Effects of Exhaust Gas Recirculation (EGR) on Turbulent Combustion Emissions in Advanced Gas Turbine Combustors with High Hydrogen Content (HHC) Fuels

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Outline of the Presentation

• Yiguang Ju - Chemical kinetics with EGR effects, Reactor Assisted Turbulent Slot (RATS) burner studies at atmospheric pressure

• Bob Lucht and Jay Gore: High-pressure Premixed Axisymmetric Reactor Assisted Turbulent (PARAT) burner, initial measurements

• Michael Mueller – Advanced numerical modeling of the RATS and PARAT burners
Effects of CO₂ and H₂O Diluents on Laminar & turbulent flame speeds, Chemical kinetics, Emissions

• What happens to the burning rate when diluents (CO₂, H₂O, etc.) are introduced? Four effects:
  – **Dilution** – Reduce reactant concentrations, reduce reaction *rates*
  – **Thermal** – Reduce flame temperature, reducing rate *coefficients*
  – **Transport** – thermal/mass diffusivity (Lewis number) and **Radiation**
  – **Chemical** – Reactions of “diluent” with fuel, oxidizer, and intermediates (e.g. CO₂+H→CO+OH and HCO+M=H+CO, H₂O+O=2OH)

Research accomplishments

• Flame speed measurements of HHC fuels with CO₂/H2O additions
• High pressure kinetic mechanism (HP-Mech) for HHC fuels with EGR
• Turbulent flame speed and structure measurements with H₂O/CO₂ dilution
• Radiation effect of CO₂/H₂O
• HO₂ diagnostics using Faraday Rotational Spectroscopy
Laminar flame speeds: Experimental Design

H₂, CH₄, CH₂O, C₂H₂, C₂H₄, and C₂H₆ fuels with H₂O or CO₂ dilutions

- Two validated experiments
  - Cylindrical, room temperature chamber for CO₂ dilution from 1-20 atm
  - Spherical, heated chamber for H₂O dilution from 1-10 atm
- Both experiments:
  - Centrally ignited spherically expanding flame
  - High speed schlieren imaging
  - Passive custom pressure-release valves

- Electrodes
- Oven
- Heater
- Heated tube
- Fan
- Pressure release tank
- Vaporized liquid or solid components, vacuum pump
- Gaseous components, vacuum pump, vent
- Secondary inlet for gaseous components

- Focus Lens
- High-Speed Camera
- Collimating Lens
- Decollimating Lens
- 100 W Mercury Lamp
- 100 μm Pinhole
- Primary Inlet
- Secondary Inlet
- Combustion Chamber
- Gas-Releasing Holes
- Permanent Magnet
- Iron Plate
- Quartz Window
- Primary Tube
- Secondary Tube
- Mixture components, vacuum pump, vent
- Heated tube
- Vaporized liquid or solid components, vacuum pump
- Gaseous components, vacuum pump, vent
- Heater
For example: $\text{C}_2\text{H}_4$ with H$_2$O dilution

- Water vapor decreases the mass burning rate, more at high pressure
- Models disagree with experiments and each other, more at high pressure
- Similar for hydrogen and syngas flames with water vapor*

![Graph](image)

**C₂H₂ Flames with CO₂ dilution**

- CO₂ dilution decreases burning rate for lean conditions – but doesn’t affect rich conditions
- Typically, CO₂ slows flame by decreasing H through reverse reaction of CO+OH=CO₂+H
- Existing models do not have a good prediction. HP-Mech improves prediction.

Chemical effect of H2, C2H4 Flames with H2O dilution

- Water addition decreases H and O radicals relative to OH and HO2
  \[ H_2O + O = 2OH \]
- High collisional efficiency of H2O
  - Increased HO2 from H+O2+M=HO2+M
  - Increased H from HCO+M=H+CO+M
- Chemical effect increases with pressure
Task 2a A high pressure mechanism (HP-Mech) for C_0-C_2 hydrocarbon fuel with H2O and CO2

Many models available, but... not for EGR, pressure dependency...

- Most widely ones: GRI-Mech, USC Mech II, optimization based, off-design problem
- Dryer models: small hydrocarbons: H_2, CO/CH_4, CH_2O, CH_3OH, CH_3CH_2OH, not focused on EGR
- Curran models: also try to optimize the experiments such as ignition delay and flame speed
- ...

**HP-Mech**

- Addressing the pressure dependence of reactions
- EGR effect
- Using the elementary rates with high level quantum computation and/or experimentally determined, *no optimization!*
- Update the thermochemistry database (e.g. Burcat and Ruscic database).

