NO$_x$ emission analysis and flame stabilization of ammonia-hydrogen-air premixed flames

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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
Challenges with NH3 combustion

- Slow kinetics (low flame speed)
- NH3, a source of fuel NOx in flames

Standard Temperature and Pressure
Air as oxidizer

A simplified reaction mechanism

Previous Study

Chemical Kinetics Study

- Flame Speed
  - Sensitivity Analysis
  - Effect of %NH3
  - Effect of φ
  - Effect of inlet T

- Ignition Delay Time
  - Effect of %NH3
  - Effect of φ
  - Effect of inlet T

- NOx Emission
  - NOx Sensitivity Analysis
  - Effect of %NH3
  - Effect of φ
  - Effect of inlet T

Goal
• 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
Previous Study

Comparison with the experimental data

![Graph showing the comparison between theoretical and experimental flame speeds.](chart)

- Full Konnov
- Red. Mech.1
- Red. Mech.2
- Red. by Duynslaegher et al.
- Exp. Van Wonterghem et al.
- Exp. Duynslaegher et al.
Quantitative comparison with **experimental data** (% discrepancy)

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Previous Study

Perfomance Chart

Chemical Kinetics Study

Reduced Mech.

Ammonia - O2 - N2
Stoichiometric
STP condition

Normalized CPU time

Average deviation from experimental data (%)

Full Konnov Mech.
Red. Mech.1
Red. Mech.2
Duynslaegher et al.
**RESULTS**

**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\textsubscript{x} emission under the rich conditions

\[ P=17 \text{ bar}, T=673 \text{ K} \]
Combustion Chamber
Experimental Study Scope

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

Methods:
- Dump Combustor
- Bluff Body
- Disc
- Porous Block

Goal:
- Chem. Kin.
- Num. Sim.
- Exp. Std.
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
Thank You

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Previously Discussed

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

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\( \phi = 0.5 \)
P=17 atm, \( \phi = 0.5 \)

\[
\begin{align*}
\text{NH}_3 + \text{OH} &= \text{NH}_2 + \text{H}_2 \text{O} \\
\text{HNO} + \text{NH}_2 &= \text{NH}_3 + \text{NO} \\
\text{NH}_3 + \text{O} &= \text{NH}_2 + \text{OH} \\
\text{NH}_3 + \text{NH}_2 &= 2\text{NH}_2 \\
\text{N}_2\text{H}_4 + \text{OH} &= \text{NH}_3 + \text{H}_2 \text{O} \\
\text{NH}_3 + \text{M} &= \text{NH}_2 + \text{H} + \text{M} \\
\text{H}_2\text{NO} + \text{NH}_2 &= \text{HNO} + \text{NH}_3 \\
\text{HNOH} + \text{NH}_2 &= \text{HNO} + \text{NH}_3 \\
\text{NH}_3 + \text{NH}_2 &= \text{N}_2\text{H}_3 + \text{H}_2 \\
\text{NH}_2 + \text{NH} &= \text{NH}_3 + \text{N} \\
\text{N}_2\text{H}_2 + \text{NH}_2 &= \text{NH}_3 + \text{NH}_3 + \text{N} \\
\text{HONO} + \text{NH}_2 &= \text{NO} + \text{NH}_3 \\
\text{N}_2\text{H}_4 + \text{NH}_2 &= \text{N}_2\text{H}_3 + \text{NH}_3 \\
\text{NH}_3 + \text{H} &= \text{NH}_2 + \text{H}_2 \\
\text{N}_2\text{H}_3 + \text{NH}_2 &= \text{NH}_3 + \text{N}_2\text{H}_2
\end{align*}
\]
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
    - $\text{NO}_2 + \text{H} \leftrightarrow \text{NO} + \text{OH}$
    - $\text{HNO} + \text{H} \leftrightarrow \text{NO} + \text{H}_2$
    - $\text{HNO} + \text{OH} \leftrightarrow \text{NO} + \text{H}_2\text{O}$

- **Decoupling thermal NOx from total NOx**

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

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

$\phi = 0.5$
RESULTS

Reduced Mechanism

NOx Emission Prediction

\( P=17 \text{ bar}, T=673 \text{ K} \)
RESULTS

Importance of OH radical in flame speed

ϕ = 0.5, P = 17 bar, T = 673 K
RESULTS

Autoignition

Importance of radicals in autoignition and ignition initiation

φ=0.5, T=1300 K, P=17 bar

Accumulation of influential radicals close to the ignition time
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»
NH₃ as a Green Energy Source
Review

- Why ammonia?