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 CO_2 and H_2O Diluents on

Laminar & turbulent flame speeds, Chemical kinetics, Emissions

- What happens to the burning rate when diluents (CO_2, H_2O, 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. **$CO_2+H \rightarrow CO+OH$ and $HCO+M=H+CO$, $H2O+O=2OH$**)

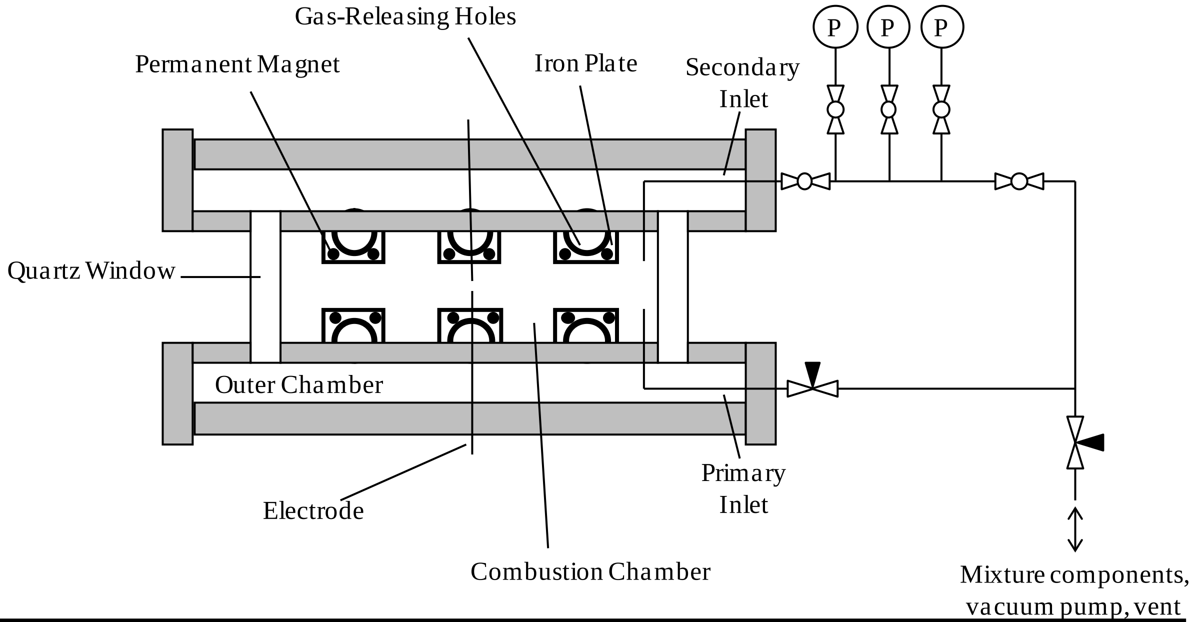
Research accomplishments

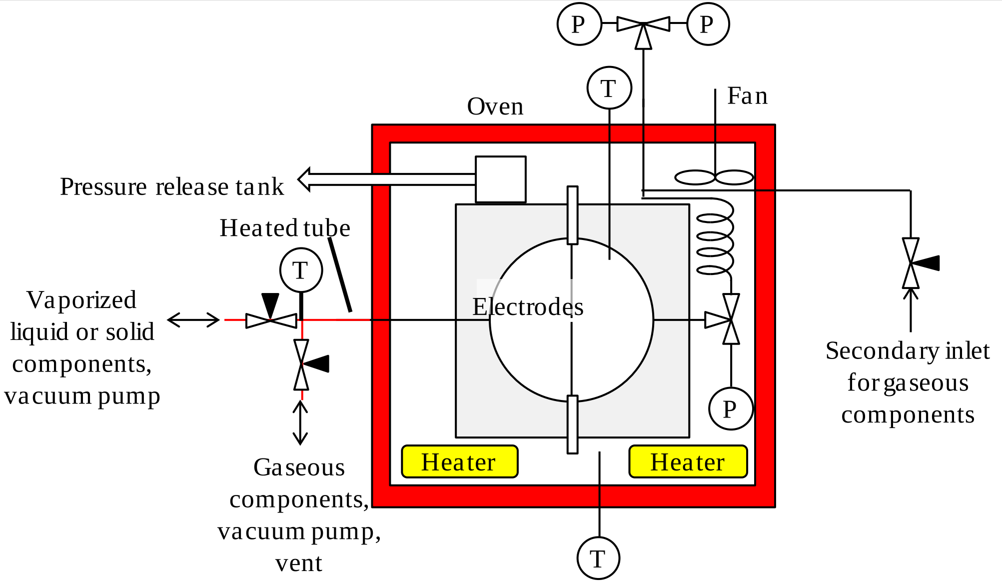
- **Flame speed measurements of HHC fuels with CO_2/H2O additions**
- **High pressure kinetic mechanism (HP-Mech) for HHC fuels with EGR**
- **Turbulent flame speed and structure measurements with H_2O/CO_2 dilution**
- **Radiation effect of CO_2/H_2O**
- **HO_2 diagnostics using Faraday Rotational Spectroscopy**

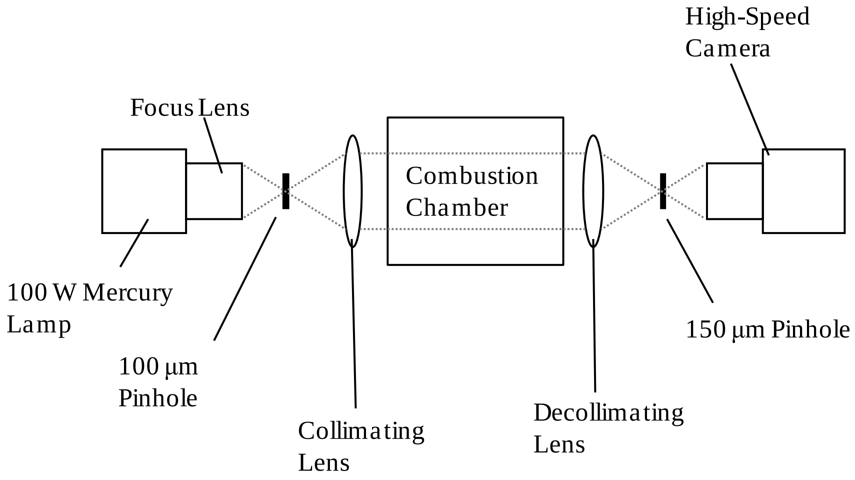
Laminar flame speeds: Experimental Design

H2, CH4, CH2O, C2H2, C2H4, and C2H6 fuels with H_2O or CO_2 dilutions

- Two validated experiments
  - Cylindrical, room temperature chamber for CO_2 dilution from 1-20 atm
  - Spherical, heated chamber for H_2O dilution from 1-10 atm
- Both experiments:
  - Centrally ignited spherically expanding flame
  - High speed schlieren imaging
  - Passive custom pressure-release valves

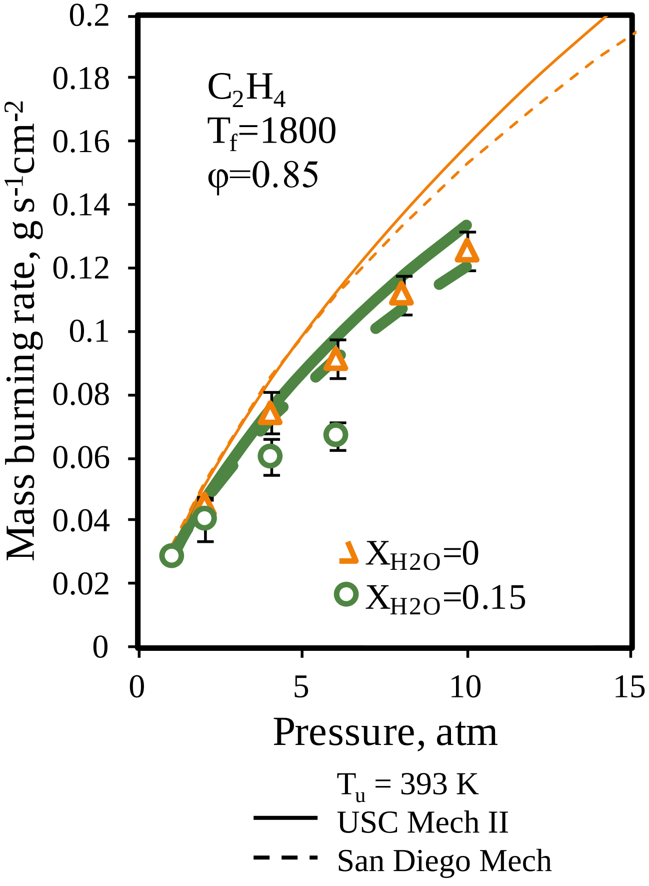






For example: C_2H_4 with H_2O dilution

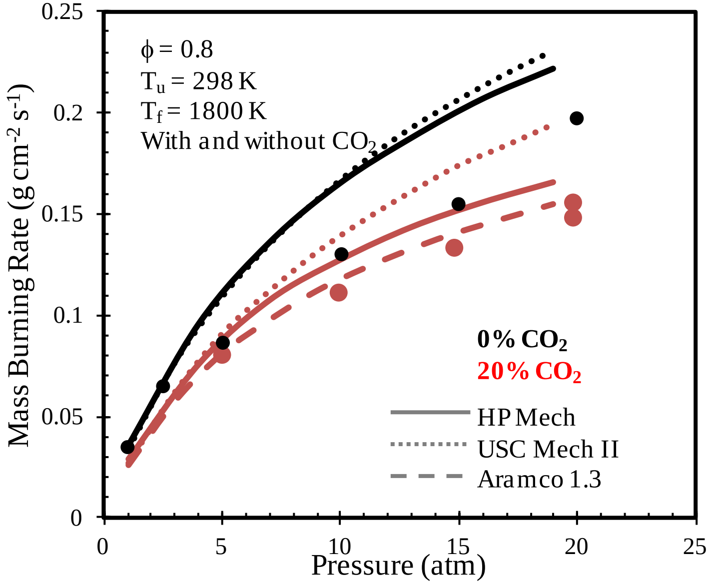
- **Water vapor decreases the mass burning rate, more at high pressure**
- **Models disagree with experiments and each other, more at high pressure**
- **Similar for hydrogen and syngas flames with water vapor***

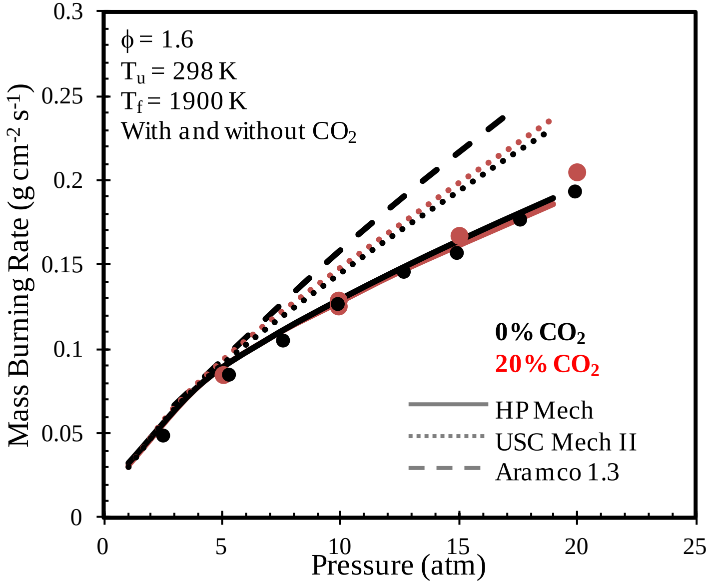


J. Santner, F.L. Dryer, and Y. Ju. "The Effects of Water Dilution on Hydrogen, Syngas, and Ethylene Flames at Elevated Pressure." *Proceedings of the Combustion Institute* 34.1 (2013): 719-726.

