An Experimental and Modeling Study of NO$_x$- CO Formation in High Hydrogen Content (HHC) Fuels Combustion in Gas Turbine Applications

(DE-FE0012005)

Tanvir Farouk
Bihter Padak

University of South Carolina, Columbia, SC 29208, USA

Fred Dryer

Princeton University, Princeton, NJ 08544, USA
(University of South Carolina, SC 29208, USA)

2016 University Turbine System Research Workshop
Blacksburg, VA

November 1$^{\text{st}}$ – 3$^{\text{rd}}$, 2016
Project Participants

University of South Carolina and Princeton University

PI: Dr. Tanvir Farouk, Assistant Professor
University of South Carolina – Mechanical Engineering

  • Sheikh Farhan Ahmed – Graduate Student
  • Fahd Ebna Alam – Graduate Student

Co-PI: Dr. Bihter Padak, Assistant Professor
University of South Carolina – Chemical Engineering

  • Nazli Asgari – Graduate Student

Co-PI: Dr. Frederick Dryer, Professor
Princeton University – Mechanical and Aerospace Engineering

  • Mac Haas – Technical Staff
Objectives

• Detailed and validated coupled HHC + NO\textsubscript{x} kinetic model

• New experimental speciation data for the oxidation kinetics of HHC fuel compositions in presence of impurities.

• Understanding of CO, NO and NO\textsubscript{2} formation and interactions in hot and cold flow interactions.

• Detailed and reduced kinetic models for HHC fuels including detailed fuel compositions and NO\textsubscript{x}.

*Improved, higher fidelity tools for engineering design!*
Tasks

• Study of reactivity and speciation data for NO$_x$ under various conditions

• Studies of CO, NO, NO$_2$ formation and conversion for NO - NO$_2$ in mixing layers

• Studies of high pressure HHC fuel kinetics using a High Pressure Laminar Flow Reactor (HPLFR)

• Kinetic assessment, validation and development of a comprehensive HHC fuel + NO$_x$ kinetic mechanism
Presentation Outline

• Research Team Members

• Project Objectives

• Research Tasks

• Year 3 progress

  - Measurement of NO\textsubscript{x} Perturbed Oxidation Experiments
  - Kinetic Modeling of NO\textsubscript{x} formation in HHC Fuels
  - Coupled CFD + Kinetics Modeling and Simulations
    - Tanvir Farouk (Fred Dryer)

  - Experiments for Speciation Measurements
    - Bihter Padak

• Summary
• Predictions of \( \text{NO}_x \) to address strict emission standards

• Trace emittents – \( \text{NO}_x \) influences the global and intricate combustion dynamics

• Fuel impurities – source of fuel (C\(_1\), C\(_2\) …) – emissions

Unless one considers the **interactions of small species and emittents**, particularly on natural gas combustion the resulting model will likely have poor fidelity to be considered for engineering applications.
Measurement of NO\textsubscript{x} perturbed oxidation experiments
Influence of Trace Nitrogen Oxides on Natural Gas Oxidation

Nominal Feed Condition

- CH$_4$ = 9800 ppm (± ~2%)
- C$_2$H$_6$ = 200 ppm (± ~4%)
- O$_2$ = 10150 / 20300 / 40600 ppm (± ~2%)
- φ = 2.0 / 1.0 / 0.5
- Ar = Balance
- Q$_{total}$ = 1300 sccm
- NO = 25 ppm (± 1 ppm)
- T = 819 ± 5 K

P = 10 atm  
T = 820 K

BUT WHY THESE MODELS?

Kinetic Models

<table>
<thead>
<tr>
<th>Model</th>
<th># of Species</th>
<th># of Elementary Rxn</th>
</tr>
</thead>
<tbody>
<tr>
<td>GRI MECH 3.0 (2000)</td>
<td>54</td>
<td>325</td>
</tr>
<tr>
<td>Dagaut et al. (CST 2005)</td>
<td>148</td>
<td>1084</td>
</tr>
<tr>
<td>Konnov (C&amp;F 2009)</td>
<td>129</td>
<td>1231</td>
</tr>
<tr>
<td>Gersen et al. (PROCI 2011)</td>
<td>136</td>
<td>979</td>
</tr>
<tr>
<td>Mathieu et al. (Fuel 2016)</td>
<td>166</td>
<td>1204</td>
</tr>
</tbody>
</table>

(Haas & Dryer, JPC-A 2014)
Non-NO\textsubscript{x} Perturbed case (\(\varphi = 1.0\))

Simulation Initial Condition:
\(X_{\text{CH}_4} = 9763\) ppm
\(X_{\text{C}_2\text{H}_6} = 204\) ppm
\(X_{\text{C}_2\text{H}_4} = 1\) ppm
\(X_{\text{O}_2} = 20238\) ppm

Balance Ar

- No evidence of reaction for measured profiles of CH\textsubscript{4}, O\textsubscript{2} and C\textsubscript{2}H\textsubscript{6}.

