Turbulent Flame Speeds and NOx Kinetics of HHC Fuels with Contaminants and High Dilution Levels

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Project Overview

Second Year of Three-Year Project is Complete

Project Highlights:

1. Duration: **Oct. 1, 2010 – Sept. 30, 2013**
2. DOE NETL Award **DE-FE0004679**
3. Budget: $501,712 DOE + $125,500 Cost Share
4. Principal Investigator: Dr. Eric L. Petersen
5. Participating Organizations:
    - Rolls-Royce (Dr. Gilles Bourque)
    - The Aerospace Corporation (Dr. Mark Crofton)
    - Trinity College (Dr. John Mertens)

Project Overview

This Project Addresses Several Problems for HHC Fuels

1. Improve **NOx kinetics** for High-Hydrogen Fuels at Engine Conditions

2. Effect of **Contaminant Species** on Ignition

3. Impact of **Diluents** on Ignition Kinetics and Flame Speeds

4. Data on **Turbulent Flame Speeds**

Project Overview

There are Six Main Work Tasks for the Project

Work Tasks:

- **Task 1** – Project Management and Program Planning
- **Task 2** – Turbulent Flame Speed Measurements
- **Task 3** – Laminar Flame Speeds with Diluents
- **Task 4** – NOx Mechanism Validation Experiments
- **Task 5** – Fundamental NOx Kinetics
- **Task 6** – Effect of Impurities on Syngas Kinetics

Task 1 – Project Management and Program Planning

Project Participants

Dr. Olivier Mathieu

Christopher Aul

Anthony Levacque

Fiona Deguillaume

Sankar Ravi

Drew Plichta

Andrew Vissotski

Travis Sikes

Michael Krejci

Task 1 - Management

Interaction and Feedback from Industry Has Been Important

Industrial Advisory Panel

Rolls-Royce Canada:
Dr. Gilles Bourque

Alstom:
Dr. Felix Güthe

General Electric:
Mr. Joel Hall

Power Systems Mfg.:
Dr. Peter Stuttaford
Mr. Khalid Oumejjoud

- Mixture Compositions and Test Conditions

- Possible Contaminant Species

- Important, Related Aspects and Ultimate Usage of Models

Task 2 – Turbulent Flame Speed Measurements

Task 2 – Turbulent Speeds

Turbulent Flame Speed Measurement Requires Development of New Techniques at TAMU

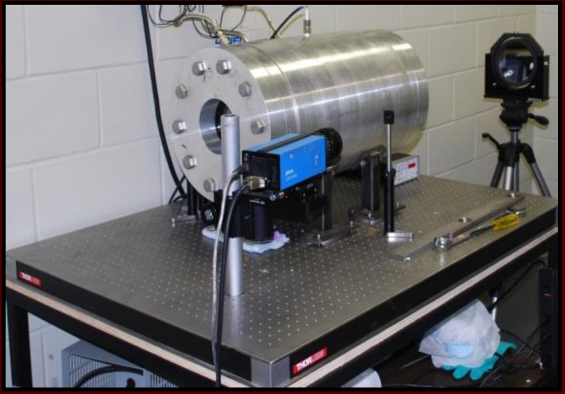
- Utilize Existing Flame Speed Hardware
- Induce Turbulence Using Fans
- Conduct Design Study Using Mockup Rig
- Design and Build New Facility Hardware

Goal: Independent Control of Length Scale (L_T) and Turbulence Intensity (u')

Task 2 – Turbulent Speeds

Design Modifications for Turbulence Production Were Optimized Using a Mock-Up Rig

Original Rig

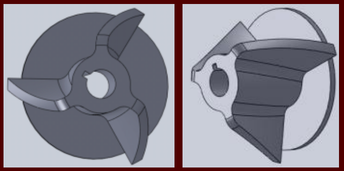


Test Matrix

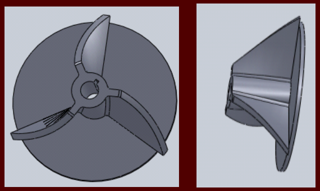
Prototype	Fan OD (in)	No of Blades	Blade Pitch
1	3	3	20
2	5	3	20
3	3	6	20
4	3	3	60

Mock-Up Rig

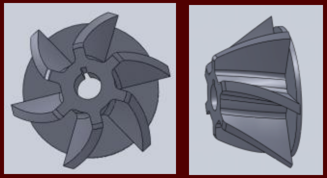
PROTOTYPE 1



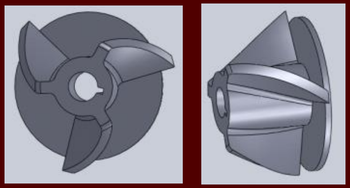
PROTOTYPE 2



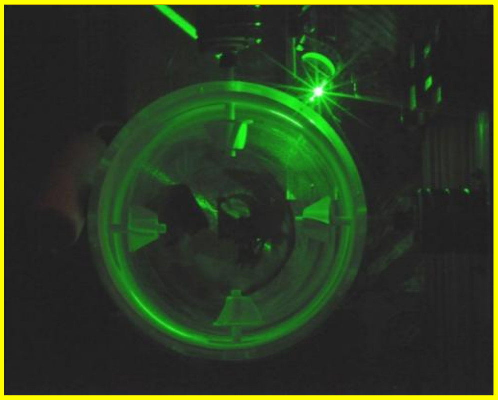
PROTOTYPE 3



PROTOTYPE 4



PIV Measurement

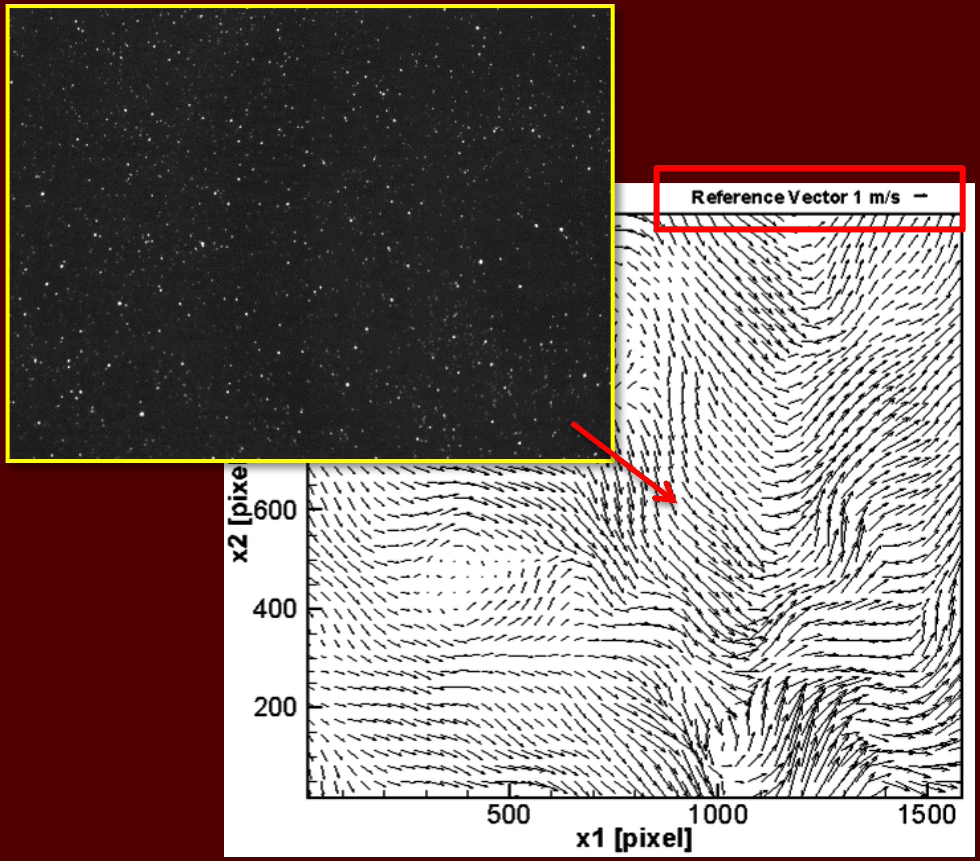


- ROI: 36 mm × 26 mm
- 8300 rpm
- Titania seed particles

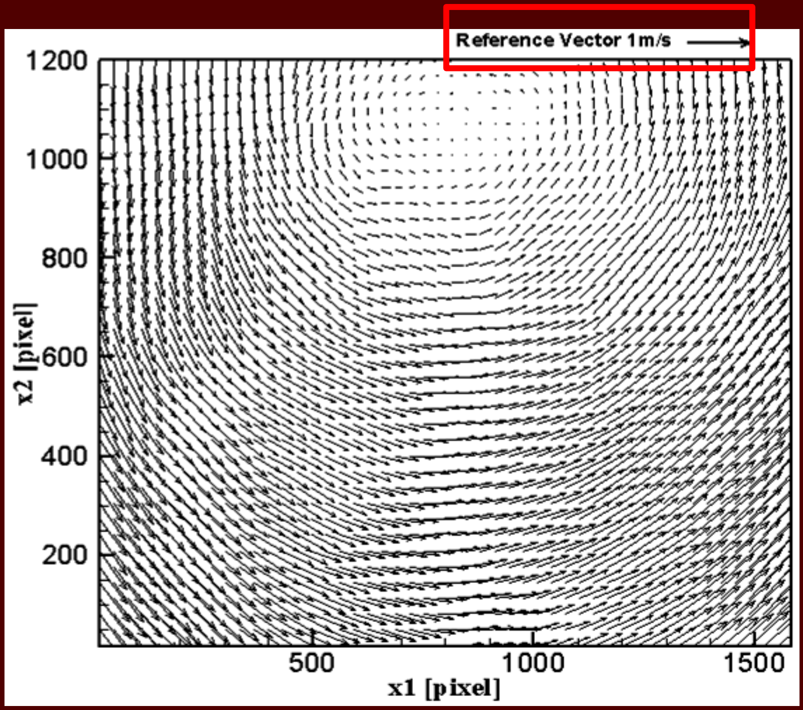
Task 2 – Turbulent Speeds

Negligible Mean Flow (<9% u_{rms}) observed for all prototypes

Raw Image with Seed Particles



Instantaneous Velocity Field



Mean Velocity Field

(Reference vector magnified 5 times)

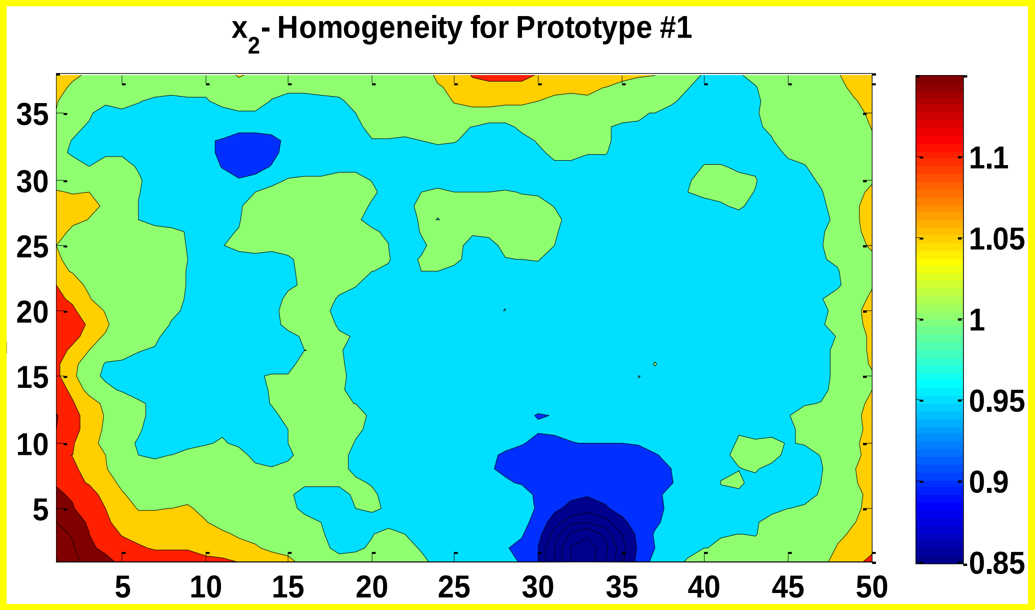
Task 2 – Turbulent Speeds

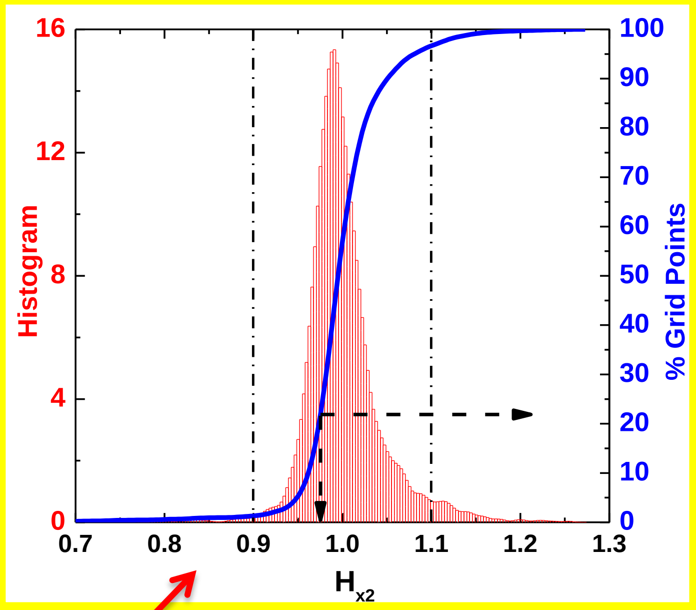
Homogenous velocity fields were observed inside the ROI

Defined as the ratio of the local RMS velocity to the spatially averaged RMS velocity *(Hwang and Eaton 2004)*,

$$H_{xi}(x_1, x_2) = u_{i,rms}(x_1, x_2)/\overline{u_{i,rms}(x_1, x_2)}$$

x_2- Homogeneity





> 95% of the grid points lie in the 0.9-1.1 range

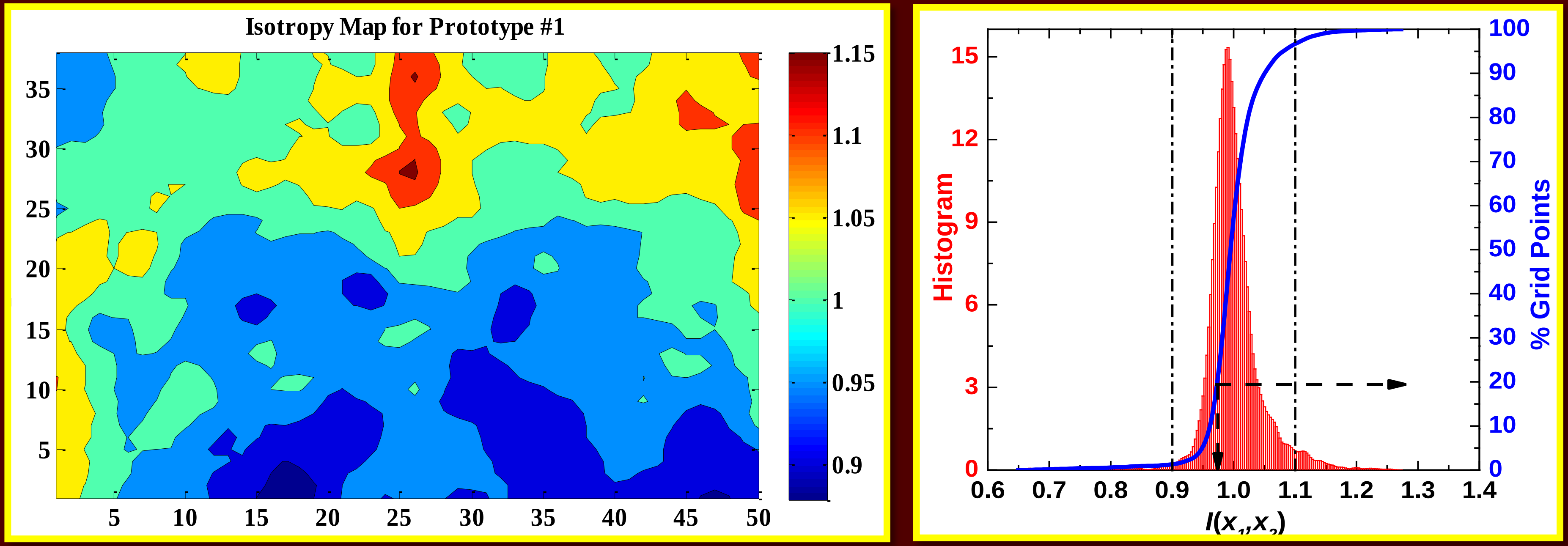
Task 2 – Turbulent Speeds

Isotropy ratios were estimated from the local RMS values

Defined as the ratio of the local RMS velocities in the two directions *(Hwang and Eaton 2004),*

$$I(x_1, x_2) = \frac{u_{1,rms}(x_1, x_2)}{u_{2,rms}(x_1, x_2)}$$

Isotropy Ratio



Task 2 – Turbulent Speeds

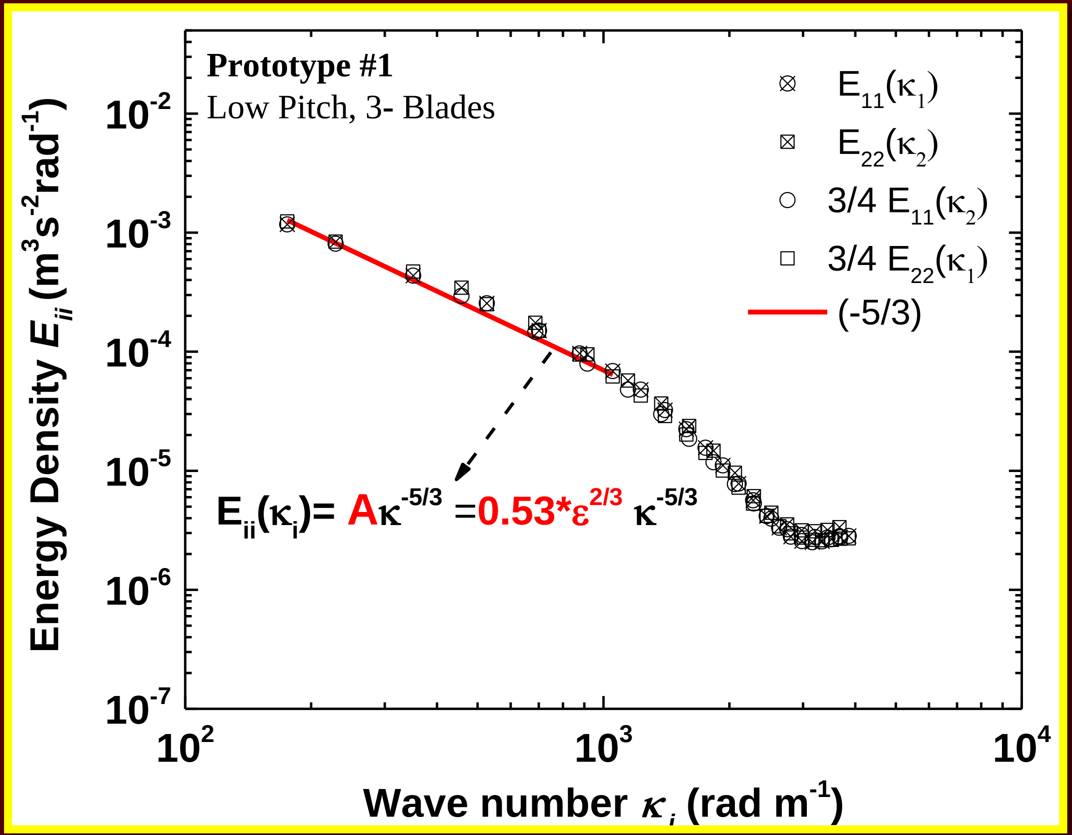
*Integral Length Scale (**L_T**) was computed using dissipation rate estimated from the 1D-energy spectrum*

$$L_T \cong \left[\frac{\left(u_{i,RMS}(x_1,x_2)u_{i,RMS}(x_1,x_2)/3\right)^{3/2}}{\varepsilon}\right]$$