C_2H_2 Flames with CO_2 dilution

- **CO_2 dilution decreases burning rate for lean conditions – but doesn't affect rich conditions**
- **Typically, CO_2 slows flame by decreasing H through reverse reaction of $CO+OH=CO_2+H$**
- **Existing models do not have a good prediction. HP-Mech improves prediction.**





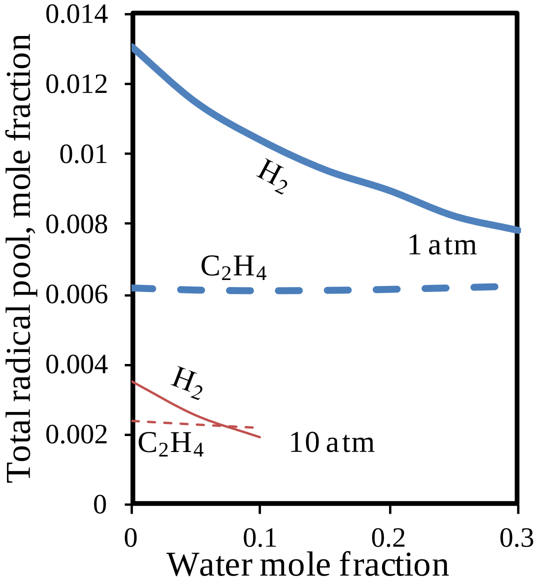
X. Shen, X. Yang, J. Santner, J. Sun, and Y. Ju. "Experimental and Kinetic Studies of Acetylene Flames at Elevated Pressures." *Proceedings of the Combustion Institute* 35 (2015).

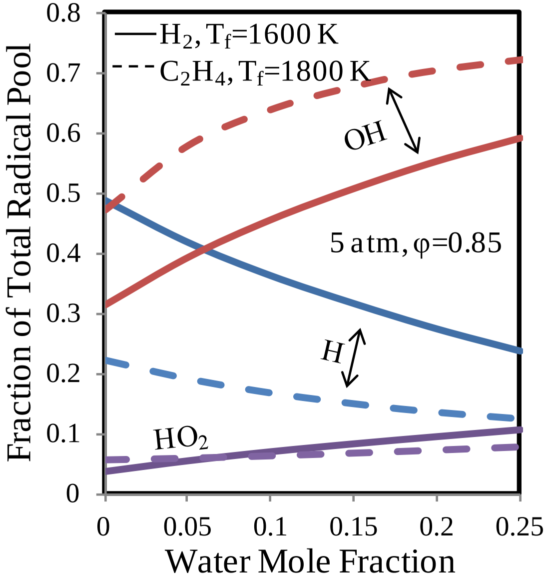
Chemical effect of H2, C_2H_4 Flames with H_2O dilution

- Water addition decreases H and O radicals relative to OH and HO_2

  $H_2O+O=2OH$

- High collisional efficiency of H_2O
  - Increased HO_2 from $H+O_2+M=HO_2+M$
  - 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+O2 = O +OH
H+O2+M=HO2+M

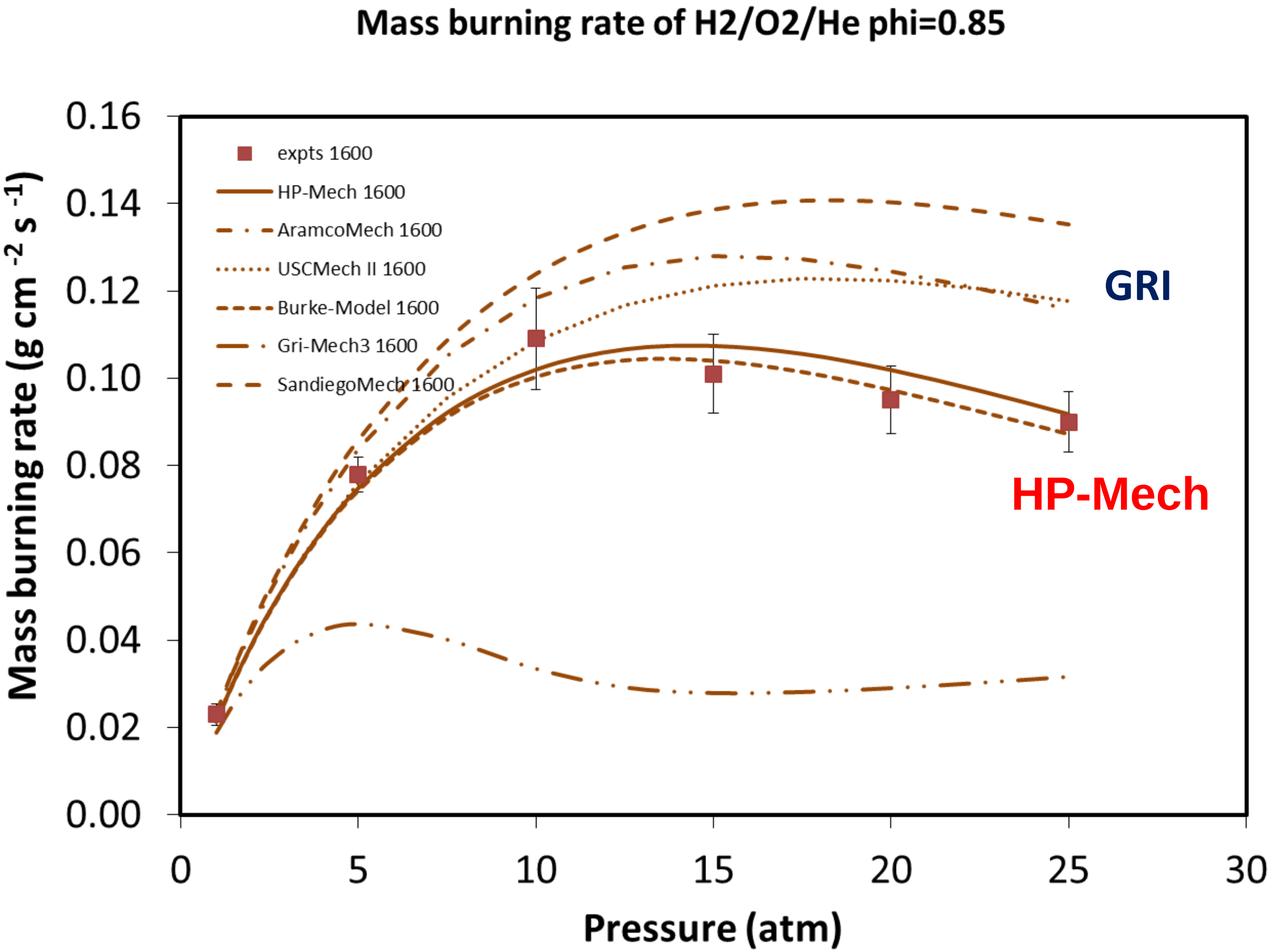
HCO+M = H+CO+M
HCO+O2 = HO2+CO

$NO+HO_2 = NO_2+OH$
$NO_2+CH_3 = NO + CH_3O$

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
  - H_2-O_2 model (Burke et al, Int. J. Chem. Kinet. 44(2012), 444–474, update or modification)
  - $CO+OH=CO_2+H$ (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)
  - $HCO+O_2=HO_2+CO$ (Klippenstein private commucation)
  - $CH+O_2$ reactions (Rohrig et al, Int. J. Chem. Kinet. 29(1997), 781-789; Bergeat et al, *Faraday Discuss.*, 119(2002), 67-77)
  - CH_2+O_2 reactions (Lee at al, *J. Phys. Chem. A*, 116 (2012), pp 9245–9254; Blitz et al, Z. Phys. Chem. 225 (2011), 957–967)
  - CH_2 relaxations (Gannon et al, J. Chem. Phys. 132(2010), 024302)
  - $H+CH_3+M=CH_4+M$ (Troe et al, J. Chem. Phys. 136(2012), 214309; Brouard et al, *J. Phys. Chem.* **93**(1989), 4047)
  - CH_3+HO_2 (Jasper et al Proc. Combust. Inst. 32, 279 (2009))
  - CH_3+OH and CH_3OH decomposition (Jasper et al, J. Phys. Chem. A 111, 3932 (2007))
  - $H+C_2H_2+M=C_2H_3+M$ and $H+C_2H_4+M=C_2H_5+M$ (Miller and Klippenstein, Phys. Chem. Chem. Phys., 6(2004), 1192 –1202)
  - $CH_2(S)+C_2H_2=C_3H_3+H$ (Gannon et al J. Phys. Chem. A 114(2010) 9413−9424; Polino et al, J. Phys. Chem. A. 117(2013):12677-92)
  - $HCCO+O_2$ (Klippenstein et al., Proc. .Combust. Inst. 29 (2002), 1209; Zou et al., Phys. Chem. Chem. Phys., 6(2004), 1697-1705)
  - C_2H_2+OH (Senosiain et al., J. Phys. Chem. A 109(2005) 6045-6055)
  - $C_2H_3+O_2$ (Klippenstein private communication; Matsugi et al, Int. J. Chem. Kinet. 46: 260–274, 2014)
  - $HCCO+OH=HCOH+CO$ (Mai et al, Chem. Phys. Lett. 592(2014) 175-181)
  - C_2H_4+O (Nguyen, et al., J. Phys. Chem. A 109(2005) 7489-7499)
  - ….