**Key reactions:**

For example

- \( H+O_2 = O + OH \)
- \( H+O_2+M=HO_2+M \)
- \( HCO+M = H+CO+M \)
- \( HCO+O_2 = HO_2+CO \)
- \( NO+HO_2 = NO_2+OH \)
- \( NO_2+CH_3 = NO + CH_3O \)
High pressure mechanism (HP-Mech) development

- **Thermochemistry:** Active Thermochemical Tables
- **Transport:** chemkin library: H, H2 and HE from Hai Wang USC Mech II
- **Reaction set:** up to C6 - reflecting the most recent advance of rate determinations
  - $\text{H}_2$-$\text{O}_2$ model (Burke et al, Int. J. Chem. Kinet. 44(2012), 444–474, update or modification)
  - $\text{CO}+\text{OH}=\text{CO}_2+\text{H}$ (Joshi et al, Int. J. Chem. Kinet. 38 (2006), 57-73)
  - HCO decomposition (Yang et al, 8th US National Combustion Meeting, Park City, Utah 2013)
  - HCO+$\text{O}_2$=HO$_2$+CO (Klippenstein private commucation)
  - $\text{CH}_2$ relaxations (Gannon et al, J. Chem. Phys. 132(2010), 024302)
  - $\text{CH}_3+\text{HO}_2$ (Jasper et al Proc. Combust. Inst. 32, 279 (2009))
  - $\text{CH}_3+\text{OH}$ and $\text{CH}_3\text{OH}$ decomposition ( Jasper et al, J. Phys. Chem. A 111, 3932 (2007))
  - $\text{H}+\text{C}_2\text{H}_2+\text{M}=$C$_2$H$_3$+M and $\text{H}+\text{C}_2\text{H}_4+\text{M}=$C$_2$H$_5$+M (Miller and Klippenstein, Phys. Chem. Chem. Phys., 6(2004), 1192 –1202)
  - C$_2$H$_2$+OH (Senosiain et al., J. Phys. Chem. A 109(2005) 6045-6055)
  - ....

Hydrogen flames-1

Mass burning rate of H2/O2/He phi=0.85

H+O2+M dominate pressure dependence

9th US National Combustion Meeting,
Cincinnati OH, May 17- 20th, 2015
H2/CO flames

Mixture composition effect at 1 atm
x%H2 and 1-x%CO x=1, 5, 25, 50

Pressure of 25% H2-75% CO
P=5, 10, 20 atm

9th US National Combustion Meeting,
Cincinnati OH, May 17-20th, 2015
Ethane flame

$C_2H_6$ flame $CO_2$ dilution effect $\phi=0.8$

$C_2H_6$ flame $CO_2$ dilution effect $\phi=1.6$

$C_2H_6$ flame $H_2O$ dilution effect $\phi=0.8$

$C_2H_6$ flame $H_2O$ dilution effect $\phi=1.6$
Objectives

• Investigate turbulent burning velocity and flame structures
  – At EGR conditions and elevated temperature
  – Systematic measurements of H$_2$O and CO$_2$ dilution
    • Effects of H$_2$O$^1$ and CO$_2$$^2$ dilution were investigated separately in previous studies only with methane/air.

• Identify chemistry/thermal/transport effects on turbulent premixed flames$^3$ in EGR conditions.

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Experiment, RATS Burner

- **Reactor Assisted Turbulent Slot burner (RATS burner)**\(^1\)
  - Heat large flow rates (1000 LPM) up to 700 K with CO2/H2O/N2 dilutions
  - \(~ 55 \text{ cm} \) heated length, 100 × 10 mm exit cross-section (\(D_H \approx 18 \text{ mm}\))
  - Two turbulence generators\(^2,3\), homogeneous isotropic turbulence confirmed by hot-wire anemometry
  - High Reynolds number (\(Re_{bulk} > 10,000\))

\(^3\) Venkateswaran, P. et. al., *Combustion and Flame*, 158, 2011, 1602-1614
Determination of turbulent flame speed, $S_T$

Find inner edge

Stack perimeters from 500 images

PDF of Flame Perimeters

Single Image of OH PLIF

Find inner edge


$S_T = \frac{Uw}{L_p}$

$L_p$ (4th order polynomial fit)
Effects on flame speed with EGR dilution

- Both CO$_2$ and H$_2$O addition decrease turbulent burning velocity, $S_T$

- Strong decrease in laminar flame speed $S_L$
  - Drop from 70.6 cm/s to 28.4 cm/s for 20% H$_2$O
  - Drop from 70.6 cm/s to 36.8 cm/s for 10% CO$_2$

- $S_T/S_L$ increases with dilution for both CO$_2$ and H$_2$O addition
  - More pronounced increase for CO$_2$, however

