Outline

• Effects of pressure and diluents on flames.
• Identification of target conditions.
• Overview of characteristic time and length scales.
• CFD simulations of turbulent time and length scales.
• Chemical kinetic mechanisms.
• LES simulations with varying O₂ concentrations.
Effect of Pressure on Laminar Flame Speed

- Cantera with GRI 3.0 used to calculate premixed laminar flame speed.
- Flame speed with 31%O2/69%CO2 lower than air mainly due to lower diffusivity.
  \[ S_L \propto \sqrt{RR \cdot D} \]
  \[ RR = \text{Reaction Rate} \]
  \[ D = \text{Molecular Diffusivity} \]
  \[ D \propto \frac{1}{P} \]
- Overall reaction order for CH4/O2/CO2 is ~ 1.4
Cantera Non-Premixed Laminar Flame Profiles

- Temperature and OH profiles through flame region.
- Flame thins due to decrease in $\alpha$ being faster than decrease in $S_L$.
- Peak in OH mole fraction decreases due to three-body recombination reactions.

$\delta_L = \frac{\alpha}{S_L}$ \quad \alpha = k/\rho C_p

Opposed Diffusion \hspace{1cm} CH4+(.31O2 .69CO2) \hspace{1cm} Phi=1 \hspace{1cm} GRI 3.0

- Sep$= 2$cm
- $V_F=V_O=27$ cm/s

Axial Position (m)

Strain Rate (1/s)

Temperature (K)

OH (mole fraction)

Axial Position (m)

Axial Position (m)
Extinction strain rate increases with pressure due to flame thinning. Higher strain rate equates to higher turbulence at quenching.

- Significant discrepancy between GRI 3.0 and Aramco. GRI predicts faster kinetics.
- Ignition delay time ranges from 1-3 msec at Allam cycle conditions.
Allam Cycle

- Goal is to estimate some characteristic combustion scales for high pressure oxy-fuel flames for direct-fired sCO2 cycles.
- Target is the Allam cycle conditions (O₂ 15% to 30% molar concentration)*.

Table 1. ALLAM CYCLE KEY POINTS (ISO CONDITIONS)

<table>
<thead>
<tr>
<th>Point</th>
<th>Pressure (Bar)</th>
<th>Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbine Inlet (A)</td>
<td>300</td>
<td>1150</td>
</tr>
<tr>
<td>Turbine Outlet (B)</td>
<td>30</td>
<td>775</td>
</tr>
<tr>
<td>CO2 Compressor Inlet (D)</td>
<td>30</td>
<td>20</td>
</tr>
<tr>
<td>CO2 Compressor Outlet (E)</td>
<td>80</td>
<td>65</td>
</tr>
<tr>
<td>CO2 Pump Inlet (F)</td>
<td>80</td>
<td>20</td>
</tr>
<tr>
<td>CO2 Pump Outlet (G)</td>
<td>300</td>
<td>55</td>
</tr>
<tr>
<td>Combustor Inlet (I)</td>
<td>300</td>
<td>750</td>
</tr>
</tbody>
</table>

* Allam, et al., Energy Procedia 37, 2013, 1135-1149
Borghi Combustion Diagram

- Borghi Diagram indicates regime of combustion (wrinkled flames, corrugated flames, stirred reactor, etc.

\[ \text{need: } \frac{u'}{S_L} \text{ and } \frac{l_T}{\delta_L} \]

P=300 bar
50 MW Thermal Input
\( \phi = 0.95 \)

\( \text{CO}_2 \) (43.6 kg/s, T=1015K)
\( \text{CO}_2 \) (14.0 kg/s, T=1015K)
\( \text{O}_2 \) (4.2 kg/s, T=1015K)
\( \text{CH}_4 \) (1 kg/s, T=496 K)

combustor

Gas Turbines
IC Engines

C. Sorusbay, “Turbulent Premixed Combustion in Engines”, Istanbul Technical University
Characteristic Scales and Dimensionless Numbers