Hydrogen flames-1



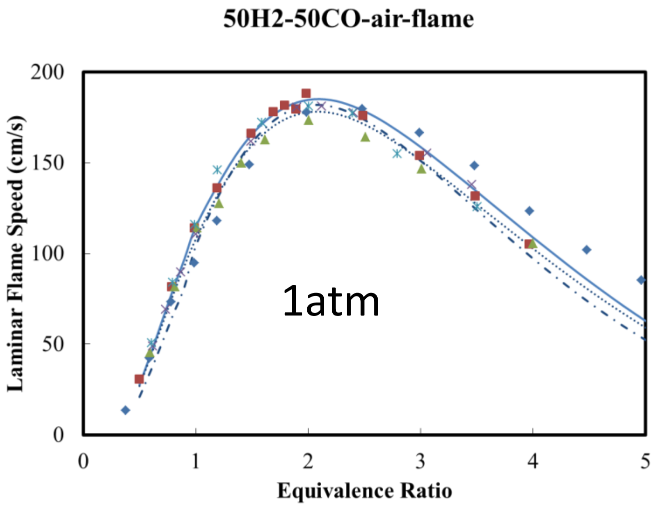
GRI

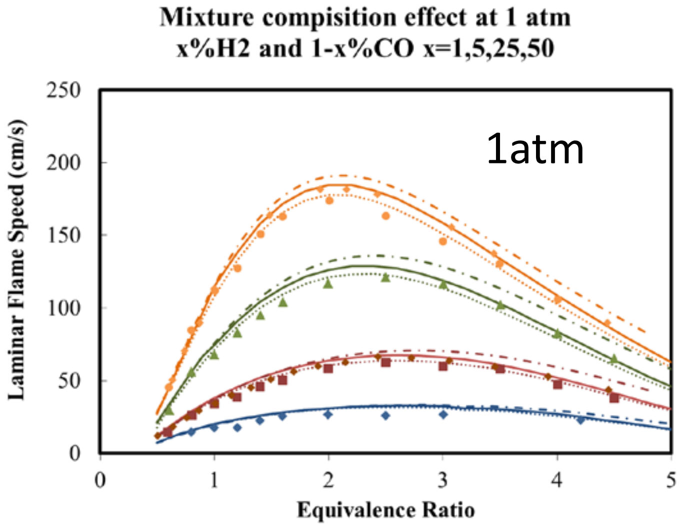
HP-Mech

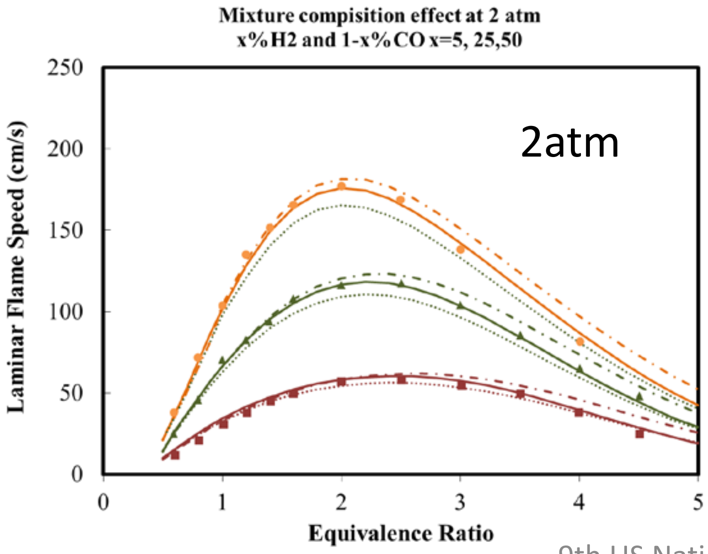
H+O2+M dominate pressure dependence

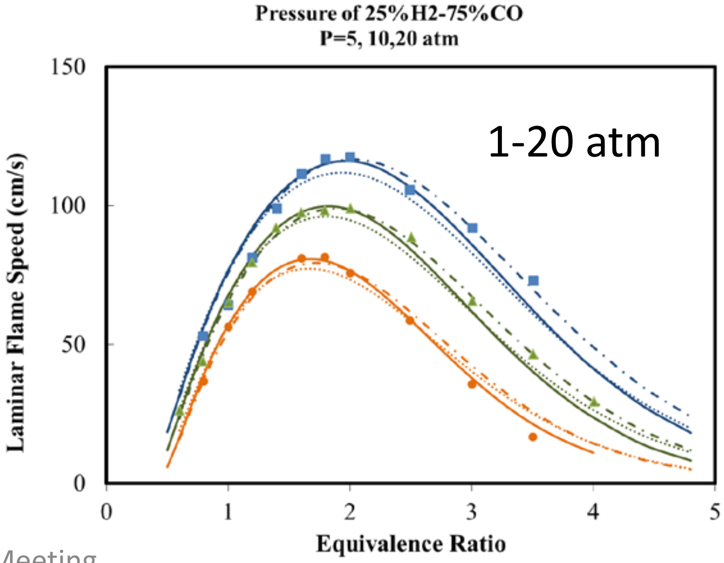
H2/CO flames

HP-Mech ——
USC Mech II ……
Aramco Mech ·–·–

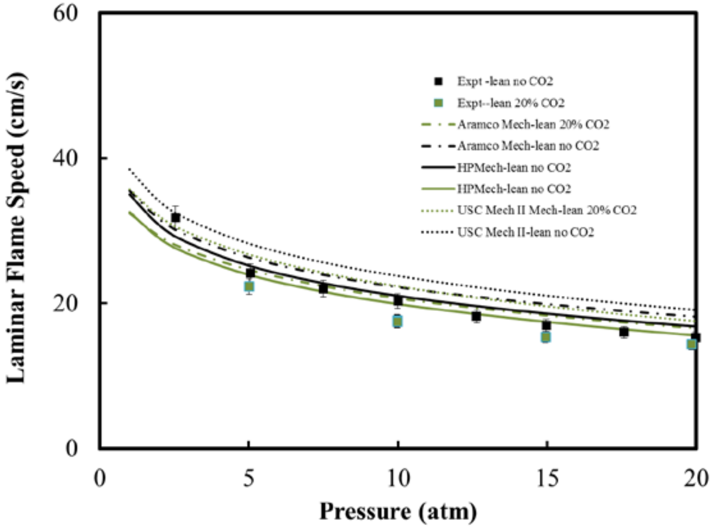

50H2-50CO-air-flame

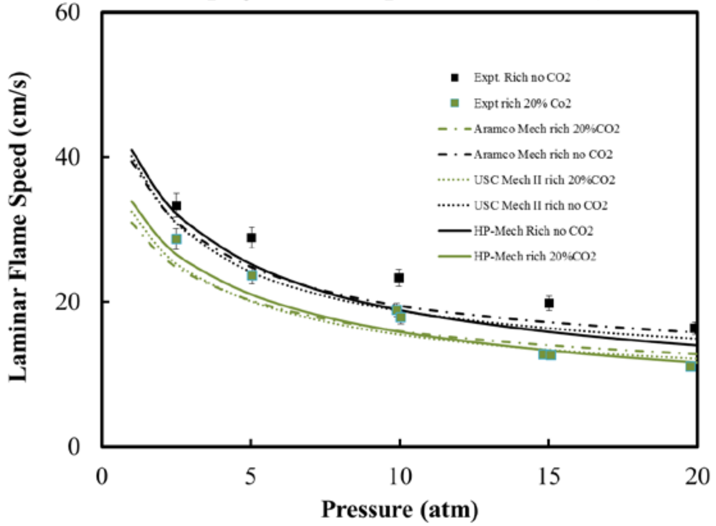

Mixture compisition effect at 1 atm
x%H2 and 1-x%CO x=1,5,25,50

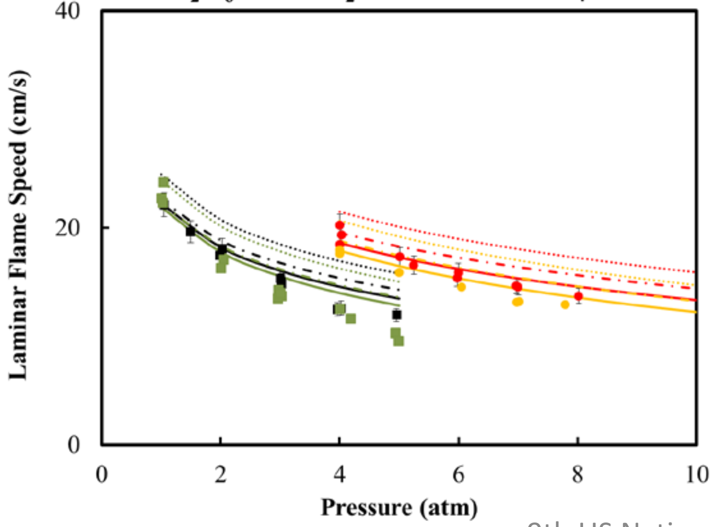

Mixture compisition effect at 2 atm
x%H2 and 1-x%CO x=5, 25,50

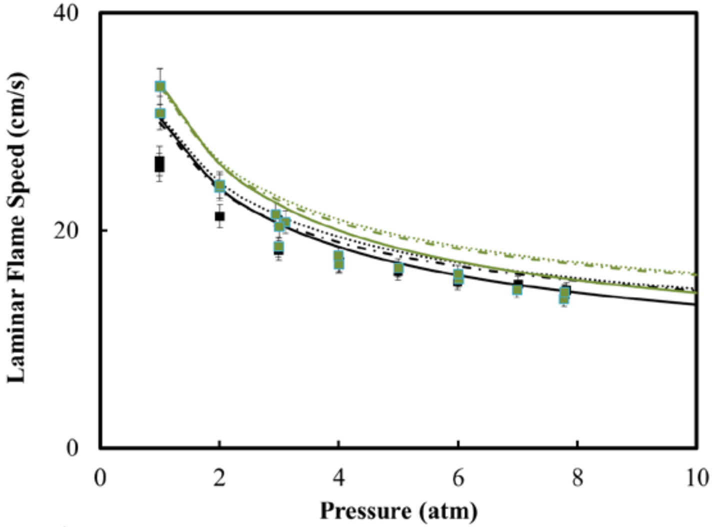

Pressure of 25%H2-75%CO
P=5, 10,20 atm

Ethane flame


C_2H_6 flame CO_2 dilution effect ϕ=0.8


C_2H_6 flame CO_2 dilution effect ϕ=1.6


C_2H_6 flame H_2O dilution effect ϕ=0.8


C_2H_6 flame H_2O dilution effect ϕ=1.6

Task 4. EGR Kinetic Effect on Turbulent CH_4 Flames

Investigation of EGR Effects on Turbulent Flame Structure in RATS Burner

Objectives

- Investigate turbulent burning velocity and flame structures
  - At EGR conditions and elevated temperature
  - Systematic measurements of H_2O and CO_2 dilution
    - Effects of H_2O[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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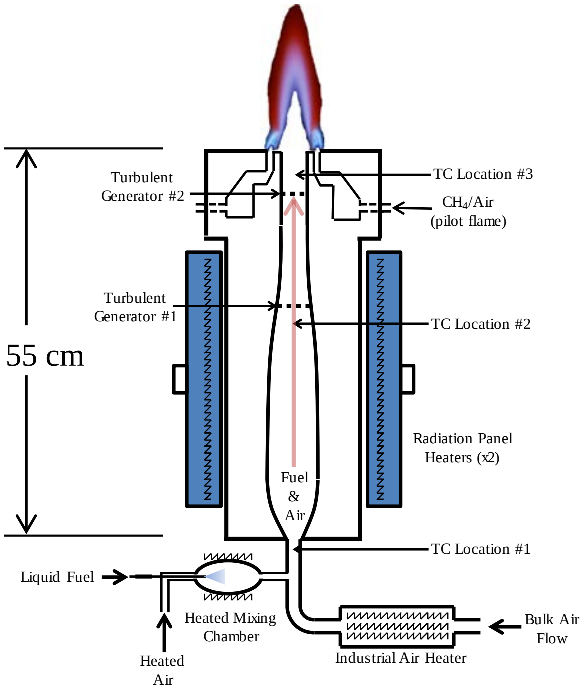
[1] H. Kobayashi, et al., Proc. Combust. Inst. 32 (2009) 2067-2614.