- Why does normally $S_T/S_L$ increases with dilution?
- How do we know the effects are thermal or kinetic?
EGR Dilution effect at Constant Temperature: Corrugated Flames

- $\text{H}_2\text{O}$ dilution has almost no discernable effect on $L_p$, $S_T$, or $S_T/S_L$.
- Thermal effects were clearly the dominant factor for $\text{H}_2\text{O}$ dilution.
- $\text{CO}_2$ dilution produces ($\sim 10\%$) decrease in $S_T$, kinetic effect.
- Turbulence reduces the kinetic effect of $\text{CO}_2$ on burning velocity.
- $\text{CO}_2$ dilution increases turbulence-turbulent flame speed coupling due to the combined chemistry and transport effect ($1/Le$). (Promoted instability)

$\mathbf{S_T/S_L \sim \left( \frac{u'}{S_L} \right)^{0.5} \left( \frac{1}{Le} \right)^{0.5}}$

- $\uparrow 10\% \text{ H}_2\text{O}$ results in $u'/S_L \uparrow 2\%$ and $1/Le \downarrow 8\%$
- $\uparrow 10\% \text{ CO}_2$ results in $u'/S_L \uparrow 18\%$ and $1/Le \uparrow 8\%$

$U = 7.5 \text{ m/s}$
$T_0 = 450 \text{ K}$
$\phi = 0.9$
$T_{\text{max}} = 2025 \text{ K}$

- $\text{Kobayashi 2002}$
- $\text{H}_2\text{O}$ addition
- $\text{CO}_2$ addition
EGR Dilution at Constant Temperature: Thin Reaction Zone

- \( \text{H}_2\text{O} \) again has no significant effect on \( L_p, S_T, \) or \( S_L \)
- Turbulence increases the decrease of \( S_T \) with \( \text{CO}_2 \) addition, enhance the turbulence-chemistry coupling.
- Turbulent flame speed deviates from the conventional \( S_T \) correlation.
Conclusions

1. H$_2$O and CO$_2$ dilution have strong thermal, transport, and chemistry effects on the turbulent flame speed of methane. The conventional $S_T/S_L$ vs. $u'/S_L$ correlation may not apply.

2. Thermal effects are the dominant factor in affecting burning velocity for both H$_2$O and CO$_2$ dilution.

3. At constant adiabatic flame temperature, H$_2$O dilution does not produce significant impacts on the normalized burning velocity $S_T/S_L$ due to the opposing effects of kinetics and transport.

4. For CO$_2$ dilution, in the corrugated flame regime, the competition between transport effect and chemistry effect results in an increase in $S_T/S_L$, thus stronger dependence of turbulent flame speed on Reynolds number.

5. In the thin reaction zone, CO$_2$ addition results in stronger chemistry effect at higher Reynolds number and an approximately constant $S_T/S_L$, deviating from the conventional turbulent flame speed correlation.
Future Plans

- Development of HP-Mech with NOx at high pressure.
- CH\textsubscript{4}/air + CO\textsubscript{2}, H\textsubscript{2}/air + H\textsubscript{2}O/CO\textsubscript{2} will be further investigated in turbulent premixed flames at higher pressure. ($S_T$ and flame structures)
- Studies of the transport effects on turbulent flame structure

Big problem:

Comparison of predicted peak OH concentrations of hydrogen flames by seven different kinetic models.

Radicals prediction is not constrained in existing models!

Large uncertainty to predict NOx emissions!

\[ N_2 + O = NO + N \]
\[ N + OH = NO + H \]
High-Pressure PARAT Burner Studies
Robert Lucht and Jay Gore
Purdue University

- Design and fabrication of PARAT burner
- Initial measurements at atmospheric pressure
- Planned high-pressure measurements
<table>
<thead>
<tr>
<th>High Pressure Lab System</th>
<th>Maximum Flow Capacity</th>
<th>Max Operating Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Natural Gas Heated High Pressure Air</td>
<td>9 lbm/s 4 kg/s</td>
<td>700 psi / 1100 K 1500 F</td>
</tr>
<tr>
<td>Electric Heated Air or Nitrogen</td>
<td>1 lbm/s 0.5 kg/s</td>
<td>600 psi / 800 K 1000 F</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>5 lbm/s 2 kg/s</td>
<td>1,500 psi</td>
</tr>
<tr>
<td>Liquid Aviation Fuel (Kerosene)</td>
<td>1 lbm/s 0.5 kg/s</td>
<td>1,500 psi</td>
</tr>
<tr>
<td>Natural Gas</td>
<td>1 lbm/sec 0.5 kg/s</td>
<td>3500 psi</td>
</tr>
</tbody>
</table>
Laser Diagnostics for High-Pressure Test Rig

