Ammonia Combustion with Near-Zero Pollutant Emissions

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Supported by the Iowa Energy Center

Motivation for NH_3

Why use NH_3 for heating and power when cheap natural gas is available?

- 60% of the Northeast U.S. heated with fuel oil
- NH_3 for remote heating and power
  (to replace propane on farms, mountain/rural communities, cell towers, etc.)
- NH_3 can be used to sequester CO_2 and makes more sense to transport than natural gas
- NH_3 can come from fossil fuels, biomass, wind, nuclear, etc.
- High thermal efficiency of gas turbines, professional users

Challenges

- NH_3 is technically non-flammable (in liquid form), has high auto-ignition temp (630 C), and low reactivity.
  (Flame speed of NH_3 ~ 6-8 cm/s, CH_4 ~ 40 cm/s, H_2 ~ 140-150 cm/s)

- NH_3 is a source of NO_x in flames.

- NH_3 is a potential contaminant, especially for marine life (e.g., 97% efficiency may not be enough)

- Modern challenge is near-zero pollutant emissions
  (actually an advantage for NH_3 if CO_2 is a pollutant)

Scope and Objectives

Ammonia swirl-stabilized flame study (40 KW)

- H_2/NH_3, CH_4/NH_3 mixtures
- Strategies for 100% NH_3 combustion & low emissions

Study of NH3 Chemistry

- Flame speed analysis
- Flame structure
- NO chemistry

Swirl-Stabilized Turbulent Flame

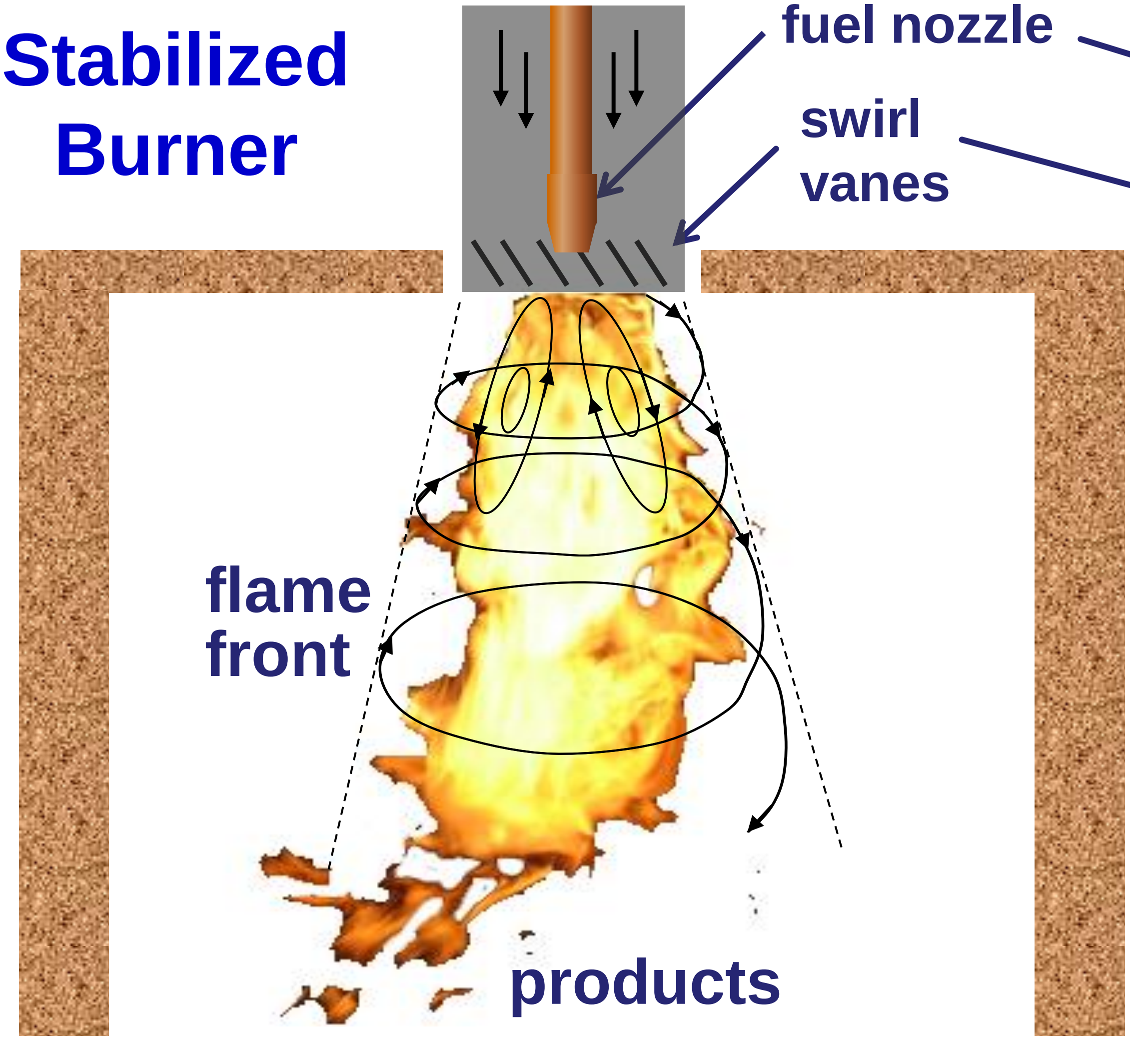
Domestic Oil Heating Furnace (40 KW)

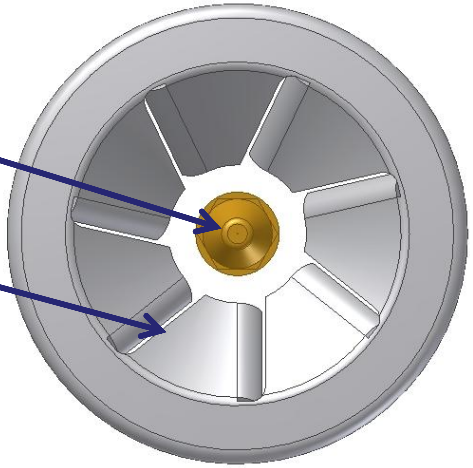
- Dimensions & heating capacity
- Equipped with thermocouple & pressure transducers.
- Custom built swirl-plate stabilizer.
- Easily movable fuel nozzle.
- Laser diagnostics accessible flame.
- Exhaust section: Chilled water-line & Sampling Locations with a optical accessible window.

- **Key feature**: Self-sustained Heat Exchanger.

Experimental Set-Up

Swirl-Stabilized Burner



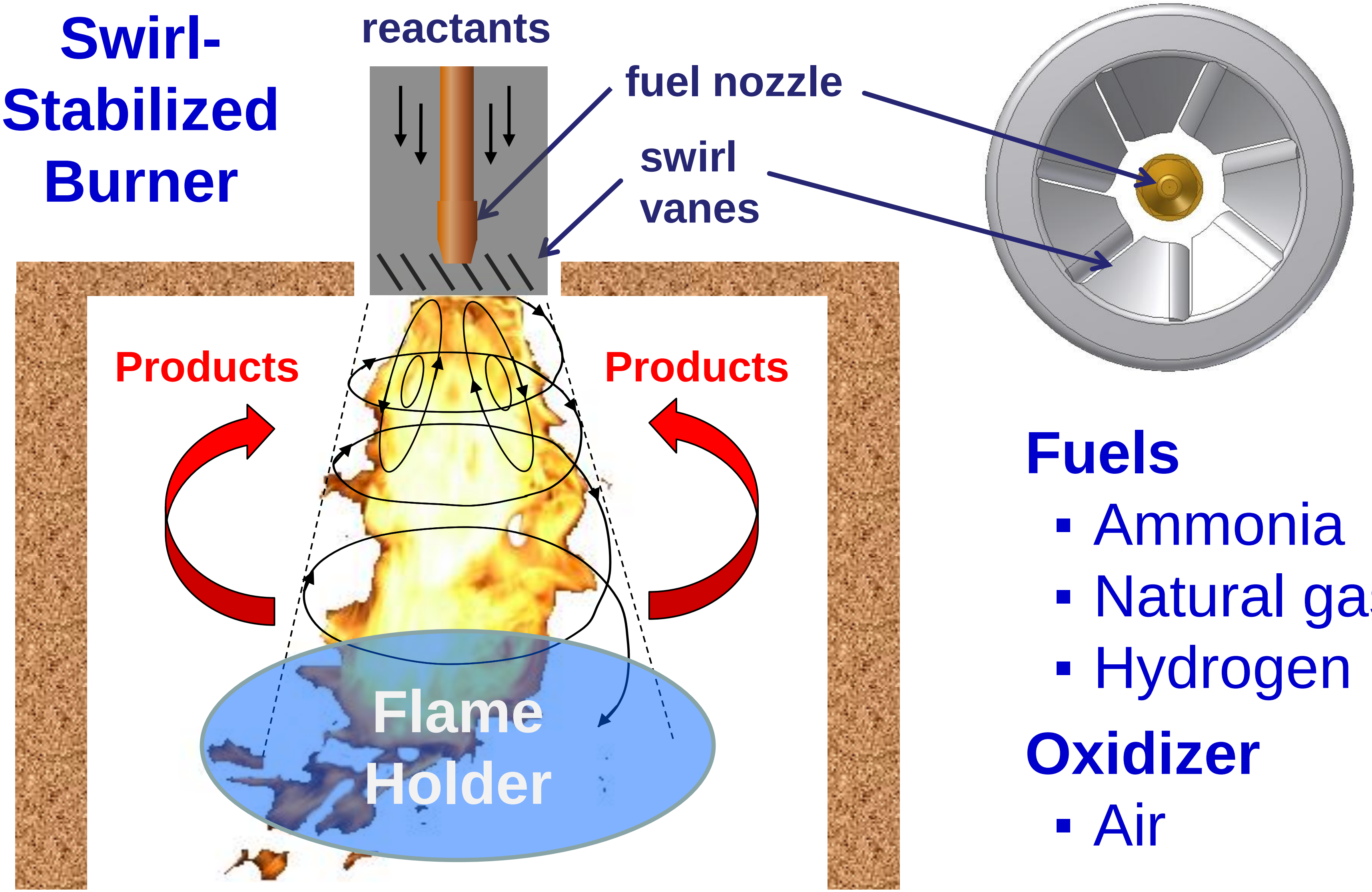


Fuels
- Ammonia
- Natural gas
- Hydrogen

Oxidizer
- Air

Combustion Optimization

Swirl-Stabilized Burner



Fuels
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Oxidizer
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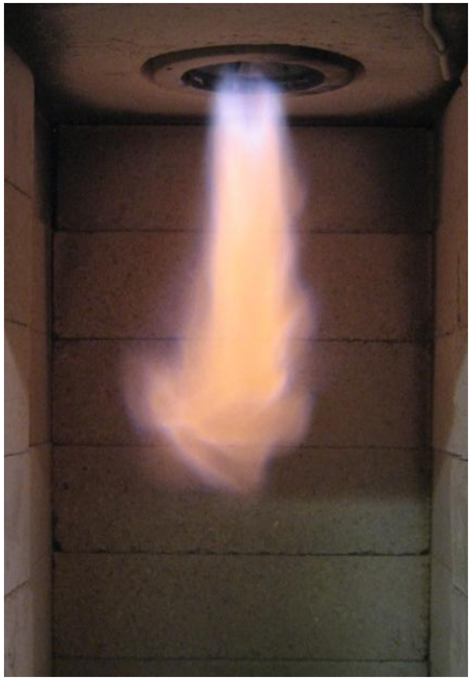
Flame Comparisons

Fuel Oil (28 kW)

60% NH_3 by Energy in H_2 (15 KW)

34% NH_3 by Energy in CH_4 (5 kW)