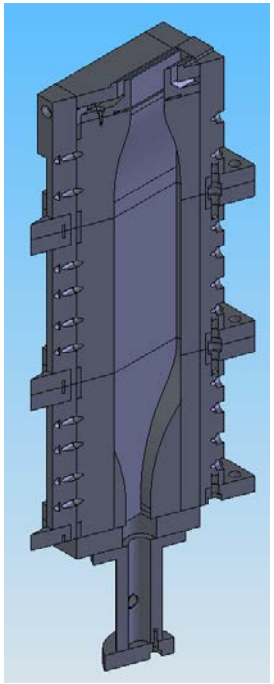
[2] H. Kobayashi, et al., Proc. Combust. Inst. 31 (2007) 1451-1458.

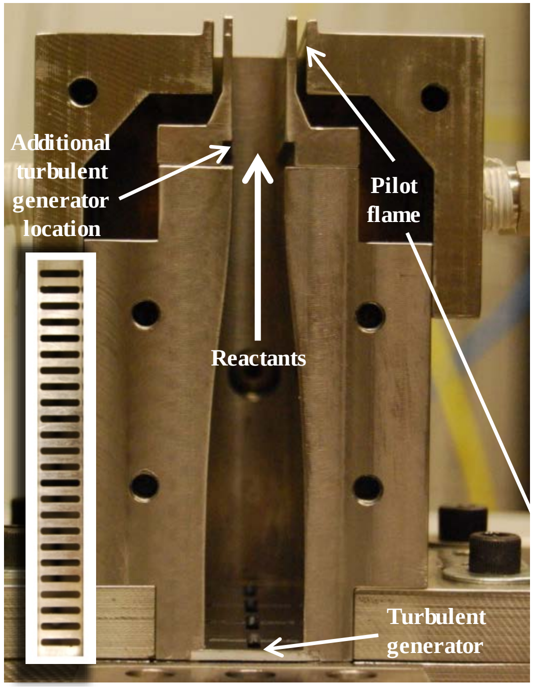
[3] J. F. Driscoll, Prog. Energy Combust. Sci. 34 (2008) 91-134.

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 cm heated length, 100 × 10 mm exit cross-section ($D_H \approx 18$ mm)
  - Two turbulence generators[2,3], homogeneous isotropic turbulence confirmed by hot-wire anemometry
  - High Reynolds number ($\text{Re}_{\text{bulk}} > 10{,}000$)







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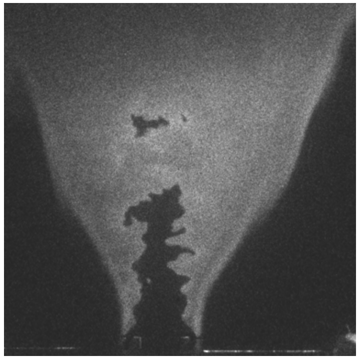
[1] S. H. Won, B. Windom et al, Combust. Flame 161 (2014) 475-483.

[2] Coppola, G., and Gomez, A., *Experimental Thermal and Fluid Science*, Vol. 33, 2009, pp. 1037-1048.

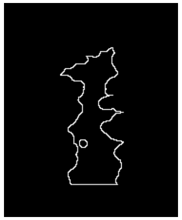
[3] Venkateswaran, P. *et. al., Combustion and Flame., 158, 2011, 1602-1614*

Determination of turbulent flame speed, S_T



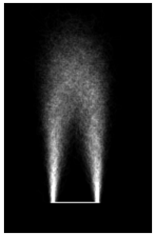
Single Image of OH PLIF

Find inner edge



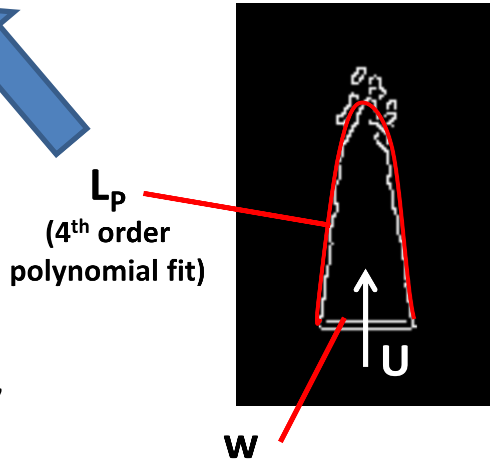
Flame perimeter from single image

Stack perimeters from 500 images

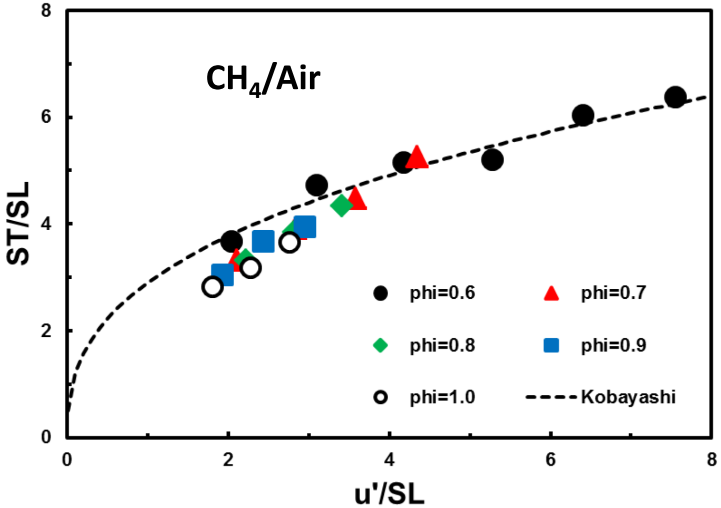


PDF of Flame Perimeters

Find inner edge



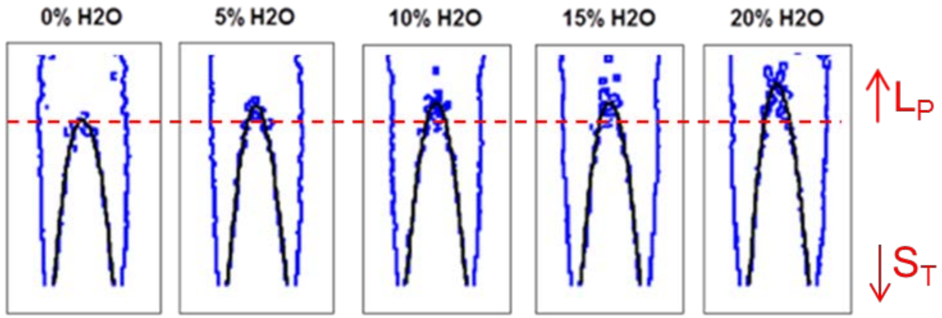
$$S_T = \frac{Uw}{L_P}$$

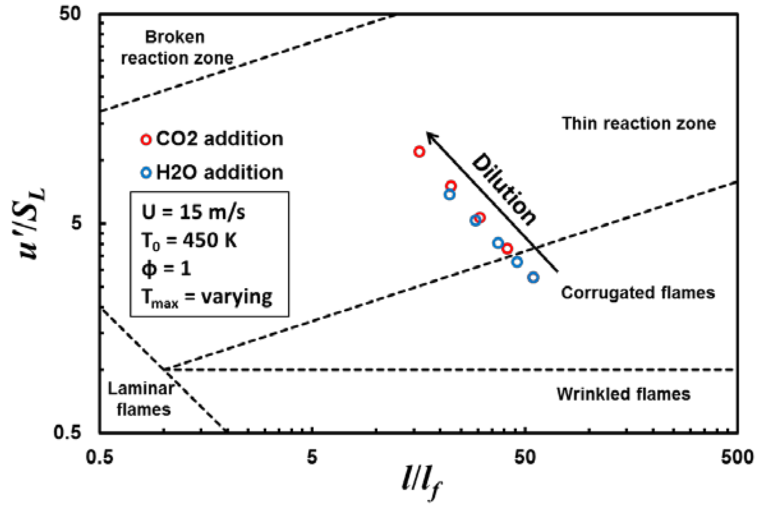


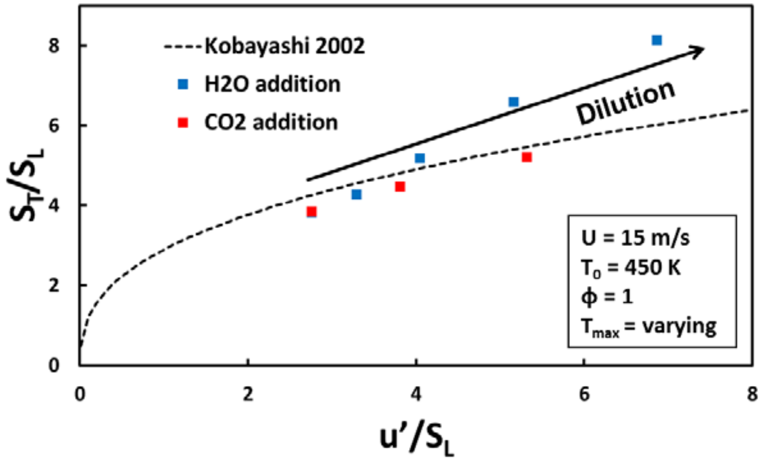
"PDF method" gives similar results to method seen in H. Kobayashi, *Exp. Therm. Fluid Sci.* 26 (2002) 375-387

Effects on flame speed with EGR dilution

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





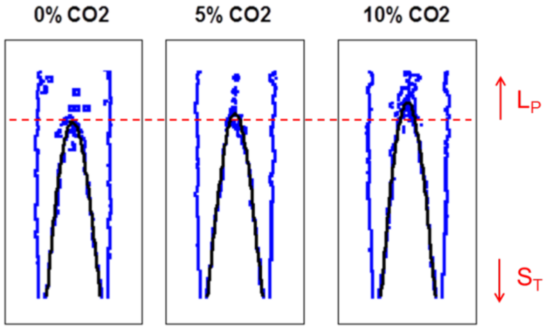


- Both CO_2 and H_2O addition decrease turbulent burning velocity, S_T
- Strong decrease in laminar flame speed S_L
  - Drop from 70.6 cm/s to 28.4 cm/s for 20% H_2O
  - Drop from 70.6 cm/s to 36.8 cm/s for 10% CO_2
- S_T/S_L increases with dilution for both CO_2 and H_2O addition
  - More pronounced 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

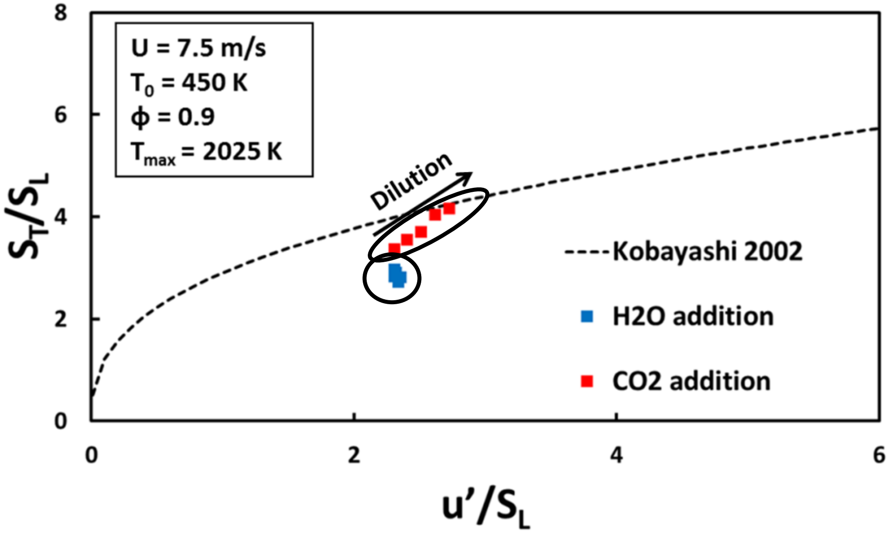
- H_2O dilution has almost no discernable effect on L_P, S_T, or S_T/S_L
- Thermal effects were clearly the dominant factor for H_2O dilution
- CO_2 dilution produces (~10%) decrease in S_T, **kinetic effect**
- Turbulence **reduces the kinetic effect** of CO_2 on burning velocity
- CO2 dilution increases turbulence-turbulent flame speed coupling due to the combined chemistry and transport effect (Le). (Promoted instability)



