NO_x emission analysis and flame stabilization of ammonia-hydrogen-air premixed flames

Hadi Nozari

Koç University İstanbul, Turkey

Arif Karabeyoğlu

SPG Inc, San Mateo CA

Koç University İstanbul, Turkey

Work Split

SPG Inc, San Mateo

- Power generation system development
- Large scale testing

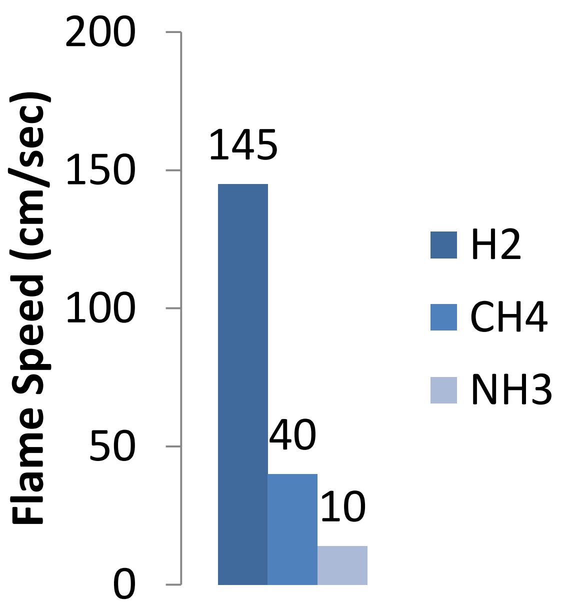
KOC University, Istanbul

- Fundamental aspects of NH3 cracking and combustion
- Small scale testing

Review

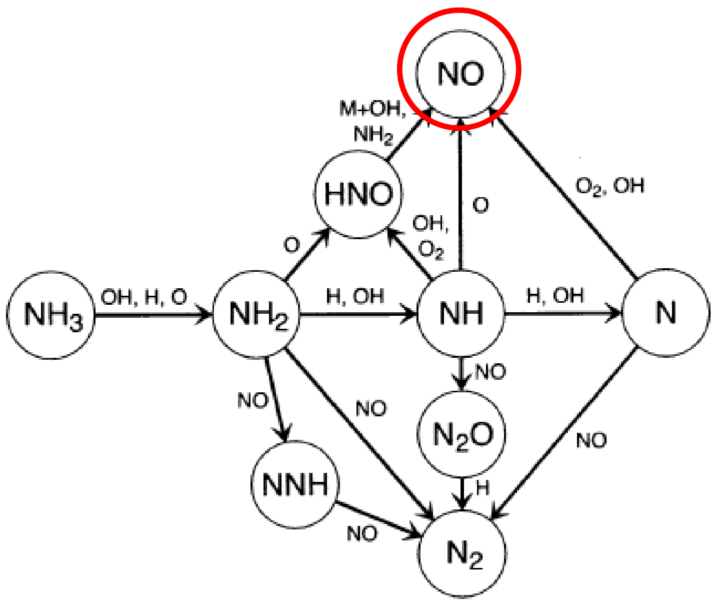
Challenges with NH3 combustion

- Slow kinetics (low flame speed)



Standard Temperature and Pressure
Air as oxidizer

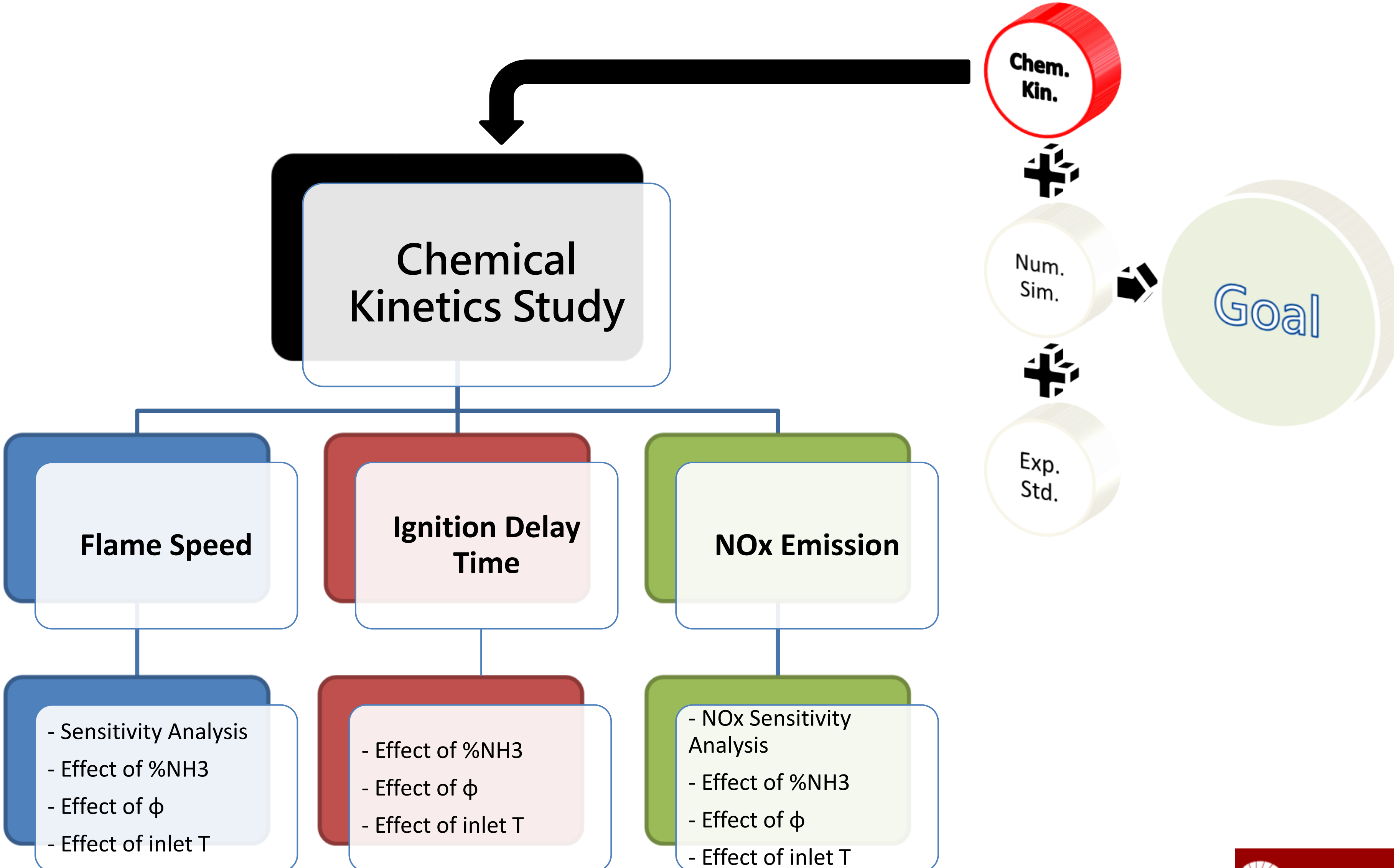
- NH3 , a source of fuel NOx in flames



A simplified reaction mechanism

«Ammonia – It's Transformation and Effective Utilization» AIAA 2008
Ref: Miller, J. A. et al. , Combust. Sci. Tech., 34:149–176 (1983)