Experimental Procedure

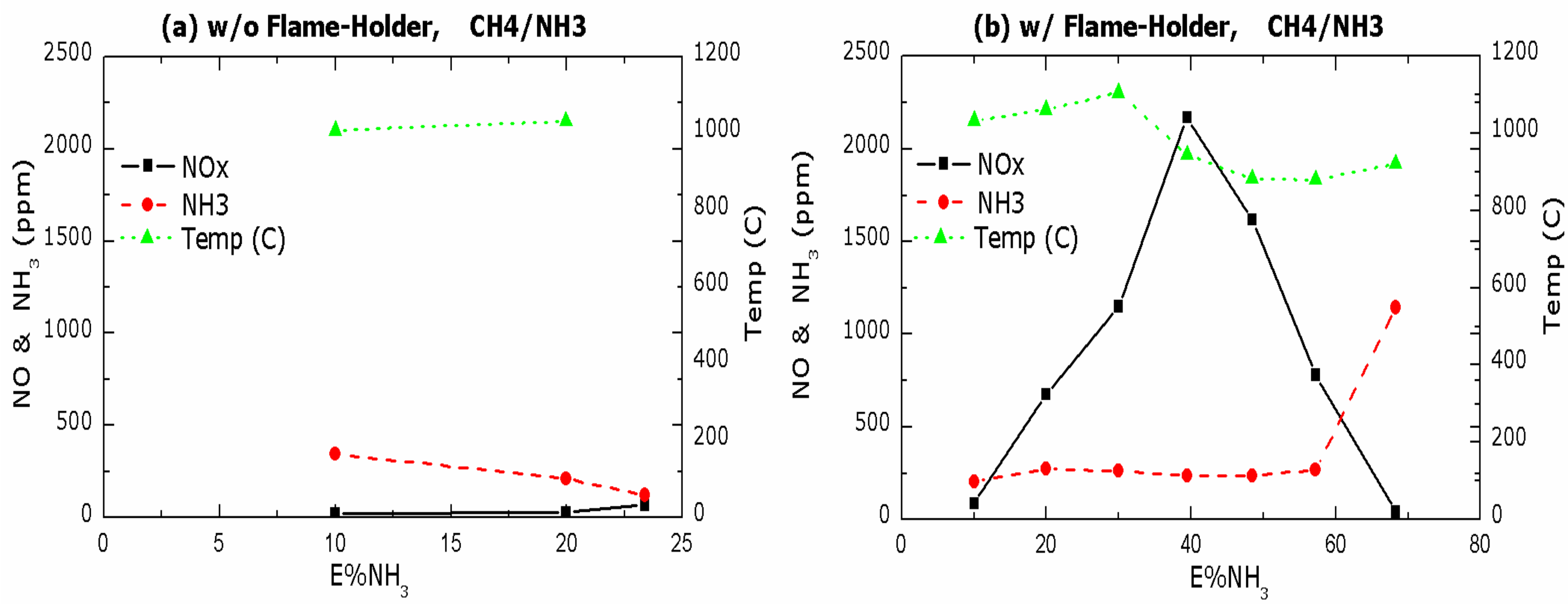
Study of Natural Gas (CH_4) and Hydrogen (H_2) Replacement by NH_3

Effects of:

1. Preheated Air Temperature
2. Equivalence Ratio
3. Heat-Rate
4. Different Fuel Nozzle Positions
5. Swirl Geometries
6. Burner Configurations

Results: CH_4/NH_3 Fuel mixture

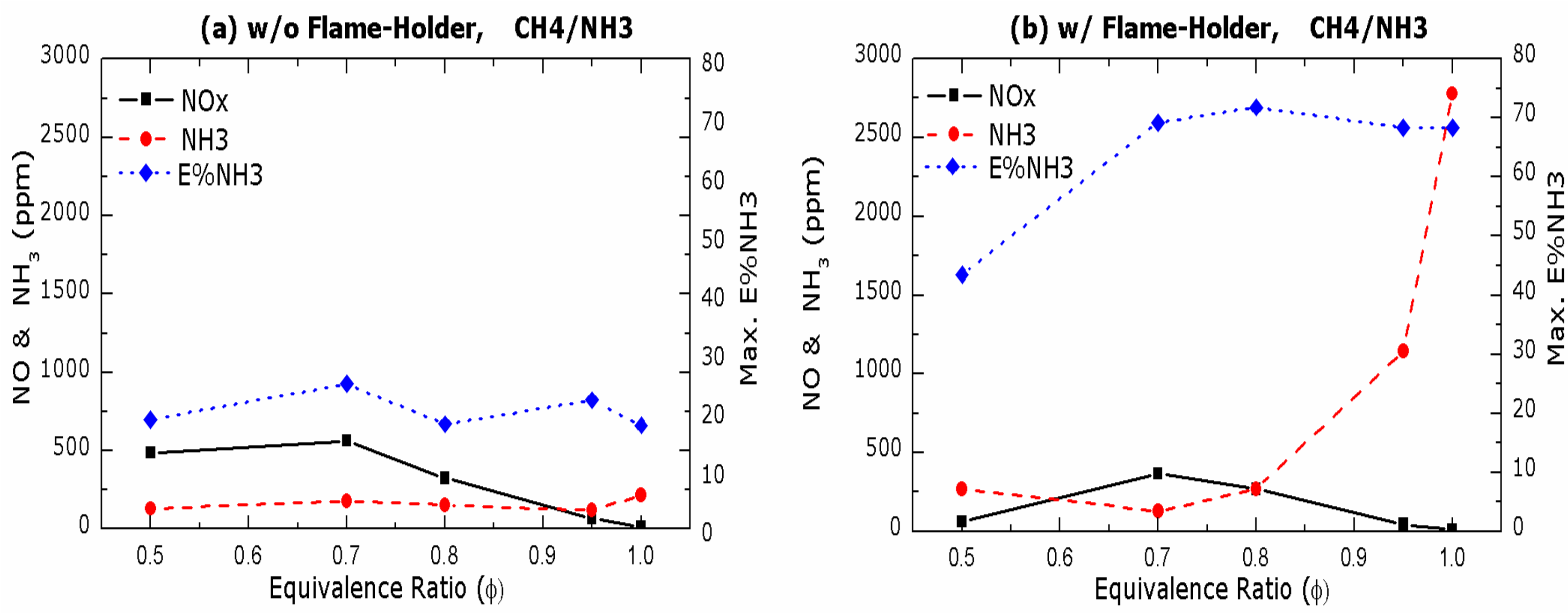
CH_4/NH_3/Air @ T_{air} = 300 C & Phi = 0.95, HR ~ 16 KW



NH_3 limited without a flame holder, but emissions sensitive to flame holder.

Results: CH_4/NH_3 Fuel mixture

CH_4/NH_3/Air @ T_{air} = 300 C, Q_total ~ 560 slpm, HR ~ 16 KW



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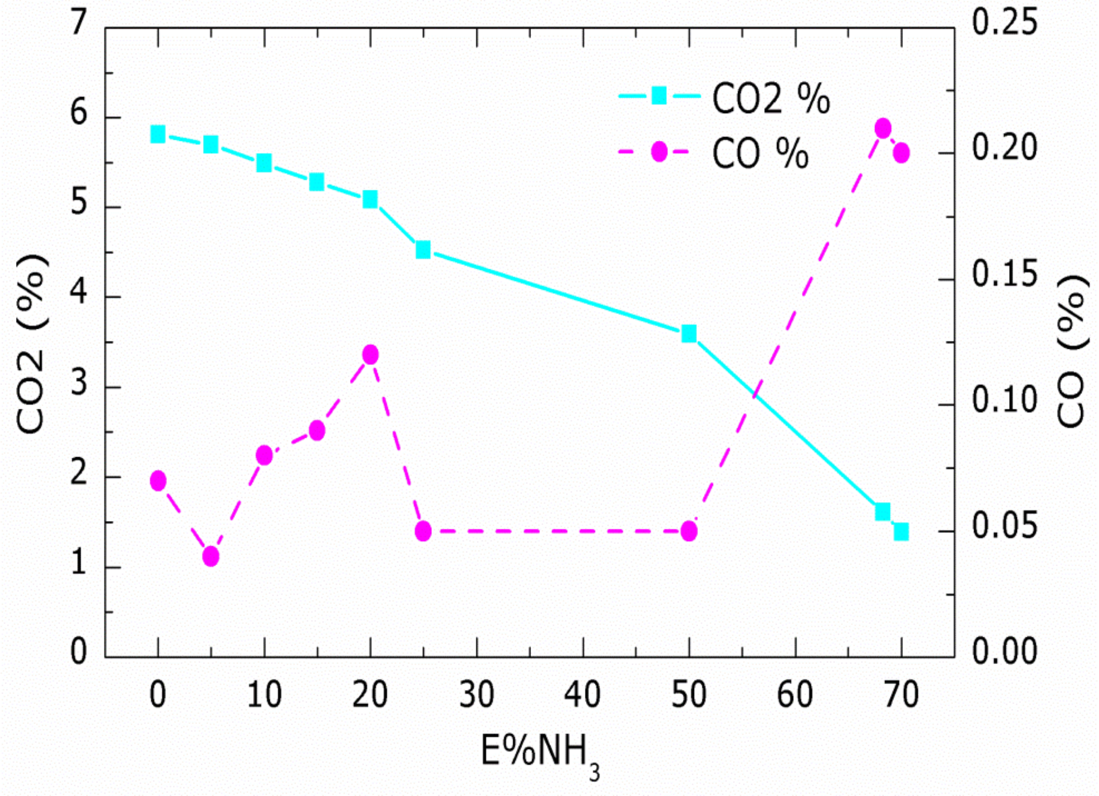
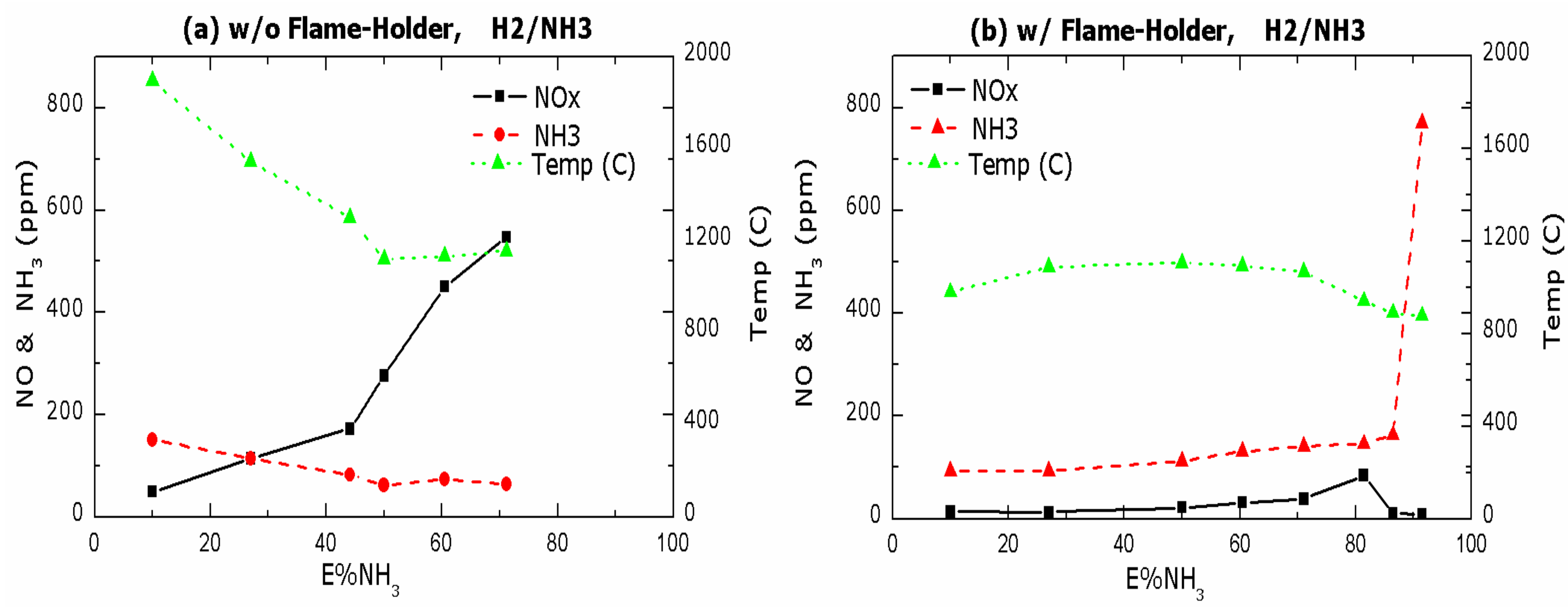


H_2/NH_3 Fuel mixture

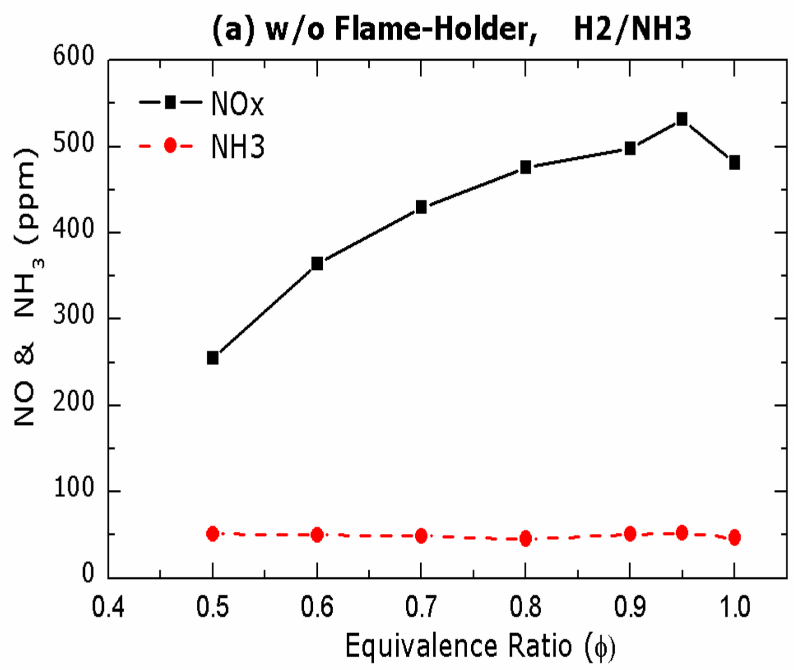
H_2/NH_3/Air @ T_{air} = 300 C & Phi = 0.95, HR ~ 15 KW

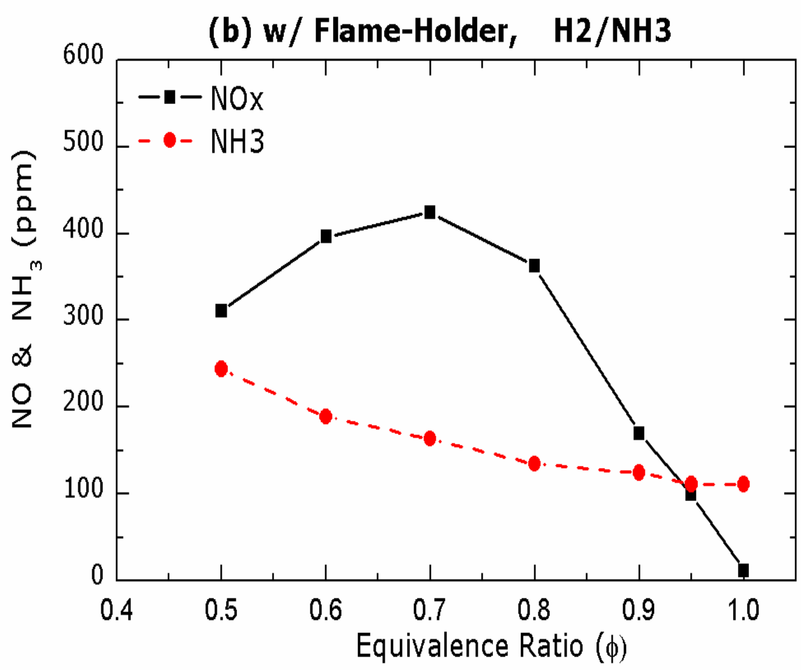


- Uniform temperature & low NO_x with Flame-Holder.

