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

PI: Wenting Sun
Co-PI: Devesh Ranjan, Tim Lieuwen, and Suresh Menon

School of Aerospace Engineering
Georgia Institute of Technology
Atlanta, GA 30332


UTSR Project: DE-FE0025174    PM: Seth Lawson
2017 UTSR Project Review Meeting
Overview of the Scientific Problem

• What fundamental combustion properties/knowledge we need in order to design combustor for SCO$_2$ oxy-combustion?
  – Kinetics and dynamics

Autoignition delays
and
flame dynamics of jet in crossflow

Conceptual 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%)
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 (complete)

Key features:

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

Eight optical windows

Contoured valve for vacuum

Single piece test section (2.1 m)

Diaphragm section (single or double)
Task 1: Development of a High Pressure Shock Tube (complete)

• Mechanism of operation

Shock Tube Schematic

Time (t)

Location (x)

Diaphragm

1. High Pressure
2. Low Pressure

Rarefaction Fan
Contact Surface
Shock Front

Reflected Shock

Lab-Frame Reflected Shock

Lab-Frame Incident Shock

First shock in Jan. 2017

<table>
<thead>
<tr>
<th>Location (x)</th>
<th>Time (ms)</th>
<th>Pressure (atm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>5</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>10</td>
</tr>
</tbody>
</table>

Measured P, calculated T

\[ T_2 = 500 \text{ – } 2000 \text{ K} \]
\[ P_2 > P_1 \]

\[ T_5 = 1000 \text{ – } 4000 \text{ K} \]
\[ P_5 > P_2 \]
Study of High Pressure Autoignition
- Facilities: mixture preparation

High accuracy Baratrons (0.05%) to measure partial pressure for mixture preparation

Magnetic stir to promote mixing

Turbo molecular pump

MicroGC to monitor compositions
Example of Pressure Traces

Unique features for high quality data
Challenges of High Pressure Shock Tube

• Shock tube is not just a tube
• Boundary layer
  – from moving shock
• For polyatomic gases, BL is much thicker
• ID of shock tube must be large
  – 150 mm

Argon as test gas

J. Hargis & E. Petersen, AIAA J, 2017
Challenges of High Pressure Shock Tube

- Test time needs to be long
  - Long enough to capture autoignition
  - Avoid bifurcation region
  - Longer tube, longer test time (21 m)
- A failed example
  - CH₄/O₂/Ar/CO₂=1:4:16:79
  - P=40 bar, T=1488 K
  - No autoignition captured
Facility Validation

• Low pressure autoignition measurement and validation
  – P = 20 atm, T = 1641 K
  – CH$_4$/O$_2$/Ar=1:4:95

• Agrees well with simulation using Aramco 2.0 (as expected)

• Experiments vs. Stanford results
  – Agreed at similar conditions
  – e.g., CH$_4$/O$_2$/Ar (2/4/96)
  – Stanford: 13.19 bar 1760 K $\tau_{ig} = 67 \mu$s
  – GT: 16.5 bar 1737 K $\tau_{ig} = 57 \mu$s
Facility Validation

- CH$_4$/O$_2$/Ar=2:4:94
- P=30 bar
- T= 1366 K
- Excellent between PMT signal (OH$^*$ emission) and simulation with Aramco 2.0

![Graph showing comparison of pressure and temperature with different models.](Image)
Headaches from $\text{SCO}_2$ !?
Real Gas Effect in Shock Tube

- Negligible effect on thermodynamic properties (P, T) in region of interest
  - Small difference (<10 K) in high T (>1000 K) region
  - Kogekar et al., CNF 2017; Tang et al., IJCK 2006; Davidson et al., IJC 1996;

- It does NOT mean negligible effect on chemical reactions
  - Real gas non-unity activity coefficient (or fugacity) (negligible above 1100 K)
  - unknowns

Graph showing ignition delay time against 1000/T (K^-1) for n-dodecane/air at 80 atm.
CO₂ Decomposition

- CO₂ decomposition → CO₂ → CO + O
- Favored at high T, low P
- May affect autoignition measurement
  - Loose demarcation

![Graph showing peak O concentration (ppm) vs. pressure (atm) for different temperatures. The graph includes lines for USC Mech II, GRI 3.0, and Aramaco 2.0, with a shaded safe region.](graph.png)
Task 2: Investigation of Natural Gas and Syngas Autoignition in sCO$_2$ Environment

- No study before in region of interest
- A new regime to explore!
- CO$_2$ has negligible chemical effect
  - Based on 1 to 15 atm results and simulation using GRI 3.0 and Aramco 1.3
  - GT 17 atm expt. Agreed with Aramco 1.3 using same mixture with Hargis et al.