(Summation over Index)

Need ε for L_T

ϵ estimated by linear fit in the *Inertial subrange*
(Meng et al. 2009)



Task 2 – Turbulent Speeds

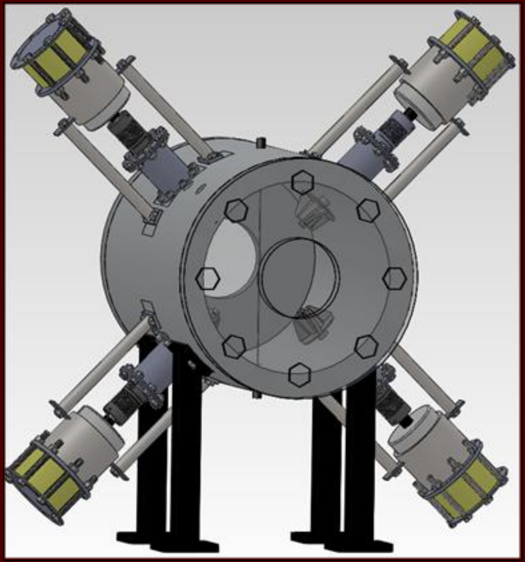
Independent control of the various turbulence parameters was achieved

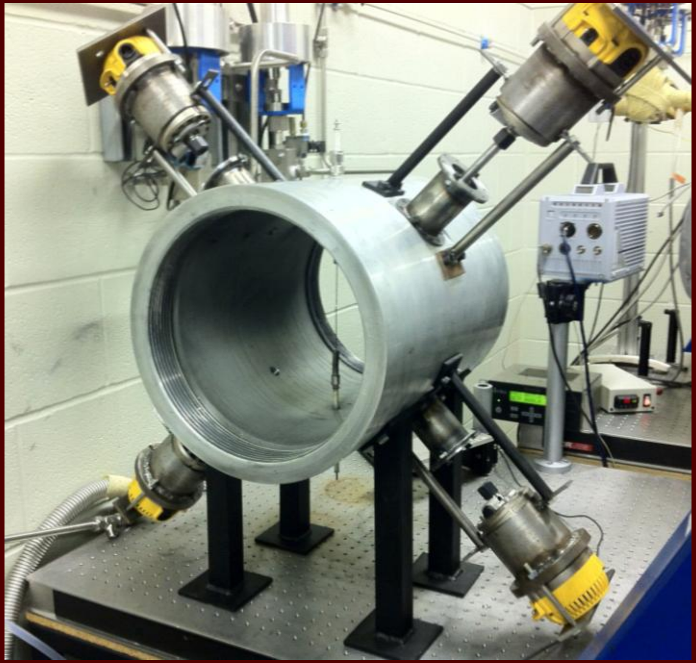
- **Central placement ensured homogenous flow fields**
- **Deviation from isotropy was observed with higher no of blades**
- **Vary u′ → Change RPM**
- **Different L_T → Use impellers with different blade pitch**

Effect of fan OD will be assessed in final vessel using LDV

Task 2 – Turbulent Speeds

Final Configuration is Set and Nearing Completion





- Central symmetric placement – 4 fans
- 3-bladed impellers with two pitch angles: 20° and 75°
- Attainable u′ range: 0- 3.5 m/s in HIT environment
- L_T will be varied between 30 mm and 50 mm

Task 2 – Turbulent Speeds

***Year 3** Will Include Shakedown of New Turbulent Flame Speed Capability and New Experiments*

- Finish Installation of New Hardware
- Characterize Turbulence Generation of New Facility
- Perform Shakedown Experiments Using H_2-Air Mixtures
- Obtain Data for H_2-CO Syngas Mixture

Task 3 – Laminar Flame Speeds with Diluents

Task 3 – S_L with Diluents

High-H_2 Fuels with High Levels of Dilution are being Studied

- Year 1 Measurements:
  - Baseline H_2-Air Flame Speeds
  - Baseline CO-H_2 Flame Speeds

- Year 2 Tests included H_2O dilution (below)

- Other Diluents for Year 3: CO_2, N_2?

Task 3 – S_L with Diluents

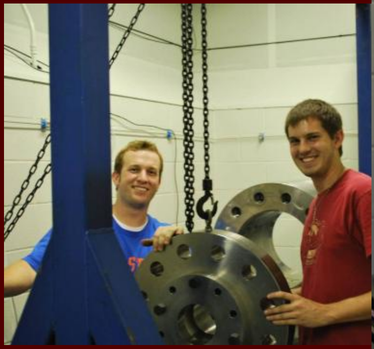
New High-Temperature High-Pressure Flame Speed Vessel is Now Operational

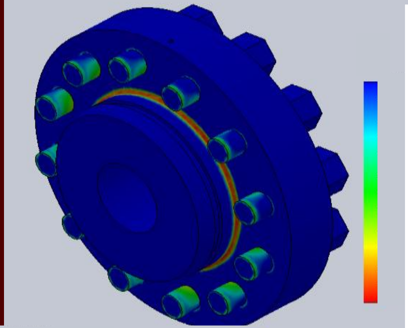
Design Parameters:

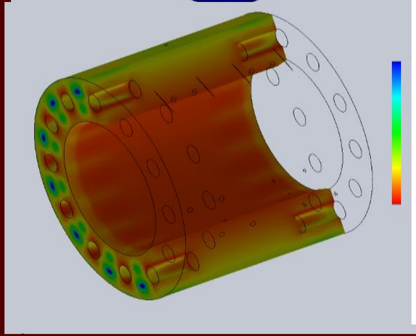
- *Max initial pressure:* ***30 atm***
- *Max initial temperature:* ***600 K***

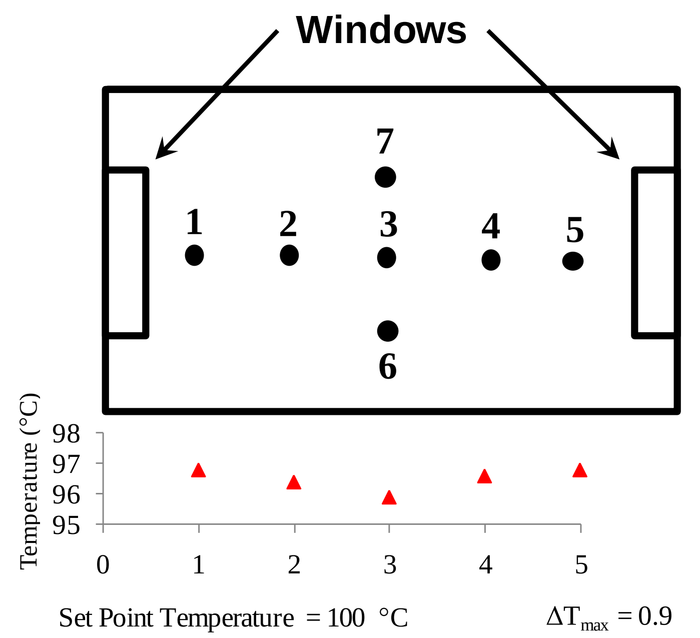
Vessel Dimensions:

- *Outer Dia.: 54.6 cm*
- *Inner Dia.:* ***31.8 cm***
- *External Length: 63.5 cm*
- *Internal Length:* ***27.9 cm***
- *Window Port Dia.: 12.7 cm*
- *Approximate Wt: 1800 lbs*









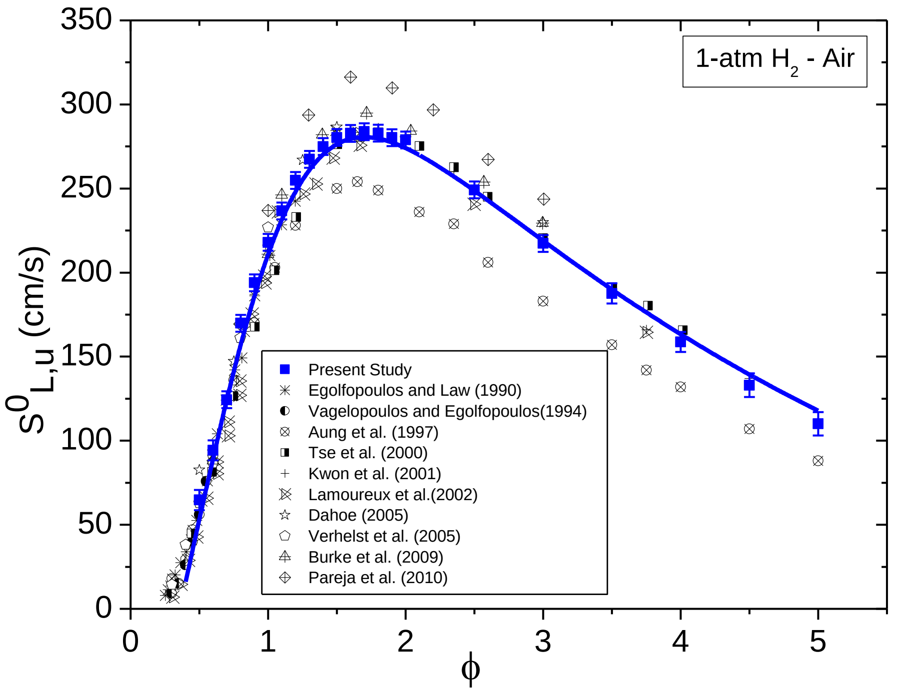
Mechanism

NUIG H_2-CO Chemistry Forms Basis of the Mechanism

- Kinetic mechanism developed at C^3
  - H_2 /CO/O_2 based on Ó Conaire et al.
  - Several significant updates based on recent experimental and kinetic data

- Simulations performed using Chemkin Pro
  - Grid independent solutions ≈ 1000 pts
  - Multi-component transport & thermal diffusion

H_2-Air Results



Task 3 – S_L with Diluents

Ongoing Experiments to Include H_2O Using a Design of Experiments Approach

- 4 Factors with 3 Levels Each

- L-9 Taguchi Matrix

- \- Temperature (323, 373, 423 K)

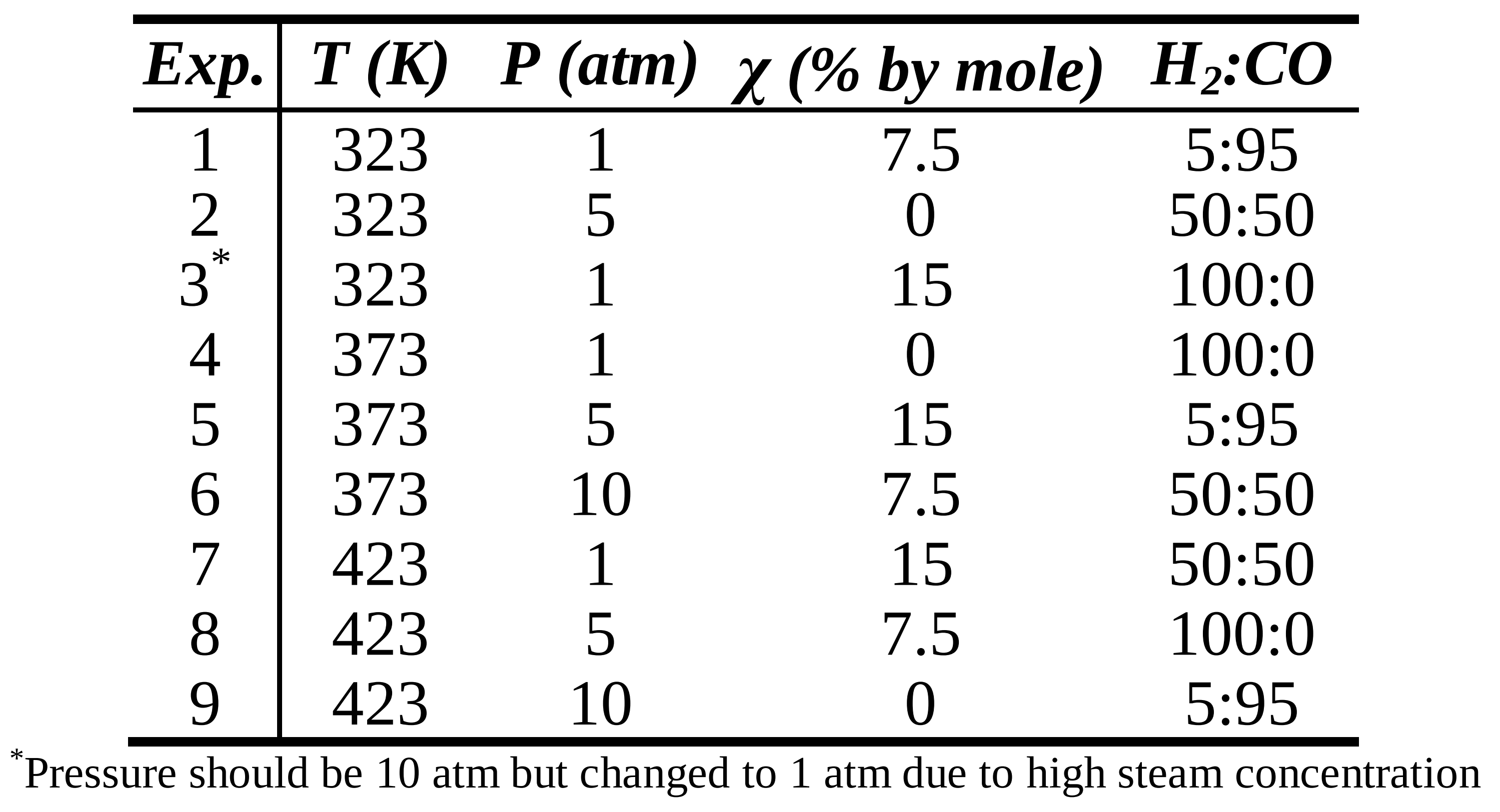
  \- Pressure (1, 5, 10 atm)

  \- Water Content (0, 7.5, 15%)

  \- H_2:CO Mixture (5:95, 50:50, 100:0)

Task 3 – S_L with Diluents

Design of Experiments Approach Utilized



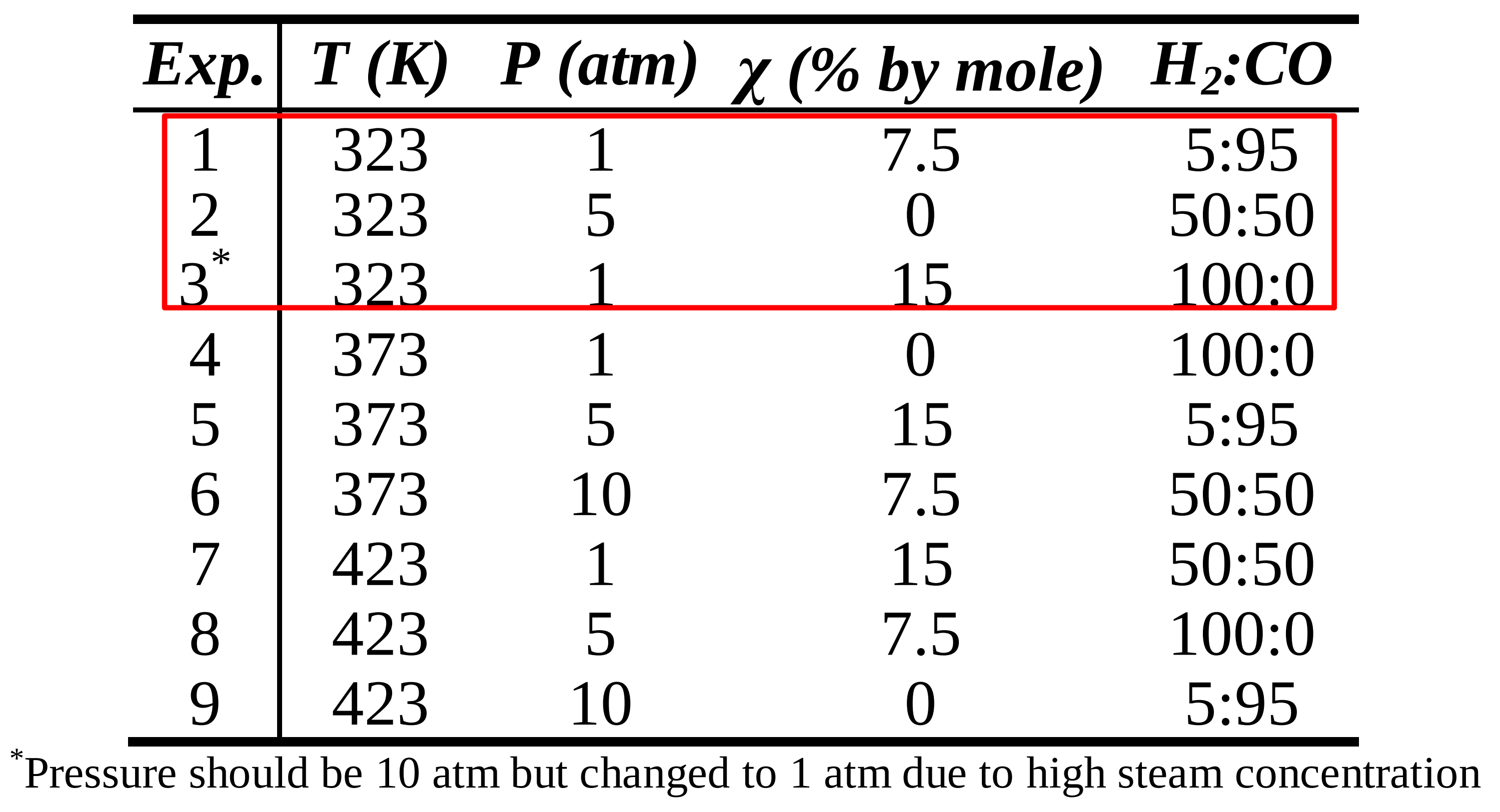
Exp.	***T* (K)**	***P* (atm)**	**χ (% by mole)**	**H_2:CO**
1	323	1	7.5	5:95
2	323	5	0	50:50
3*	323	1	15	100:0
4	373	1	0	100:0
5	373	5	15	5:95
6	373	10	7.5	50:50
7	423	1	15	50:50
8	423	5	7.5	100:0
9	423	10	0	5:95