- Included here for completeness…

\[ K_a = \frac{\tau_{\text{chem}}}{\tau_K} = \frac{\delta_L^2}{l_K^2} \quad \text{Karlovitz Number (chemical time / Kolmogorov time)} \]

\[ Da = \frac{\tau_{\text{turb}}}{\tau_{\text{chem}}} = 0.247 \left( \frac{k}{\varepsilon} \right) \left( \frac{S_L^2}{\alpha} \right) \quad \text{Damkohler Number (turbulent time / chemical time)} \]

\[ \delta_L = \frac{\alpha}{S_L} \quad \text{Laminar flame thickness (thermal diffusivity / laminar flame speed)} \]

\[ l_K = \left( \frac{\nu^3}{\varepsilon} \right)^{1/4} \quad \text{Kolmogorov length scale (kinematic viscosity / turbulent dissipation rate)} \]

\[ l_T = 0.2 \frac{k^{1/2}}{\varepsilon} \quad \text{Integral length scale (turbulent kinetic energy / turbulent dissipation rate)} \]

\[ u' = \sqrt{\frac{2k}{3}} \quad \text{Turbulent fluctuating velocity} \]

\[ K > 1 \text{ means the smallest eddies can enter and thicken the flame front} \]

\[ Da >> 1 \text{ means the chemistry is fast compared to turbulent mixing} \]
50 MW Conceptual Combustor

SSME Preburner type combustor - 21 coaxial injectors, 4M Cells

- Flow split of CO₂ between injectors and wall purge was varied to produce cases 1 to 3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂ mole fraction</td>
<td>0.31</td>
<td>0.18</td>
<td>0.09</td>
</tr>
<tr>
<td>Uₚ (m/s)</td>
<td>30</td>
<td>35</td>
<td>70</td>
</tr>
<tr>
<td>lₖ (m)</td>
<td>1.9e-3</td>
<td>2.2e-3</td>
<td>2.0e-3</td>
</tr>
<tr>
<td>U’ (m/s)</td>
<td>7.5</td>
<td>10.7</td>
<td>23.8</td>
</tr>
<tr>
<td>Sₗ (m/s)</td>
<td>0.58</td>
<td>0.082</td>
<td>0.05</td>
</tr>
<tr>
<td>τₐₚ (s)</td>
<td>9.2e-4</td>
<td>1.6e-3</td>
<td>2.5e-3</td>
</tr>
</tbody>
</table>
Turbulent Time and Length Scales

Two Limiting Cases:

Case 1: 25% of CO2 by mass mixed in with O2 ($X_{O2}=0.31, \phi=0.95$)

Case 3: Fully mixed (100% of CO2 mixed in with O2) ($X_{O2}=0.09, \phi=0.95$)

Steady RANS k-e
DRM19 reduced CH4 mechanism
No Combustion model

Case 1
25% of CO2 with O2 ($X_{O2}=0.31$)
75% of CO2 through purge
$l_T=1.9$ mm
$U'=7.5$ m/s

Case 3
100% of CO2 with O2 ($X_{O2}=0.09$)
$l_T=2.0$ mm
$U'=23.8$ m/s
Borghi Diagram for Oxy-Combustion

• Three cases shown for 300 bar oxy-combustion define a range of conditions (O₂ from 9-31%) spanning the thickened, corrugated flame regime and stirred reactor.

• Significantly outside the range of gas turbine and IC engine operation.
  • Re# and/or Ka# significantly larger than gas turbines or IC engines.

• Requires assessment of appropriate turbulent combustion models.
Chemical Kinetic Mechanisms

• No detailed mechanisms validated at sCO2 conditions. Best available is likely Aramco Mech (U. Galway). Validated with flame-speed up to 60 bar and ignition delay to 260 bar. Likely better than GRI 3.0.

• Huge mechanism, 103 species, 480 reactions after reduction to C2 and smaller.

• Need for compact skeletal mechanisms amenable to CFD modeling (10-30 species maximum).