Survey of studies of natural gas/syngas kinetics

- Natural Gas
- Syngas

Operating region of sCO$_2$ power cycle combustor

We are here now

Too early to make conclusion

Validation

Critical P of CO$_2$

Pressure effect

CO$_2$ concentration (mole fraction)

0 0.2 0.4 0.6 0.8 1

0 10 100 1000

Pressure (atm)

e.g.:
Autoignition with high CO$_2$ concentration: 15 bar

- CH$_4$/O$_2$/Ar/CO$_2$ = 5:10:40:45
- P = 15 bar
- T = 1409 K
Autoignition with high CO$_2$ concentration: 41 bar

- CH$_4$/O$_2$/Ar/CO$_2$ = 5:10:40:45
- P = 41 bar
- T = 1535 K
Autoignition with high CO$_2$ concentration:
105 bar

- CH$_4$/O$_2$/Ar/CO$_2$ = 3:6:24:67
- P = 105 bar
- T = 1310 K

More data needed, simulation vs. expt. for comparison only
No conclusion, no recommendation yet
Task 3: Development of a Compact and Optimized Chemical Kinetic Model for SCO$_2$ Oxy-combustion

- USC Mech II (111 species) is used as a starting point for future optimized mechanism

- A 27 species reduced mechanism$^1$ for natural gas and syngas is developed (still too large for CFD)

- A new 13 species model was developed with optimization
  - Covers 900 K to 1800 K, 150 atm to 300 atm
  - Max 12% deviation

Task 4: Analytical modeling of Supercritical Reacting Jets in Crossflow

- Analytical framework for reacting jets in cross-flow
  - connect flow dynamics to flame dynamics
  - Modeling explicit flame position dynamics
  - Modeling spatially integrated heat release dynamics as a function of flame position

- Understanding flow dynamics of a jet in cross-flow
  - provide key inputs to the velocity field used in the analytical model
Position Dynamics PDE

\[
\frac{\partial \xi}{\partial t} + (u - u_D(x, \xi)) \frac{\partial \xi}{\partial x} - v = \mathcal{D} \left( \frac{\partial^2 \xi}{\partial x^2} - s_D(x, \xi) \right) \left[ 1 - \left( \frac{\partial \xi}{\partial x} \right)^2 \right]
\]

- **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 propagation-like term from diffusion**

- **Decompose all quantities into a steady time-average and time-dependent perturbation**

\[
\xi = \xi_0(x) + \xi_1(x,t) \\
u = u_0(x) + u_1(x,t) \quad v = v_0(x) + v_1(x,t) \\
u_D = u_{D,0} + u_{D,1} \quad s_D = s_{D,0} + s_{D,1}
\]
Flame Position Dynamics

\[
\frac{\partial \xi_1(x, t)}{\partial t} + \left( u_0(x) - u_{D,0}(x) - 2s_{D,0}(x) \right) \frac{\partial \xi_1(x, t)}{\partial x} - \mathcal{D} \frac{\partial^2 \xi_1}{\partial x^2} \\
= \left( v_1(x, t) - u_1(x, t) \frac{d \xi_0(x)}{dx} \right) + \xi_1 \left( \frac{\partial u_{D,0}}{\partial \xi_0} \frac{d \xi_0(x)}{dx} - \frac{\partial s_{D,0}}{\partial \xi_0} \left[ 1 - \left( \frac{d \xi_0(x)}{dx} \right)^2 \right] \right)
\]

- **Governing Physics**
  - Wrinkle convection
  - Diffusion, similar to premixed flame stretch
  - Reactive type dynamics