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

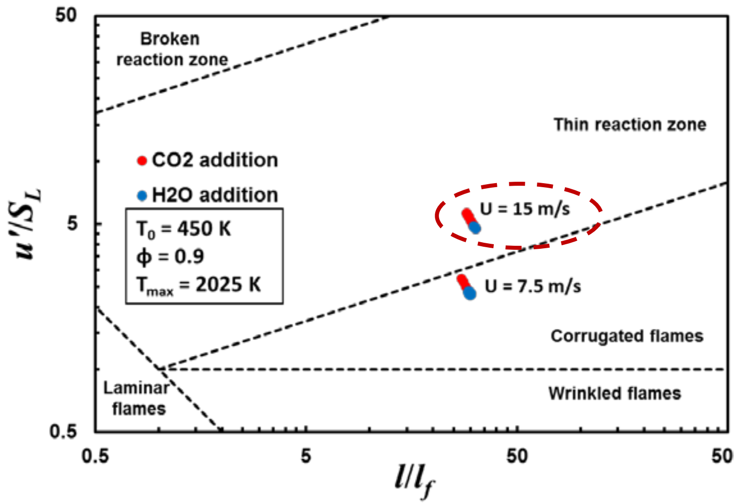
↑ 10% H_2O results in u'/S_L ↑ 2% and 1/Le ↓ 8%

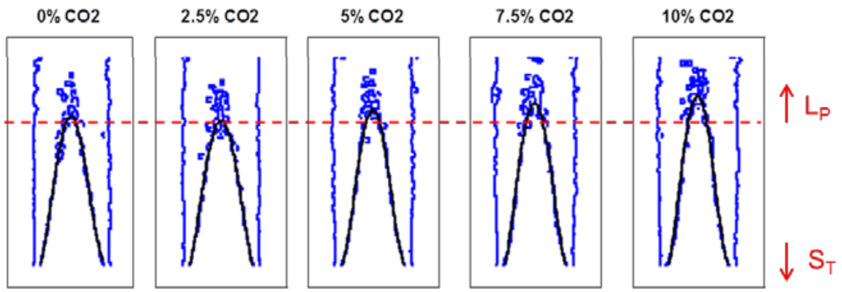
↑ 10% CO_2 results in u'/S_L ↑ 18% and 1/Le ↑ 8%

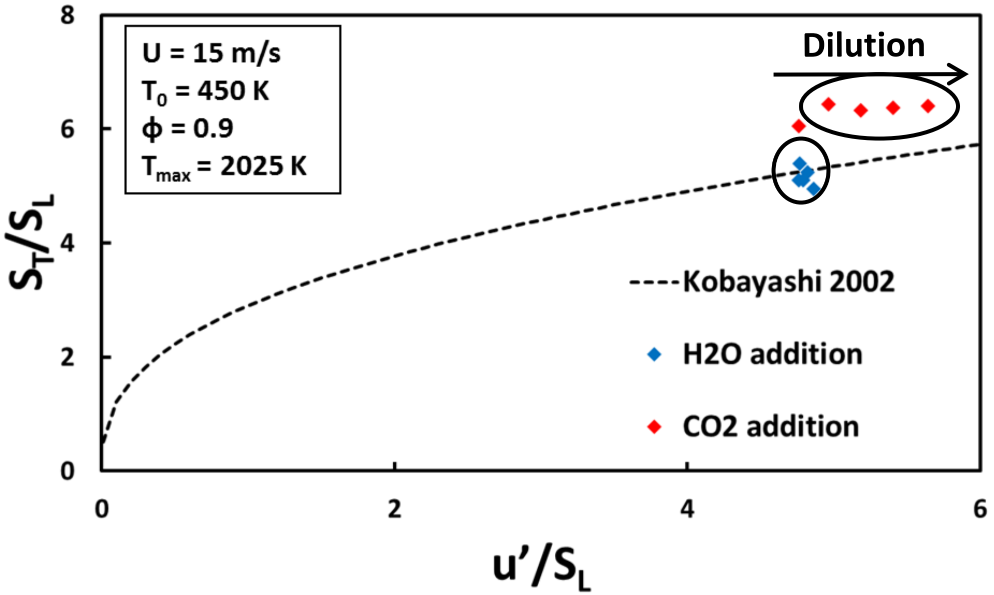


EGR Dilution at Constant Temperature: Thin Reaction Zone

- H_2O again has no significant effect on L_P, S_T, or S_L
- Turbulence increases the decrease of S_T with CO_2 addition, enhance the turbulence-chemistry coupling.
- Turbulent flame speed deviates from the conventional S_T correlation.





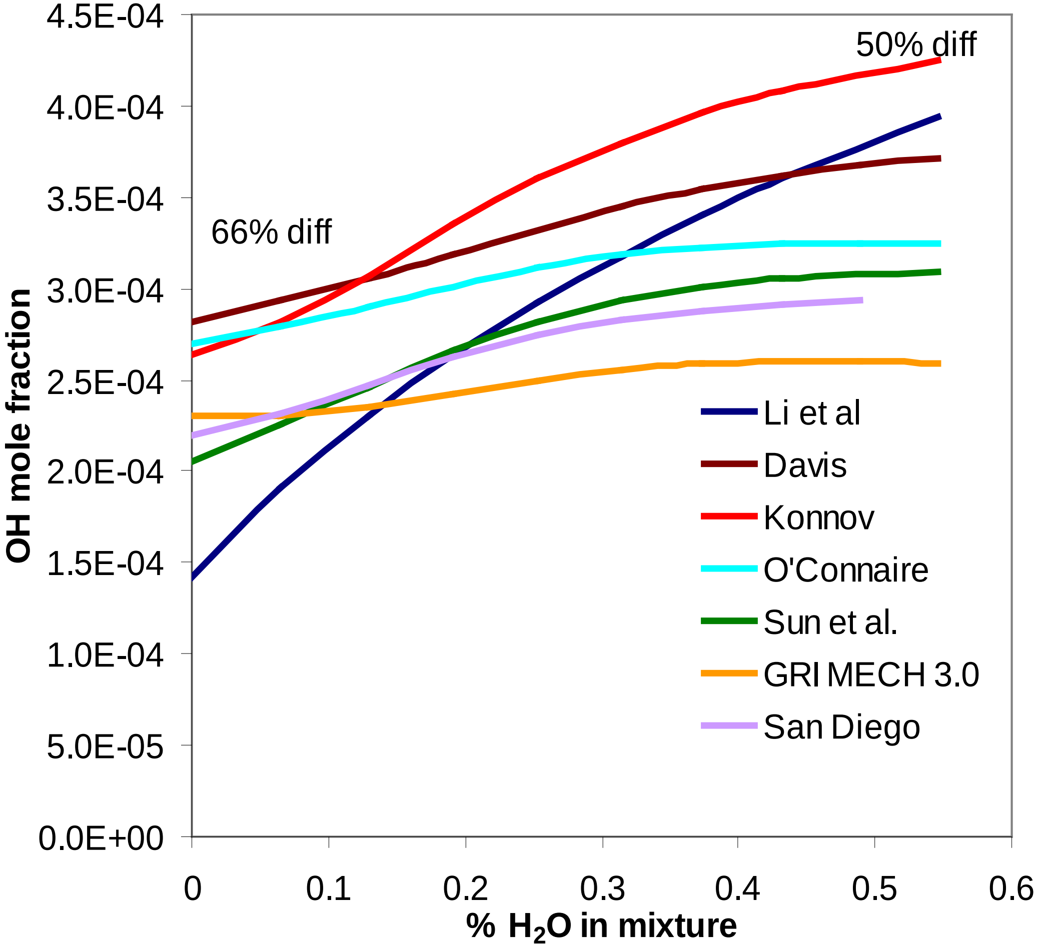


Conclusions

1. **H_2O 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_2O and CO_2 dilution.**
3. **At constant adiabatic flame temperature, H_2O 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_4/air + CO_2, H_2/air + H_2O/CO_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!