H_2/NH_3 Fuel mixture

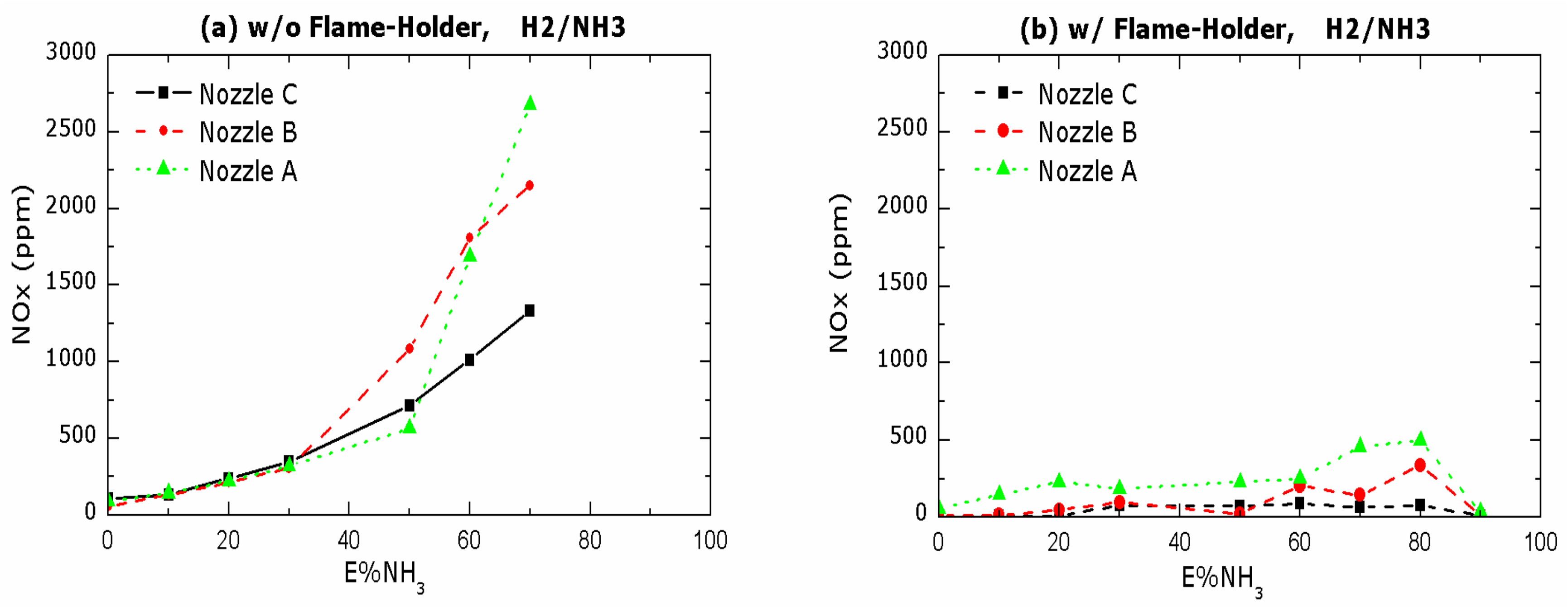
H_2/NH_3/Air, T_{air} = 300 C , Q_total ~ 300 slpm, E%NH_3 ~ 50





Effect of Nozzle Position

H_2/NH_3/Air, T_{air} = 300 C , Q_total ~300 slpm, Equiv Ratio ~ 0.95



Reference condition “C” used for all tests

100% NH3 Combustion?

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- Redesigned fuel nozzle
- E%NH_3 = 100
- Inlet Air 25 C
- Equiv Ratio ~ 0.95
- Heat Rate ~ 16.15 KW
- NO_x < 3-5 ppm (Ultra Low)
- NH_3 ~ 800 - 1300 ppm
  (99.9% combustion efficiency)

What have we learned thus far?

- Yes 100% NH_3 combustion is feasible
- Yes low emissions are feasible
- Maybe ultralow emissions are feasible
- All depends on the combustor design

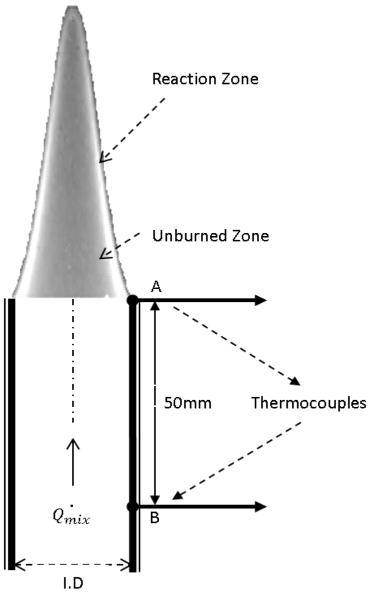
What's needed ?

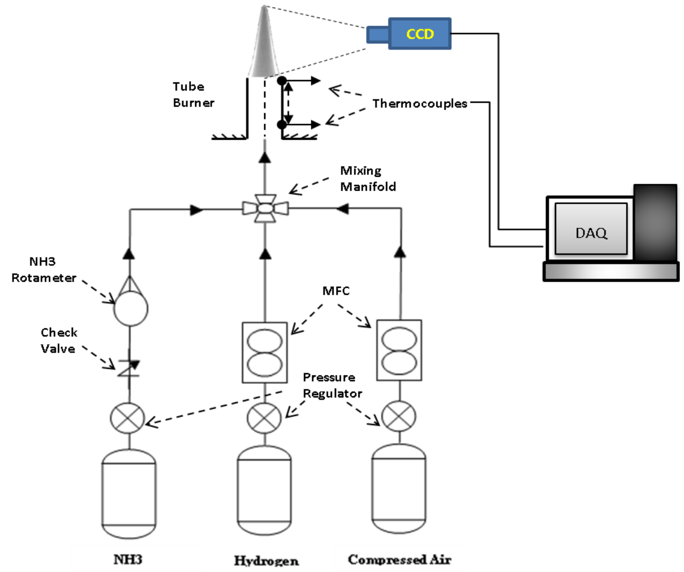
- Predictive modeling tools (next study)
- Optimization of cracking and catalytic reduction (future work)

Chemical Kinetics Mechanisms

- Miller and Bowman – 19 species and 73 reactions
- Lindstedt – 22 species, 97 reactions
- GRI-Mech3.0 – 53 species and 325 reactions
- Tian – 84 species and 703 reactions
- Konnov – 127 species and 1207 reactions
- Konnov (without C) 31 species 241 reactions

Experimental setup

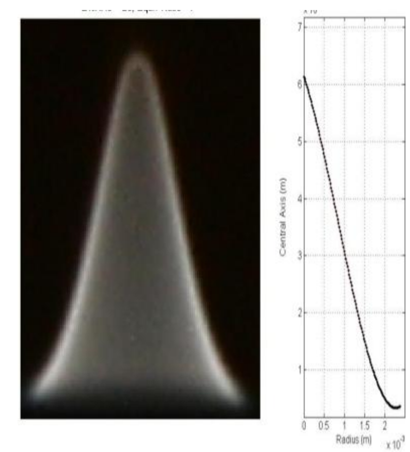




Equiv ratio (Ø)
0.5 – 1.1

E%NH_3	$\dot{Q}_{mix}$ $(slpm)$	I.D (mm)
0	12	4.65
20	2	4.65
50	2	4.65
80	2	11.11

Average of 25 pictures



E%NH_3 = 20 at Ø = 1.0, for H_2-NH_3-Air

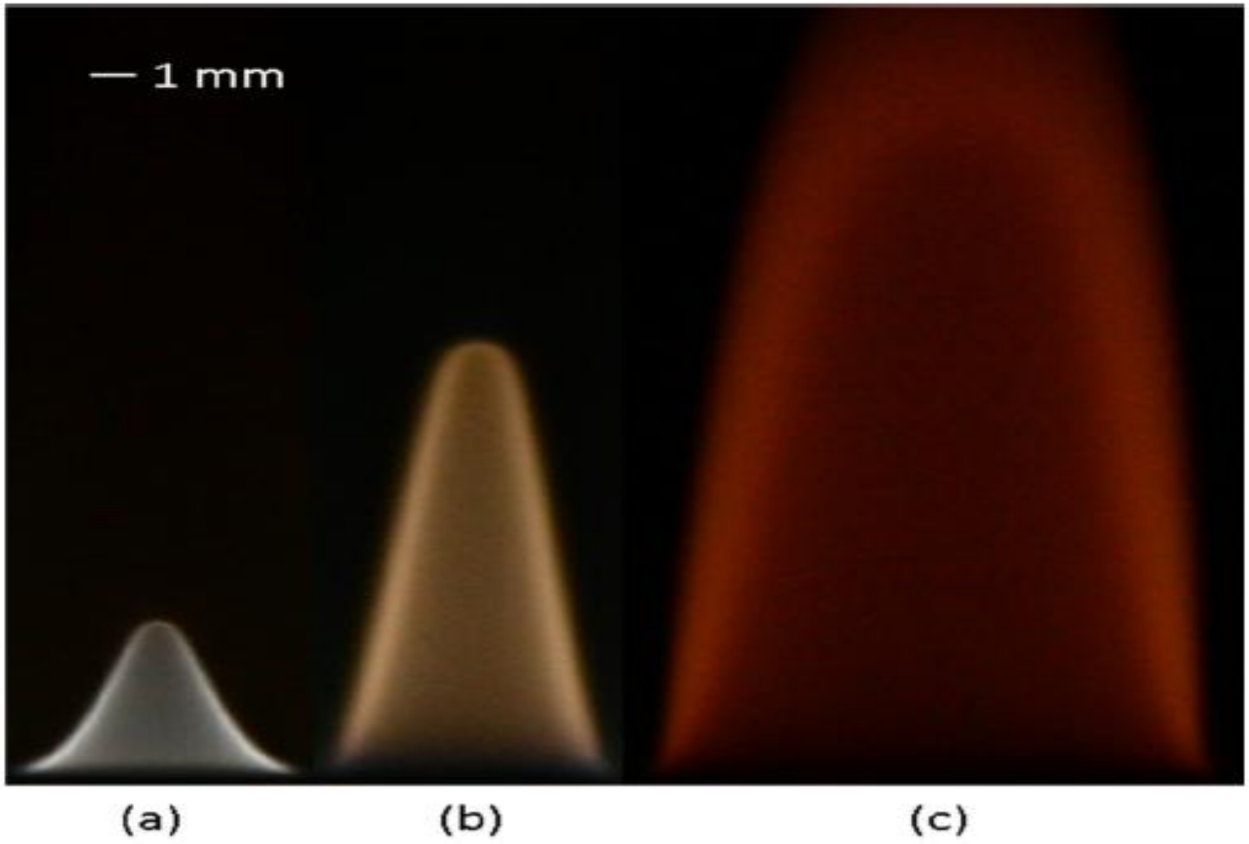
At each condition;

- Flame speed is measured.

$$S_l = \frac{\dot{Q}_{mix}}{A_{flame}}$$

- Heat loss ($\dot{Q}_{heat\ loss}$) to the tubing is estimated.