- **High Pe limit**
  - Diffusion time-scale large compared to convection time-scale
  - Diffusion based convection – 1/Pe^2
  - Diffusion based propagation – 1/Pe
Global Flame Dynamics

- For acoustically compact flames, spatially integrated heat release is the dynamics relevant quantity

\[ \dot{Q}(t) = \int_{\text{flame}} \dot{m}_F'' \, \mathcal{H}_R \, dA = \int_{\text{flame}} \rho_u \mathcal{D} \left| \nabla Z_0 \right|_{Z_{st}} \, \mathcal{H}_R \sqrt{1 + \left( \frac{\partial \xi}{\partial x} \right)^2} \, dx \]

\[ = \int_{\text{flame}} \dot{m}'_{F,0} \, \mathcal{H}_R \, dA_0 + \int_{\text{flame}} \dot{m}'_{F,1} \, \mathcal{H}_R \, dA_1 + \int_{\text{flame}} \dot{m}''_{F,1} \, \mathcal{H}_R \, dA_0 \]

- Time-average heat release

\[ \dot{m}''_{F,0} = \rho_u \mathcal{D} \frac{1}{\sqrt{1 + \left( \frac{\partial \xi}{\partial y} \right)^2}} \left. \frac{\partial Z_0}{\partial y} \right|_{Z_{st}} \quad dA_0 = \sqrt{1 + \left( \frac{\xi_{0,x}}{\xi_{0,y}} \right)^2} \]

- Weighted Area Dynamics
  - Note that for premixed flame with constant flame speed, this weighting was constant = flame speed

\[ dA_1 = \frac{\xi_{0,x}}{\sqrt{1 + \left( \xi_{0,y} \right)^2}} \xi_{1,x} \]

\[ \dot{m}''_{F,1} = -\rho_u \mathcal{D} \frac{1}{\sqrt{1 + \left( \frac{\xi_{0,x}}{\xi_{0,y}} \right)^2}} \left[ \frac{1 + \left( \xi_{0,x} \right)^2}{\xi_{0,x}} \left( \frac{\partial Z_0}{\partial y} \right)_{Z_{st}} \xi_{1,x} + \frac{\partial^2 Z_0}{\partial y^2} \xi_{1,y} \right] \]

- Mass burning rate dynamics
Experiment Data Processing

- Vortex Tracking
- Extract Phase roll-off from experimental data
  - Further data reduction and smoothing required to get meaningful information
- Physical parameters
  - Convection speed
  - Differences in leeward and windward side