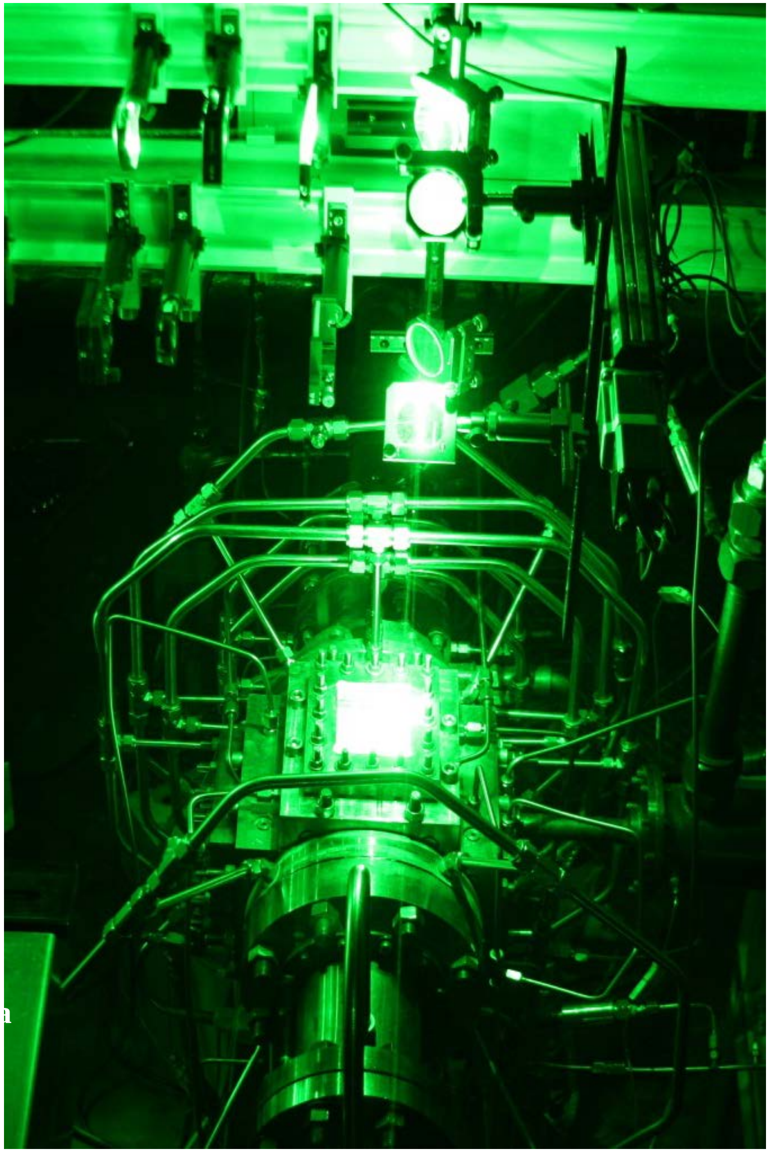
N2+O=NO+N
N+OH=NO+H

High-Pressure PARAT Burner Studies
Robert Lucht and Jay Gore
Purdue University

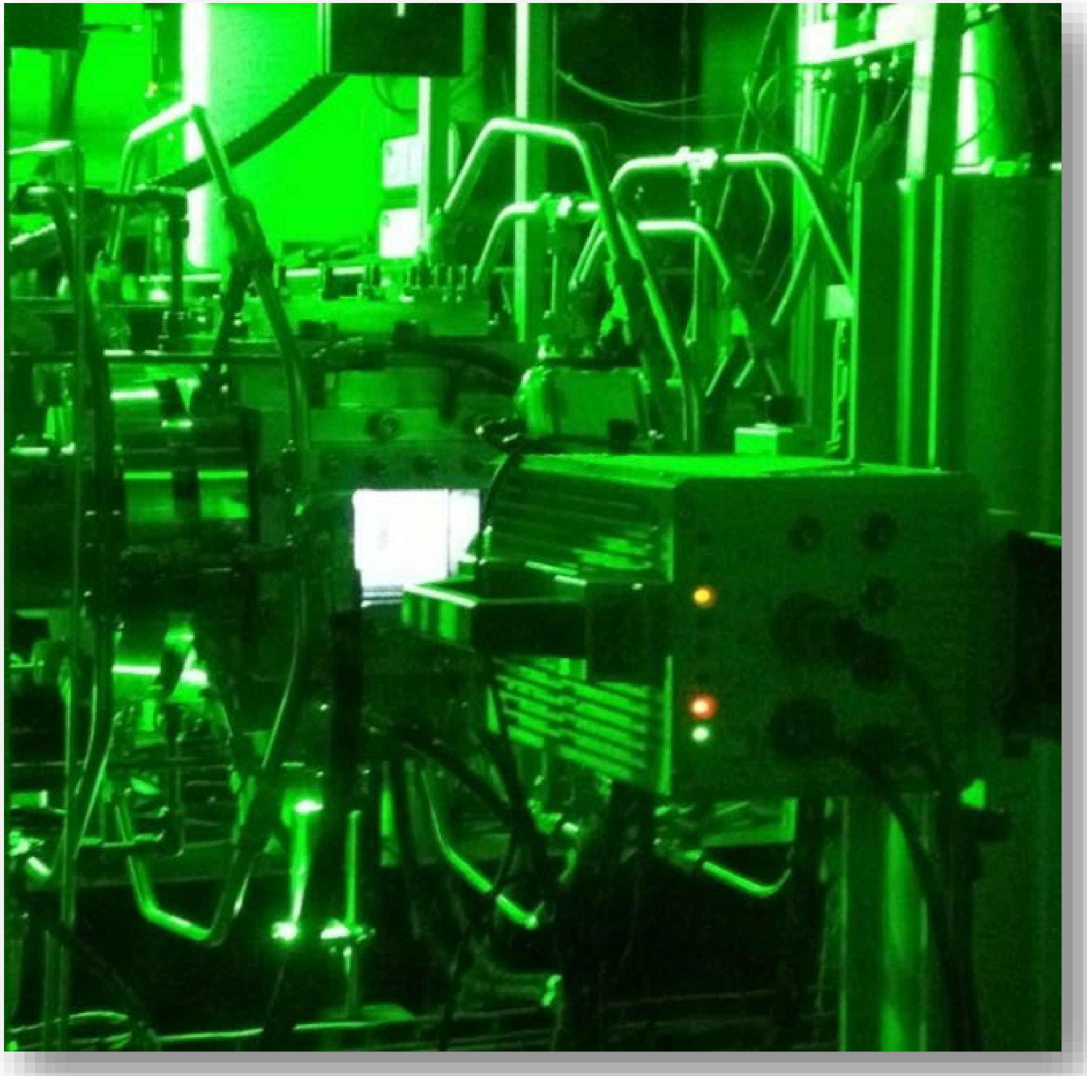
- Design and fabrication of PARAT burner
- Initial measurements at atmospheric pressure
- Planned high-pressure measurements

Purdue Gas Turbine Combustion Facility (GTCF)

High Pressure Lab System	Maximum Flow Capacity	Max Operating Condition
Natural Gas Heated High Pressure Air	9 lbm/s 4 kg/s	700 psi / 1100 K 1500 F
Electric Heated Air or Nitrogen	1 lbm/s 0.5 kg/s	600 psi / 800 K 1000 F
Nitrogen	5 lbm/s 2 kg/s	1,500 psi
Liquid Aviation Fuel (Kerosene)	1 lbm/s 0.5 kg/s	1,500 psi
Natural Gas	1 lbm/sec 0.5 kg/s	3500 psi

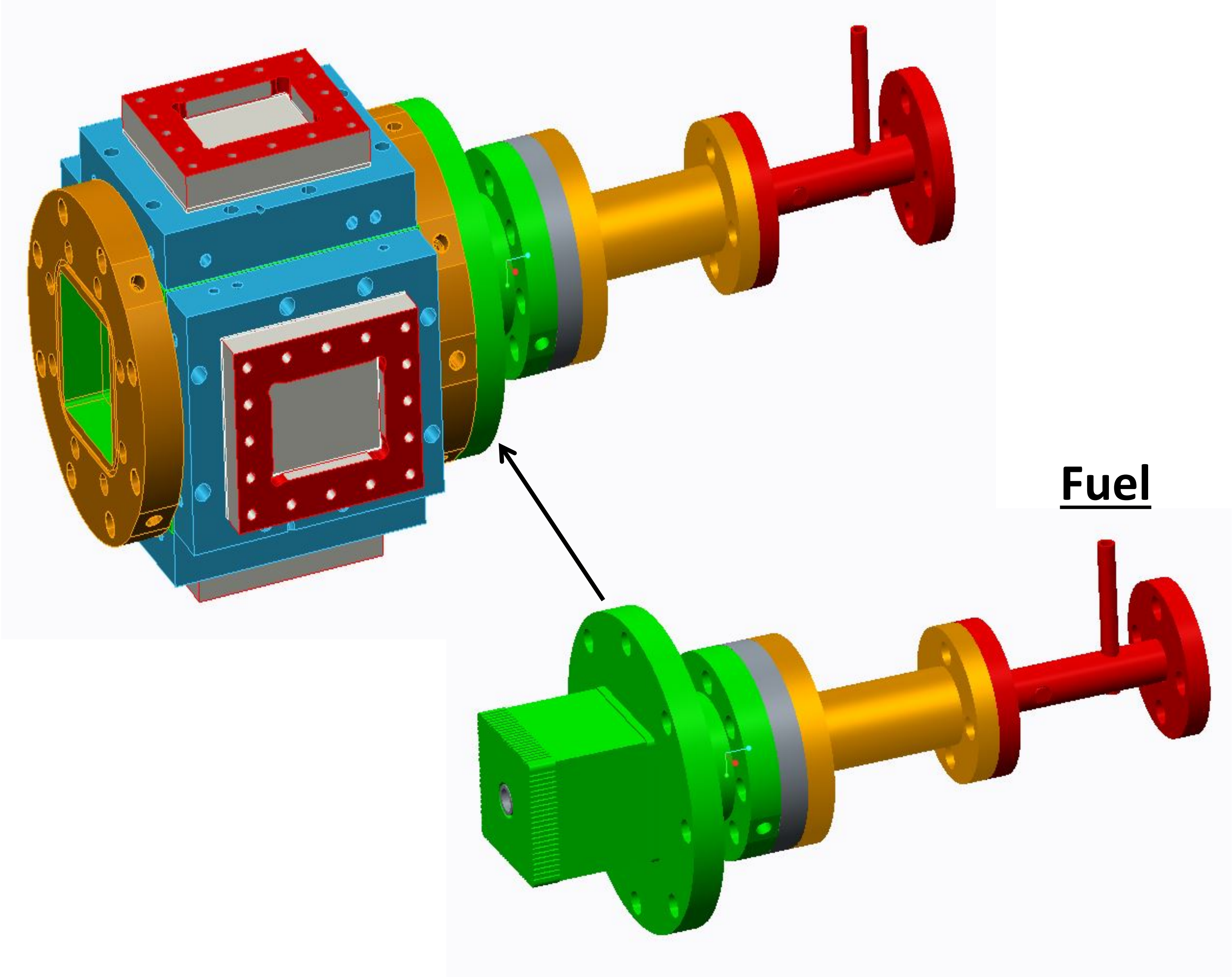


Laser Diagnostics for High-Pressure Test Rig

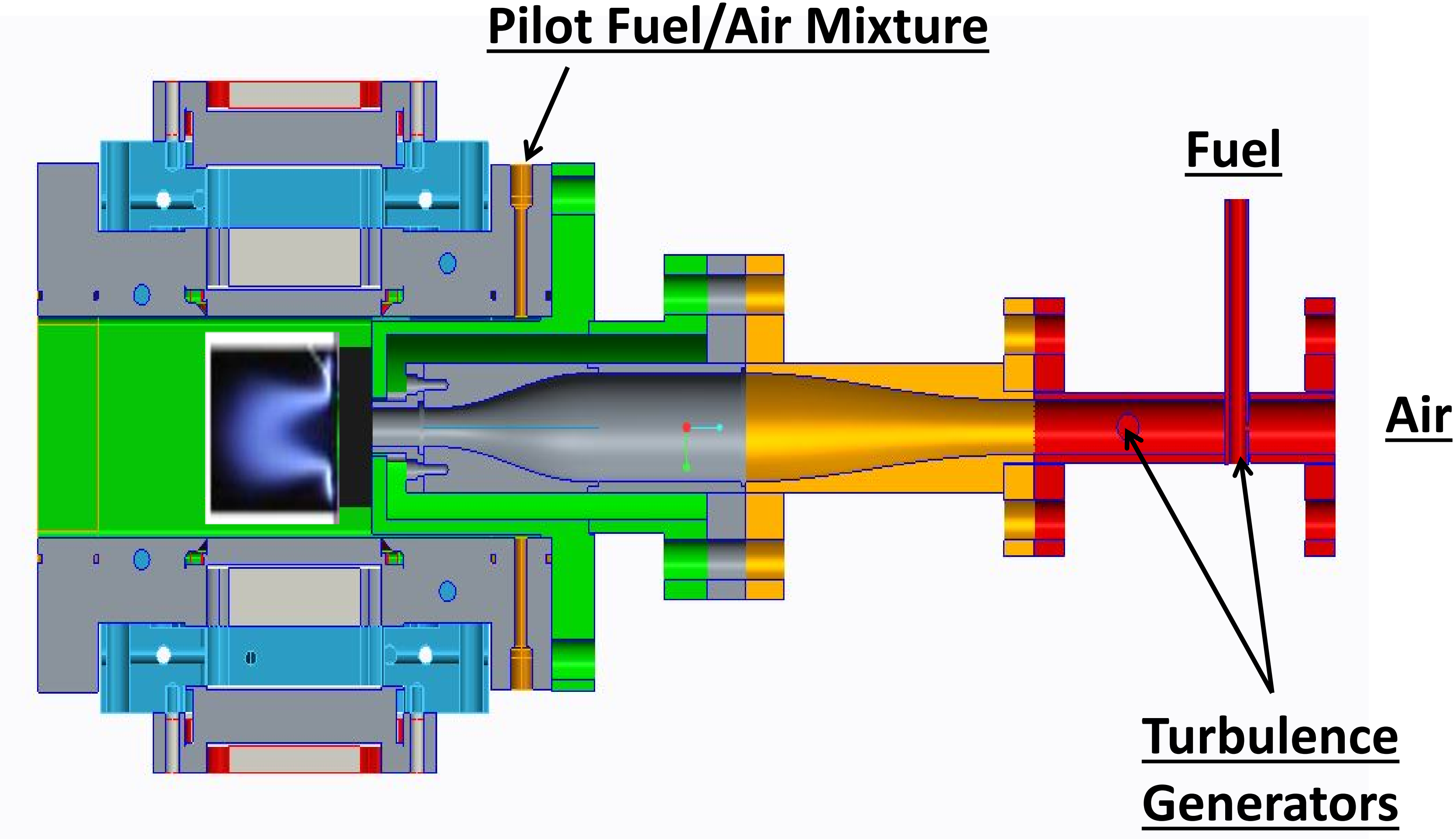


- 10 kHz stereo PIV
- 10 kHz OH PLIF
- Pulse burst laser is being delivered this week for PIV, PLIF at data rates up to 100 kHz