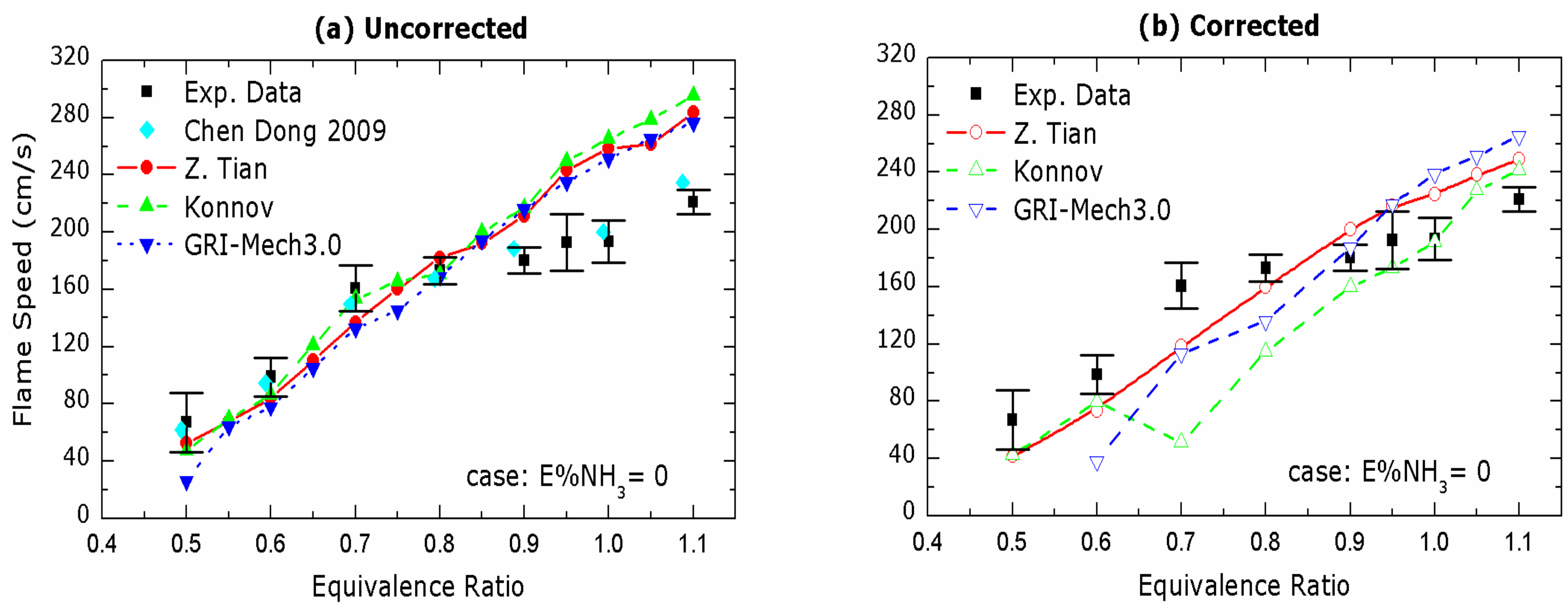
E%NH_3 : 20% 50% 80%



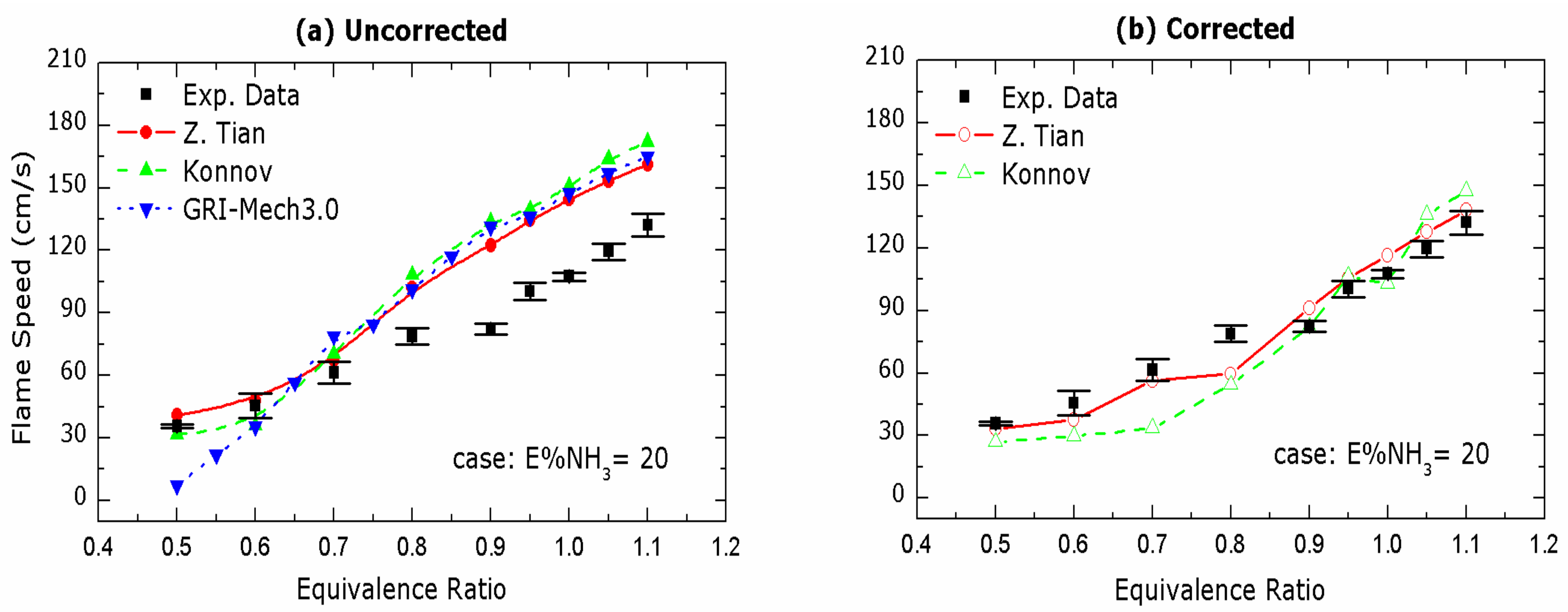
Instantaneous laminar flame images at Ø = 1.0, for E%NH_3 of (a) 20, (b) 50 and (c) 80.

Results

E%NH_3 = 0 (pure H_2-Air)

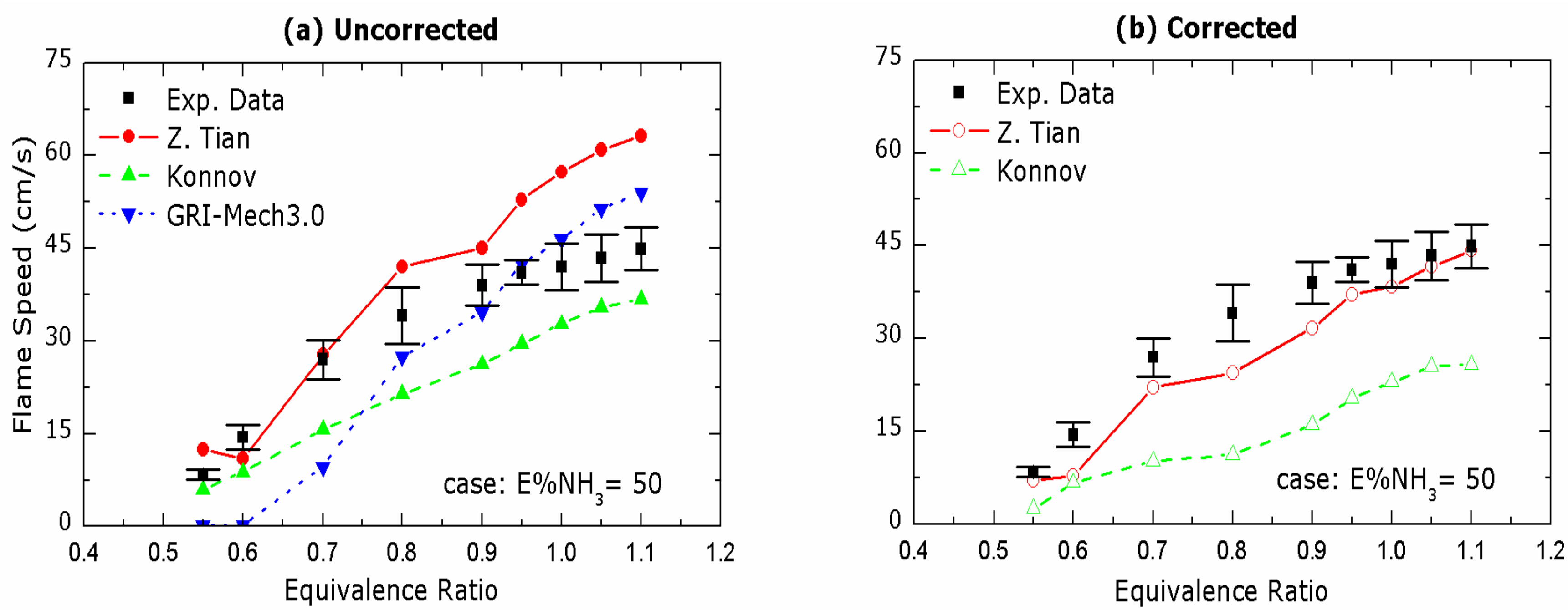


E%NH_3 = 20



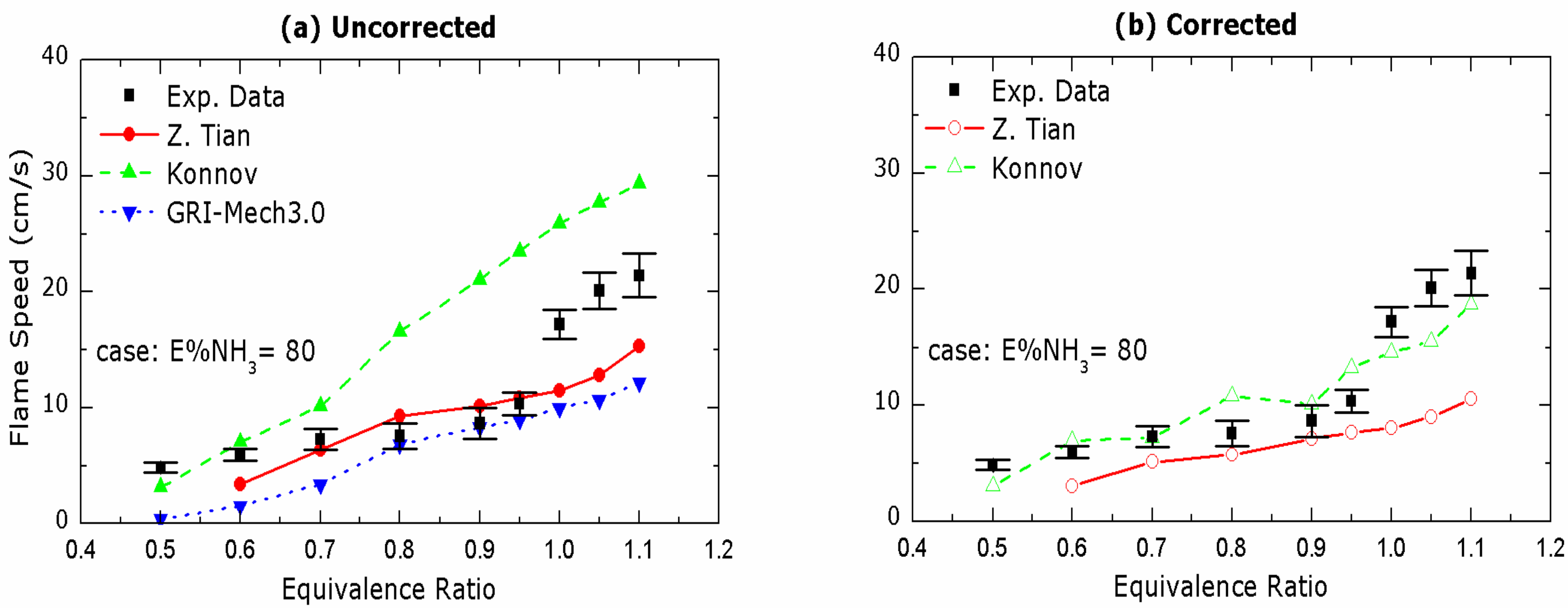
- Overall, Z. Tian mechanism is in better agreement.