*Pressure should be 10 atm but changed to 1 atm due to high steam concentration

Taguchi L9 Matrix

Task 3 – S_L with Diluents

Design of Experiments Approach Utilized



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6	373	10	7.5	50:50
7	423	1	15	50:50
8	423	5	7.5	100:0
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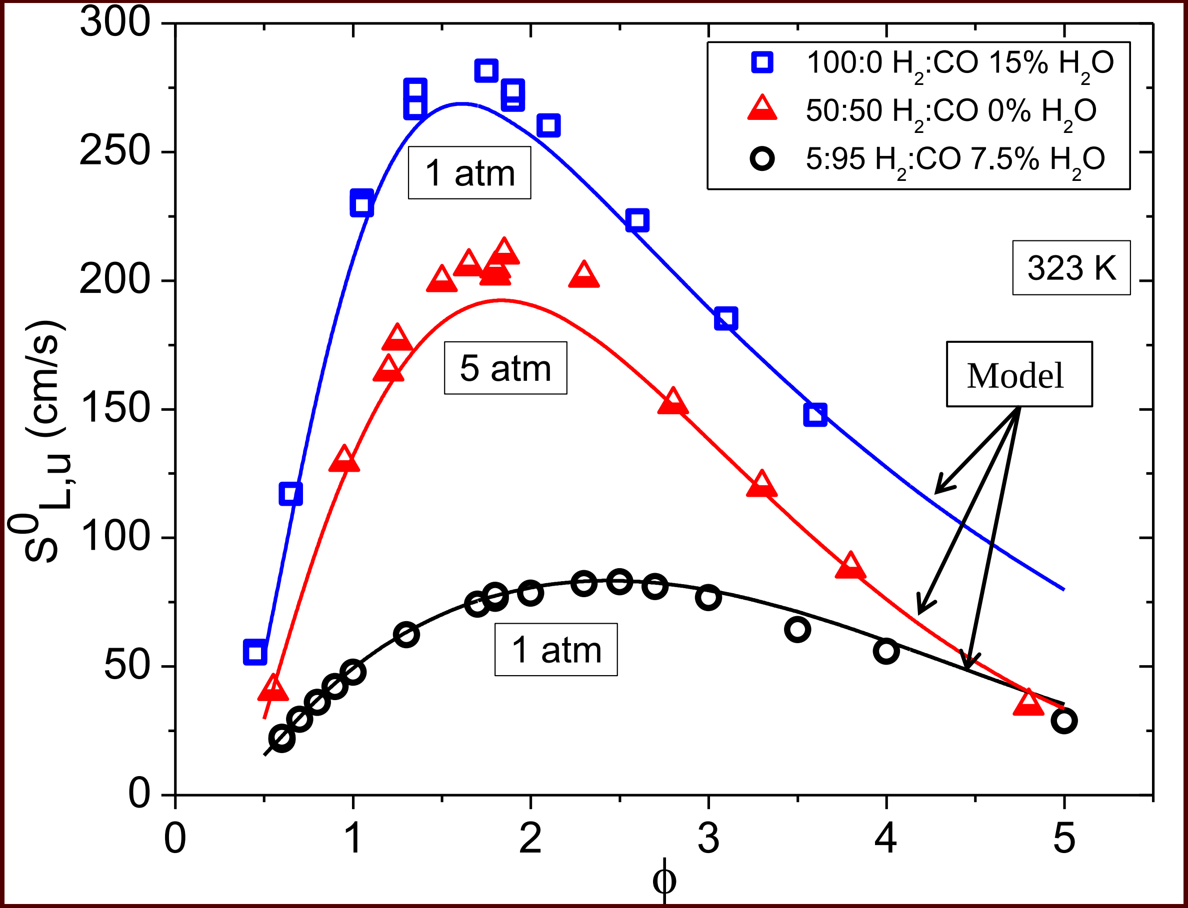
[*] Pressure should be 10 atm but changed to 1 atm due to high steam concentration

Taguchi L9 Matrix

Task 3 – S_L with Diluents

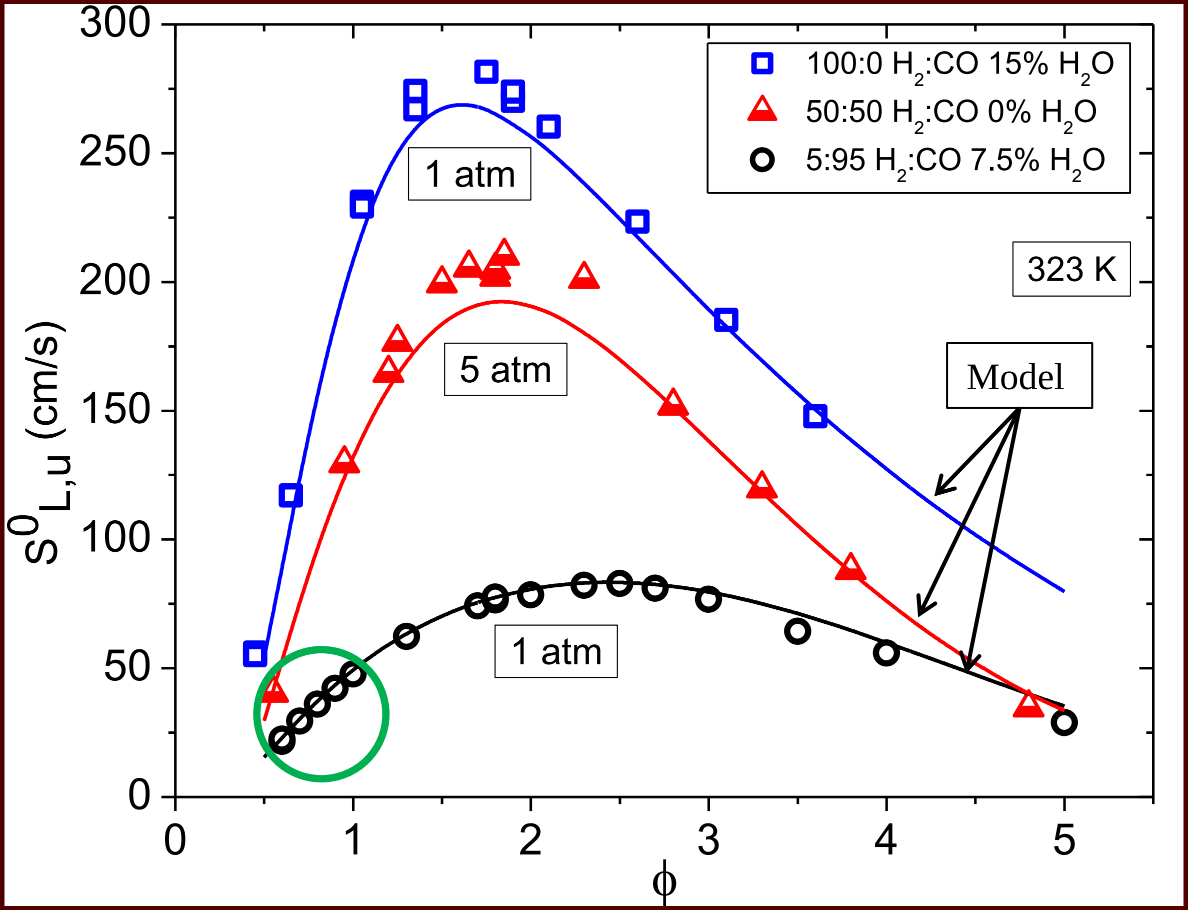
Results: Combos 1 - 3



Carbon monoxide increase causes a reduction in velocity and the mixture becomes less influenced by the equivalence ratio

Task 3 – S_L with Diluents

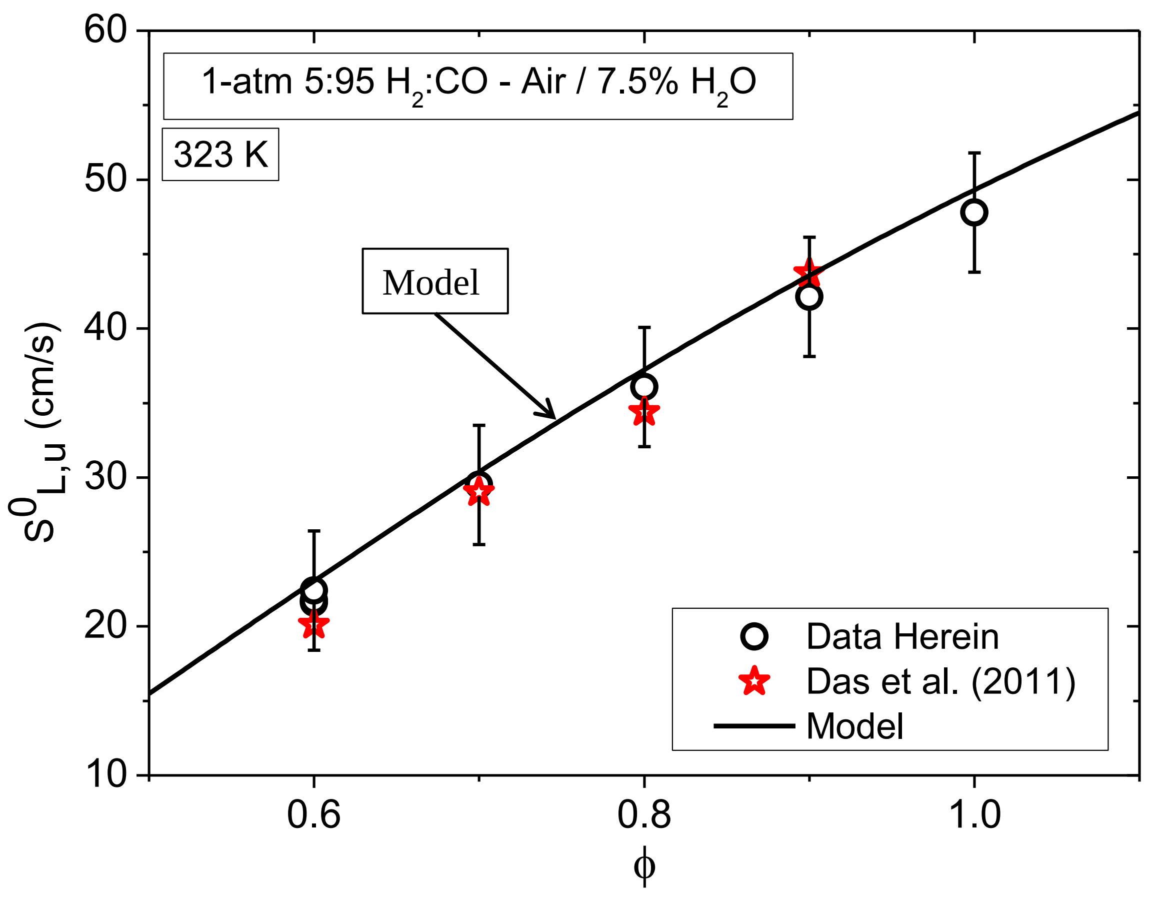
Results: Combos 1 - 3



Carbon monoxide increase causes a reduction in velocity and the mixture becomes less influenced by the equivalence ratio

Task 3 – S_L with Diluents

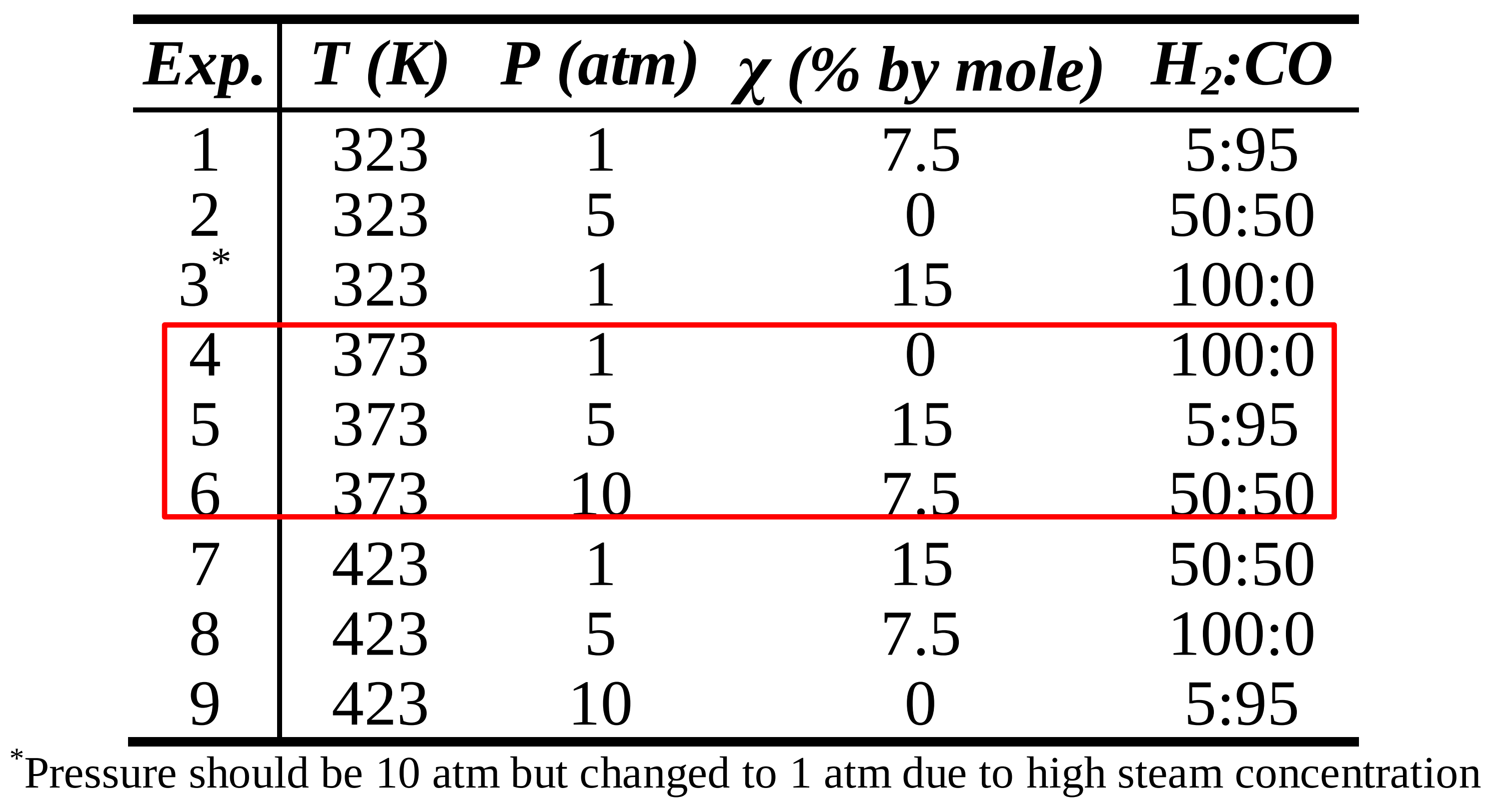
Good Agreement with Available Data (Das, Sung et al., 2011)



Good agreement with Das et al. (2011) and the model (solid line)

Task 3 – S_L with Diluents

Results: Combos 4 - 6



Exp.	T (K)	P (atm)	χ (% by mole)	H_2:CO
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7	423	1	15	50:50
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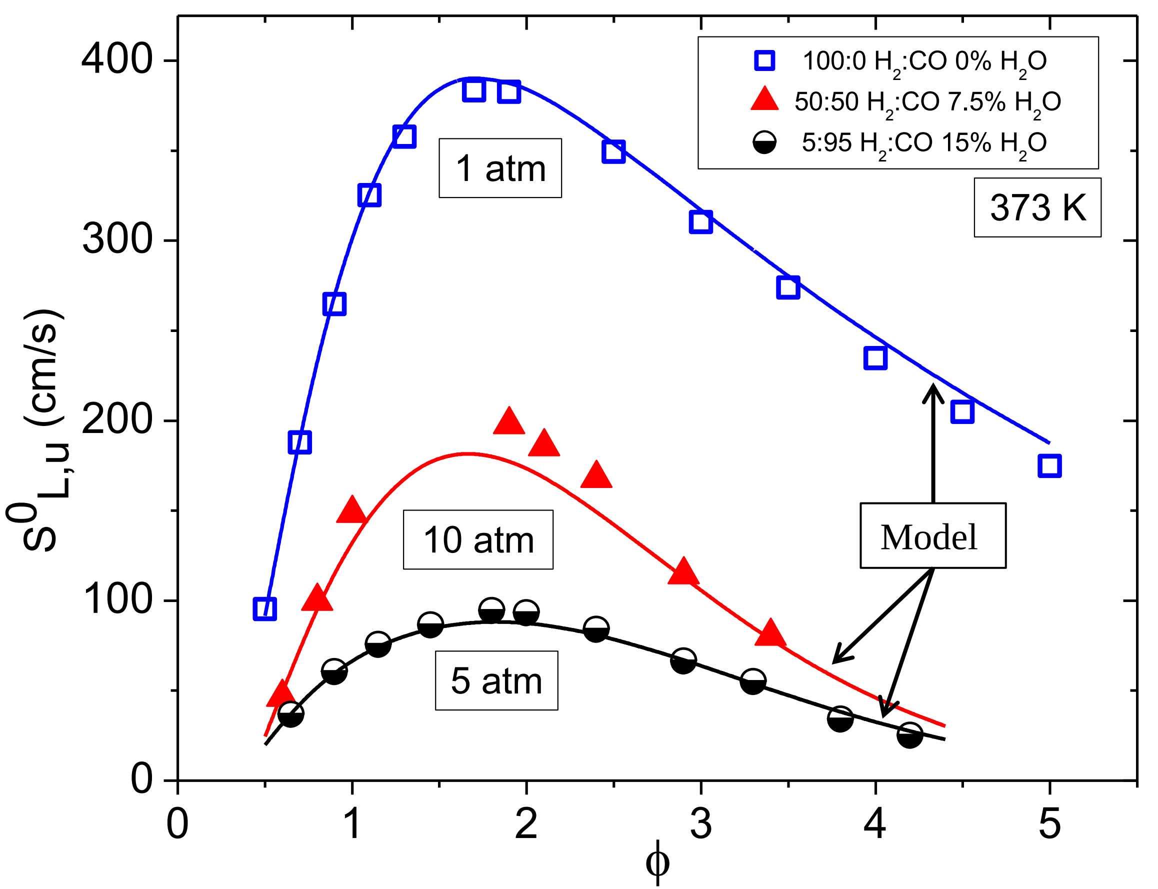
9	423	10	0	5:95