Assembly of PARAT Burner into the Windowed High-Pressure Test Rig



Cross-sectional View of PARAT Burner into the Windowed High-Pressure Test Rig

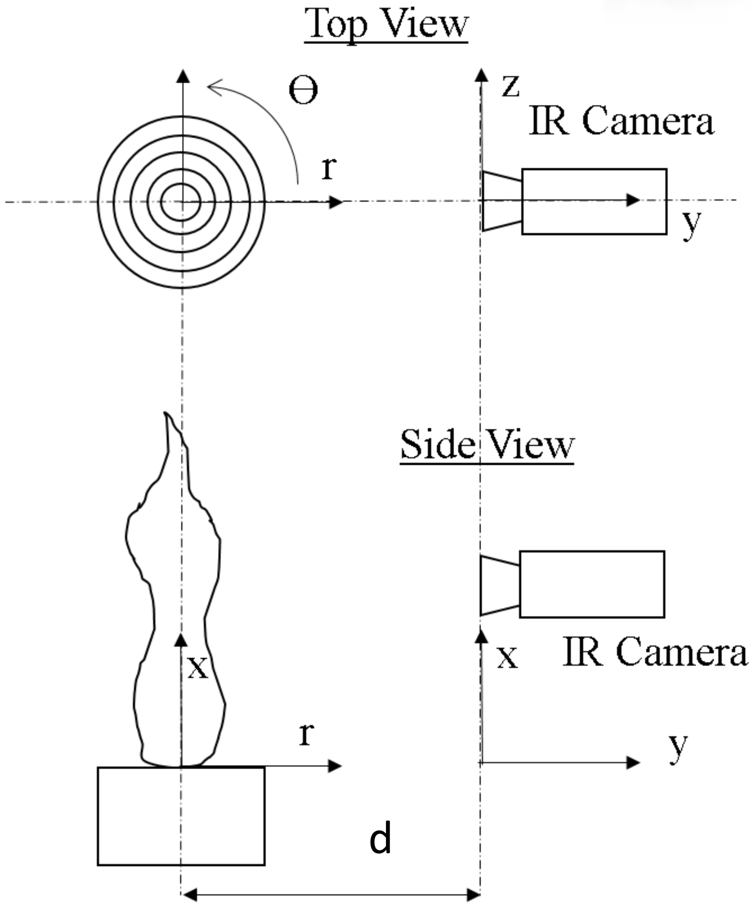


Initial Operation of the PARAT Burner at Atmospheric Pressure: Operating Conditions

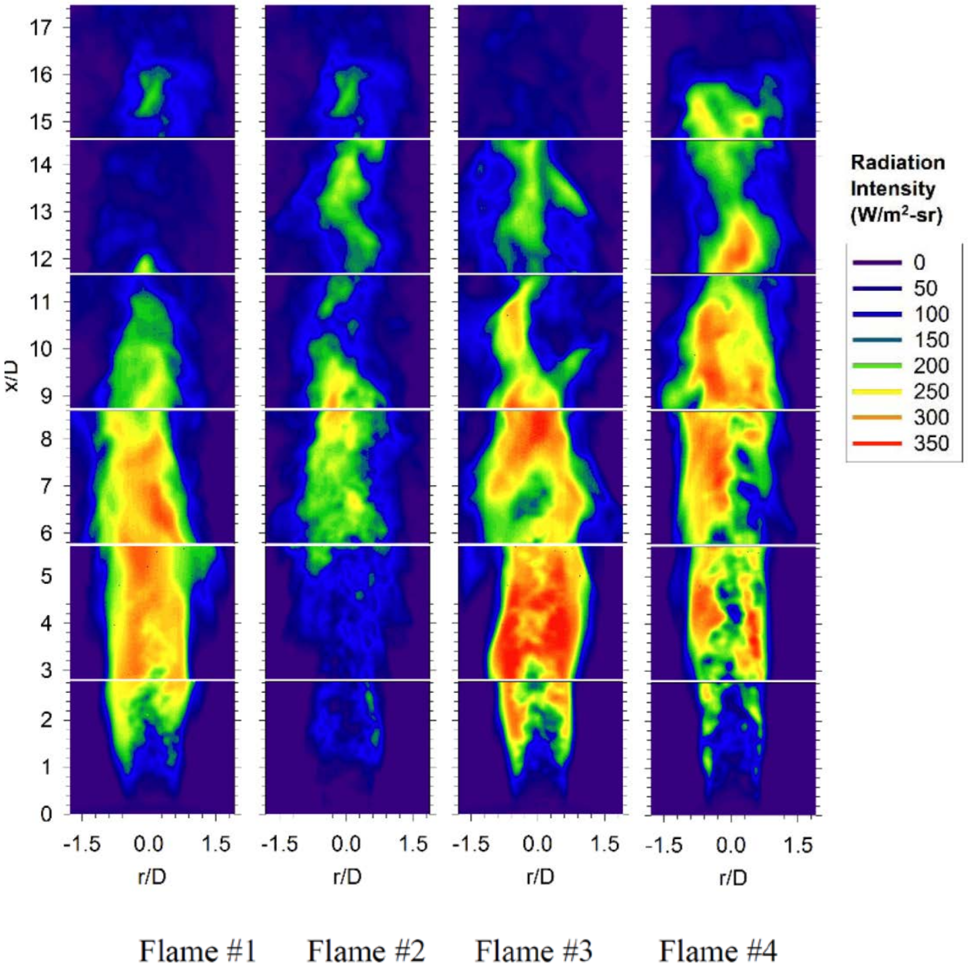
	Without EGR		With EGR	
Flame No.	1	2	3	4
Re	10000	20000	10000	10000
Equivalence ratio	0.8	0.8	0.8	0.8
CO_2 percentage by mass%	0.0	0.0	10.0	20.0
Air flow rate (l/min)	122.2	244.4	107.6	93.4
CH_4 flow rate (l/min)	10.3	20.5	10.1	9.9
CO_2 flow rate (l/min)	0.0	0.0	8.3	16.2
CO_2/CH_4 mass flow rate ratio	0.0	0.0	2.26	4.5
H_2 flow rate (l/min)	2.0	2.0	2.0	2.0

IR Imaging of PARAT Burner Flames

- **Turbulent lean premixed methane flame**
  - Re = 8950
  - Burner diameter (D) = 15 mm
- **FLIR Infrared Camera**
  w/ band pass filters
  - H_2O: 2.58 ± 0.03 μm
  - H_2O and CO_2 2.77 ± 0.1 μm
  - CO_2 4.38 ± 0.08 μm
- **Distance between camera and flame**
  d = 0.5 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

	Without EGR		With EGR	
Flame No.	1	2	3	4
Re	10000	20000	10000	10000
Equivalence ratio	0.8	0.8	0.8	0.8
CO_2 percentage by mass%	0.0	0.0	10.0	20.0
Air flow rate (l/min)	122.2	244.4	107.6	93.4
CH_4 flow rate (l/min)	10.3	20.5	10.1	9.9
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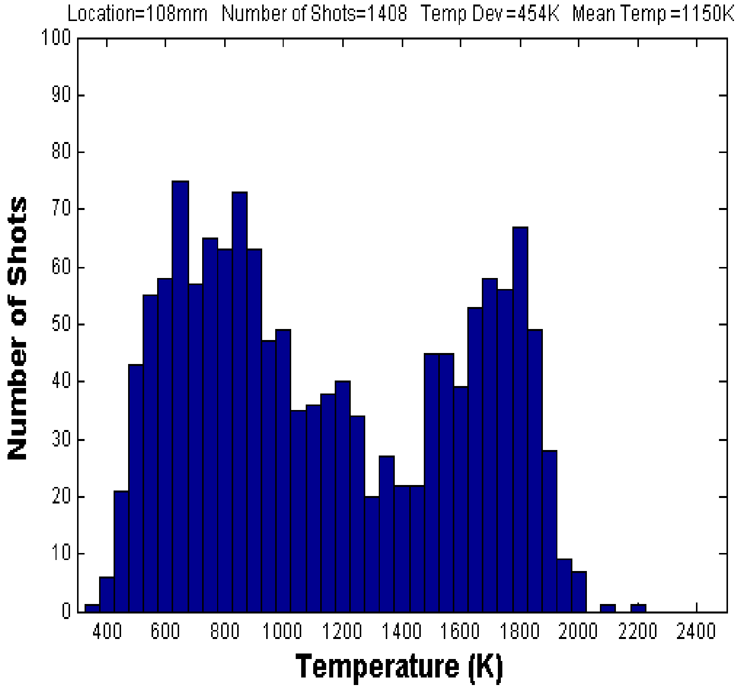
CO_2/CH_4 mass flow rate ratio	0.0	0.0	2.26	4.5
H_2 flow rate (l/min)	2.0	2.0	2.0	2.0

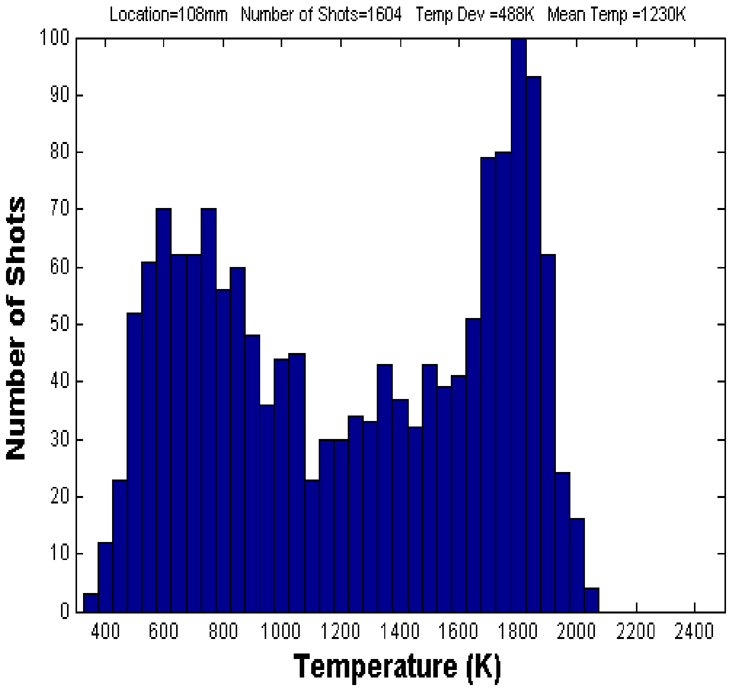
CARS Measurements in Atmospheric Pressure PARAT Burner Flames: Temperature PDFs Along Centerline