E%NH_3 = 50



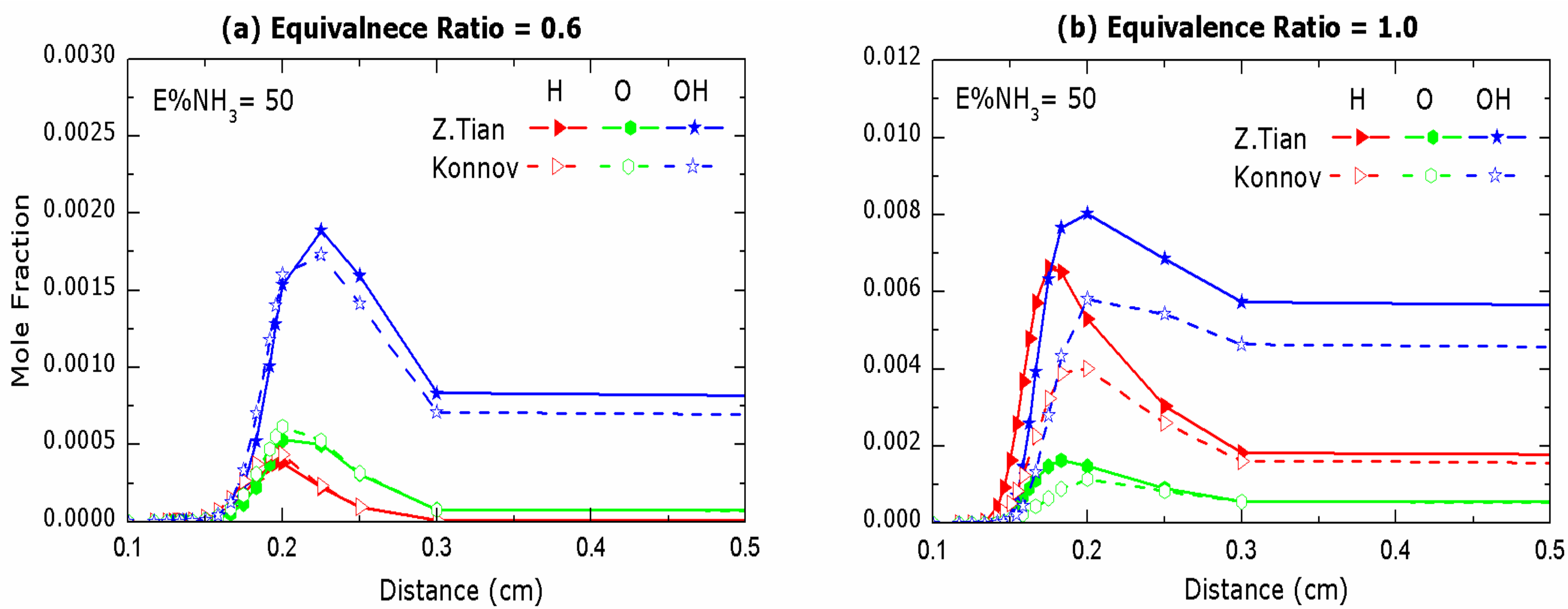
- Overall, Z. Tian mechanism is fairly comparable with experimental data.

E%NH_3 = 80



- Konnov mechanism emerged as the best-fit mechanism for higher E%NH_3.

Effects of Radicals on Flame Speed

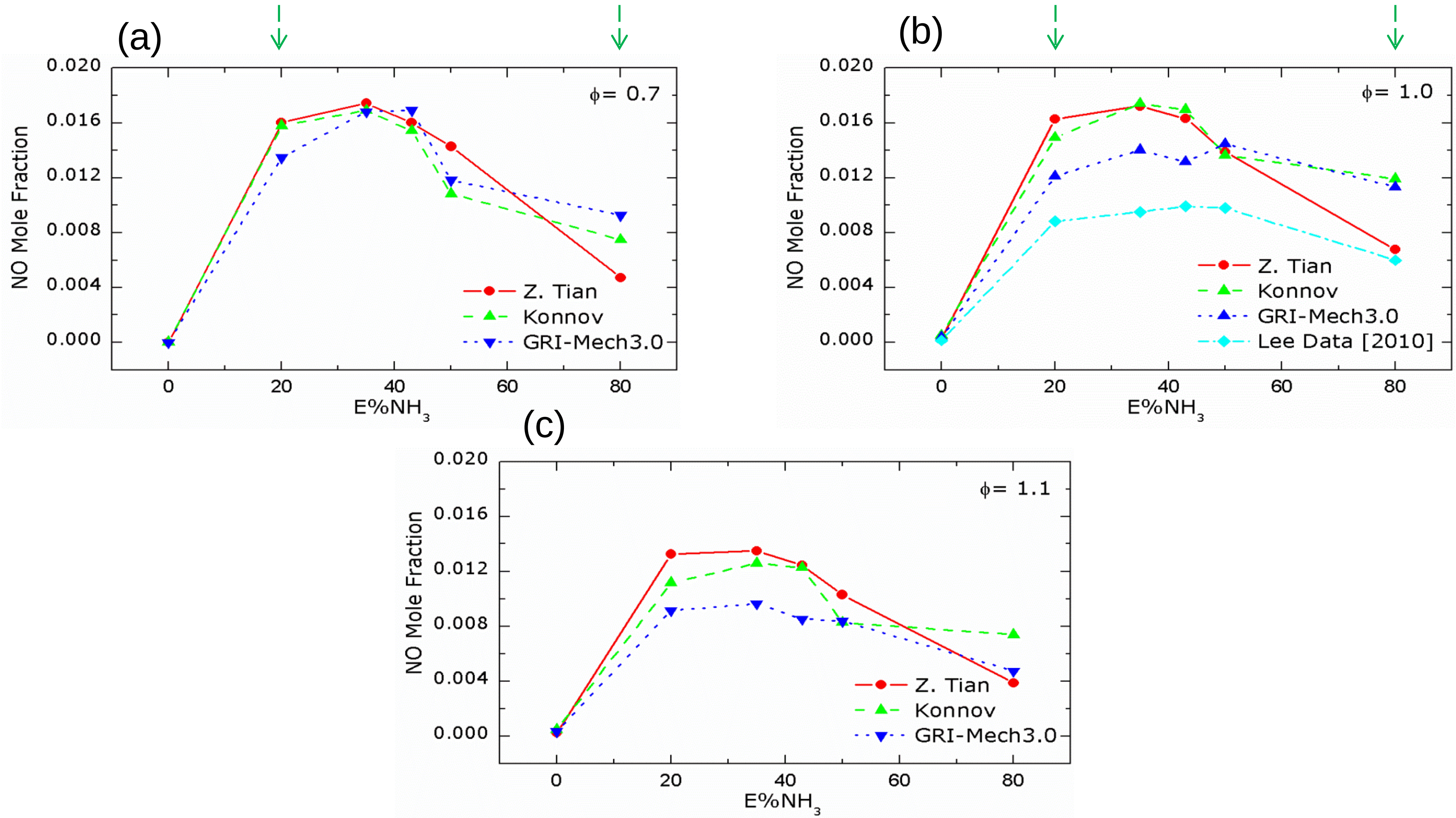


Submitted in Fuel, 2011

- Free radicals O, H & OH determines flame speed for H_2/NH_3 mixtures.

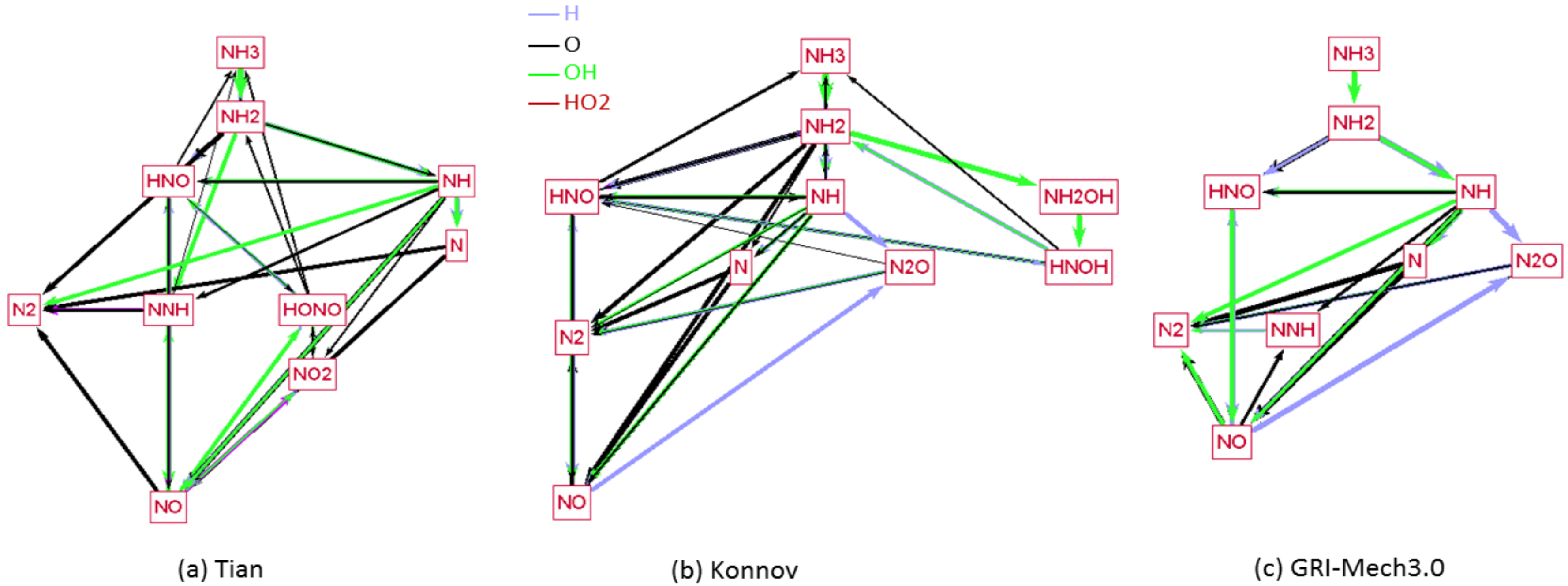
Results: NO mole fraction

Sensitivity & ROP Analysis: NO & NH_3



Results: Sensitivity Analysis

Equivalence ratio 0.7, E%NH_3 =20



NH_3 oxidation:

$$NH_3 + OH \leftrightarrow NH_2 + H_2O \quad \text{(Rxn \# 1)}$$
$$NH_3 + H \leftrightarrow NH_2 + H_2 \quad \text{(Rxn \# 2)}$$
$$NH_3 + O \leftrightarrow NH_2 + OH \quad \text{(Rxn \# 3)}$$

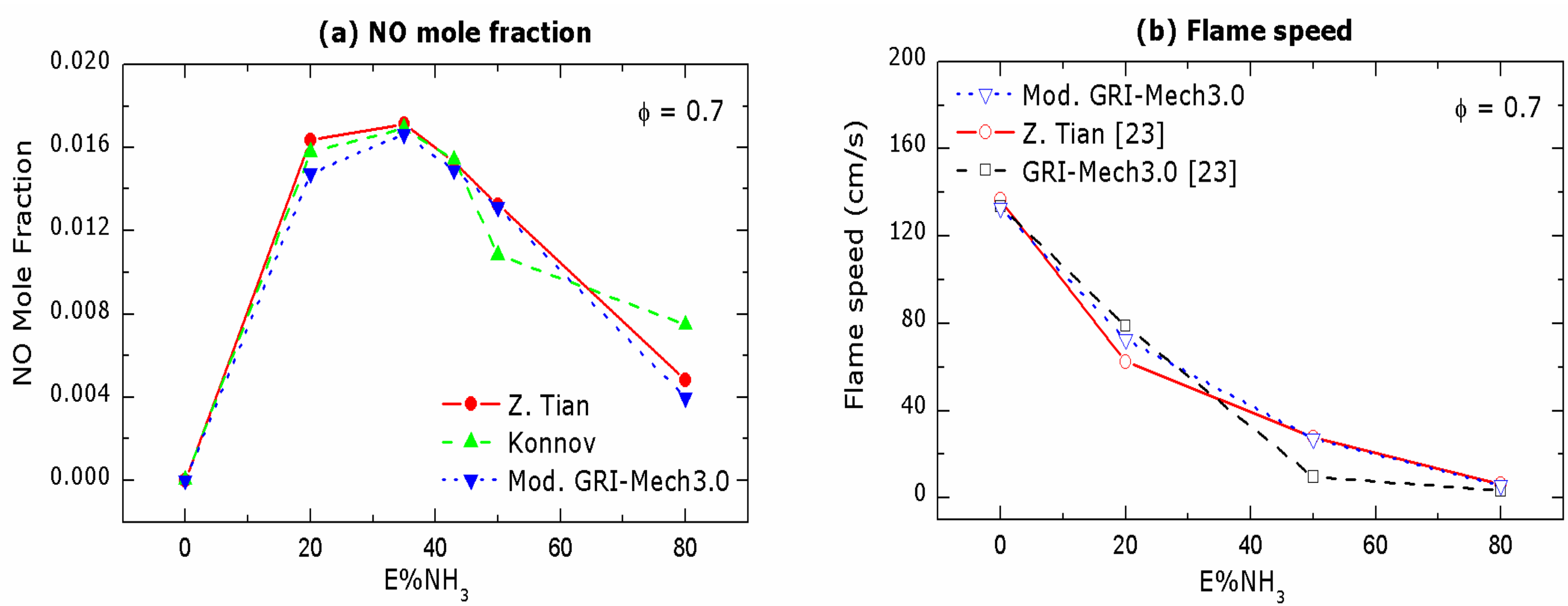
NH_2 oxidation:

$$NH_2 + OH \leftrightarrow HNO + H_2 \quad \text{(Rxn \# 4)}$$
$$NH_2 + H \leftrightarrow NH + H_2O \quad \text{(Rxn \# 5)}$$
$$NH_2 + O \leftrightarrow HNO + H \quad \text{(Rxn \# 6)}$$