Need flame speed, species profiles and induction time data for direct-fired conditions!
Mechanism Reduction

- Combination of reaction path analysis, flame-speed sensitivity and ignition delay time sensitivity.
- Optimized for Allam cycle combustor conditions
  - 300 bar
  - $T_{\text{preheat}} \sim 1000K$
  - Oxidizer: 25% $O_2$ + 75% $CO_2$
- Several skeletal mechanisms developed with 33, 29, 26 and 17 species.

Flame speed sensitivity at 300 bar

Flame Speed Sensitivity
AramcoMech 2.0 300 bar
$T=985$, CH4:.12989, O2:.27351, CO2:.5966
Mechanism Reduction

• Performance comparison of various skeletal mechanisms.
  • Flame speed and ignition delay improve with the inclusion of more species and reactions.
    • 33 species mechanism able to predict flame-speed and ignition delay fairly well.
    • 17 species able to predict flame-speed to within ~30% of detailed mechanism.

Laminar Flame Speed
P=60 bar, T=298K, CH4 + (.15O2/He)

Ignition Delay Time
Phi=1, T=985K, (.13CH4/.27O2/.60CO2)

Mechanism Reduction

- Performance comparison of various skeletal mechanisms.
  - All do very well for CO production profiles.
- CO prediction important for accurate cycle efficiency calculations.
LES Modeling: Temperature Contours

Large Eddy Simulation, Dynamic $k$-$e$ transport
17-species skeletal mechanism
No Combustion Model
$\Phi=0.95$

- Combustor exit temperature is the same for all three cases (~1520 K).
- Combustion transitions from lifted flame to stirred reactor as $O_2$ is decreased. Consistent with Borghi diagram.
  - Peak temperature decreases (2730 K to 1614 K).
  - Core velocity increases (30 m/s to 70 m/s).
LES Modeling: CO Contours

Large Eddy Simulation, Dynamic \( k-e \) transport
17-species skeletal mechanism
No Combustion Model
\( \Phi=0.95 \)

- Combustor exit temperature is the same for all three cases (1520 K).
- For 31% \( \text{O}_2 \) case, peak CO concentration well above equilibrium value (\( X_{\text{CO}}=0.25 \)).
- For all cases, peak CO is significantly higher than equilibrium.
LES Modeling: CO Summary

- Peak CO concentrations well above equilibrium levels.
- Average CO concentrations at combustor exit also well above equilibrium levels.
- Cycle efficiency calculations indicate roughly a 0.75 % pt. drop in efficiency per mole % CO in working fluid.

<table>
<thead>
<tr>
<th>Case</th>
<th>Oxidizer flow (kg/s)</th>
<th>Purge flow (kg/s)</th>
<th>O2 mole %</th>
<th>Equilibrium Flame Temp(K)</th>
<th>Equilibrium Flame CO mole %</th>
<th>LES Peak Temp(K)</th>
<th>LES Peak CO Mole %</th>
<th>LES Avg CO mole %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>16.8</td>
<td>43.6</td>
<td>31.0</td>
<td>2690</td>
<td>2.4</td>
<td>2730</td>
<td>25.0</td>
<td>3.5</td>
</tr>
<tr>
<td>2</td>
<td>30.4</td>
<td>30.0</td>
<td>18.0</td>
<td>2100</td>
<td>0.15</td>
<td>2060</td>
<td>5.0</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>60.4</td>
<td>0.0</td>
<td>9.0</td>
<td>1612</td>
<td>0.0018</td>
<td>1614</td>
<td>3.0</td>
<td>0.013</td>
</tr>
</tbody>
</table>

Equilibrium Calcs
Comb Exit: 
T=1612 K
X_CO = 0.0018 %
Concluding Remarks

- Oxy-combustion at 300 bar is somewhat uncharted territory.
  - Conditions more representative of rocket engines.
  - Limited data available.

- Need for validated detailed chemical kinetic mechanisms as well as reduced mechanisms.

- Must take care in selecting appropriate combustion models (fast mixing, flamelet, EDC, PDF, etc...).

- CO production highly sensitive to flame temperature and may be well above equilibrium.