Previous Study



SPG Advancing Propulsion & Energy

Previous Study

Chemical Kinetics Study

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

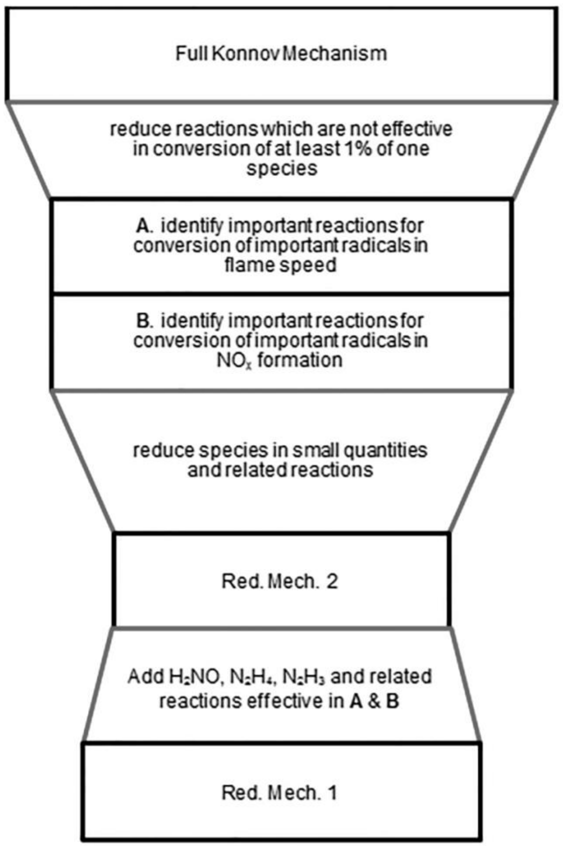
Numerical study of combustion characteristics of ammonia as a renewable fuel and establishment of reduced reaction mechanisms

Hadi Nozari[a], Arif Karabeyoğlu[a,b,*]

[a] Department of Mechanical Engineering, Koç University, Istanbul, Turkey
[b] Space Propulsion Group Inc., Palo Alto, CA, USA

- 2 reduced mechanisms for steady state conditions of engine
  - NOx predictions
  - Flame speed

Reference: Konnov mechanism



Very good agreement with the full mechanism and experimental data

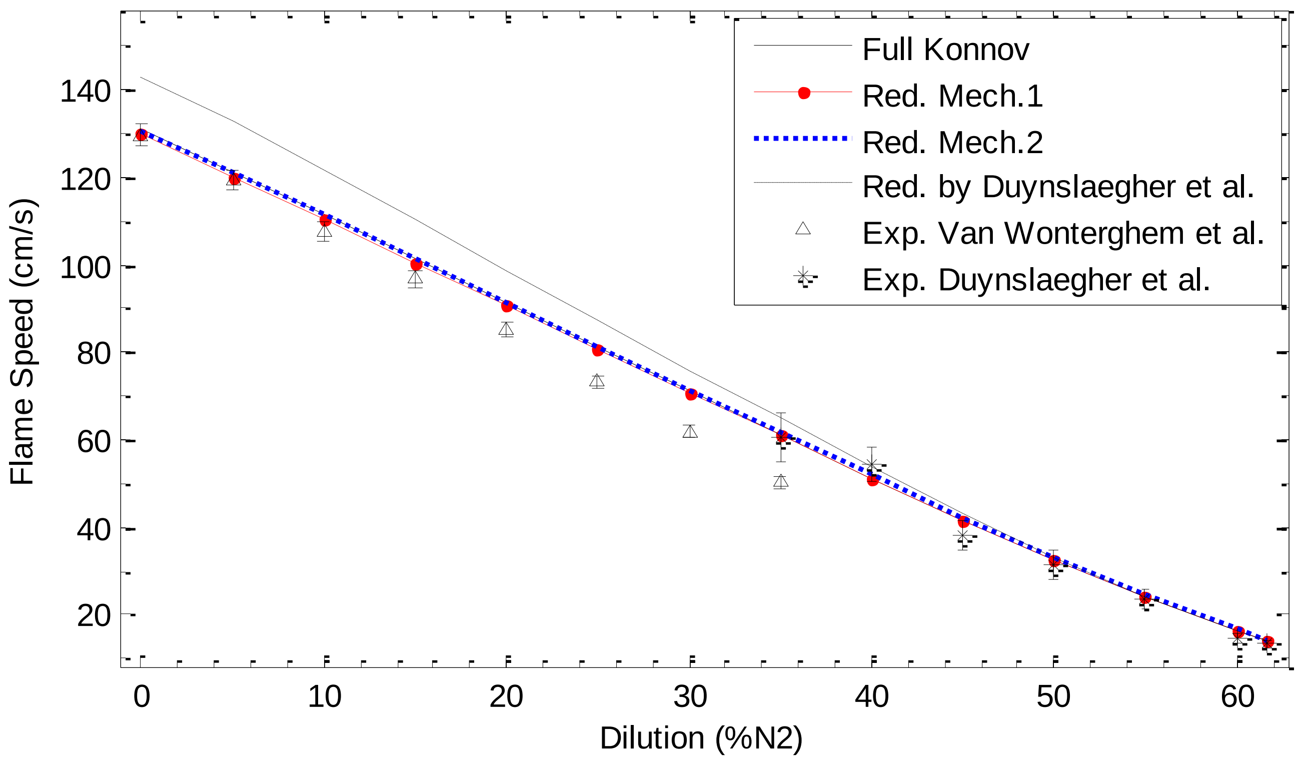
	Konnov (full)	Belgium Red.	Red. Mech. 1	Red. Mech. 2
# elements	3	3	3	3
# species	30	19	21	18
# reactions	240	80	91	80

Previous Study

Chemical Kinetics Study

Reduced Mech.

Comparison with the **experimental data**



Ammonia-O2-N2
Stoichiometric
STP condition

Previous Study

Chemical Kinetics Study

Reduced Mech.