<table>
<thead>
<tr>
<th>Case</th>
<th>R/NR</th>
<th>J</th>
<th>S</th>
<th>$Re_j$</th>
<th>$Re_{\infty}$</th>
<th>$T_{\infty}$ [K]</th>
<th>$f_F$ [Hz]</th>
<th>$A_F$ [A]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>R</td>
<td>5.05</td>
<td>0.41</td>
<td>1980</td>
<td>10520</td>
<td>1241</td>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>R</td>
<td>4.72</td>
<td>0.40</td>
<td>1990</td>
<td>11500</td>
<td>1186</td>
<td>177</td>
<td>0.6</td>
</tr>
<tr>
<td>3</td>
<td>R</td>
<td>4.69</td>
<td>0.40</td>
<td>1980</td>
<td>11480</td>
<td>1187</td>
<td>177</td>
<td>1.2</td>
</tr>
<tr>
<td>4</td>
<td>R</td>
<td>4.84</td>
<td>0.41</td>
<td>1980</td>
<td>10970</td>
<td>1218</td>
<td>177</td>
<td>1.5</td>
</tr>
<tr>
<td>5</td>
<td>R</td>
<td>4.83</td>
<td>0.41</td>
<td>1980</td>
<td>11060</td>
<td>1211</td>
<td>250</td>
<td>0.9</td>
</tr>
<tr>
<td>6</td>
<td>R</td>
<td>4.78</td>
<td>0.40</td>
<td>1990</td>
<td>11280</td>
<td>1203</td>
<td>250</td>
<td>1.5</td>
</tr>
<tr>
<td>7</td>
<td>R</td>
<td>4.60</td>
<td>0.39</td>
<td>1990</td>
<td>11170</td>
<td>1179</td>
<td>340</td>
<td>0.6</td>
</tr>
<tr>
<td>8</td>
<td>R</td>
<td>4.67</td>
<td>0.40</td>
<td>1980</td>
<td>11490</td>
<td>1191</td>
<td>340</td>
<td>1.5</td>
</tr>
<tr>
<td>9</td>
<td>R</td>
<td>23.23</td>
<td>0.40</td>
<td>4420</td>
<td>11480</td>
<td>1191</td>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>R</td>
<td>22.40</td>
<td>0.40</td>
<td>4400</td>
<td>11780</td>
<td>1179</td>
<td>177</td>
<td>0.6</td>
</tr>
<tr>
<td>11</td>
<td>R</td>
<td>25.19</td>
<td>0.42</td>
<td>4400</td>
<td>10420</td>
<td>1247</td>
<td>177</td>
<td>1.2</td>
</tr>
<tr>
<td>12</td>
<td>R</td>
<td>23.59</td>
<td>0.41</td>
<td>4380</td>
<td>11200</td>
<td>1203</td>
<td>177</td>
<td>1.5</td>
</tr>
<tr>
<td>13</td>
<td>R</td>
<td>23.75</td>
<td>0.40</td>
<td>4400</td>
<td>11150</td>
<td>1206</td>
<td>250</td>
<td>0.9</td>
</tr>
<tr>
<td>14</td>
<td>R</td>
<td>23.89</td>
<td>0.40</td>
<td>4400</td>
<td>11230</td>
<td>1199</td>
<td>250</td>
<td>1.5</td>
</tr>
<tr>
<td>15</td>
<td>R</td>
<td>23.38</td>
<td>0.40</td>
<td>4400</td>
<td>11430</td>
<td>1192</td>
<td>340</td>
<td>0.6</td>
</tr>
<tr>
<td>16</td>
<td>R</td>
<td>23.67</td>
<td>0.40</td>
<td>4400</td>
<td>11330</td>
<td>1197</td>
<td>340</td>
<td>1.5</td>
</tr>
<tr>
<td>17</td>
<td>R</td>
<td>5.08</td>
<td>1.04</td>
<td>2590</td>
<td>10660</td>
<td>1236</td>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>18</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>19</td>
<td>R</td>
<td>4.64</td>
<td>0.97</td>
<td>2590</td>
<td>11900</td>
<td>1171</td>
<td>177</td>
<td>1.5</td>
</tr>
<tr>
<td>20</td>
<td>R</td>
<td>4.68</td>
<td>1.00</td>
<td>2560</td>
<td>11490</td>
<td>1189</td>
<td>250</td>
<td>0.9</td>
</tr>
<tr>
<td>21</td>
<td>R</td>
<td>4.63</td>
<td>0.98</td>
<td>2550</td>
<td>11680</td>
<td>1178</td>
<td>250</td>
<td>1.5</td>
</tr>
<tr>
<td>22</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>23</td>
<td>R</td>
<td>4.97</td>
<td>1.02</td>
<td>2550</td>
<td>10810</td>
<td>1219</td>
<td>340</td>
<td>1.5</td>
</tr>
<tr>
<td>24</td>
<td>R</td>
<td>25.32</td>
<td>1.04</td>
<td>5750</td>
<td>10610</td>
<td>1236</td>
<td>0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Modeling Velocity Disturbances

- Using experiment database
- Data Sampling
  - w.r.t. jet centerline co-ordinate
  - at windward and leeward vortex centerlines
  - conditioned to flame location
    - Leeward flame was too diffuse
- Spatial variation of phase roll-off from Fourier modes

\[
u'(x,t) = \text{Re} \left[ \hat{A}(x) \exp\left( \frac{-i \omega x}{c_0} \right) + \hat{B}(x) \exp\left( \frac{-i \omega x}{u_0} + i \varphi(x) \right) \right] \exp(-i \omega t)
\]
Key Takeaways from Task

