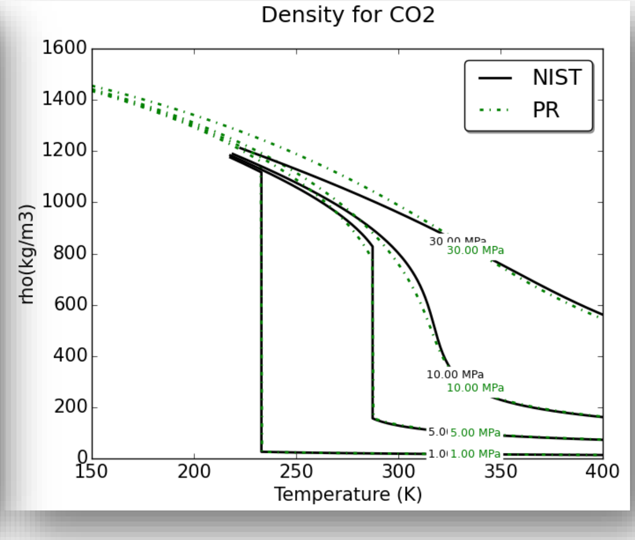
- Fluid properties assessed for methane, oxygen and carbon dioxide against reference NIST database
- Reasonable agreement for a wide range of operating conditions
- Peng Robinson cubic EoS is adequate for present study



Methane



Oxygen



Carbon dioxide