Quantitative comparison with **experimental data (% discrepancy)**

	% N_2	Konnov	Red. Mech.1	Red. Mech.2	Red. By Duynslaegher et al.
Experiments of Van Wonterghem et al.	0	1.2	0.4	0.8	10.3
	5	1.5	0.6	1.3	11.2
	10	3.6	2.9	3.5	13.1
	15	4.7	3.8	4.8	13.8
	20	7.1	6.3	7.1	15.6
	25	11.3	10.0	10.7	19.2
	30	15.1	14.7	15.2	22.8
Experiments of Duynslaegher etal.	35	1.4	1.1	1.9	7.9
	40	5.9	6.0	4.5	1.4
	45	9.5	9.1	10.5	12.6
	50	3.8	3.6	5.8	4.7
	55	1.9	1.2	3.6	3.1
	60	12.1	14.0	15.5	12.8
	61.7	3.9	5.6	7.8	5.6

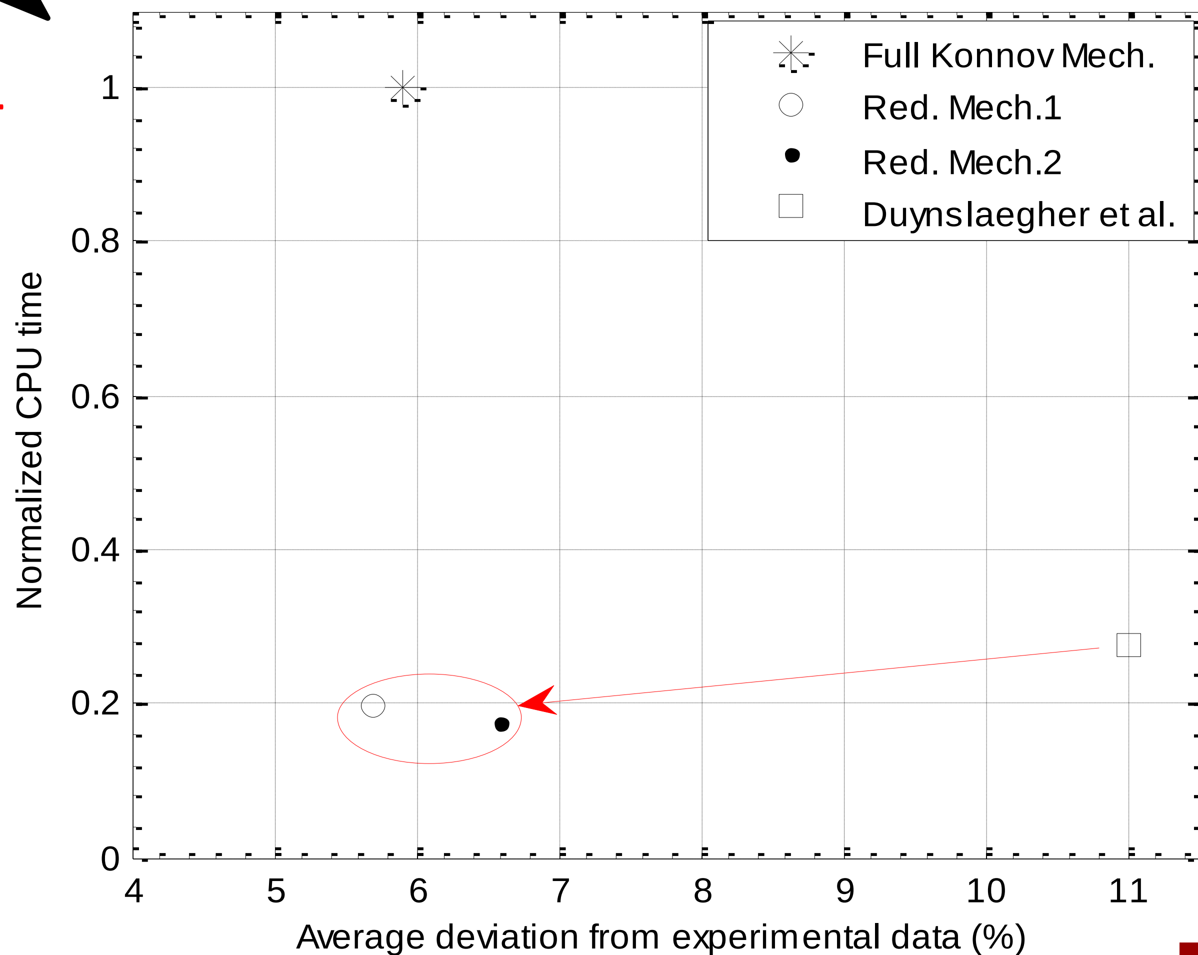
Ammonia-O2-N2
Stoichiometric
STP condition

Previous Study

Chemical Kinetics Study

Reduced Mech.

PERFORMANCE CHART



Ammonia-O2-N2
Stoichiometric
STP condition

RESULTS

Previous Study

Reduced Mech.

NOx Formation

Effect of equivalence ratio variation

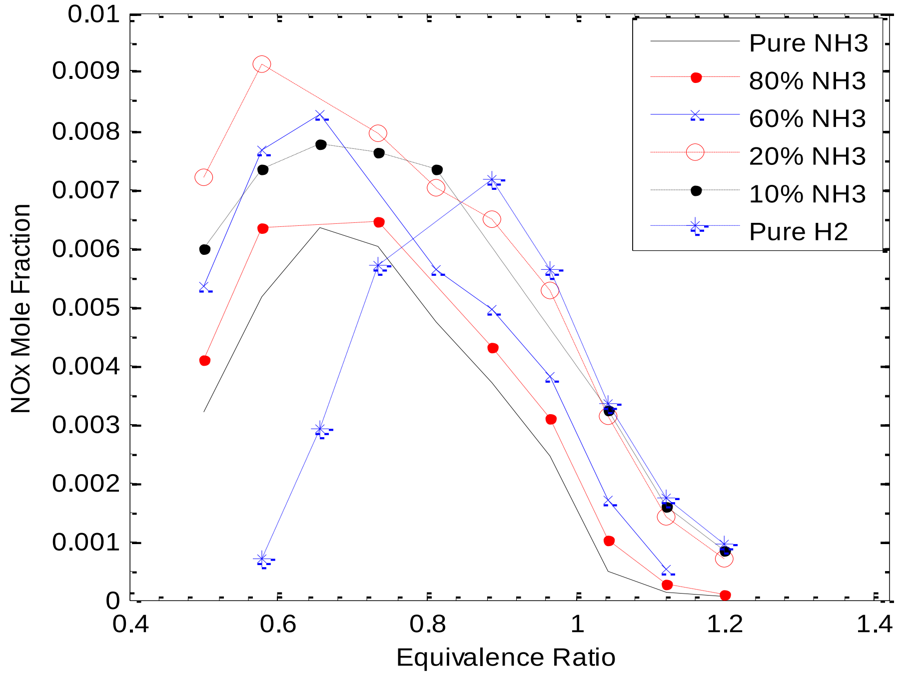
- Increasing / Decreasing trend

Two opposite effects:

1) Increase in thermal NOx by increase in adiabatic flame T
2) Decreasing fuel NOx by decreasing O/F ratio

$$NH_i + OX \rightarrow NO + H_iX$$

OX: Oxygenated species



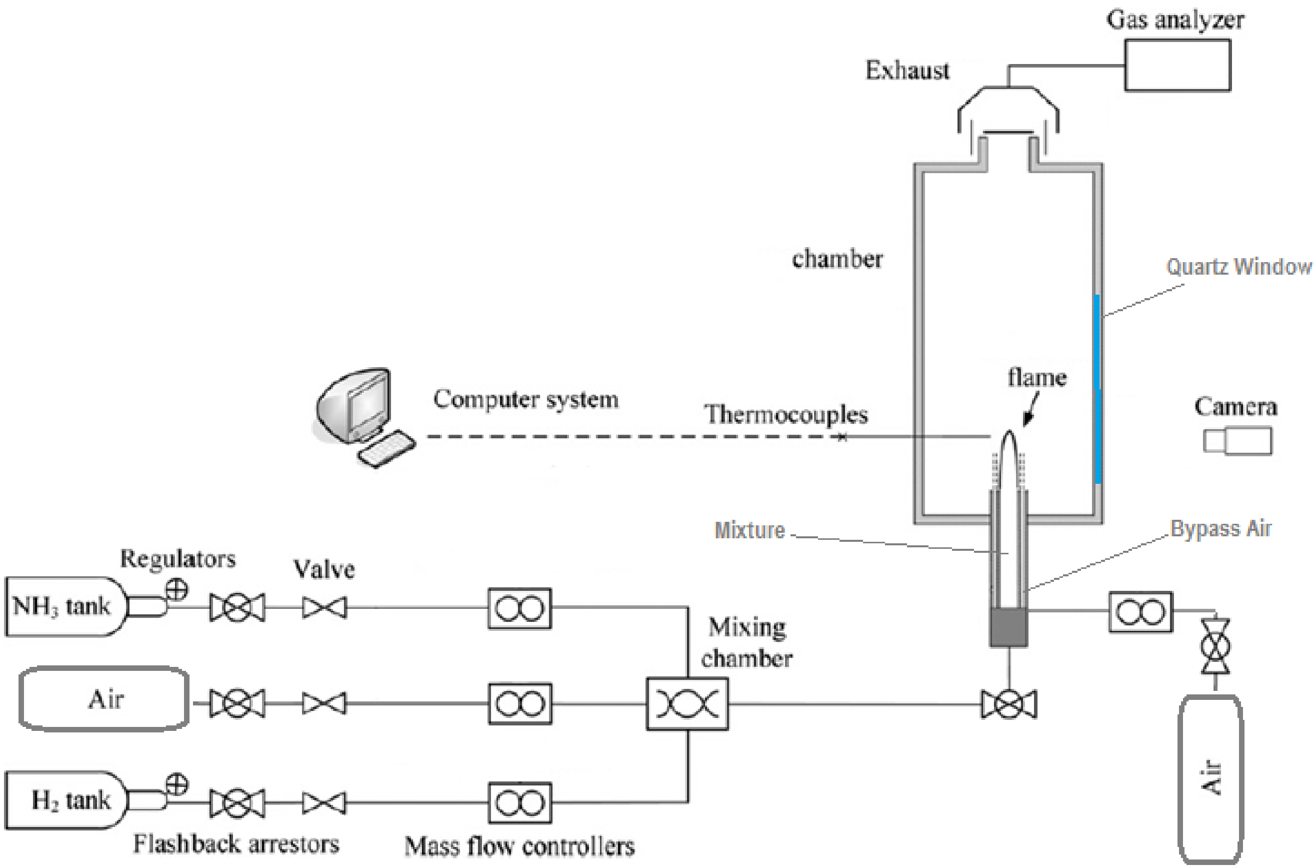
Noticeable reduction in NO_x emission under the rich conditions