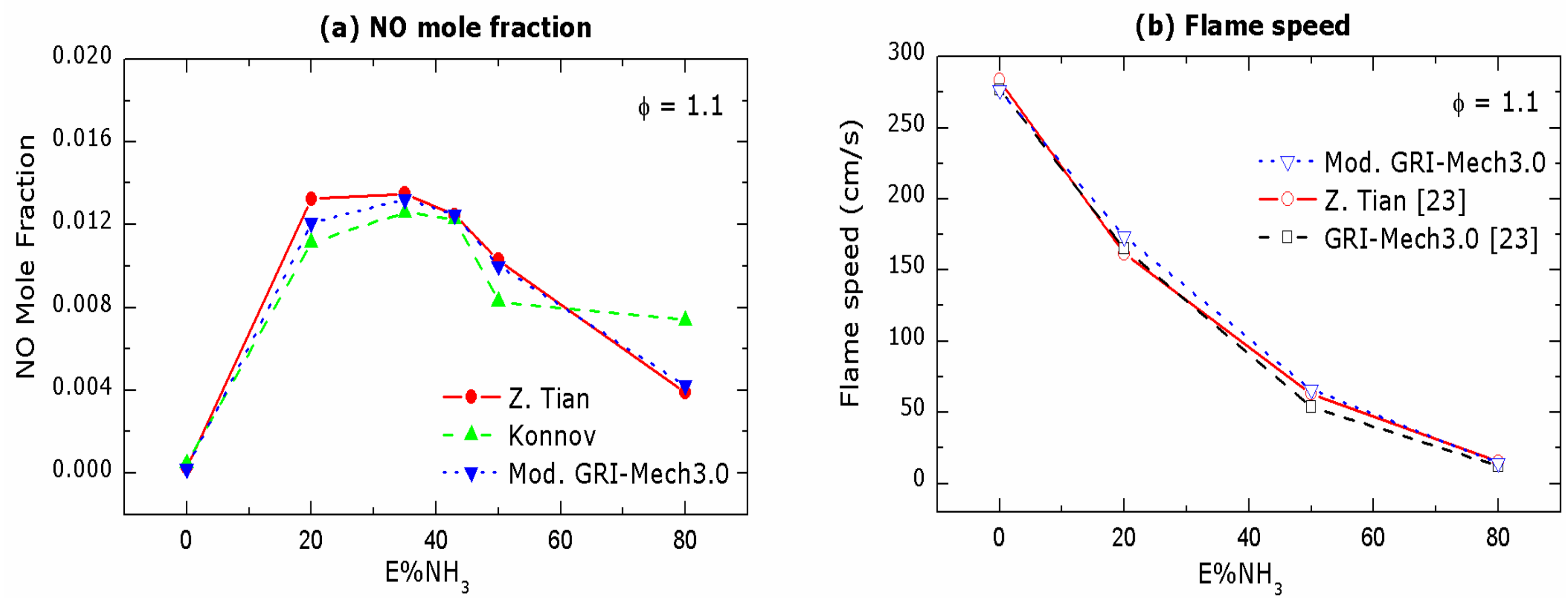
- HNO & NH are identified as NO precursors