*Pressure should be 10 atm but changed to 1 atm due to high steam concentration

Task 3 – S_L with Diluents

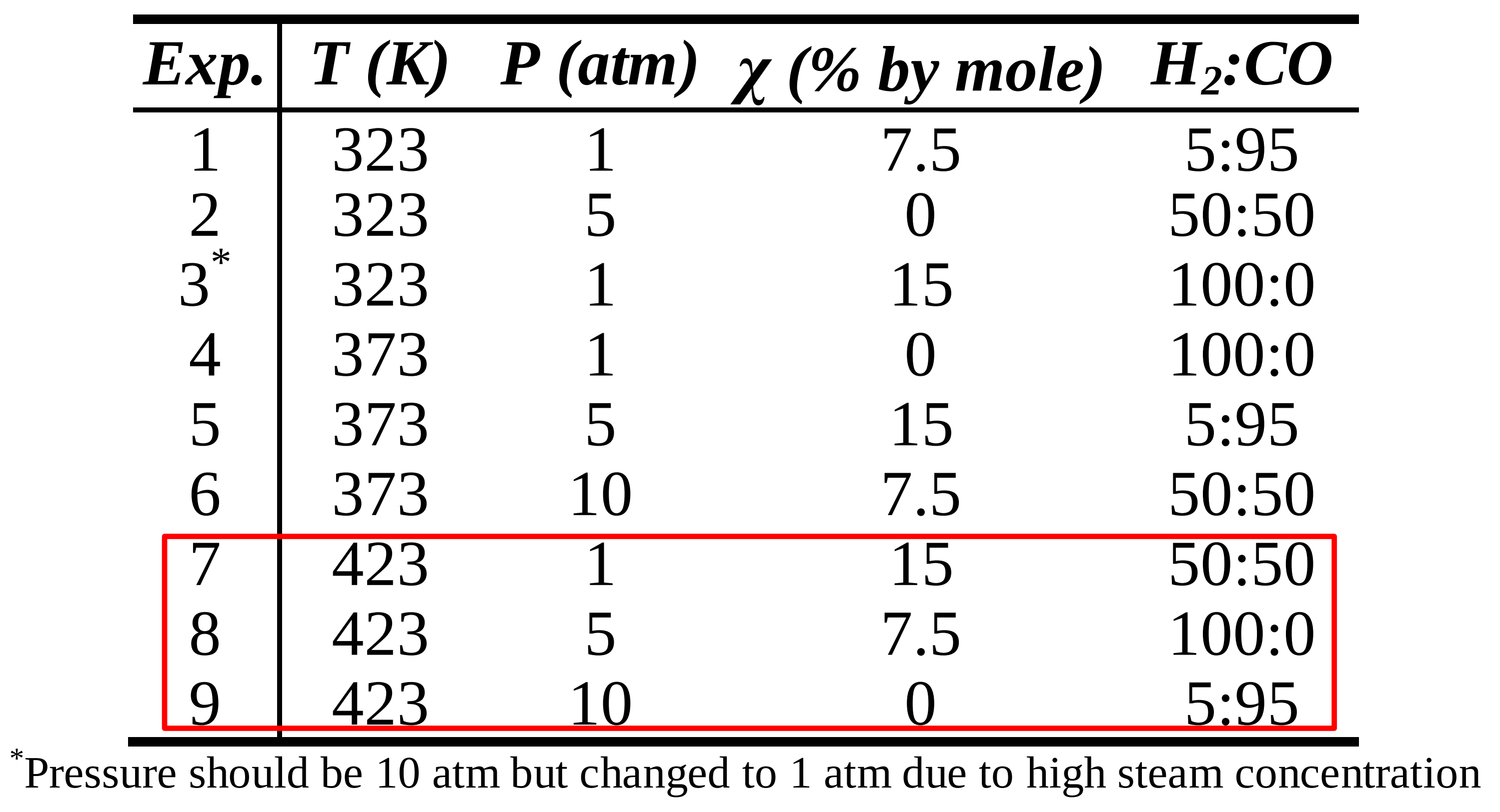
Results: Combos 4 - 6



Good agreement with the model (solid lines)

Task 3 – S_L with Diluents

Results: Combos 7 - 9



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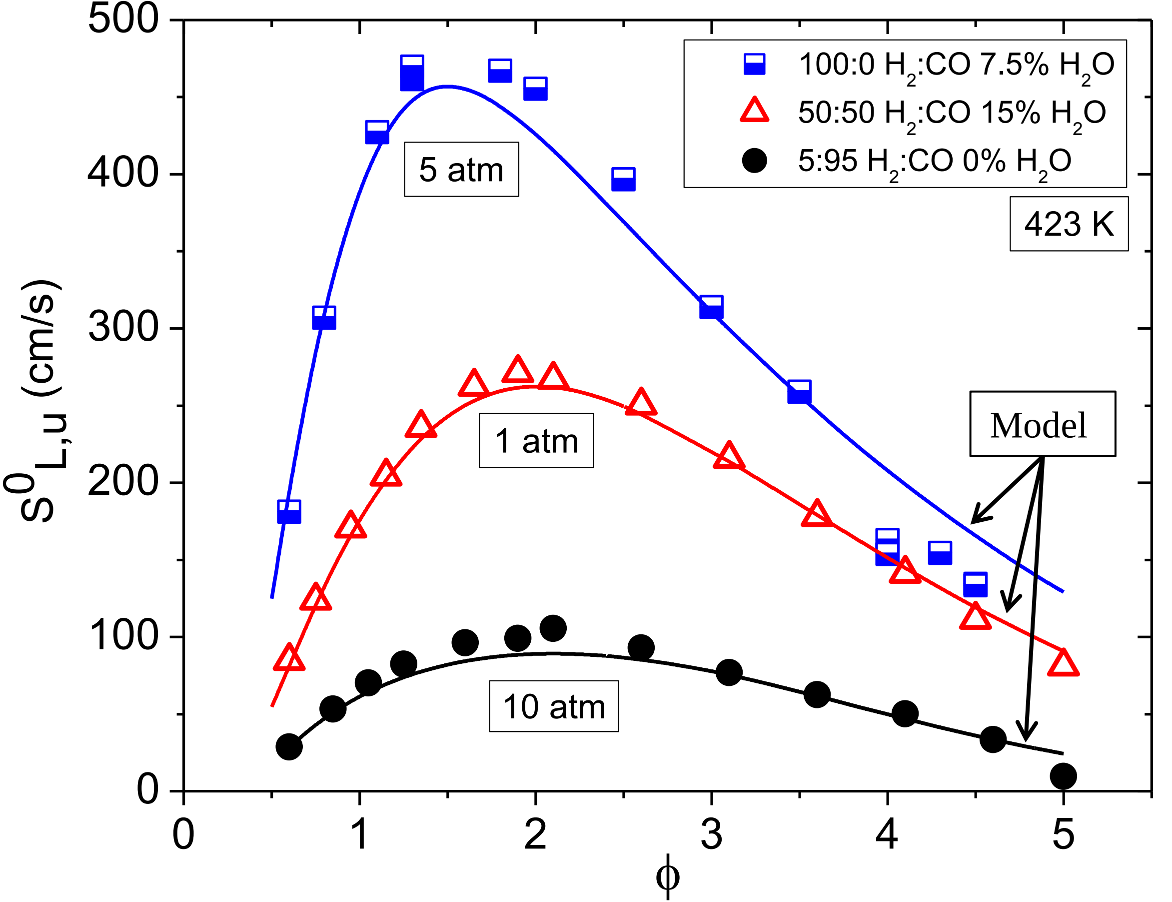
*Pressure should be 10 atm but changed to 1 atm due to high steam concentration

Task 3 – S_L with Diluents

Results: Combos 7 - 9

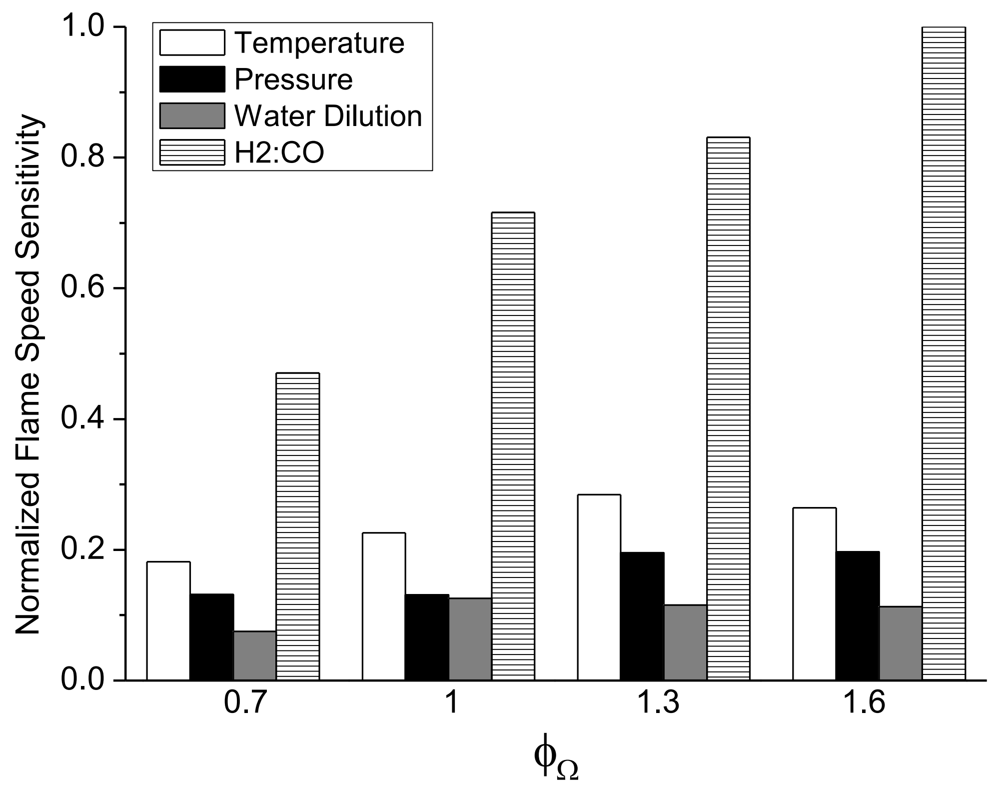


Good agreement with the model (solid lines)

Task 3 – S_L with Diluents

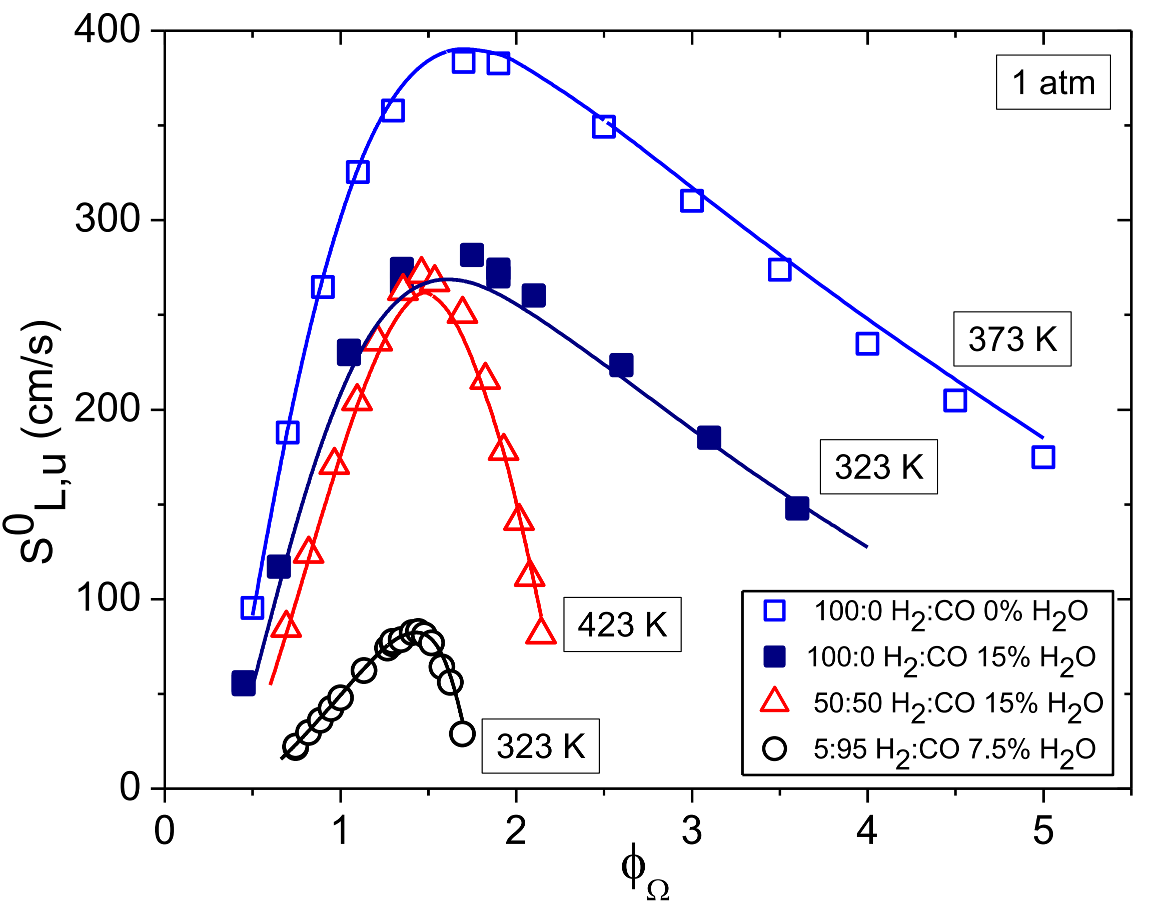
Results: Sensitivity Analysis from the Matrix

The maximum difference between the averaged parameter values (i.e., S_L) at each DOE level (i.e. 1, 2, or 3) for each factor and equivalence ratio



Task 3 – S_L with Diluents

1-atm Results Plotted with Modified ϕ_Ω Show Common Peak

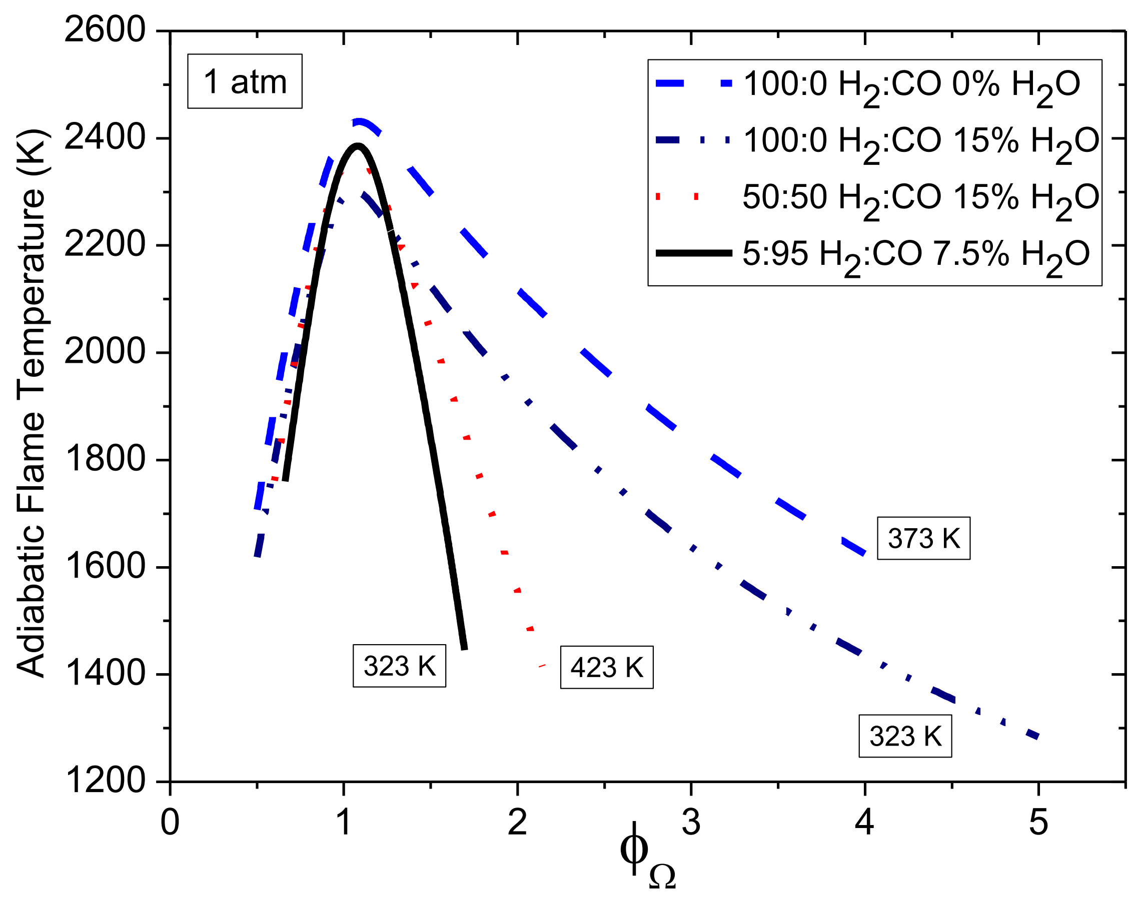


$$\Phi_\Omega = \frac{(1+X_{CO})}{\left(X_{CO}+\frac{1}{\Phi}\right)}$$

- Shifts in the peak flame speed are adjusted
- CO dilution has a strong influence