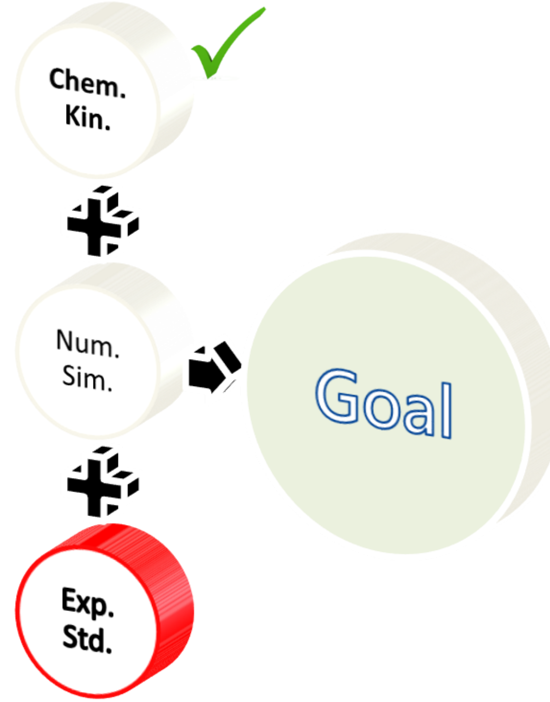
P=17 bar, T=673 K

KOÇ UNIVERSITY

IN PROGRESS

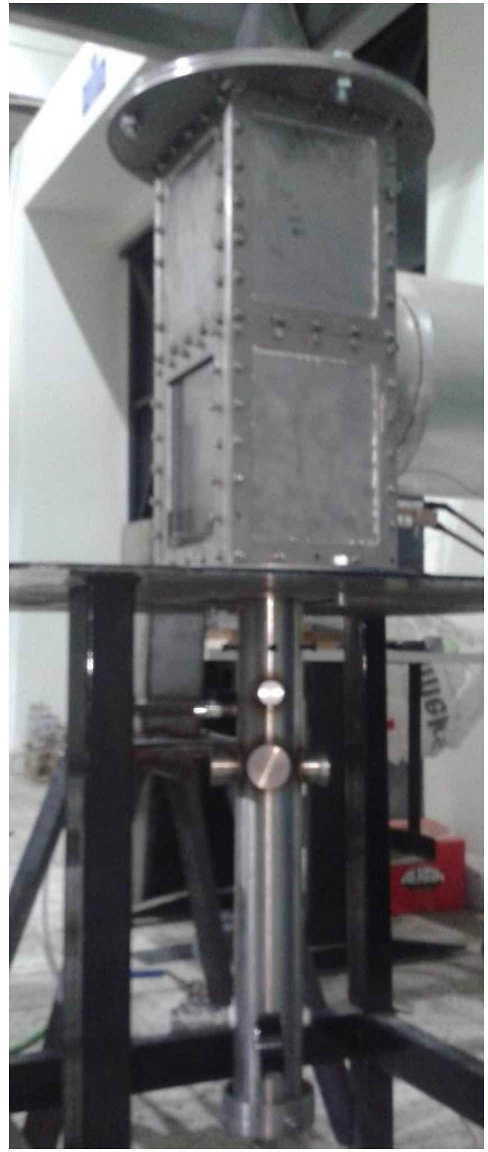
Setup Schematics

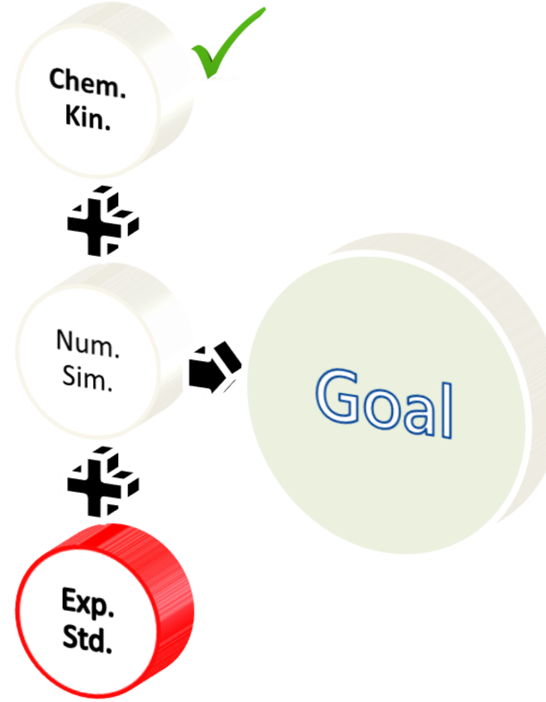




IN PROGRESS

Combustion Chamber





IN PROGRESS

Chem. Kin.

+

Num. Sim. → Goal

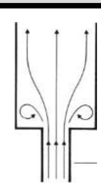
+

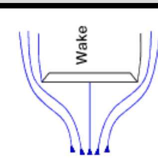
Exp. Std.

Experimental Study Scope

NOx	T	Flame Stability
vs. Equivalence Ratio	vs. Equivalence Ratio	Flame Holding Methods
vs. %NH3	vs. %NH3	Blow-Off & Flashback
vs. Flame Holding Method		

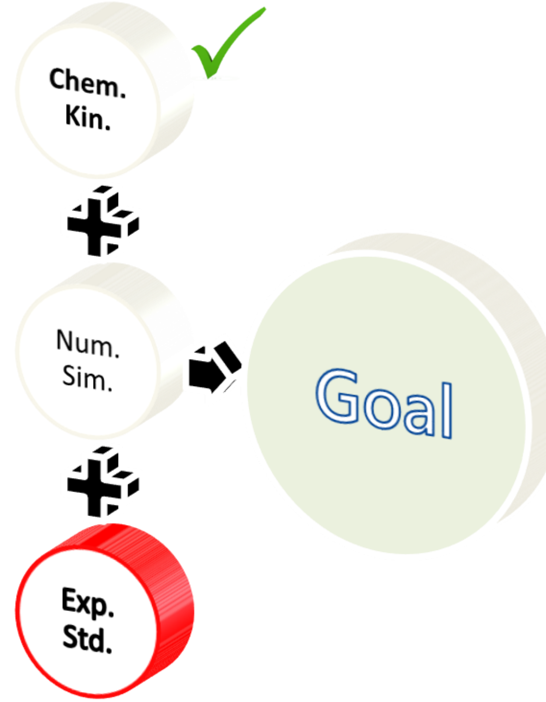
Dump Combustor → Bluff Body → Disc → Porous Block