Tian & Modified GRI-Mech3.0

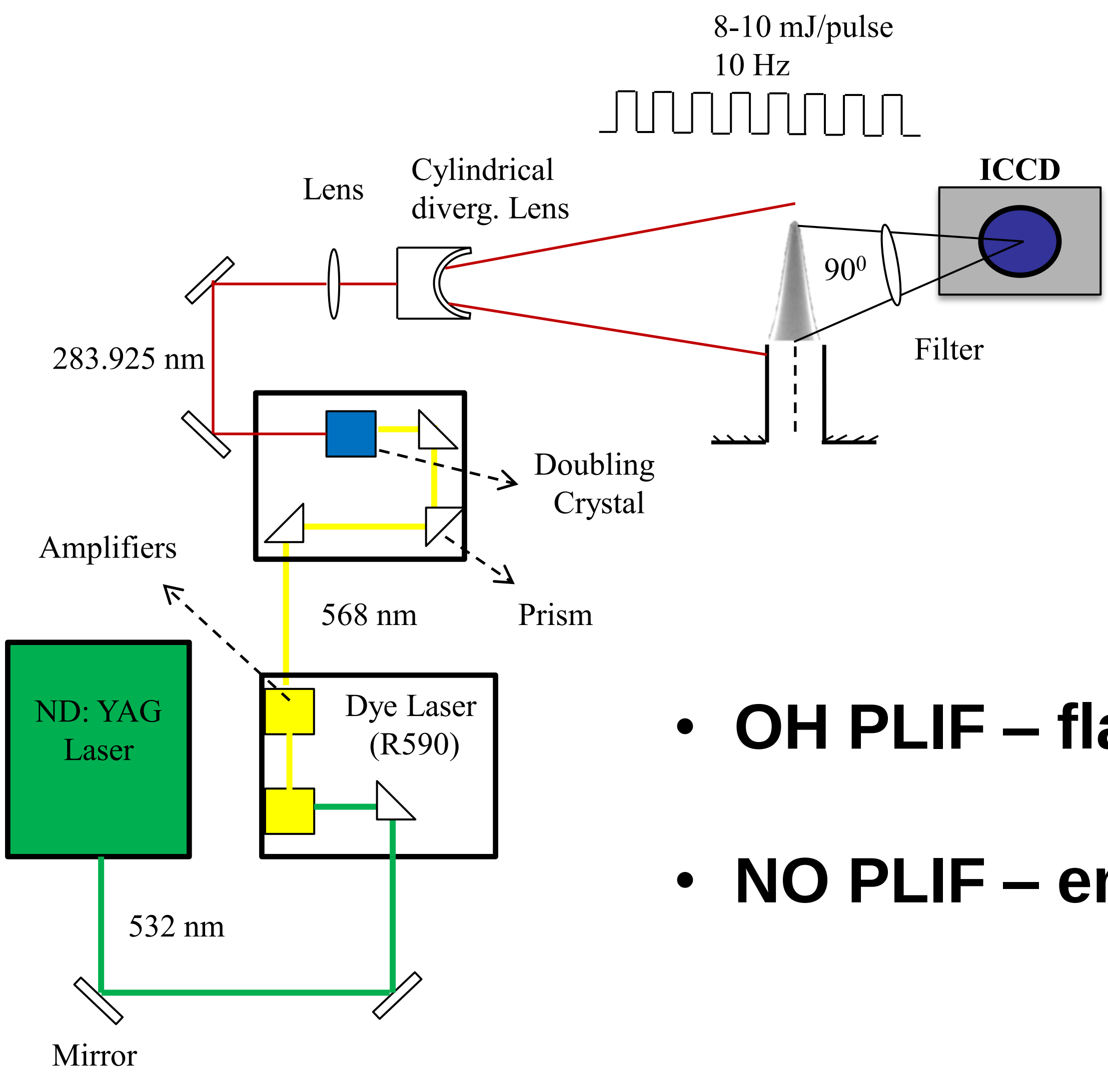
Equivalence Ratio 0.7



Equivalence Ratio 1.1



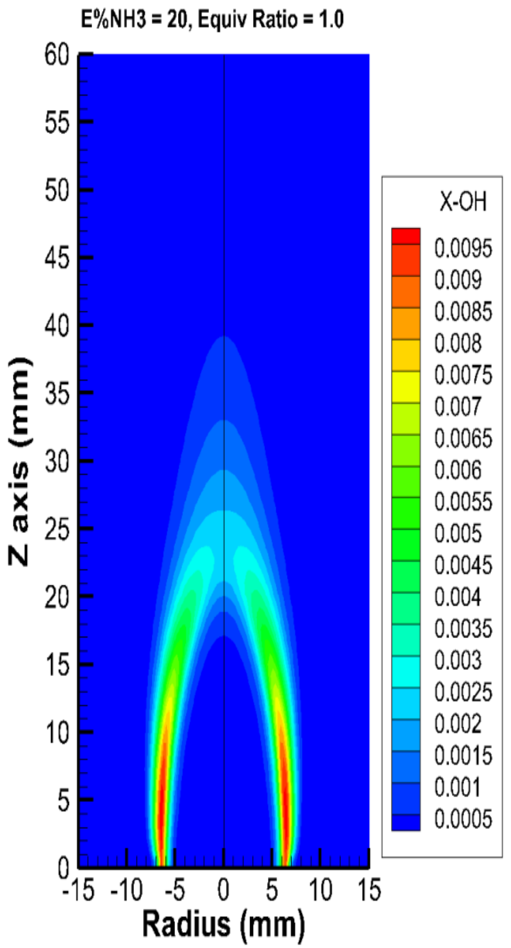
PLIF Set-Up

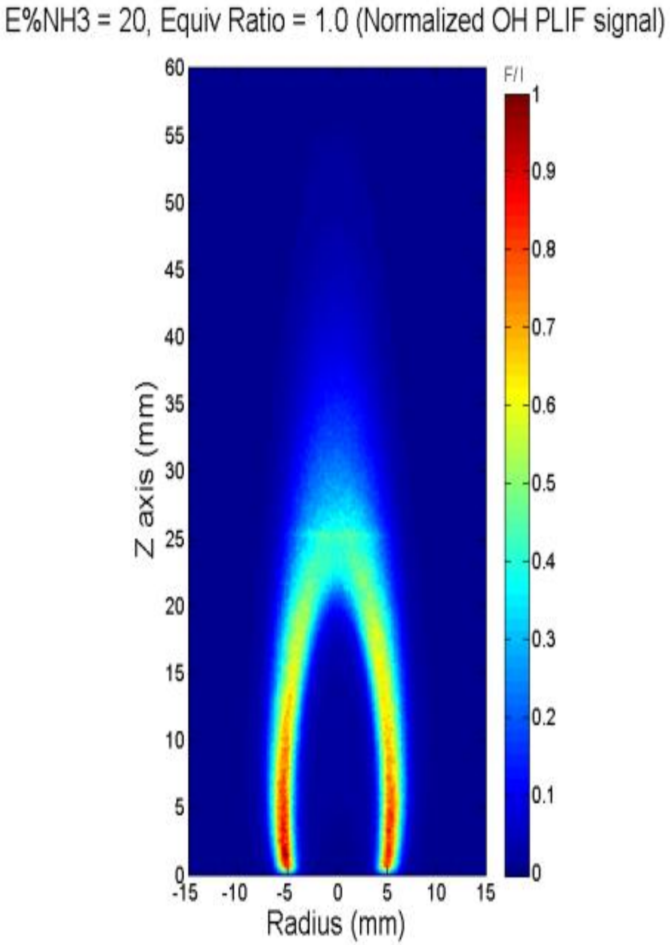


- **OH PLIF – flame structure**
- **NO PLIF – emissions**

Results - OH Flame Structure

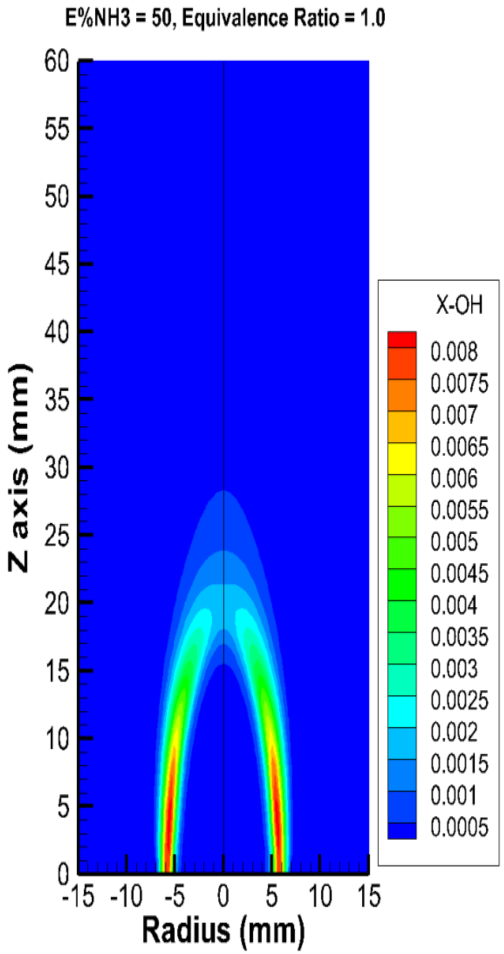
$E\%NH_3 = 20$

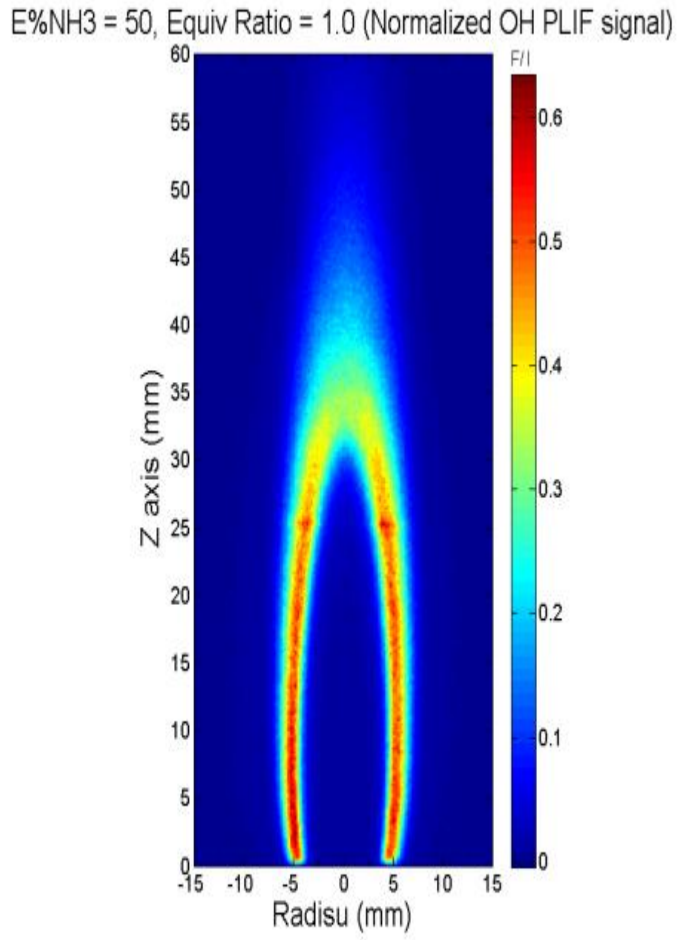




Results - OH Flame Structure

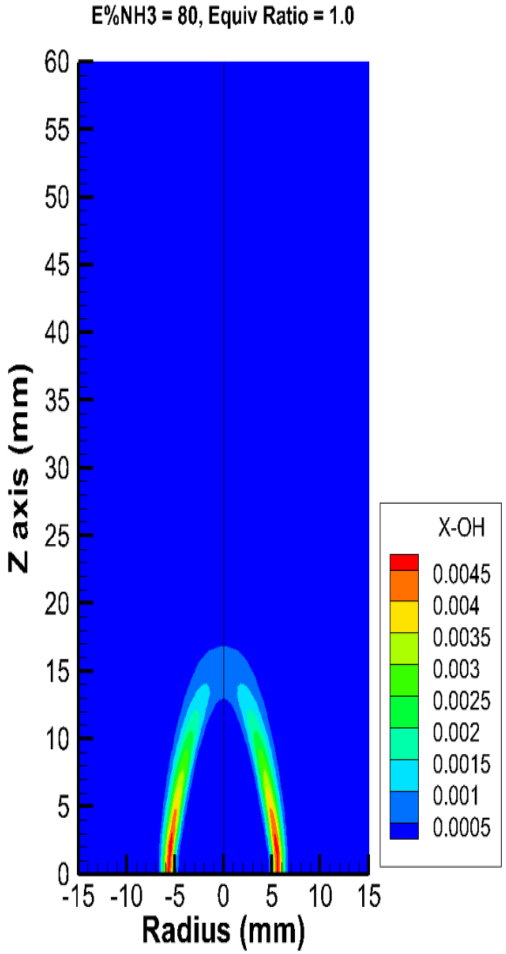
$E\%NH_3 = 50$

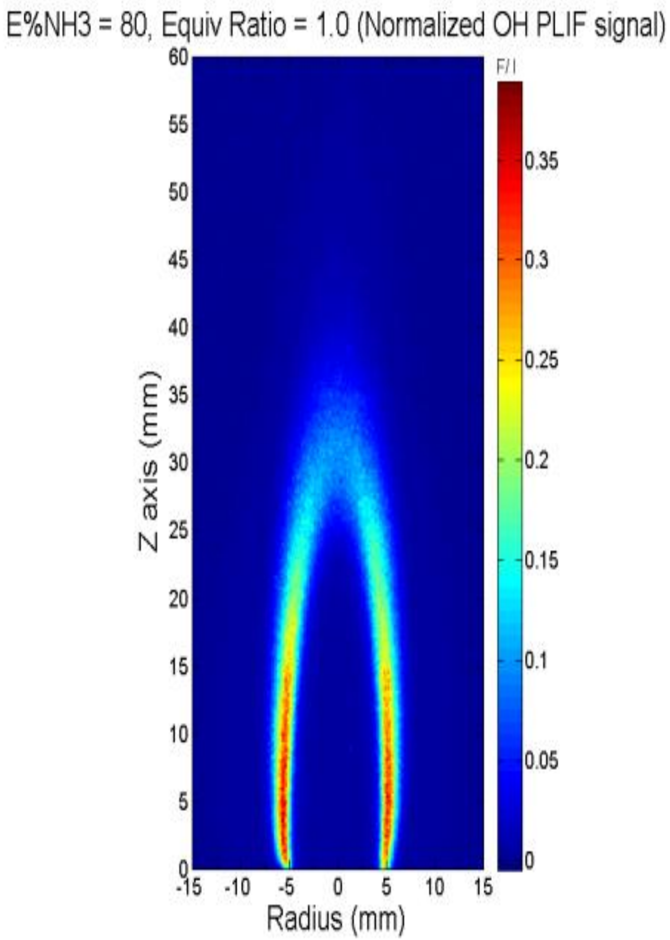




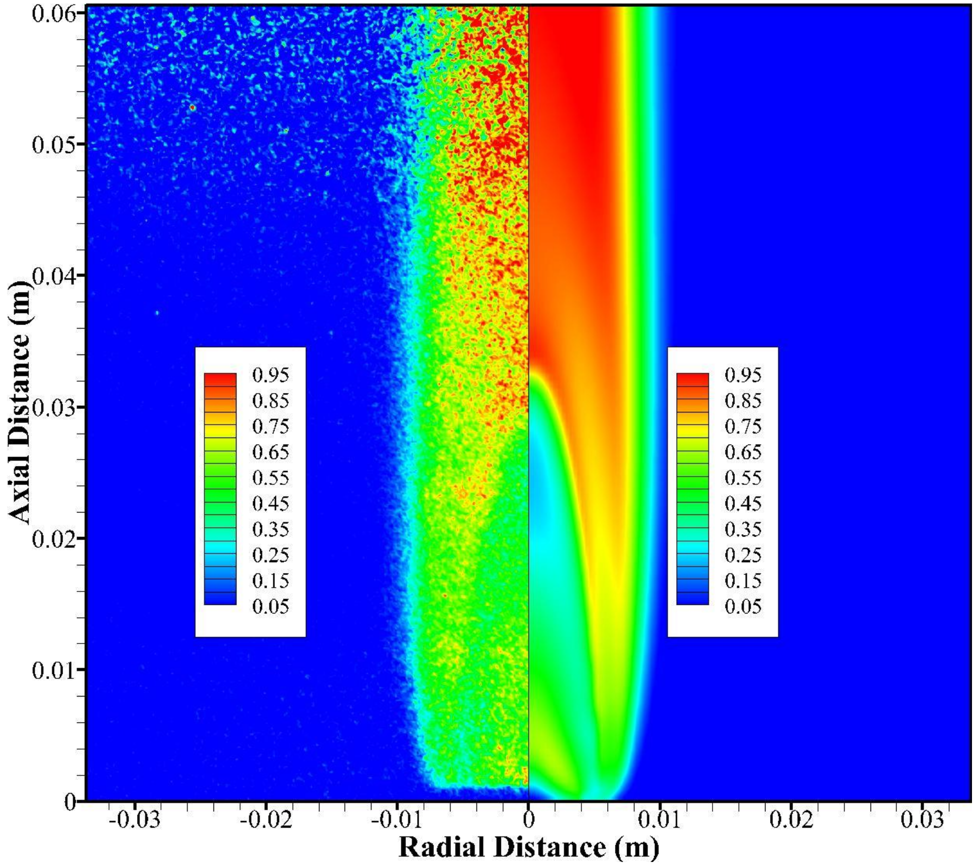
Results - OH Flame Structure

$E\%NH_3 = 80$



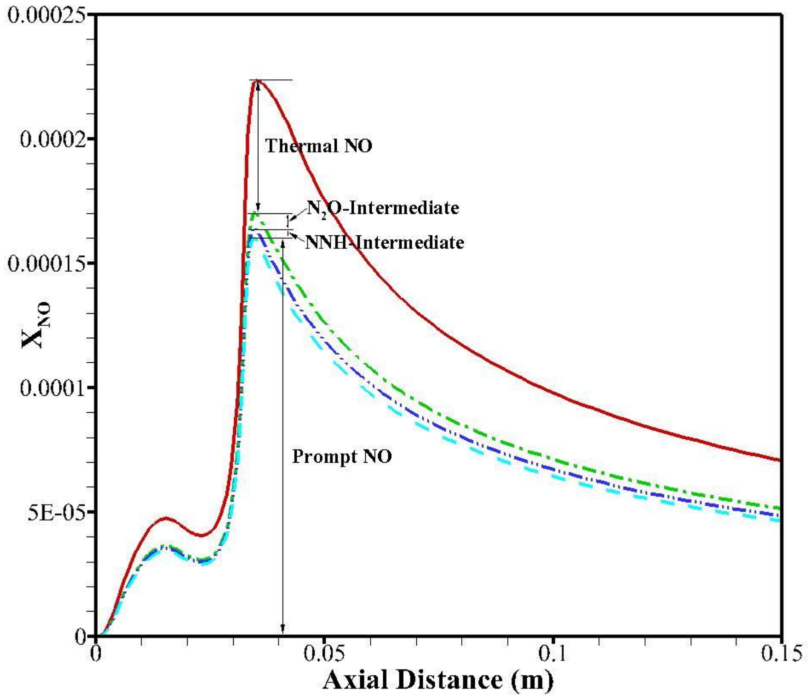


CFD vs. PLIF Images

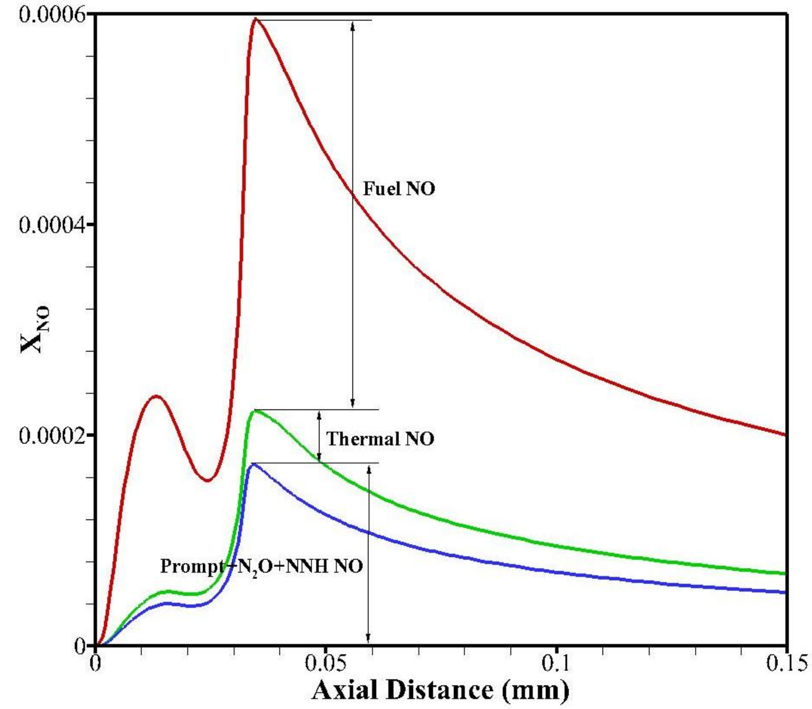


- Example comparison between experiment (left) and CFD (right)