Task 3 – S_L with Diluents

Flame Temperature for 1-atm Results



- Little influence on the fuel-lean side
- Strong influence on the fuel-rich side

Task 4 – NOx Mechanism Validation Experiments

Task 4 – NOx Mechanism

Kinetics Mechanism Validation with NOx at Engine Conditions is being Performed

- Mechanism Based on Galway C5 Mechanism
- NOx Mechanism(s) from Recent Literature Investigated
- Ignition Times with NO_2 and N_2O Precursors for Validation (and EGR-Related)
- Ammonia Oxidation and Chemical Kinetics
- **Goal: Oxidation Dataset and Suggest Mechanism at End**

Task 4 – NOx Mechanism

Texas A&M High-Pressure Shock Tube

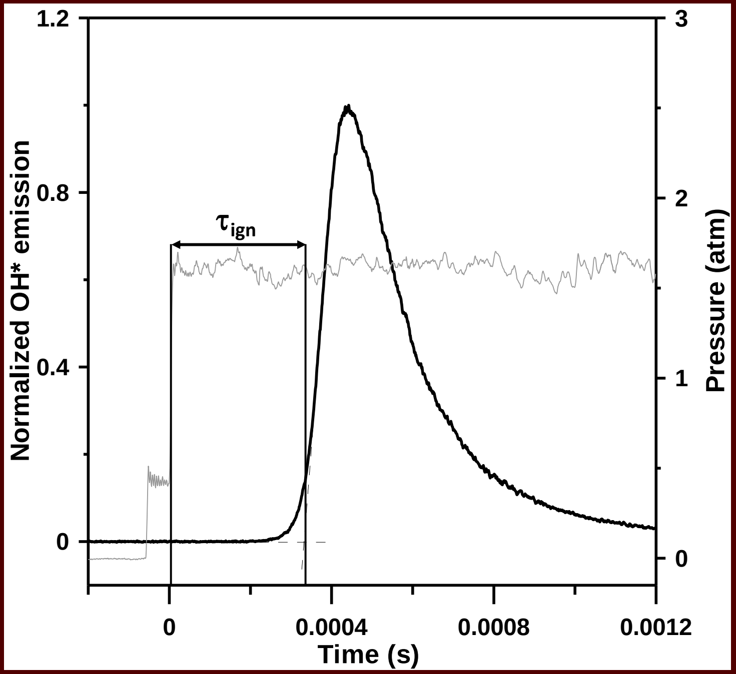
Task 4 – NOx Mechanism

Addition of NO_2 *in H_2-O_2 Mixtures*

- **Dilute conditions (98% Ar)**
- **Ignition delay time measurement at the sidewall location**
  - **OH* Emission**
  - **307 ± 10 nm**

Mostly at $\phi = 0.5$ for H_2/O_2

Mixture composition (mole fraction)	T_5 (K)	P_5 (atm)	Reference
0.01 H_2 / 0.01 O_2 / 0.98 Ar	960-1625	1.65 ± 0.15 atm	Keromnes et al.
	1085-1245	13.3 ± 1.0 atm	
	1160-1270	32.8 ± 1.5 atm	
0.01 H_2 / 0.01 O_2 / 0.0001 NO_2 / 0.9799 Ar	945-1640	1.70 ± 0.2 atm	This study
	1035-1200	12.5 ± 0.9 atm	
	1055-1235	33.7 ± 1.6 atm	
0.01 H_2 / 0.01 O_2 / 0.0004 NO_2 / 0.9796 Ar	990-1565	1.65 ± 0.25 atm	This study
	1030-1220	13.5 ± 0.7 atm	
	1020-1230	34.2 ± 0.7 atm	
0.01 H_2 / 0.01 O_2 / 0.0016 NO_2 / 0.9784 Ar	1100-1720	1.60 ± 0.15 atm	This study
	1035-1250	13.2 ± 0.6 atm	
	1050-1270	33.1 ± 0.4 atm	

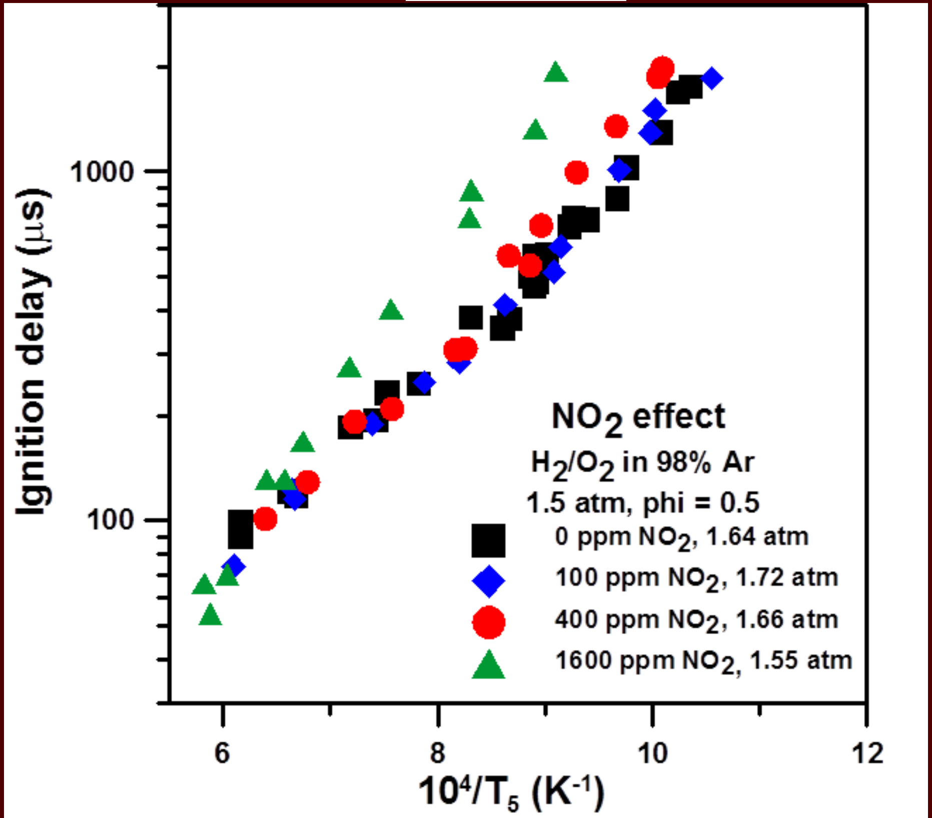


Also: ϕ = 0.3 and 1.0 without and with 100 ppm NO_2

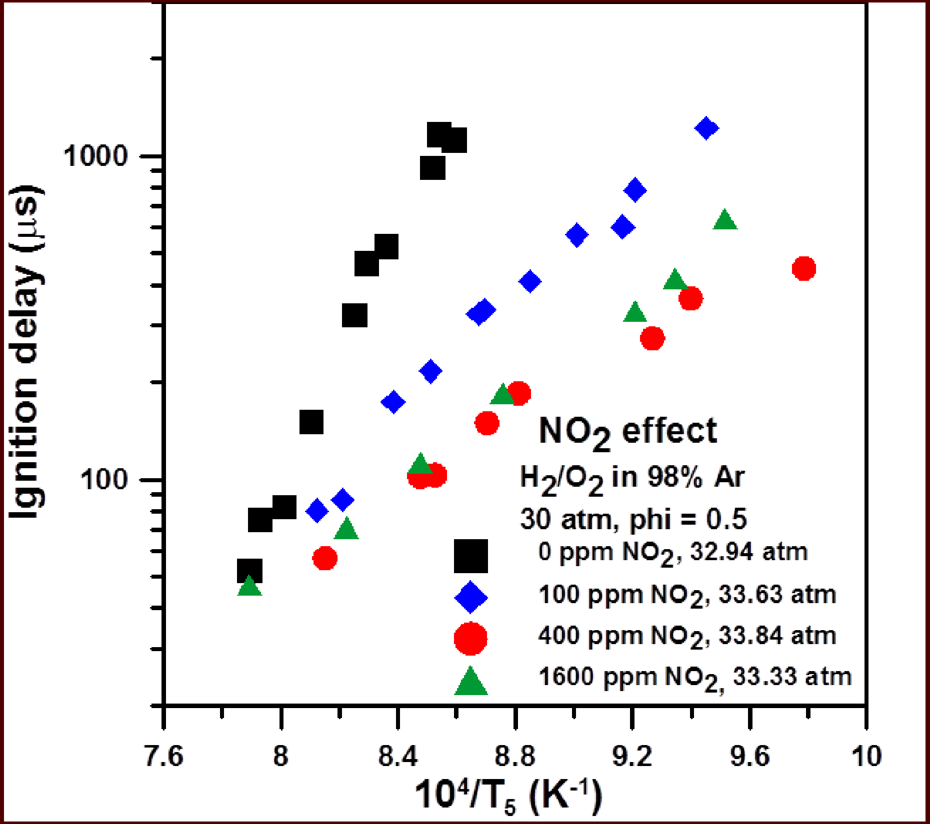
Task 4 – NOx Mechanism

Effect of NO_2 on H_2-O_2 Mixtures is Stronger at Higher Pressure

1.5 atm



30 atm



Task 4 – NOx Mechanism

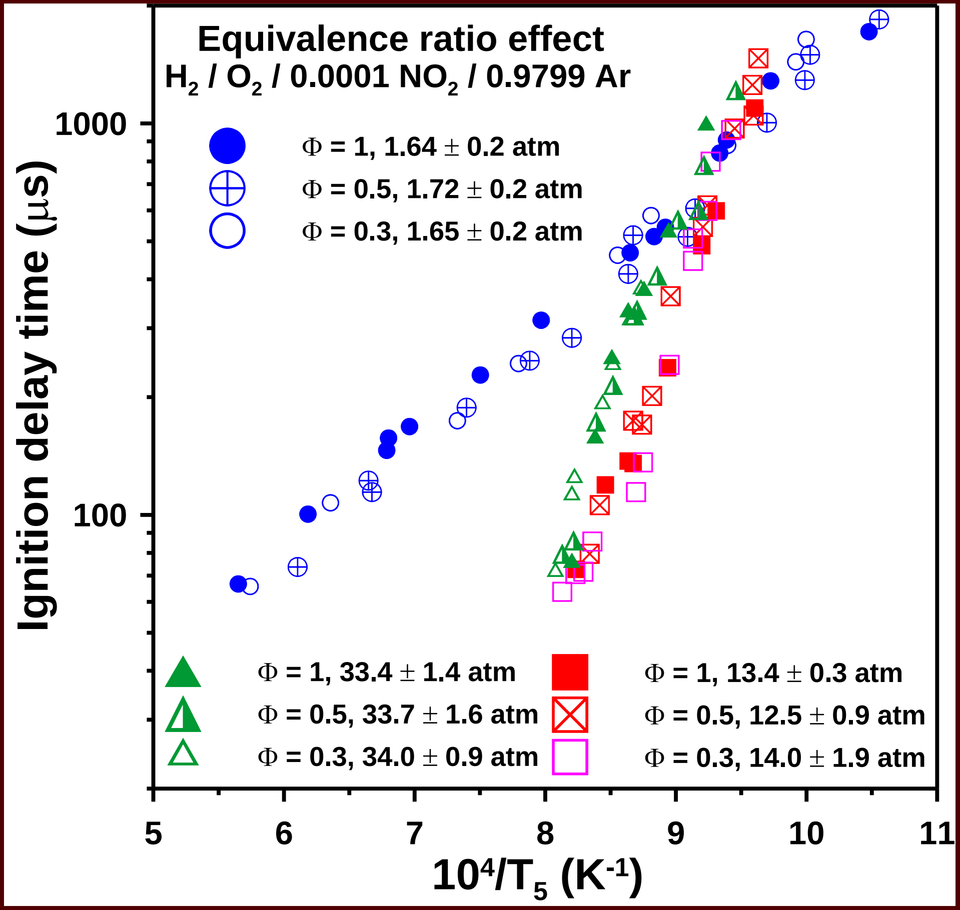
Equivalence ratio effect at 100 ppm

ϕ = 0.3, 0.5, 1.0 with 100-ppm NO_2

⇒ Nearly no effect on ϕ

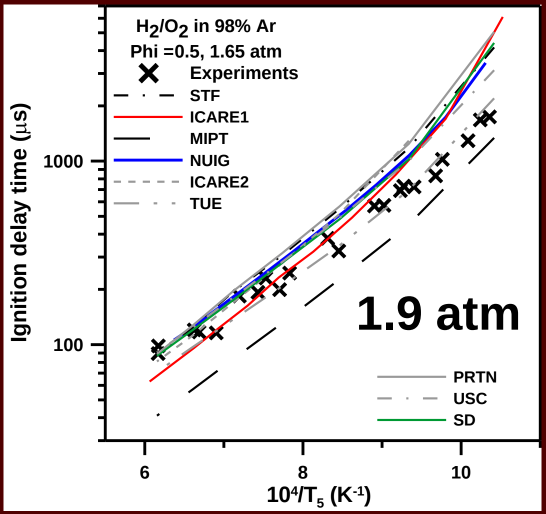
⇒ Similar to neat H_2/O_2 mixtures (Keromnes et al., 2012, Herzler and Naumann, 2009)

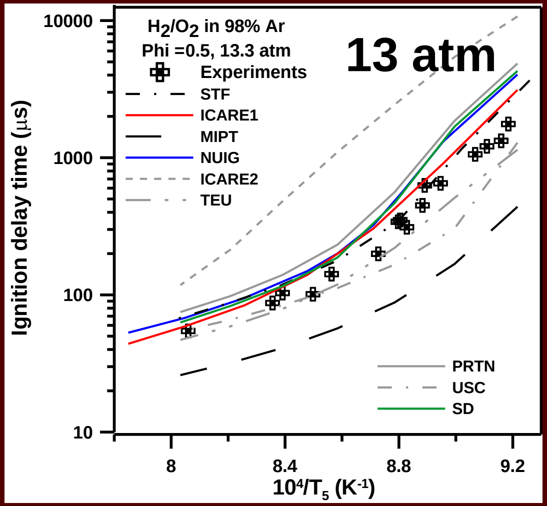
⇒ Computation showed the same for larger NO_2 concentrations

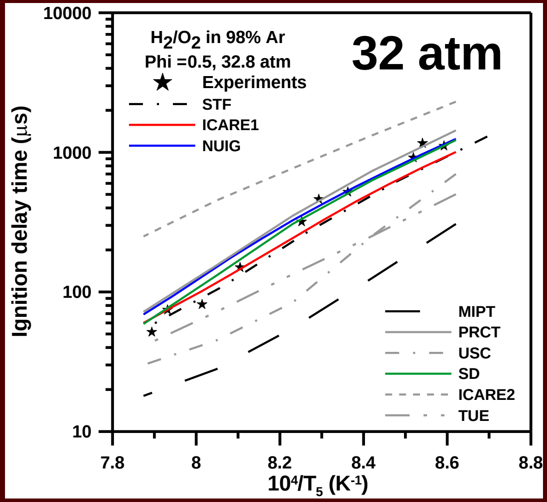


Task 4 – NOx Mechanism

Variation in H_2/O_2 Mechanisms for Baseline H_2-O_2 Data







ICARE1: Mevel *et al.* (Proceed. Combust. Inst. 32 (2009) 359–366)

ICARE2: Dayma and Dagaut (Combust. Sci. and Tech. 178 (2006), 1999-2024)

MIPT: Kosarev *et al.* (Combust. Flame 151 (2007) 61–73)

NUIG: Healy *et al.* (Combust. Flame 157 (2010) 1526-1539)

PRNT: Burke *et al.* (Int. J. Chem. Kinet. (2011), DOI: 10.1002/kin.20603)

SD: Petrova and Williams (Combust. Flame 144 (2006) 526-544)

STF: Hong *et al.* (Combust. Flame 158 (2011) 633-644)

TUE: Konnov (Combust. Flame 156 (2009) 2093-2105)

USC: Wang *et al.* (http://ignis.usc.edu/USC_Mech_II.htm, May 2007)

Task 4 – NOx Mechanism

NUIG Mechanism Chosen as Baseline H_2-O_2 Chemistry

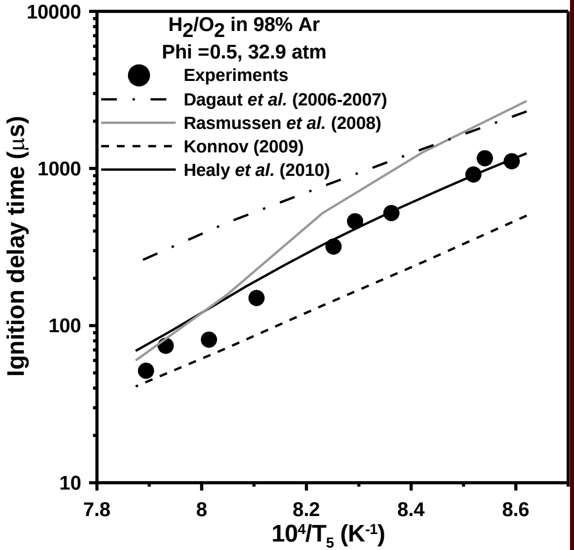
Several NOx mechanisms tested:

- **Rasmussen, Glarborg et al., 2008**
- **Konnov, 2009**
- **Dagaut, Brezinsky et al. (2006, 2007)**

Not in full agreement with the data over the range of conditions investigated

Because of H_2 chemistry? NOx chemistry?