KOÇ UNIVERSITY

IN PROGRESS



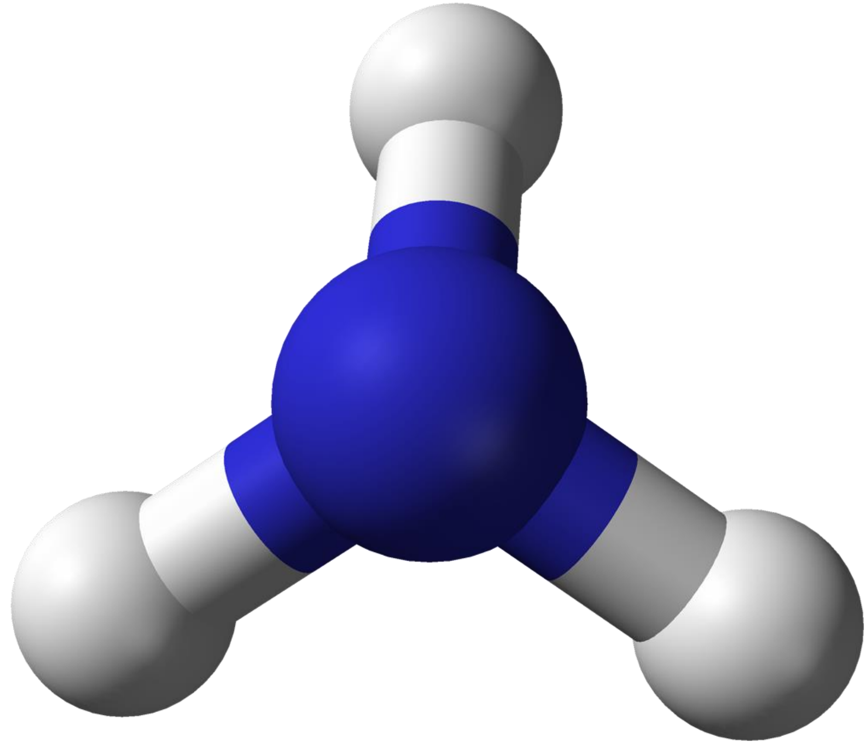
Premixed NH3-H2-Air Flame

φ=1.2 , 40% NH3 - 60% H2

φ=1.2 , 60% NH3- 40% H2

φ=1 , 40% NH3 - 60%H2

Si-C Porous Media
20 Pores Per Inch



Thank You

akarabeyoglu@ku.edu.tr
hnozari@ku.edu.tr

Previously Discussed

Chemical Kinetics Study

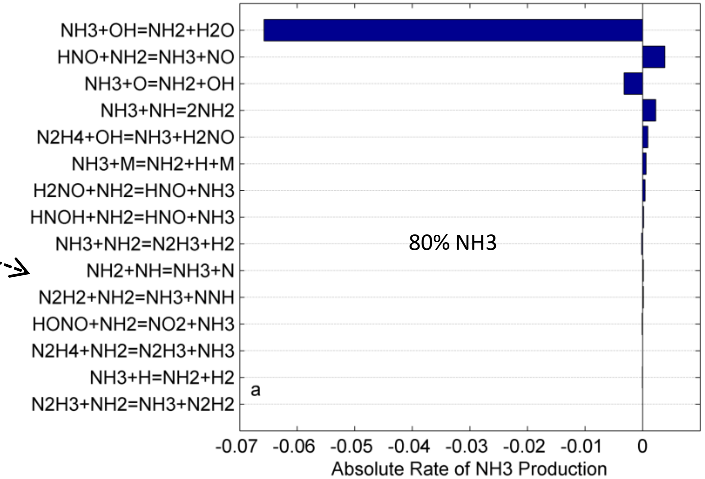
PROPULSION ENERGY 2015 AIAA

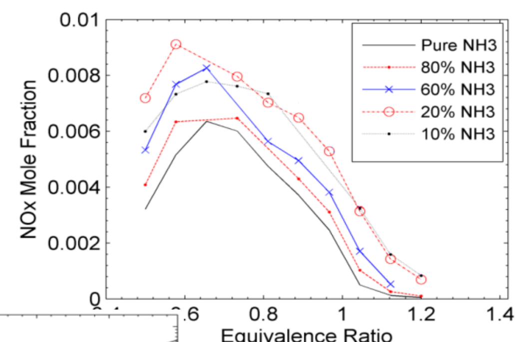
Combustion characteristics of ammonia as a renewable energy source and development of reduced chemical mechanisms

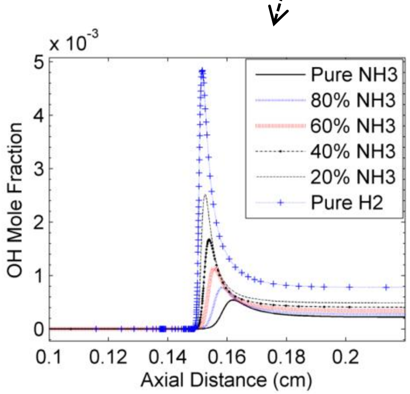
Hadi Nozari[1]
Koç University, Istanbul, Turkey

Arif Karabeyoğlu[2]
Koç University, Istanbul, Turkey
Space Propulsion Group Inc., Palo Alto CA, USA

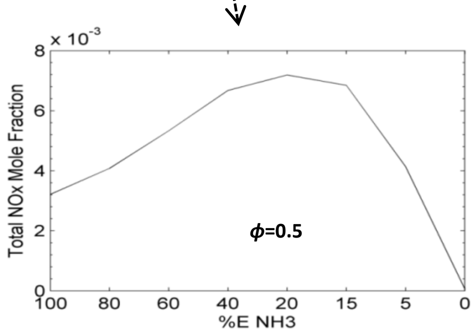
(doi: 10.2514/6.2015-3917)

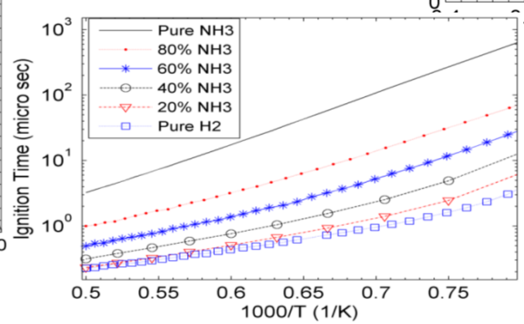






P=17 atm, ϕ=0.5





KOÇ UNIVERSITY

RESULTS

NOx Formation

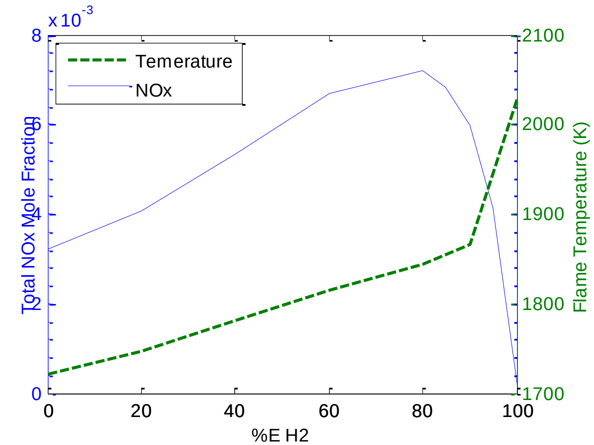
Effect of H2 addition to the mixture

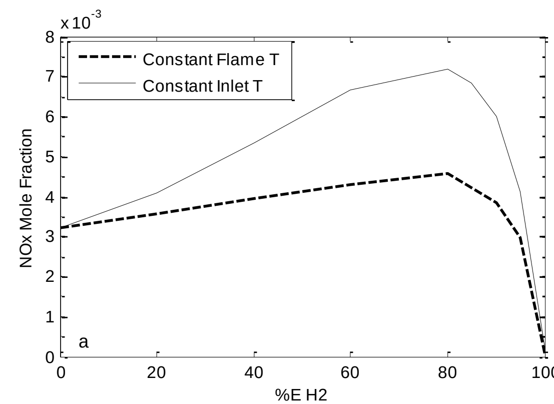
- **Constant Inlet T (400°C)**
  - Thermal NOx and Fuel NOx; the only players?
- **Constant Flame T (1730 K)**
  - General expectation: decrease in Total NOx (decreasing fuel bond N)
  - Total NOx still increasing (despite const. thermal NOx)!
  - Effect of H and HNO accumulation → Increasing ROP of some key reactions
    - $NO_2+H \leftrightarrow NO+OH$
    - $HNO+H \leftrightarrow NO+H_2$
    - $HNO+OH \leftrightarrow NO+H_2O$
- **Decoupling thermal NOx from total NOx**

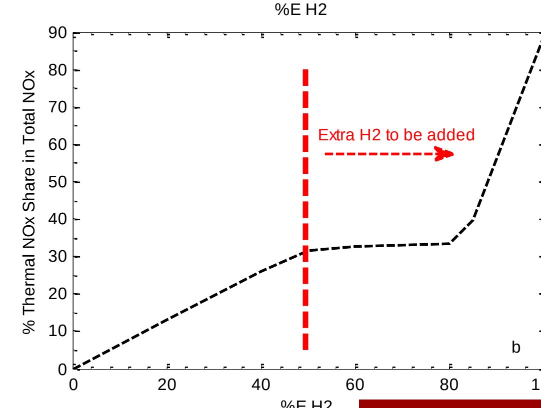
$$\frac{[\text{NOx Level @Const. Inlet T of 400°C}] - [\text{NOx Level @ Const. Flame T of 1730 K}]}{[\text{NOx Level @ Const.Inlet T of 400°C}]} \times 100 = \boldsymbol{Thermal\ NOx\ Share}$$