• PDEs for steady state and fluctuating flame position
  – Reduce the need for a full-field mixture fraction solution
• Global dynamics through spatially integrated heat release expressed in terms of flame position dynamics
  – Simplified expression for combustion dynamics modeling
• Identification of control parameter
  – From previously measured JICF data
  – Vortex tracking
  – Phase roll-off convection speed
  – Differences in speed between windward and leeward side
Task 5: LES Studies of Supercritical Mixing and Combustion

- **Mixing** and flame stability
- Systematic variation of design parameters
  - Momentum ratios for fuel and oxygen, flow rate, number of sets
  - Size, spacing, and locations of injectors
- Computational modeling may be more cost effective but include its own challenges
  - Autoignition kinetics (large uncertainty, maybe wrong)
  - Turbulence-chemistry closure
  - Real gas effects

*Baseline model NOT actual design*
Recap of Last Year: Real Gas Effect

- Global (highly simplified) kinetic model
- 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
Recap of Last Year: Flame Length and Combustion Efficiency

- **Combustion is not efficient**
- Combustion efficiency estimated as:
  \[ \eta = 100 \times \frac{\dot{m}_{f,\text{in}} - \dot{m}_{f,\text{out}}}{\dot{m}_{f,\text{in}}} \approx 49\% \]
- Flame length, \( L_f \sim 14.5 \, D_{ox} \)
  - estimated as intersection of \( Z = Z_{st} \) and \( T = 1500 \, K \)
- \( \eta \) needs to be improved
  - Inflow realistic turbulence
  - Modify J and jet spacing
  - Mass flow rate changes
  - Jet-staging and distributed mixing
  - Inflow swirling
- Mixing is the key
• Fluent simulation with circumferential injections
• Mixing is challenging
Summary of Progress for Numerical Investigation

• Focus on jet mixing, LES of non-reacting mixing to identify where stoichiometric surface appear, then identify autoignon regions
  • Case 1: fuel jet behind O₂ jet by 28 mm
  • Case 2: O₂ behind fuel jet by 28 mm; Case 3: 14 mm
• LES using compressible adaptive-mesh-refinement (AMR)
  • Reduced finite-rate kinetics (from Task 3) used
  • Implemented in a PSR based network model
• Studies of reacting spatial mixing layer (SML) configuration
  • Canonical problem with some known features
  • CH₄-O₂ mixing and reactions in CO₂ background
  • Study effect of pressure, details of the kinetics
LES using AMR: Mixing in JICF

- AMR refines grid near the jet inlets.
- SGS closure accounts for AMR$^1$
Mixing Studies Using LES

- Z = 1 (fuel), Z = 0 (oxidizer); dashed black line: stoichiometric mixture fraction
- Cross flow: sCO₂ at 300 atm; Fuel jet diameter is 3 mm, O₂ jet diameter is 5 mm
- Case 1 and 3 - distance between jets is 28 mm; Case 2 - 14 mm
- A bigger and continuous zone of stoichiometry is visible when the two jets are closer indicating enhanced mixing
- Mixing dependent on injection locations & conditions – difficult to optimize
Task 5: LES Studies of Supercritical Mixing and Combustion

Equilibrium Calculations using PSR

- Points were selected from the LES as an input to PSR
- Initial concentrations of species and temperature were selected at these points.
- The equilibrium temperature, species concentrations are tabulated in the next slide.
- From the table we see that the points 7, 8 and 9 where the oxidizer and fuel have mixed we get combustion
- Shown for Case 2
## Task 5: LES Studies of Supercritical Mixing and Combustion