NO Sub-mechanisms

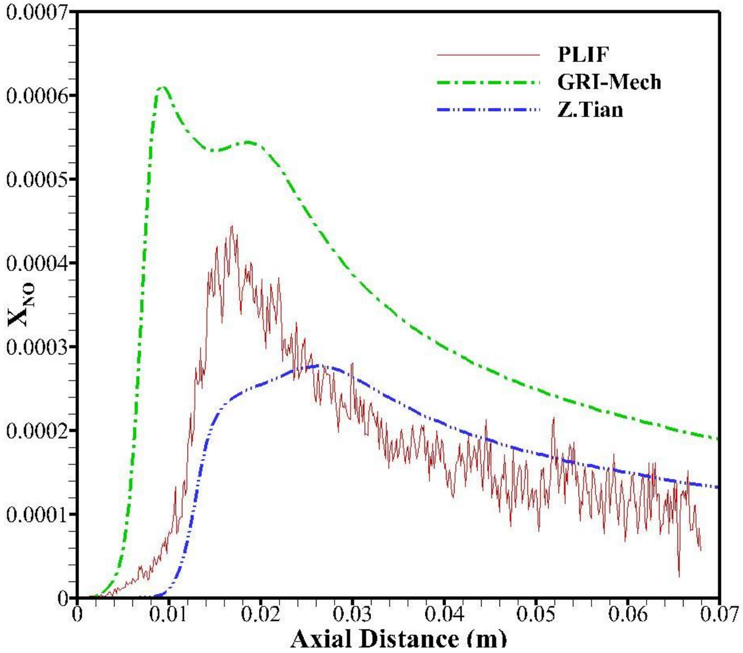


CH4 without NH3

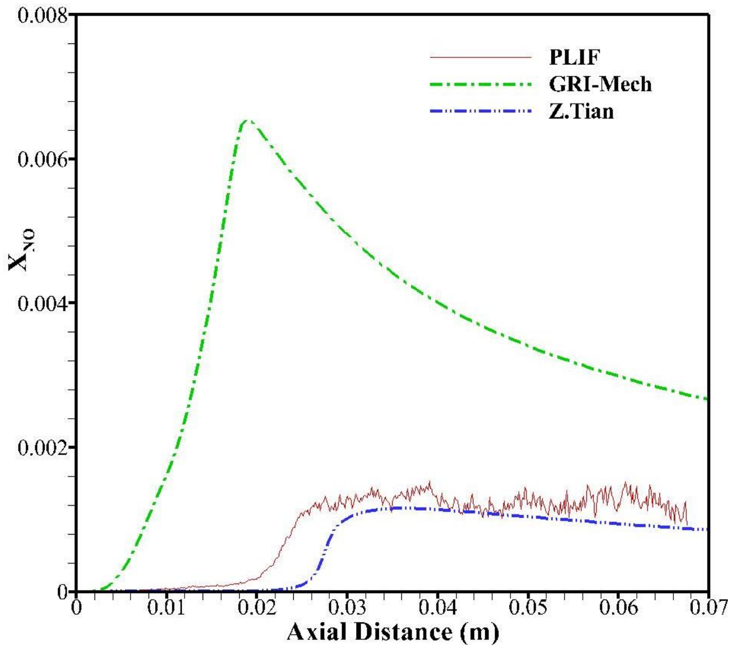


CH4 with 1% NH3

Quantitative Comparisons

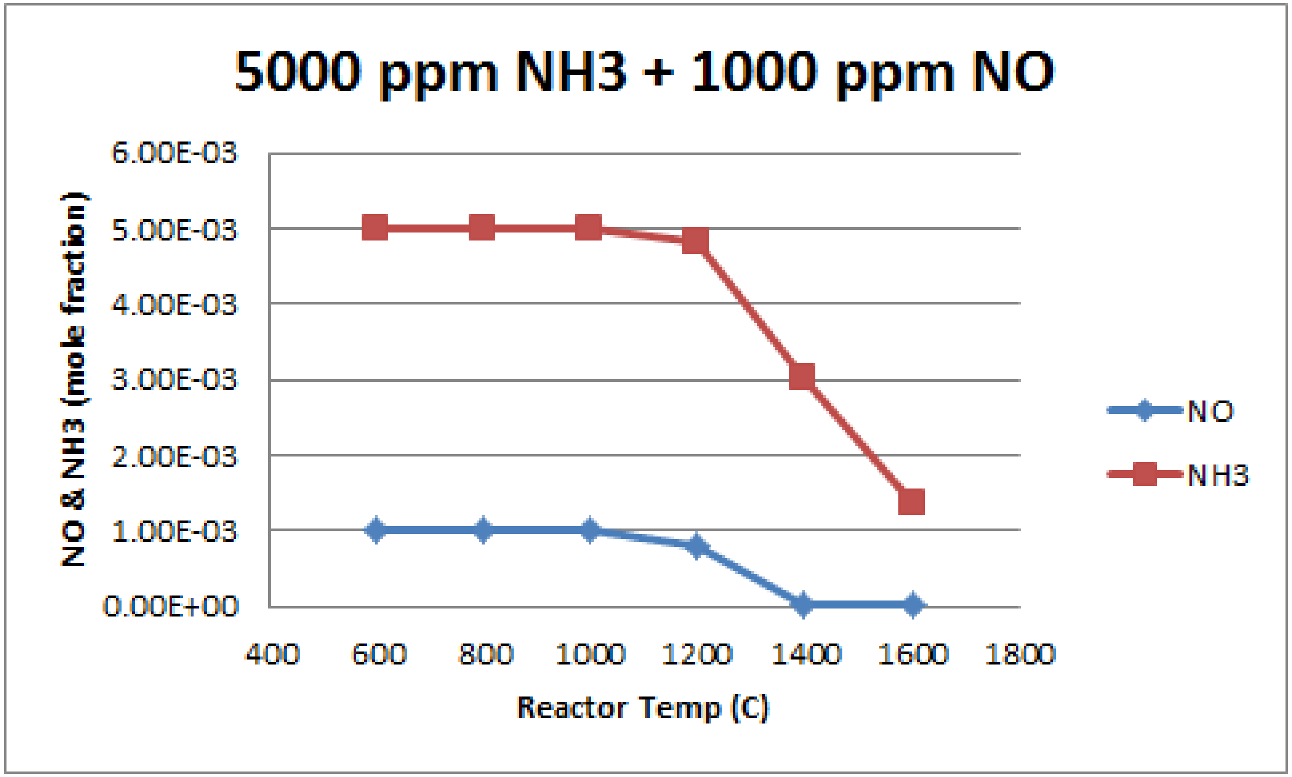


H2/CO with 1% NH3



H2/CO with 30% NH3

Simulation of Reforming



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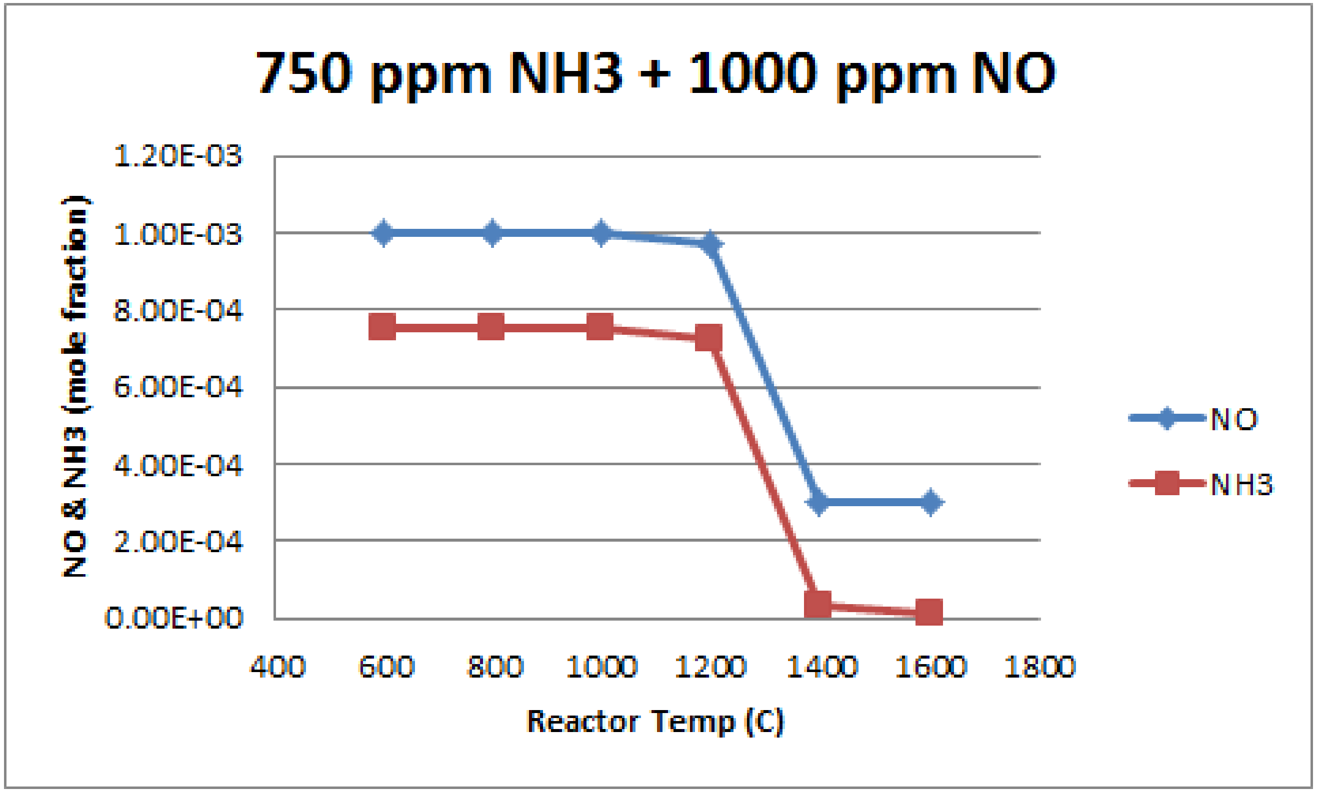

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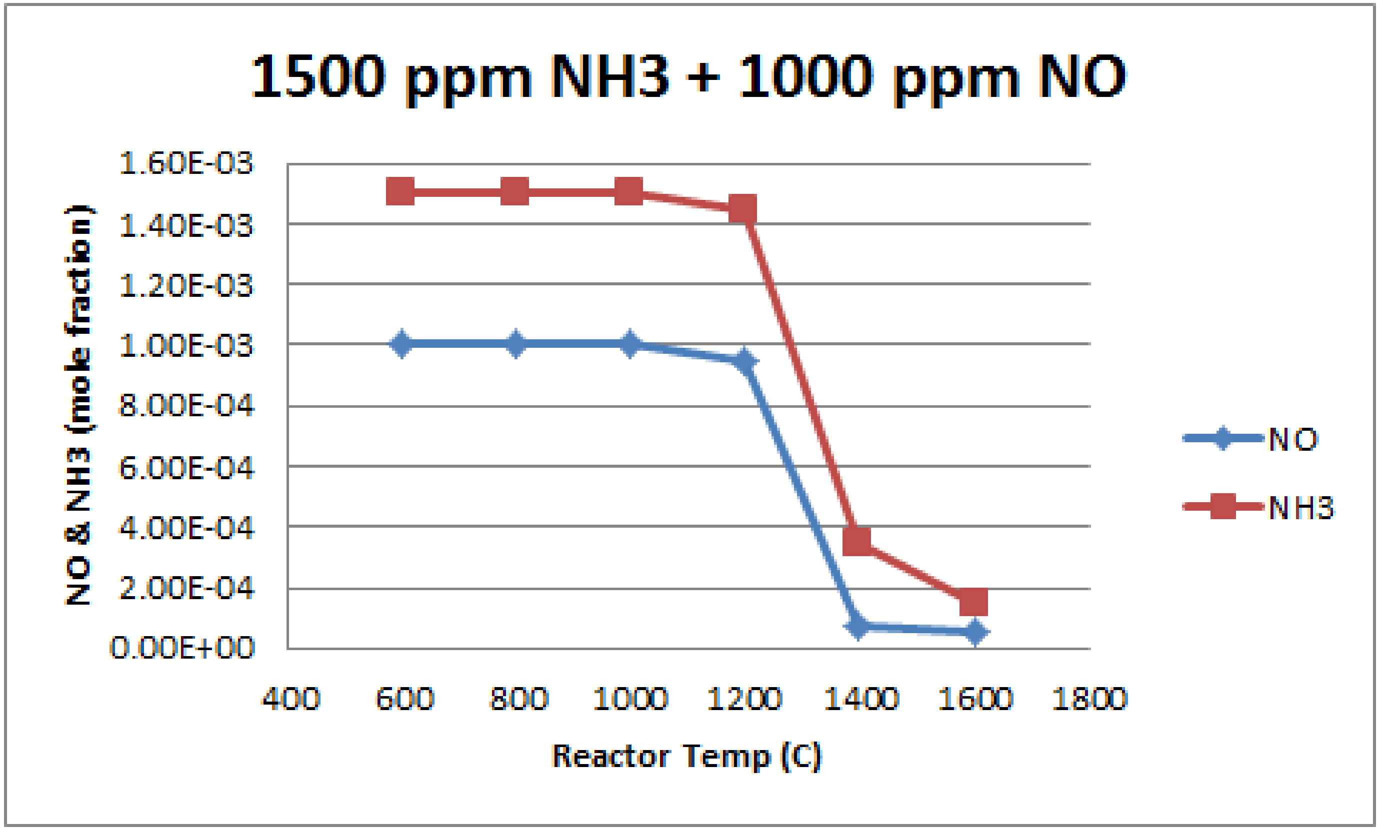

Summary

- Tian mechanism validated for range E%NH_3 = 0 to 50%
- Konnov mechanism best fit for E%NH_3 = 80%.
- GRI-Mech 3.0 not recommend for lean conditions and high E%NH_3 mixtures.
- O, H & OH play decisive role in determining laminar flame speed of the H_2/NH_3 mixtures.

Acknowledgments

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Thank You !!!

Questions !!!