  - Thermal NOx share increase with increasing H2 % (Flame T)

ϕ=0.5





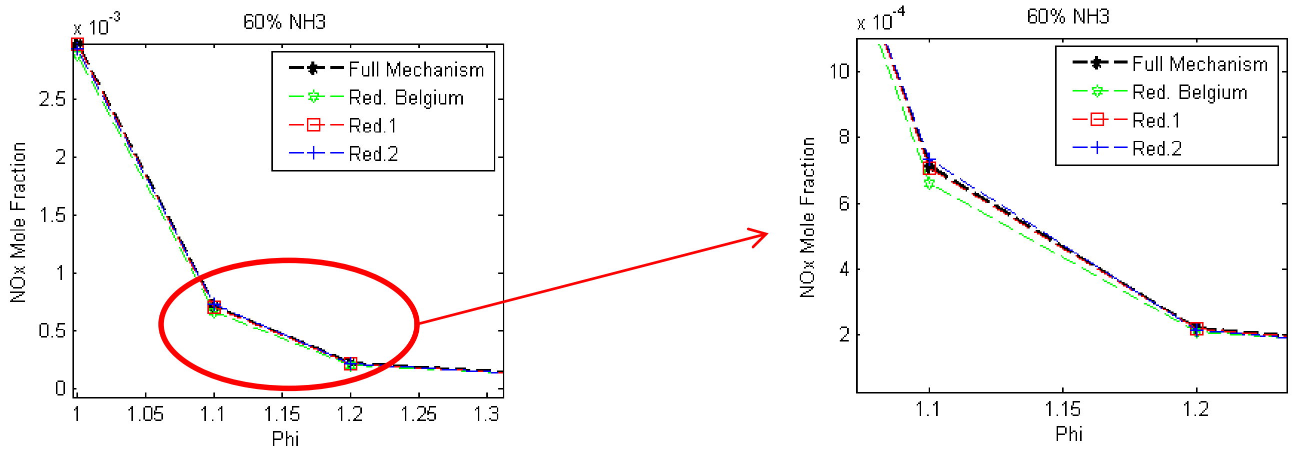


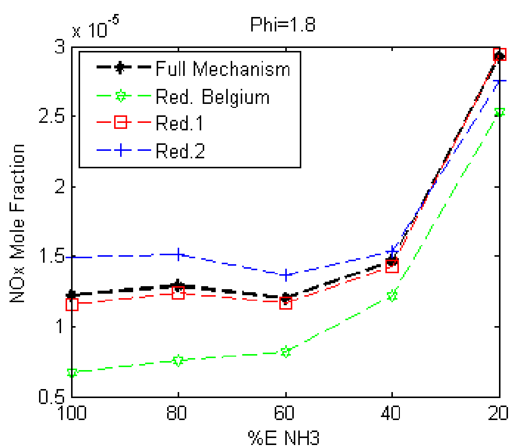
KOÇ UNIVERSITY

RESULTS

Reduced Mechanism

NOx Emission Prediction

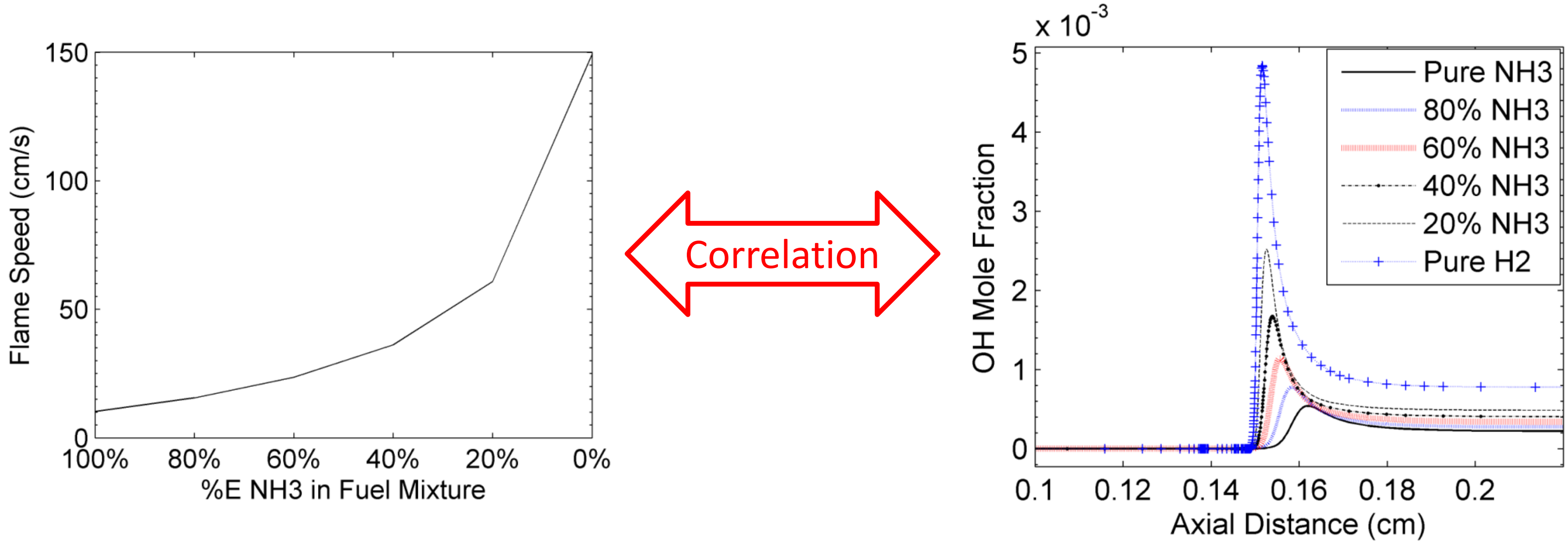




P=17 bar, T=673 K

RESULTS

Importance of OH radical in flame speed



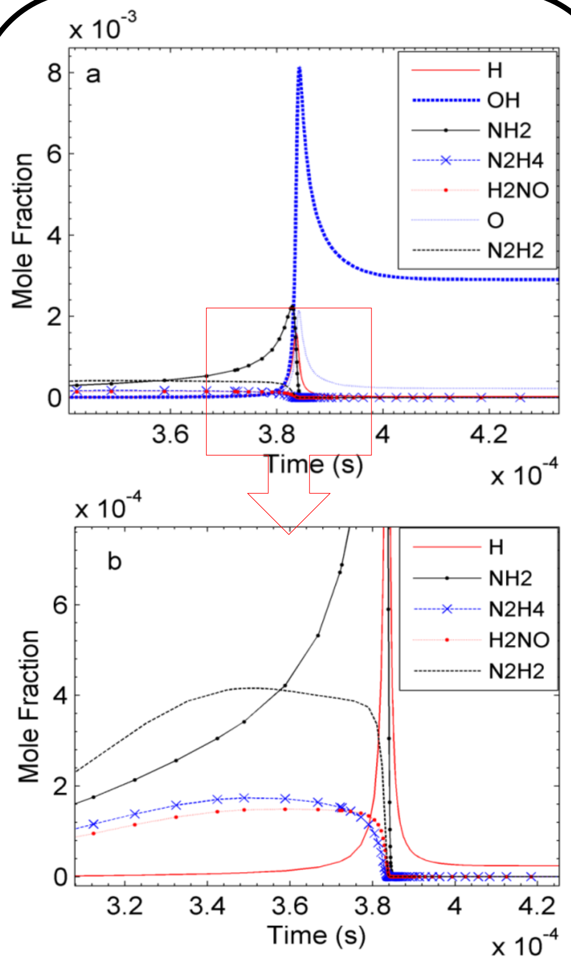
ϕ = 0.5, P=17 bar, T= 673 K

KOÇ UNIVERSITY

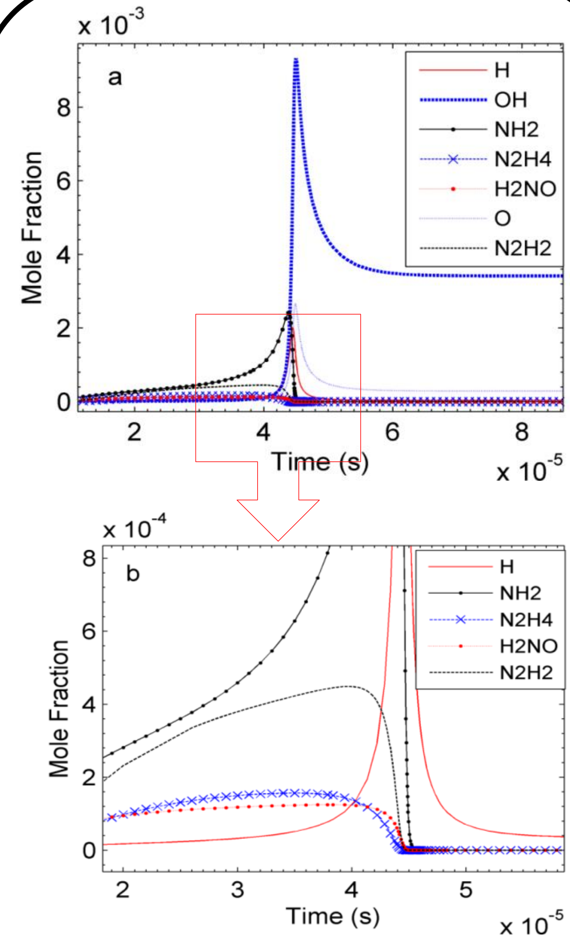
RESULTS

Autoignition

Importance of radicals in autoignition and ignition initiation



100%NH_3



80%NH_3

Accumulation of influential radicals close to the ignition time

ϕ=0.5, T=1300 K, P=17 bar