⇨ Test against new H_2/O_2 data (Keromnes, Curran, Petersen et al., 2012)



- **Poor agreement against our H_2/O_2 data**
- **Several H_2 mechanisms tested (see Mathieu et al., accepted in *Int. J. Hydrogen Energy*, 2012)**
- **Healy, Curran, et al. (2010) selected as base H_2 mechanism**

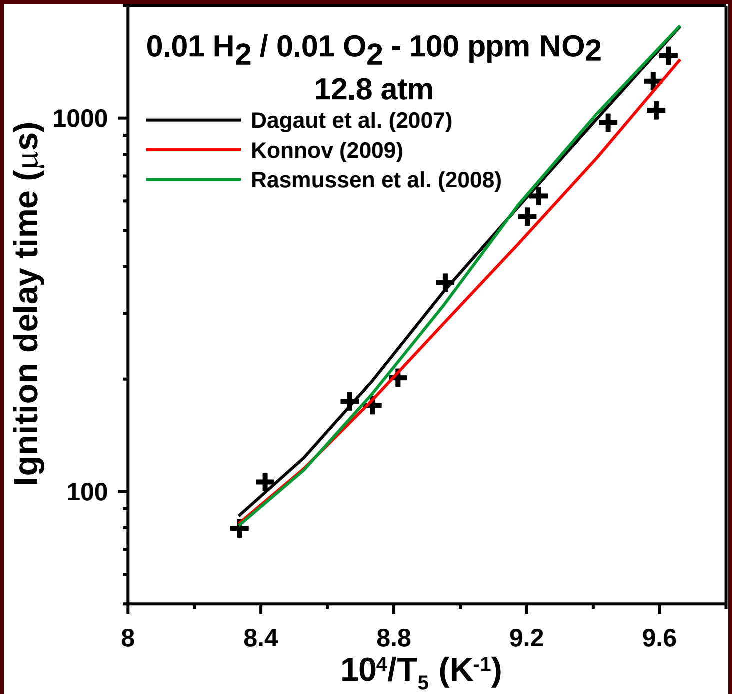
Task 4 – NOx Mechanism

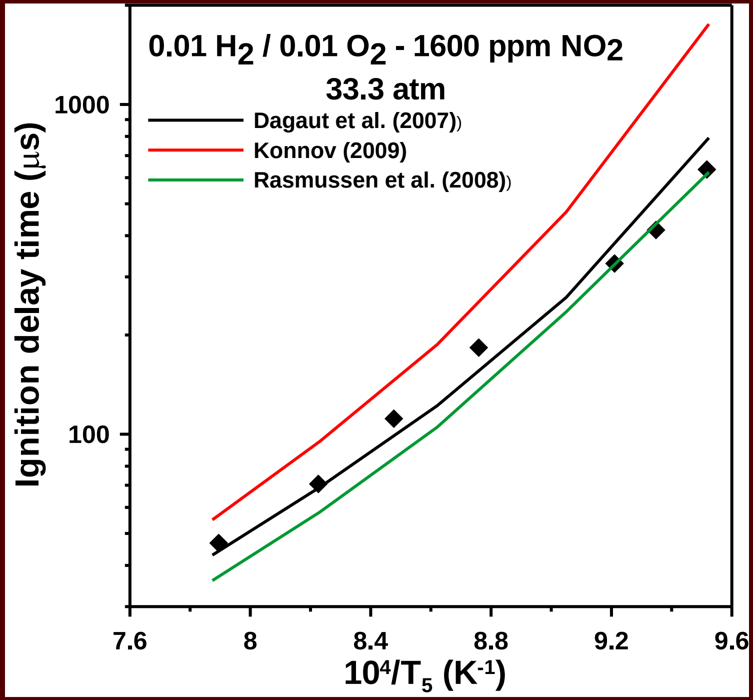
NO_2 mechanism selection

NOx mechanisms merged with the H_2/O_2 Mechanism:

- **Rasmussen, Glarborg *et al.*, 2008**
- **Konnov, 2009**
- **Dagaut, Brezinsky *et al.* (2006, 2007)**

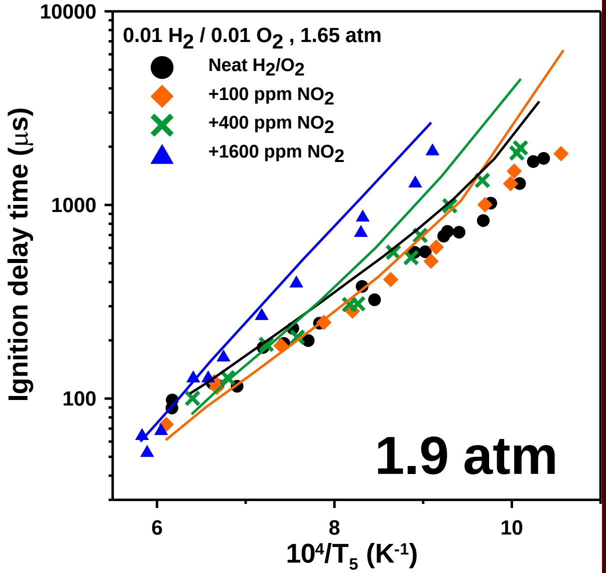
Updated $H_2 + NO_2 \rightleftarrows HONO + H$: Rate from Parks, Lin et al. (1998)

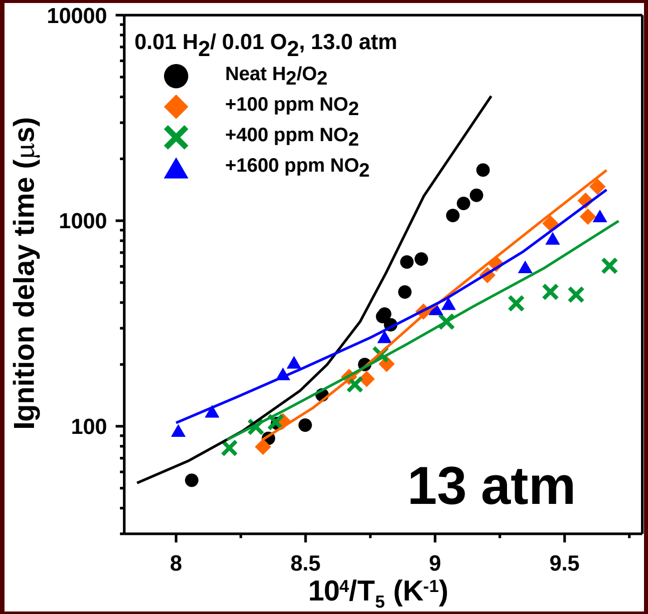


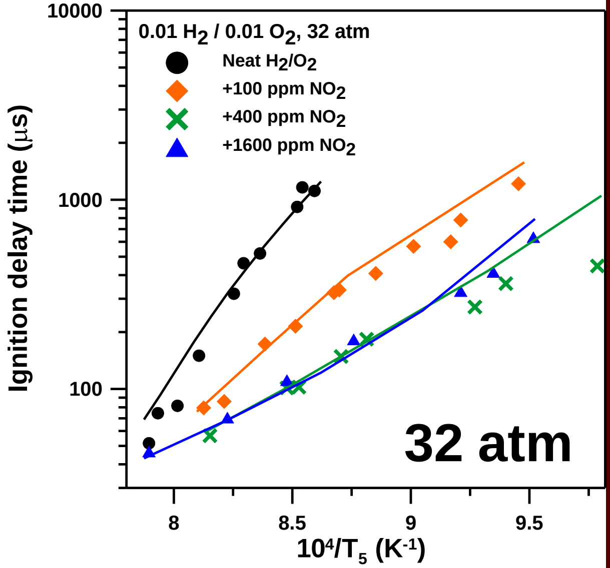


Task 4 – NOx Mechanism

NO_2 Mechanism Performs Well Over Range of Data





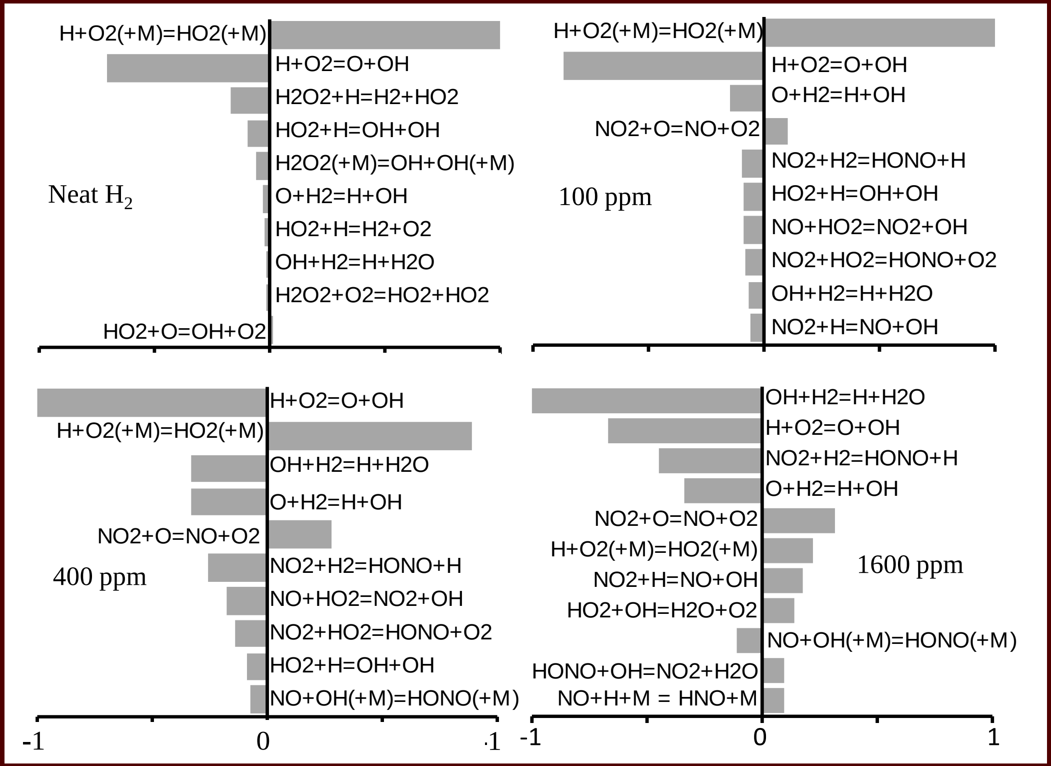


Good predictions against the new data

Task 4 – NOx Mechanism

Ignition Sensitivity Analyses for NO_2 Addition

13.5 atm,
1110 K



400-ppm NO_2 addition:

$H + O_2 \rightleftarrows O + OH$ (promoting)
$H + O_2 + H + M \rightleftarrows HO_2 + M$ (inhibiting)

$NO_2 + H_2 \rightleftarrows HONO + H$ more important => H production
$NO_2 + HO_2 \rightleftarrows HONO + O_2$

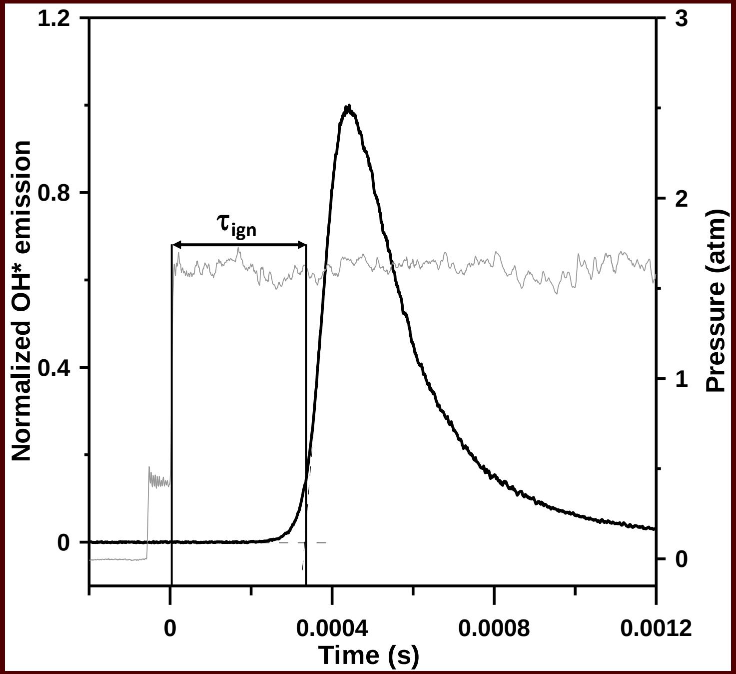
Then $HONO + M \rightleftarrows OH + NO + M$

Task 4 – NOx Mechanism

Ignition Delay Time from OH Emission*

- **Dilute conditions (98-97.84% Ar)**
- **Measurement at the sidewall location**
  - **307 ± 10 nm**

Mixture composition (mole fraction)	**T_5 (K)**	**P_5 (atm)**	**Reference**
0.01 H_2 / 0.01 O_2 / 0.98 Ar	960-1625	1.65 ± 0.15 atm	Keromnes et al.
	1085-1245	13.3 ± 1.0 atm	
	1160-1270	32.8 ± 1.5 atm	
0.01 H_2 / 0.01 O_2 / 0.0001 N_2O / 0.9799 Ar	950-1660	1.60 ± 0.17 atm	This study
	1090-1230	13.1 ± 0.3 atm	
	1150-1260	31.8 ± 1.1 atm	
0.01 H_2 / 0.01 O_2 / 0.0004 N_2O / 0.9796 Ar	940-1675	1.67 ± 0.25 atm	This study
	1075-1220	12.6 ± 0.8 atm	
	1145-1300	31.4 ± 1.0 atm	
0.01 H_2 / 0.01 O_2 / 0.0016 N_2O / 0.9784 Ar	950-1660	1.62 ± 0.20 atm	This study
	1080-1225	13.1 ± 0.6 atm	
	1125-1235	32.4 ± 1.0 atm	



Task 4 – NOx Mechanism

*Effect the N_2O concentration at around **1.7 atm***

No discernible effect of 100 ppm N_2O addition

Above 100ppm: N_2O additions ↘ τ_{ign} at high temperatures

@1650 K: τ_{ign} = 95 µs for neat H_2 and 45 µs with 1600 ppm N_2O

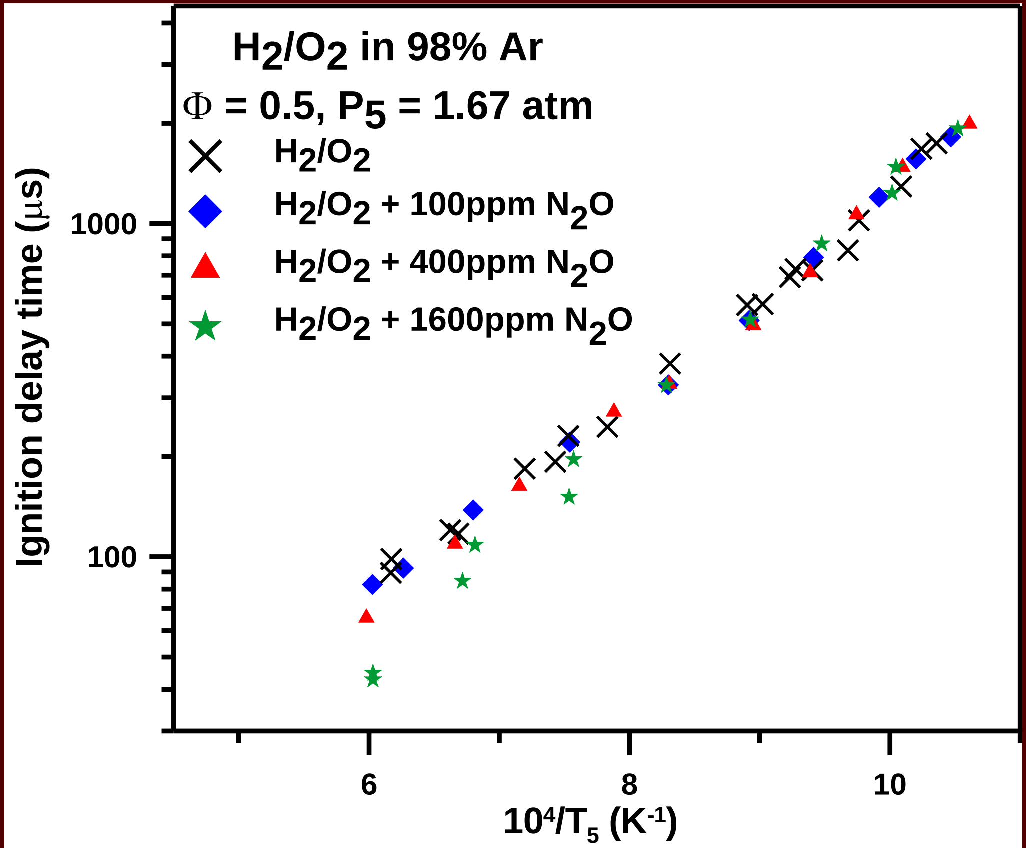
N_2O additions induced a change in the apparent activation energy (Ea): Ea ↗ with $[N_2O]$

57 kJ/mol for the neat H_2/O_2 mixture,

58 kJ/mol with 100ppm N_2O,

60.8 kJ/mol with 400 ppm N_2O,

69.5 kJ/mol with 1600 ppm N_2O.



Task 4 – NOx Mechanism

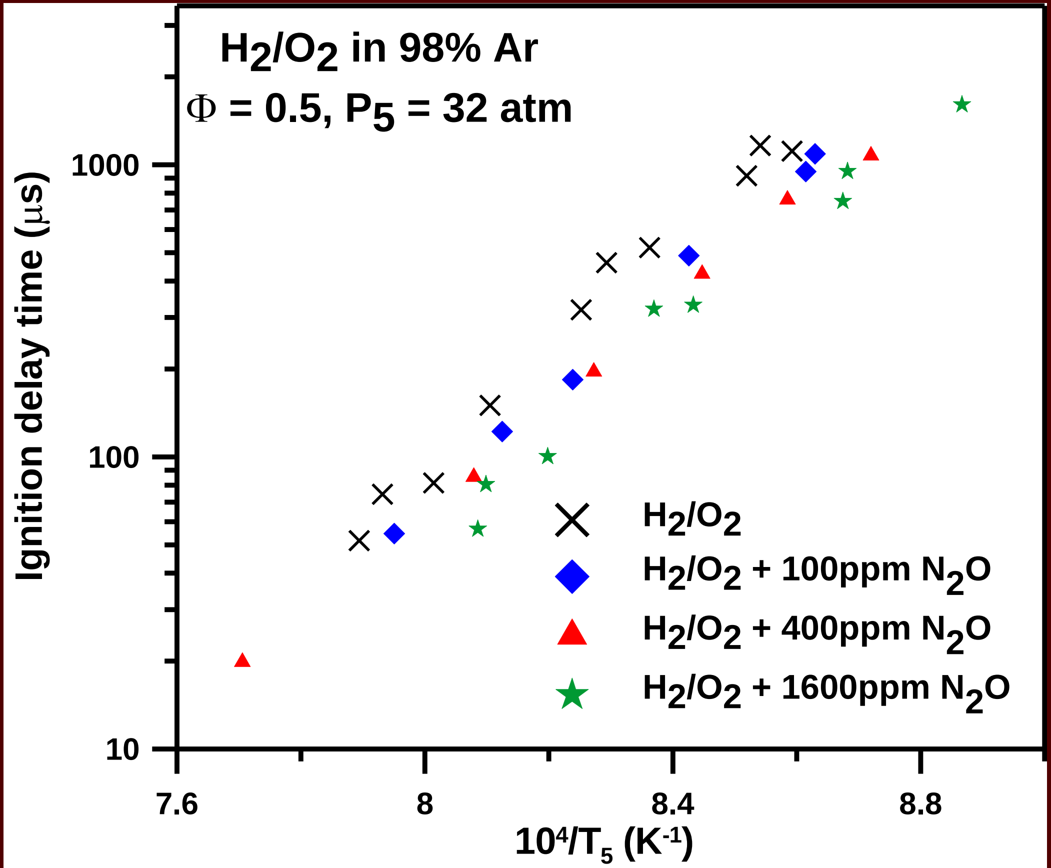
*Effect the N_2O concentration at around **32 atm***

N_2O additions: ➘ τ_{ign} on the whole range of temperatures

@ 1235 K: τ_{ign} =

- **150 μs for neat H_2,**
- **114 μs with 100 ppm N_2O,**
- **98 μs with 400 ppm N_2O,**
- **58 μs with 1600 ppm N_2O.**

No significant change in Ea



Task 4 – NOx Mechanism

N_2O Mechanism Selected from Mevel et al.