Axial Location

108 mm



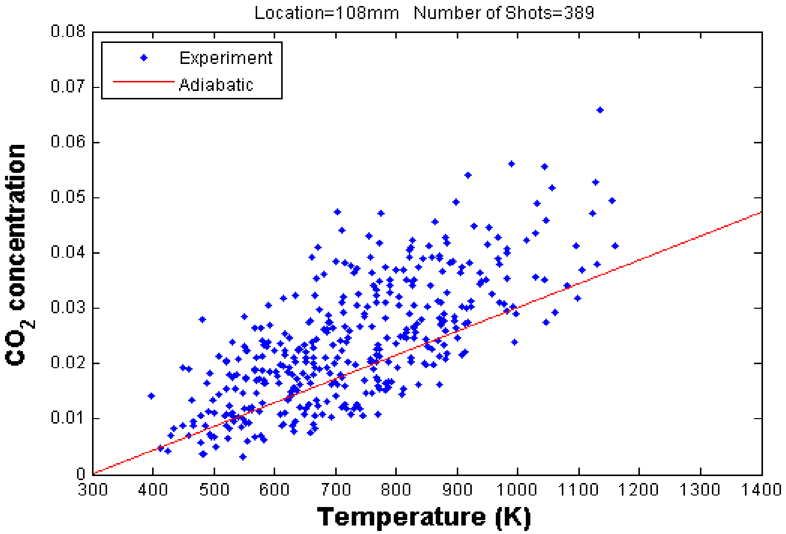
113 mm



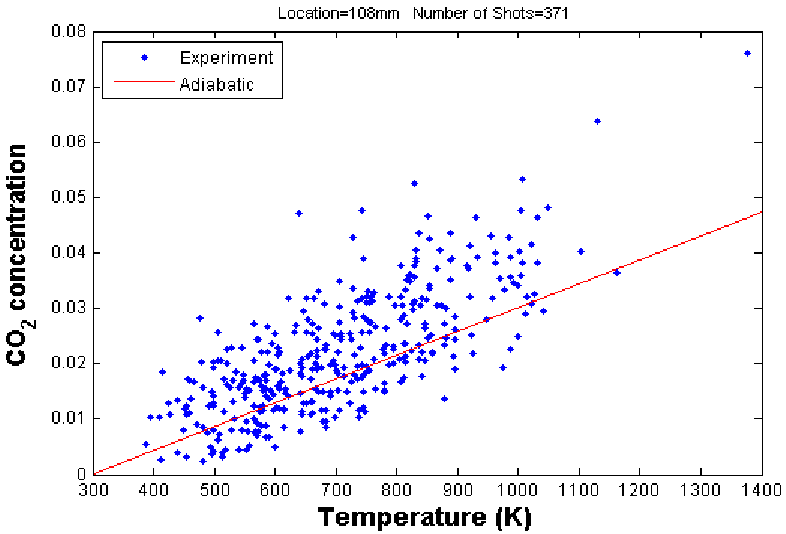
CARS Measurements in Atmospheric Pressure PARAT Burner Flames: Temperature PDFs Along Centerline

Axial Location

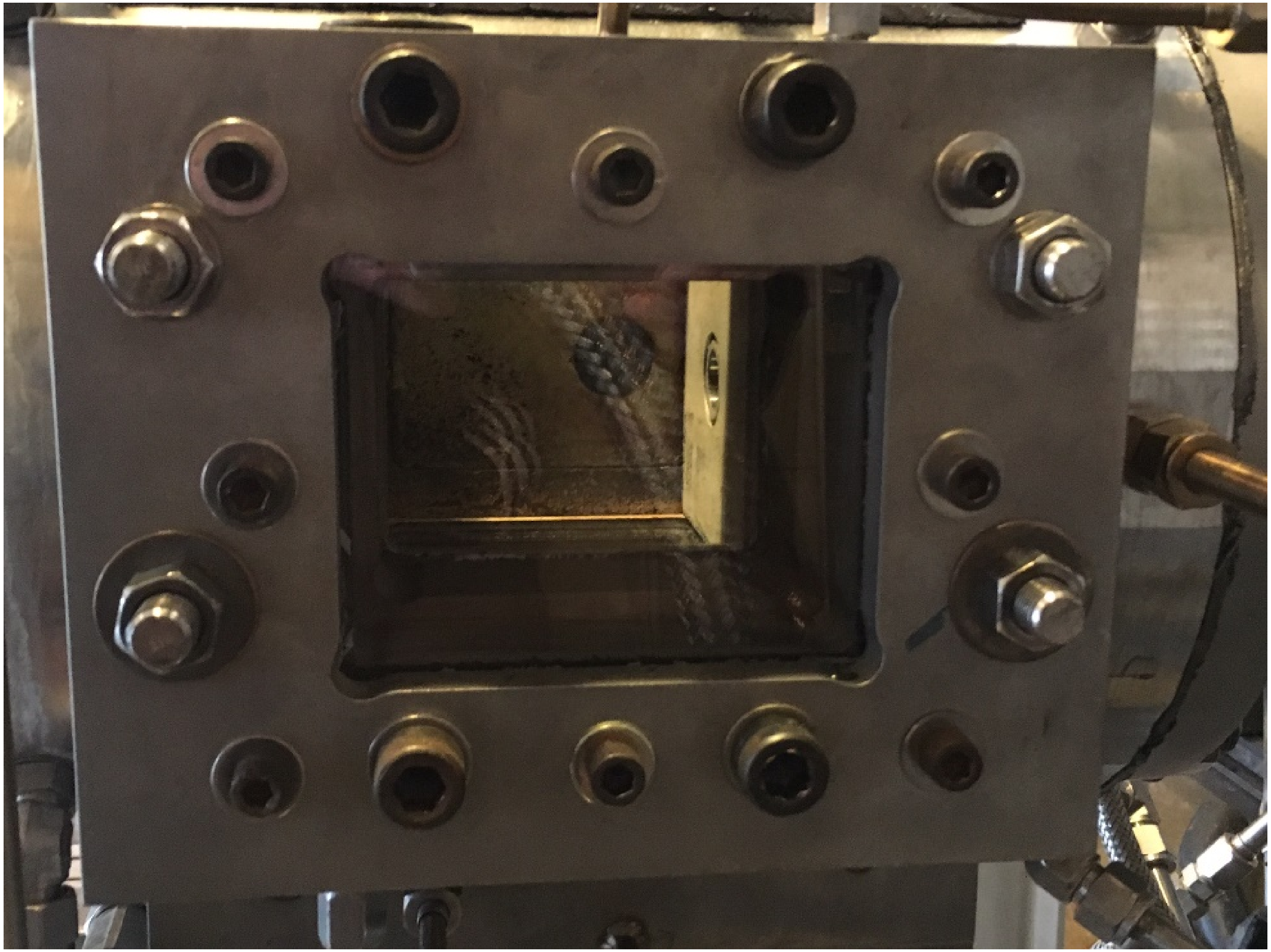
108 mm



113 mm



CARS Measurements at High Pressure: PARAT Burner Now Installed in HP Test Rig

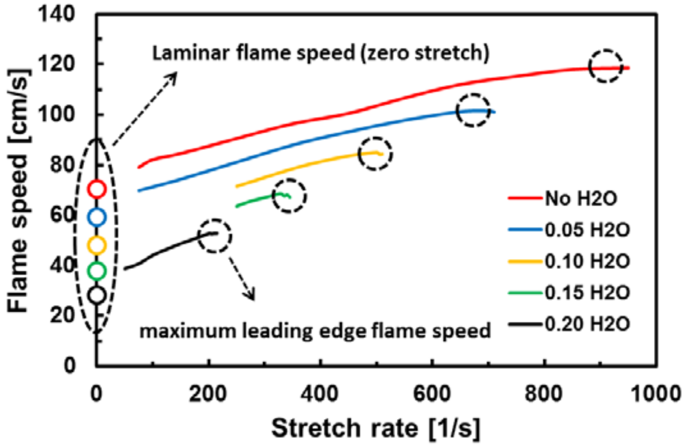


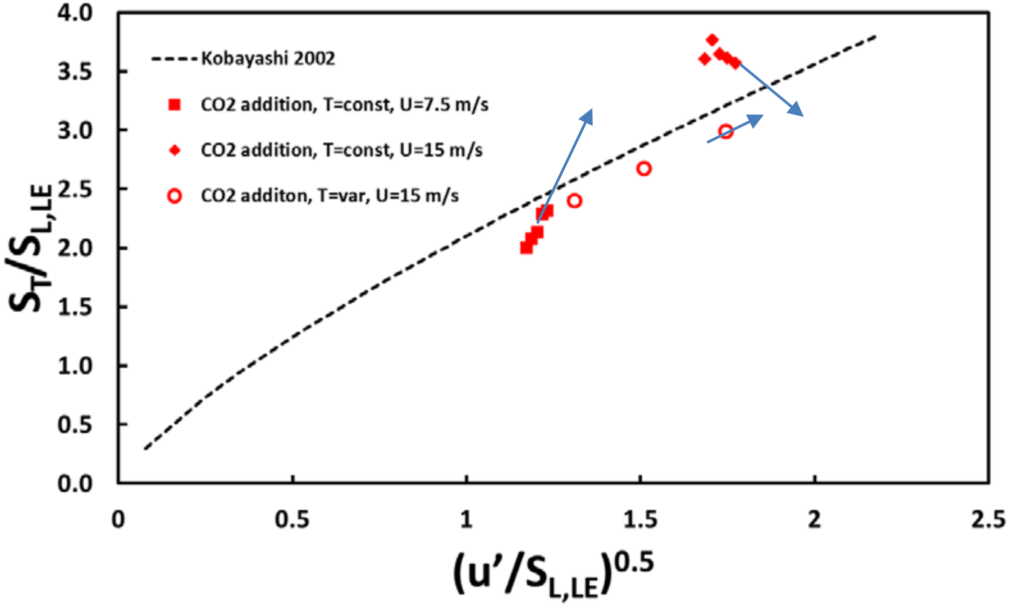
High-Pressure PARAT Burner Studies Future Work

- Initial tests for operability
- High-speed stereo PIV, OH PLIF for comparison with numerical modeling
- Nox, CO emission measurements for comparison with numerical modeling

Correlation of Turbulent Flame Speed using leading edge flame speed

- In the corrugated flame regime, where the Lewis number effect is important. CO_2 dilution leads to an increase in $S_T/S_{L,LE}$
- In the thin reaction zone, however, $S_T/S_{L,LE}$ now decreases with CO_2 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?