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>361.22</td>
<td>0.989</td>
<td>0.0</td>
<td>0.011</td>
<td>361.22</td>
<td>0.989</td>
<td>0.0</td>
<td>0.011</td>
</tr>
<tr>
<td>2</td>
<td>385.95</td>
<td>0.980</td>
<td>0.0</td>
<td>0.02</td>
<td>385.93</td>
<td>0.980</td>
<td>0.0</td>
<td>0.020</td>
</tr>
<tr>
<td>3</td>
<td>695.79</td>
<td>0.325</td>
<td>0.0</td>
<td>0.675</td>
<td>645.30</td>
<td>0.313</td>
<td>0.0</td>
<td>0.687</td>
</tr>
<tr>
<td>4</td>
<td>363.14</td>
<td>0.0</td>
<td>0.999</td>
<td>0.001</td>
<td>363.14</td>
<td>0.0</td>
<td>0.999</td>
<td>0.001</td>
</tr>
<tr>
<td>5</td>
<td>364.06</td>
<td>0.0</td>
<td>0.998</td>
<td>0.002</td>
<td>364.06</td>
<td>0.0</td>
<td>0.998</td>
<td>0.002</td>
</tr>
<tr>
<td>6</td>
<td>474.49</td>
<td>0.0</td>
<td>0.948</td>
<td>0.052</td>
<td>483.78</td>
<td>0.0</td>
<td>0.947</td>
<td>0.053</td>
</tr>
<tr>
<td>7</td>
<td>654.53</td>
<td>0.028</td>
<td>0.545</td>
<td>0.427</td>
<td>1184.11</td>
<td>0.0</td>
<td>0.546</td>
<td>0.454</td>
</tr>
<tr>
<td>8</td>
<td>697.67</td>
<td>0.044</td>
<td>0.414</td>
<td>0.542</td>
<td>1446.9</td>
<td>0.0</td>
<td>0.325</td>
<td>0.675</td>
</tr>
<tr>
<td>9</td>
<td>807.32</td>
<td>0.042</td>
<td>0.236</td>
<td>0.722</td>
<td>1464.7</td>
<td>0.0</td>
<td>0.151</td>
<td>0.849</td>
</tr>
<tr>
<td>10</td>
<td>1026.6</td>
<td>0.005</td>
<td>0.076</td>
<td>0.919</td>
<td>1104.5</td>
<td>0.0</td>
<td>0.064</td>
<td>0.936</td>
</tr>
<tr>
<td>11</td>
<td>859.22</td>
<td>0.100</td>
<td>0.015</td>
<td>0.885</td>
<td>762.65</td>
<td>0.059</td>
<td>0.0</td>
<td>0.941</td>
</tr>
</tbody>
</table>
2D Spatial Mixing Layer

- Splitter plate: 1.2 mm
- CH$_4$ jet of 3 mm, 30 m/s, 300 K
- O$_2$ jet of 5 mm, 30 m/s, 300 K
- Outer jets of CO$_2$ at 50 m/s, 500 K
- 1 atm, 200 atm and 300 atm cases
- 5-species reduced kinetics from Task 3
- New analysis shows that vapor-liquid equilibrium (VLE) can occur under supercritical conditions
Vapor-Liquid Equilibrium in Supercritical Mixtures

- Single species: the phase is uniquely defined by the equilibrium diagram
- Subcritical regime: jet exhibits atomization, droplets, and sharp gas/liquid interface
- Supercritical regime: Interface is diffused and no droplet formation
- Mixtures: VLE exists at interface for given \((p, T)\) and composition \(z_i\).
- JICF can have local VLE regions in
  - \(\text{CH}_4-\text{CO}_2\), \(\text{O}_2-\text{CO}_2\) interfaces
  - \(\text{CH}_4-\text{O}_2-\text{CO}_2-\text{H}_2\text{O}\) regions
- Critical properties of each component play a crucial role to determine VLE
- Need to include VLE effects to account for mixture effects
Future of Task 5

• Revisit the earlier supercritical JICF mixing case, accounting for presence of VLE to reassess the problems seen in the past.
• Continue spatial mixing layer studies with different conditions
  • Binary mixing under supercritical conditions
  • Reacting cases under supercritical conditions
• Autoignition studies will require more detailed kinetics
  • 19 species chemistry from Task 3 available
Summary of Year 2 Achievement

• High pressure shock tube commissioned
  – System validation (vs simulation, previous work)
  – Measurement of autoignition delays with high CO$_2$ concentration (above critical pressure of CO$_2$)

• Different optimized reduced kinetic models developed and implemented in CFD

• Governing equation developed for theoretical framework

• LES investigation of JICF
  – Not efficient on mixing
  – Sensitive to kinetic models
  – Jet mixing, quick estimation of autoignition location
  – Vapor-liquid equilibrium plays important role
Thank you! & Questions?

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