Several NOx mechanism merged with the H_2/O_2 Mechanism:

ICARE1: Mevel *et al.* (Proceed. Combust. Inst. 32 (2009) 359–366)

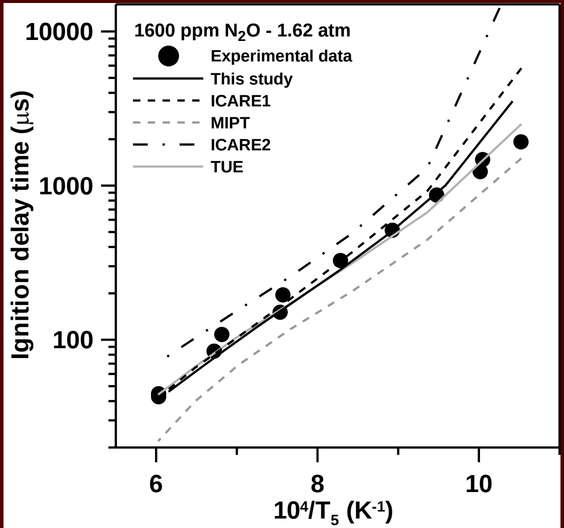
with different reaction rates from Literature for:

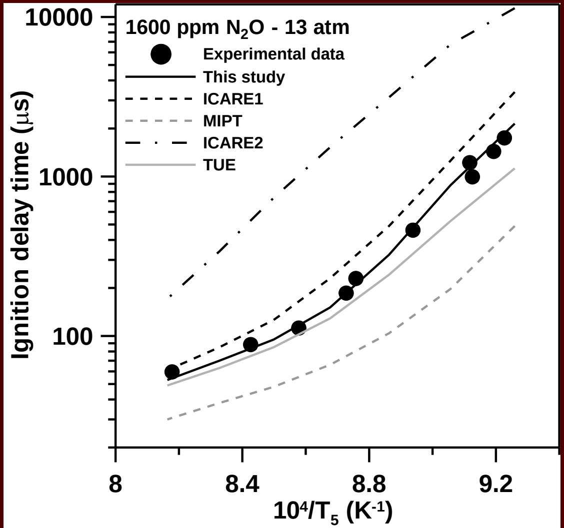
- **$N_2O + M \rightleftarrows N_2 + O + M$**
- **$N_2O + H \rightleftarrows N_2 + OH$**

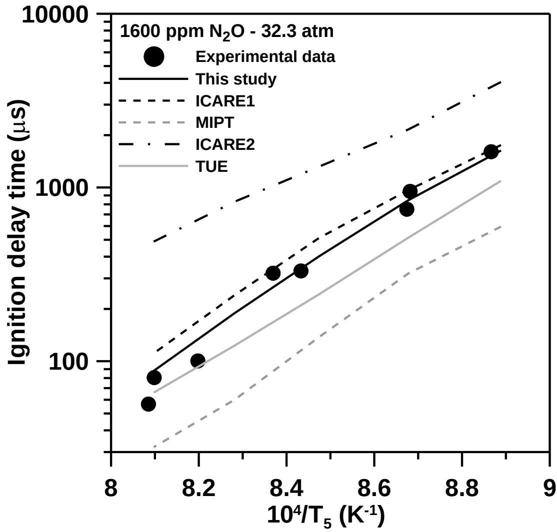
ICARE2: Dayma and Dagaut (2006)4)

MIPT: Kosarev *et al.* (2007)

TUE: Konnov (2009)



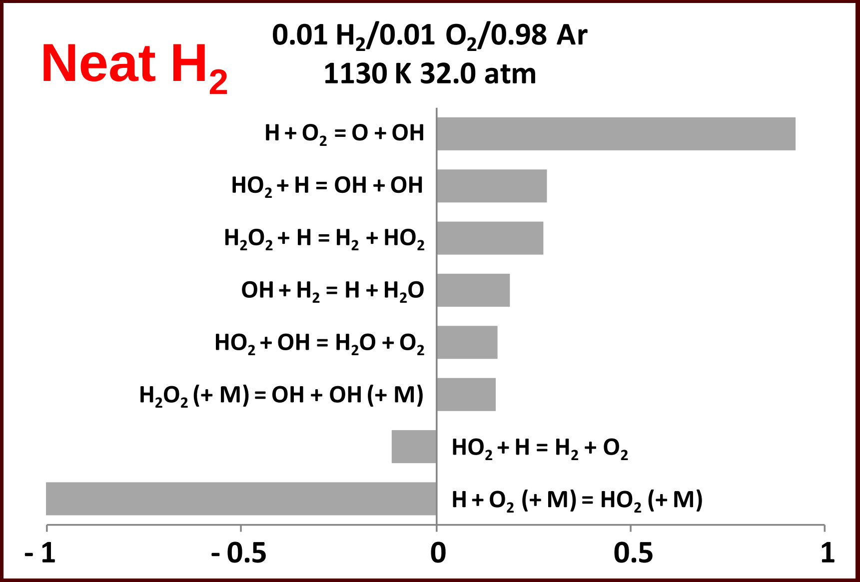




Good predictions against the new data

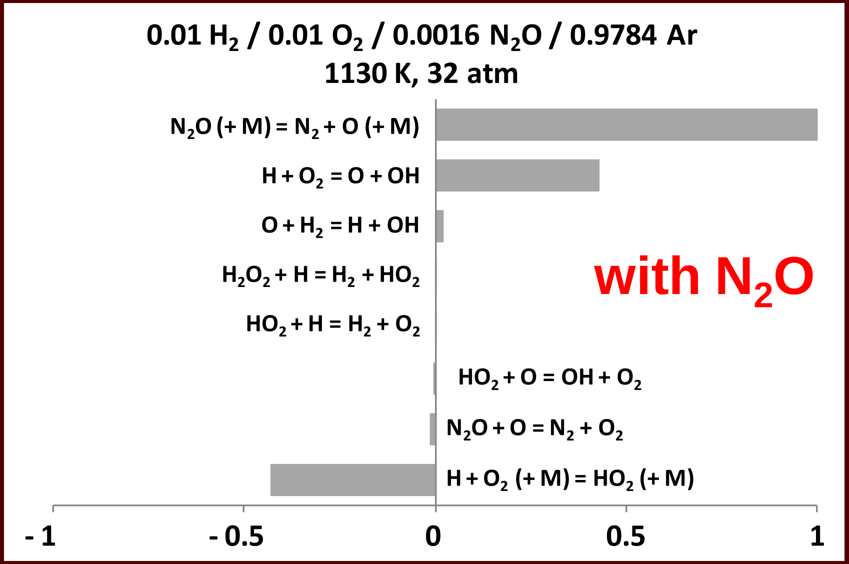
Task 4 – NOx Mechanism

Sensitivity analyses for N_2O-Based Experiments



Neat H_2

0.01 H_2/0.01 O_2/0.98 Ar
1130 K 32.0 atm



0.01 H_2 / 0.01 O_2 / 0.0016 N_2O / 0.9784 Ar
1130 K, 32 atm

with N_2O

- **Neat H_2:**
  $H + O_2 + M \rightleftarrows HO_2 + M$ followed by $H + O_2 \rightleftarrows O + OH$ (promoting) .

- **1600 ppm N_2O addition:**
  $N_2O + M \rightleftarrows N_2 + O + M$ most sensitive reaction

The O-atoms released via $N_2O + M \rightleftarrows N_2 + O + M$ will react through $O + H_2 = H + OH$ and then promote the overall reactivity.

Task 4 – NOx Mechanism

This Task is Nearly Complete

- Additional Work on NH_3 Performed (not shown)
- Compile Overall NOx Mechanism Based on NO_2, N_2O, NH_3 Results

Task 6 – Effect of Impurities on Syngas Kinetics

Task 6 – Impurities

Trace Impurities are Being Studied

- Trace Species (H_2S, NH_3, HCN, NOx, HC fuel, other?)
- Laminar Flame Speeds Using Established Methods
- Dilute Shock-Tube Experiments (Ignition and Time Histories)
- Pertinent Mixtures of Interest to Industry

Task 6 – Impurities

- **Baseline mixtures:**
  - Neat H_2 ($H_2/O_2/Ar$)
  - Baseline syngas (BS), with H_2/CO = 1
- **Addition of components/impurities found in biomass-derived syngas to BS:** BS-CO_2, -H_2O, -CH_4 and -NH_3
- **Study of a mixture representing an average Biomass-derived syngas** (Biosyn and Biosyn-NH_3)
- **3 pressures:** 1.7, 13.0 and 32 atm
- Φ = 0.5

Mixture name	% H_2	% CO	% O_2	% CH_4	% CO_2	% H_2O	% NH_3	% Ar
Neat H_2	1.0	0.0	1.0	0.0	0.0	0.0	0.0	98.0
BS	0.5	0.5	1.0	0.0	0.0	0.0	0.0	98.0
BS-CH_4	0.406	0.406	1.113	0.075	0.0	0.0	0.0	98.0
BS-CO_2	0.46	0.46	0.93	0.0	0.15	0.0	0.0	98.0
BS-H_2O	0.444	0.444	0.889	0.0	0.0	0.223	0.0	98.0
BS-NH_3	0.5	0.5	1.0	0.0	0.0	0.0	0.02	97.98
Biosyn	0.29659	0.29659	0.95013	0.08924	0.15748	0.20997	0.0	98.0
Biosyn-NH_3	0.29659	0.29659	0.95013	0.08924	0.15748	0.20997	0.02	97.98

Composition averaged from 23 bio-syngas

Task 6 – Impurities

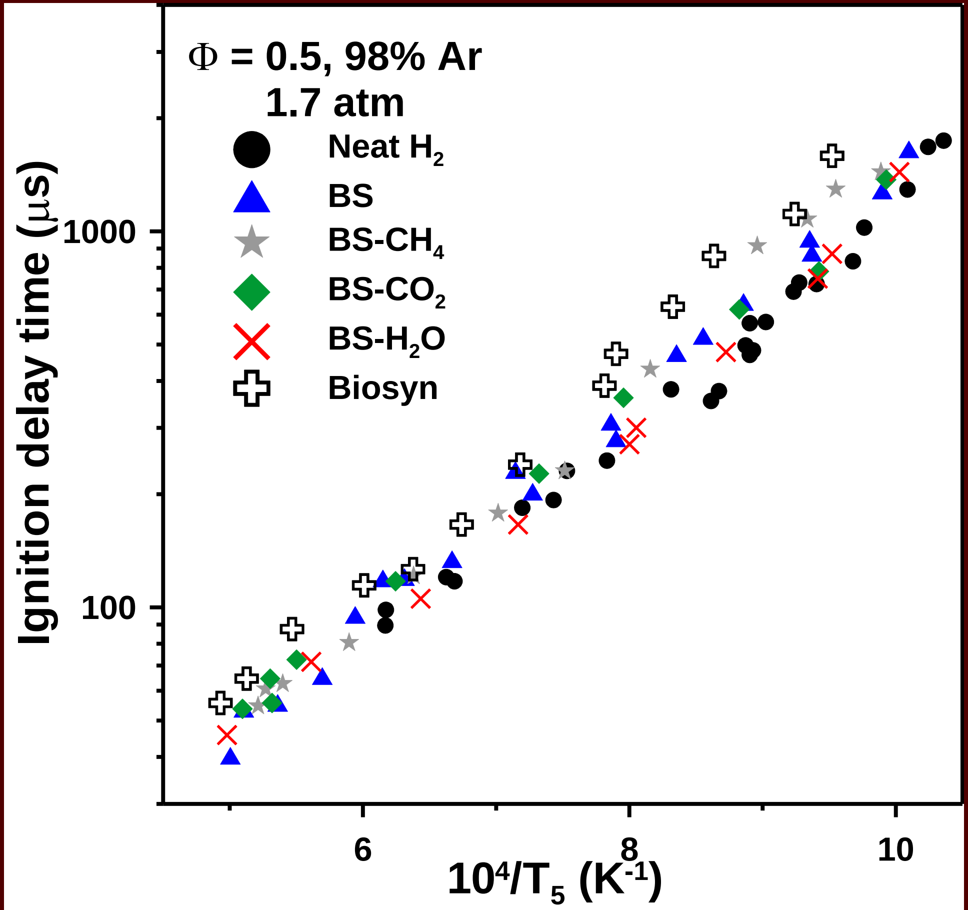
*Syngas composition effect at around **1.7 atm***

Small differences between Neat H_2 and BS

Compared to BS:

- **No effect of CO_2 addition**
- **H_2O seems to slightly ↘ τ_{ign}**
- **CH_4 ↗ τ_{ign}, mostly at LT**

Difference can be relatively important between BS and Biosyn

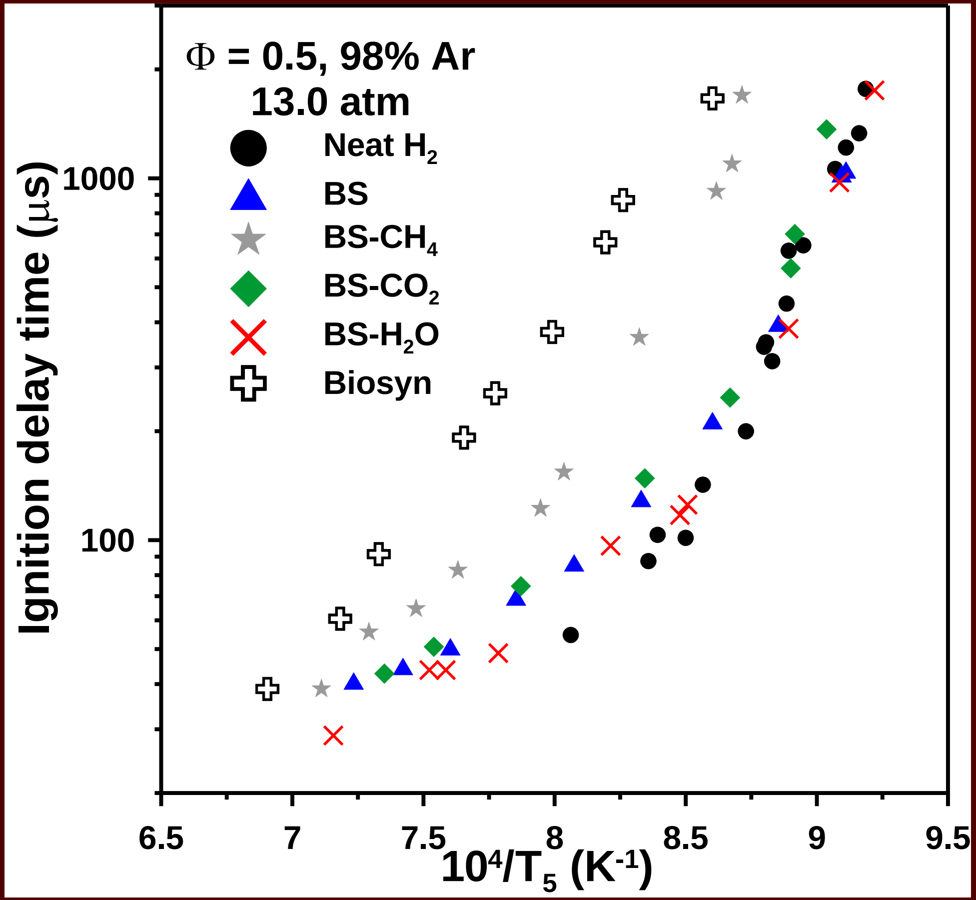


Task 6 – Impurities

*Syngas composition effect at around **13 atm***

- Longer τ_{ign} for BS at HT compared to Neat H_2
- No discernible effect of CO_2 addition
- Slight ↘ in τ_{ign} with H_2O addition
- Very important effect of CH_4 addition (BS-CH_4, Biosyn)