- 10 kHz stereo PIV
- 10 kHz OH PLIF
- Pulse burst laser is being delivered this week for PIV, PLIF at data rates up to 100 kHz
Assembly of PARAT Burner into the Windowed High-Pressure Test Rig
Cross-sectional View of PARAT Burner into the Windowed High-Pressure Test Rig
## Initial Operation of the PARAT Burner at Atmospheric Pressure: Operating Conditions

<table>
<thead>
<tr>
<th></th>
<th>Without EGR</th>
<th>With EGR</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Flame No.</strong></td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td><strong>Re</strong></td>
<td>10000</td>
<td>20000</td>
</tr>
<tr>
<td><strong>Equivalence ratio</strong></td>
<td>0.8</td>
<td>0.8</td>
</tr>
<tr>
<td><strong>CO₂ percentage by mass%</strong></td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td><strong>Air flow rate (l/min)</strong></td>
<td>122.2</td>
<td>244.4</td>
</tr>
<tr>
<td><strong>CH₄ flow rate (l/min)</strong></td>
<td>10.3</td>
<td>20.5</td>
</tr>
<tr>
<td><strong>CO₂ flow rate (l/min)</strong></td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td><strong>CO₂/CH₄ mass flow rate ratio</strong></td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td><strong>H₂ flow rate (l/min)</strong></td>
<td>2.0</td>
<td>2.0</td>
</tr>
</tbody>
</table>
IR Imaging of PARAT Burner Flames

- Turbulent lean premixed methane flame
  - \( \text{Re} = 8950 \)
  - Burner diameter \( (D) = 15 \text{ mm} \)

- FLIR Infrared Camera
  - w/ band pass filters
  - \( \text{H}_2\text{O} \): \(2.58 \pm 0.03 \mu\text{m}\)
  - \( \text{H}_2\text{O} \) and \( \text{CO}_2 \): \(2.77 \pm 0.1 \mu\text{m}\)
  - \( \text{CO}_2 \): \(4.38 \pm 0.08 \mu\text{m}\)

- Distance between camera and flame
  - \( d = 0.5 \text{ m} \)

- Sampling frequency=430 Hz
IR Imaging of PARAT Burner Flames

Infrared images of the CO$_2$ (4.3 micrometer band) for the four different flames at a representative exposure time of 20 µs

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<td>Equivalence ratio</td>
<td>0.8</td>
<td>0.8</td>
</tr>
<tr>
<td>CO$_2$ percentage by mass%</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Air flow rate (l/min)</td>
<td>122.2</td>
<td>244.4</td>
</tr>
<tr>
<td>CH$_4$ flow rate (l/min)</td>
<td>10.3</td>
<td>20.5</td>
</tr>
<tr>
<td>CO$_2$ flow rate (l/min)</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>CO$_2$/CH$_4$ mass flow rate ratio</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>H$_2$ flow rate (l/min)</td>
<td>2.0</td>
<td>2.0</td>
</tr>
</tbody>
</table>
CARS Measurements in Atmospheric Pressure
PARAT Burner Flames: Temperature PDFs Along Centerline

Axial Location

108 mm

113 mm
CARS Measurements in Atmospheric Pressure
PARAT Burner Flames: Temperature PDFs Along Centerline

Axial Location

108 mm                                113 mm
CARS Measurements at High Pressure: PARAT Burner Now Installed in HP Test Rig
High-Pressure PARAT Burner Studies

Future Work

• Initial tests for operability
• High-speed stereo PIV, OH PLIF for comparison with numerical modeling
• Nox, CO emission measurements for comparison with numerical modeling
In the corrugated flame regime, where the Lewis number effect is important, CO₂ dilution leads to an increase in \( \frac{S_T}{S_{L,LE}} \).

In the thin reaction zone, however, \( \frac{S_T}{S_{L,LE}} \) now decreases with CO₂ dilution, indicating stronger turbulence-chemistry effect.

However, the leading edge speed does not improve the correlation of turbulent flame speed with \( u' \).
Effects on flame speed with EGR dilution at constant temperature

- To remove thermal effects, we hold the adiabatic flame temperature $T_{ad}$ constant.
- The 10% CO$_2$ cases ($T_{ad} = 2025$ K) is used as a baseline—all other cases with extra N$_2$ dilution.
- Modified Damköhler scaling analysis contains elements of both transport ($Le$) and kinetics ($S_L$):
  $$\frac{S_T}{S_L} \sim \left( \frac{u'}{S_L} \right)^{0.5} \left( \frac{1}{Le} \right)^{0.5}$$
- How will the chemistry effect change when we move from the corrugated flame to thin reaction zone regime?