KOÇ UNIVERSITY

Outline

- Why ammonia?
- Challenges
- Chemical Kinetics Results
- Ongoing Experimental Research

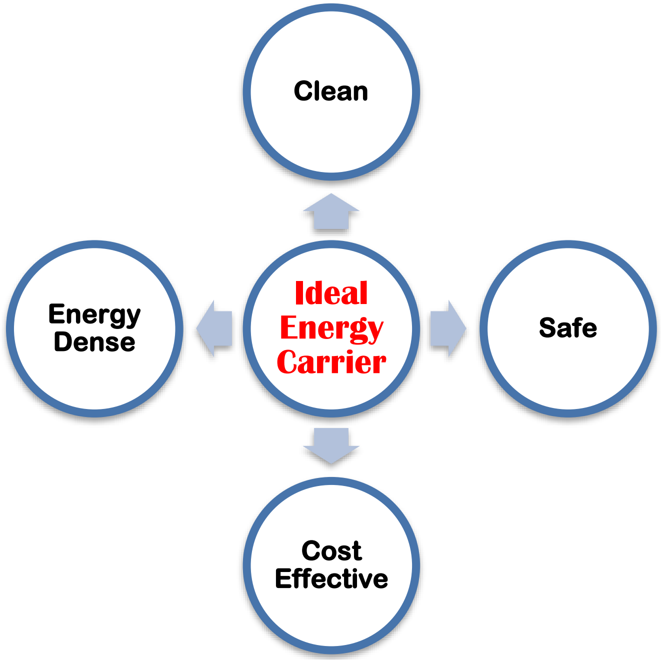
THE ENERGY PROBLEM

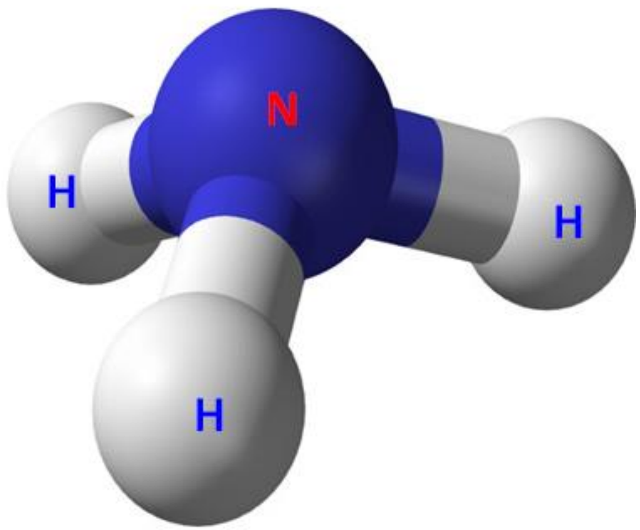
- Extensive use of fossil fuels
- Major problems: Human health and welfare, environmental issues
- A hot concern: Replacing current energy carriers
- The Intergovernmental Panel on Climate Change (IPCC) report: Atmospheric CO2 levels rose almost twice as fast in the first decade of this century

«THE WORLD MUST RAPIDLY MOVE AWAY FROM CARBON-INTENSIVE FUELS»

KOÇ UNIVERSITY

IDEAL ENERGY CARRIER





NH_3 as a Green Energy Source

Review

- Why ammonia?