Large differences in τ_{ign} between BS and Biosyn



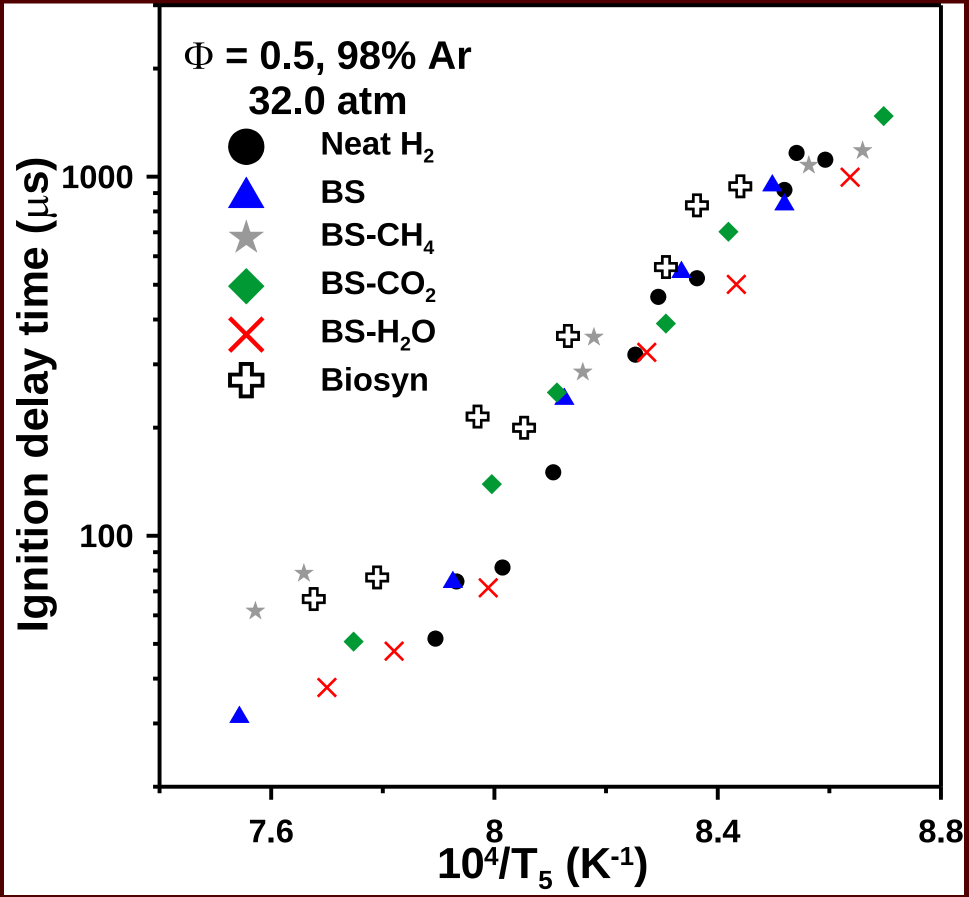
Task 6 – Impurities

*Syngas composition effect at around **32 atm***

Composition effect relatively weak at 32 atm

Most of the effects visible on HT side

Effects similar to lower pressure conditions (↗ in τ_{ign} when CH_4 is added)



Task 6 – Impurities

Pressure and NH_3 effects

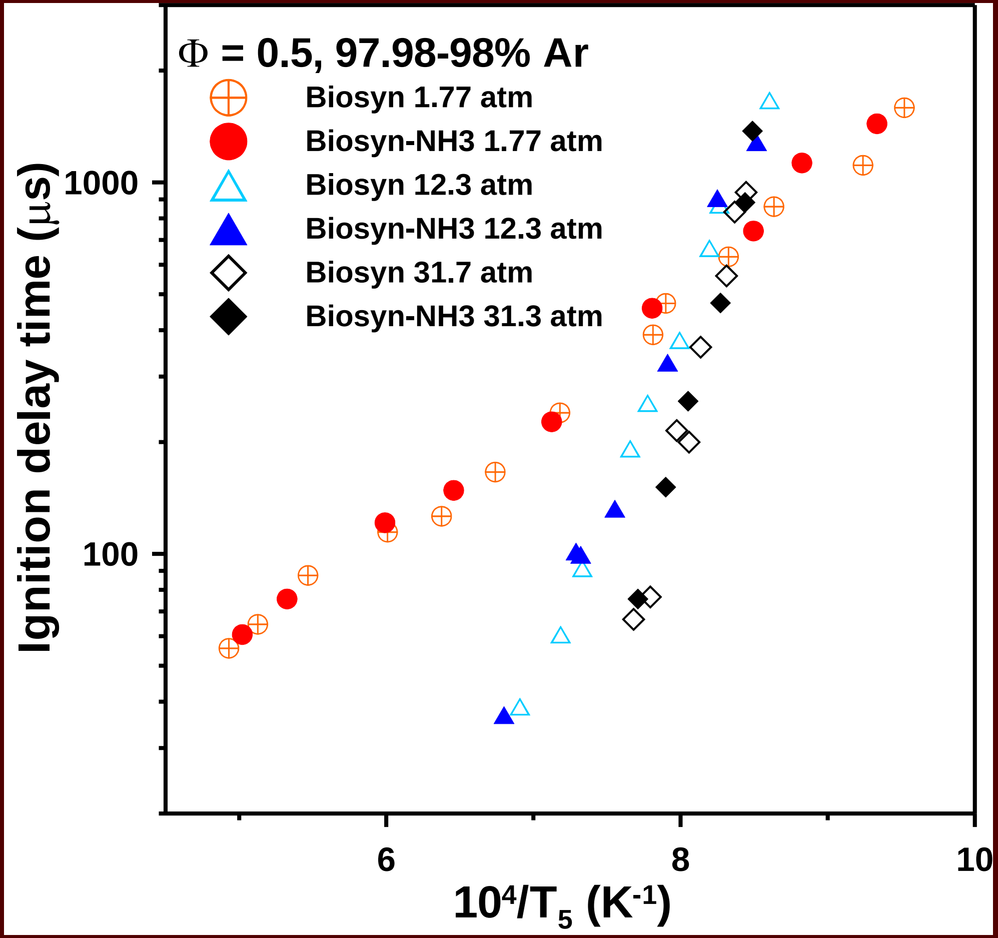
Important effect of pressure, due to H_2/O_2 chemistry

Competition between:

$H + O_2 = O + OH$ (R1) => HT/LP

$H + O_2 + M = HO_2 + M$ (R2) => LT/HP

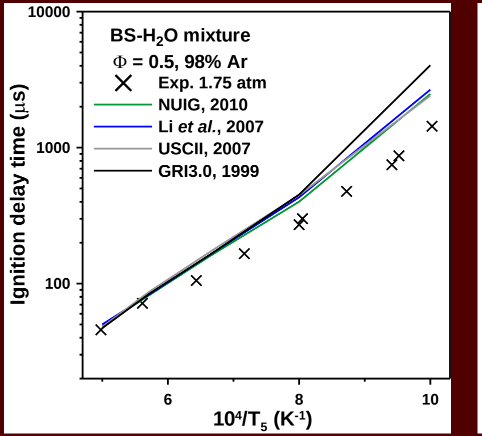
No appreciable effect of NH_3 for Biosyn

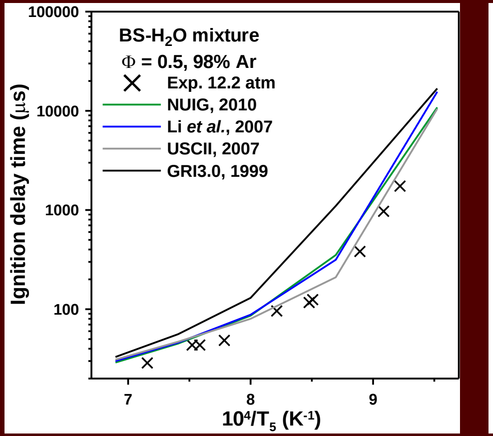


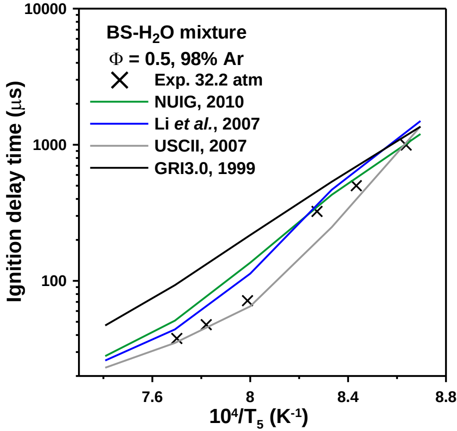
Task 6 – Impurities

Various mechanisms tested against our results

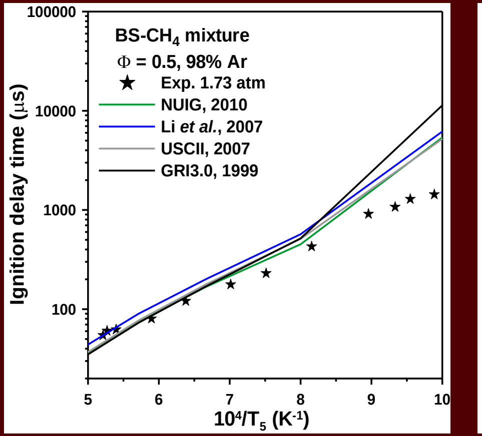
GRI 3.0, 1999 / USC II, 2007 / Li, Dryer *et al., 2007* / Galway, 2010.

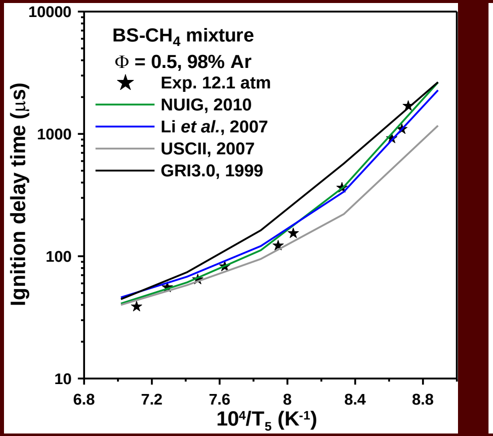


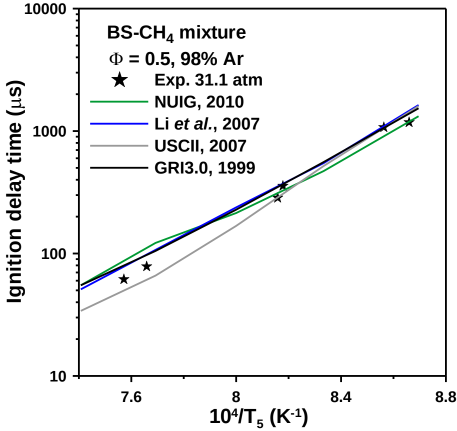




$H_2/CO/H_2O$





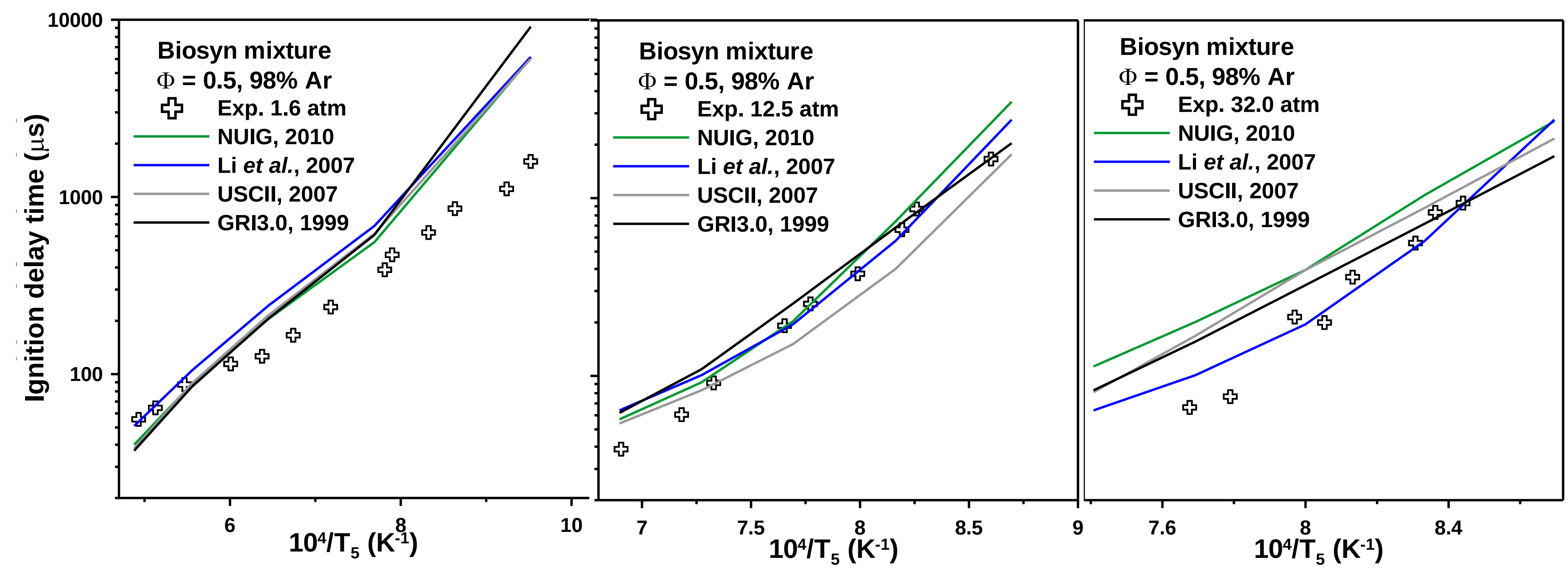


$H_2/CO/CH_4$

Task 6 – Impurities

Various mechanisms tested against our results

$H_2/CO/CO_2/H_2O/CH_4$

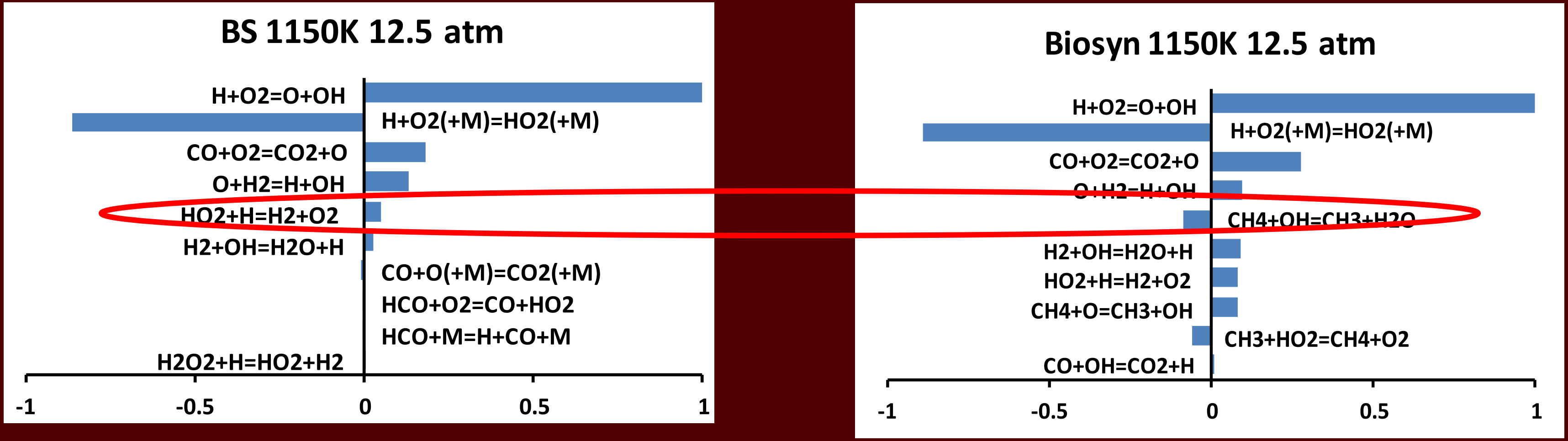


Overall, NUIG and Li *et al.* mechanisms offer the best predictions.

Task 6 – Impurities

Chemical Analysis Shows Impact of CH_4

Investigation on the effect of CH_4 addition: sensitivity analysis on OH* at 1150K, 12.5 atm



Between BS and Biosyn, only one reaction is different :

$CH_4 + OH \rightleftarrows CH_3 + H_2O$

Then reactions of smaller importance:

$CH_4 + O \rightleftarrows CH_3 + OH$**, partly compensated by** $CH_3 + HO_2 \rightleftarrows CH_4 + O_2$

Overall, inhibiting effect of CH_4, mostly via $CH_4 + OH \rightleftarrows CH_3 + H_2O$

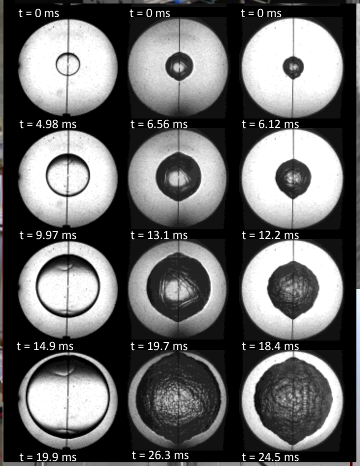
Summary

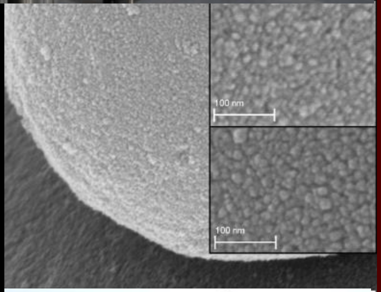
Progress Through 2^{nd} Year Has Been Covered

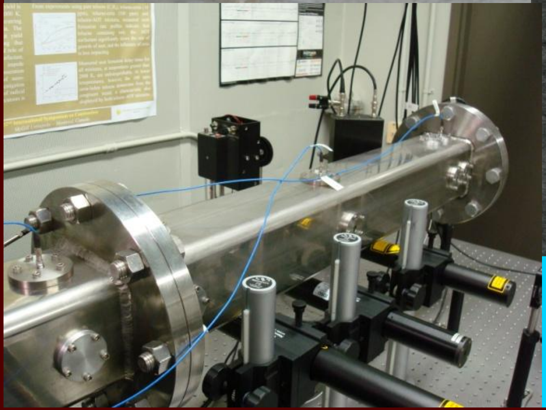
Work Tasks:

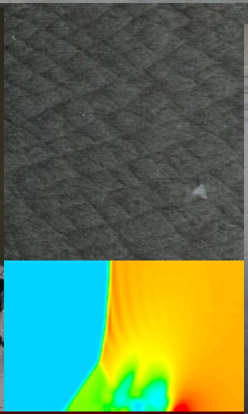
- **Task 1** – Project Management and Program Planning
- **Task 2** – Turbulent Flame Speed Measurements
- **Task 3** – Laminar Flame Speeds with Diluents
- **Task 4** – NOx Mechanism Validation Experiments
- **Task 5** – Fundamental NOx Kinetics
- **Task 6** – Effect of Impurities on Syngas Kinetics

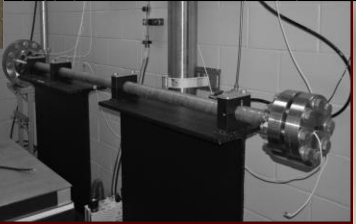
Petersen Group Research

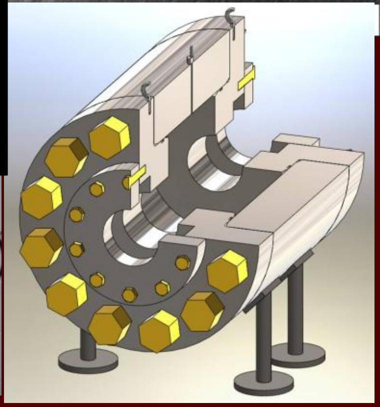












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