- Few ppm of C\textsubscript{2}H\textsubscript{4} quantified @ distinct 950 cm\textsuperscript{-1} FTIR wave number.

- Conditions of incipient of reactions. C\textsubscript{2}H\textsubscript{6} oxidation via flux through C\textsubscript{2}H\textsubscript{5} \(\leftrightarrow\) C\textsubscript{2}H\textsubscript{4}.

- GRI 3.0, CRECK & Zhao et al. is predicting reasonable @ 4.0s Rel. Plug Flow Time.

Simulation strategy: Experimentally acquired initial conditions + experimentally measured temperature imposition (CHEMKIN-PRO\textsuperscript{®}). No time-shift is applied.
Non-NO$_x$ Perturbed case ($\varphi = 1.0$)

Can time-shift improve the model predictions?

- GRI 3.0, CRECK & Zhao et al. is predicting reasonable @ 4.0s Rel. Plug Flow Time.
Time-shifted Analysis of Non-NOx Perturbed Case ($\phi = 1.0$)

Even after time-shift, other model predictions cannot be improved, suggesting varying degree of reactivity.

Konnov (2009) and Dagaut et al. (2005) are significantly divergent with drastic change in slope.

Subset of reactions describing $C_2$ chemistry in each may be responsible for the disparate predictions.

GRI 3.0 is non-reactive, like this case, for NOx perturbed reactive cases → Thus, neglected altogether.
Trace NO\textsubscript{x} Perturbed Case (φ = 1.0)

PFR-PFR Analysis (Solid Line): PFR Simulation with time-shift @ 50% CH\textsubscript{4} depletion

PSR-PFR Analysis (Dash Line): Adiabatic PSR targeting 1\textsuperscript{st} data point matching, followed by PFR simulation.

- Gersen and Mathieu models essentially bound profiles of all of the experimentally measured major species.

- However, NO\textsubscript{x} mole fraction predictions indicate near-complete destruction of NO\textsubscript{x} (NO+NO\textsubscript{2}) \( \Rightarrow \) CH\textsubscript{3}NO\textsubscript{2}
**Trace NO<sub>x</sub> Perturbed Case (φ = 0.5)**

**PFR-PFR Initialization**: Experimentally measured input at relative time, t = 0

**PSR-PFR Initialization**: Nominal condition as input to PSR. Vary residence time, τ<sub>PSR</sub> to match experimentally measured input at relative time, t = 0.
Trace NO$_x$ Perturbed Case (φ = 2.0)

Similar model predictions as stoichiometric and lean case.
Kinetic Analysis thru Flux Analysis ($\varphi = 1.0$, PSR-PFR Approach)
Kinetic Analysis # Konnov Model

- In Konnov (2009) model, there is no flux through the channel of CH$_3$O$_2$ (both NO$_x$ perturbed and non-perturbed case)

\[
\text{CH}_3 \rightarrow \text{CH}_3\text{O} (-78.3\%, \text{NO}_2) \rightarrow \text{CH}_2\text{O} (-99.5\%, \text{O}_2+\text{m})
\]

- Interestingly, CH$_3$O$_2$ species is included in the model!

**Unperturbed Condition**

- Following reactions are known to consume CH$_3$

\[
\text{CH}_3 + \text{O}_2 \leftrightarrow \text{CH}_3\text{O}_2 \quad \text{(R1)}
\]

& this reaction is not competitive with either

\[
\text{CH}_3 + \text{O}_2 \leftrightarrow \text{CH}_2\text{O} + \text{OH} \quad \text{(R2)}
\]

and/or

\[
\text{CH}_3 + \text{HO}_2 \leftrightarrow \text{CH}_3\text{O} + \text{OH} \quad \text{(R3)}
\]

- Eventually, the model predicts significant CH$_3$ consumption via CH$_2$O & CH$_3$O formation

- Both these reactions (R2 & R3) convert slowly reacting CH$_3$ to fast reacting species (CH$_2$O & CH$_3$O) plus OH radicals. This explains why the model shows reactivity!
**Kinetic Analysis # Konnov Model**

**NO\textsubscript{x} Perturbed Case**

- An important NO ⇔ NO\textsubscript{2} recycling reaction
  \[
  \text{CH}_3\text{O}_2 + \text{NO} \rightleftharpoons \text{CH}_3\text{O} + \text{NO}_2 \quad (R4)
  \]

  & the above reaction will be compared to
  \[
  \text{CH}_3 + \text{NO}_2 \rightleftharpoons \text{CH}_3\text{O} + \text{NO} \quad (R5)
  \]

**BUT, “CH\textsubscript{3}O\textsubscript{2}” Chemistry is found to be Questionable !!!**

Thus, CH\textsubscript{3}O\textsubscript{2}-mediated NO\textsubscript{x} recycling loop presents a potential bottle-neck. This leads to accumulation of NO via R5.

- Remaining NO\textsubscript{x} cycling channel
  \[
  \text{HO}_2 + \text{NO} \rightleftharpoons \text{OH} + \text{NO}_2 \quad (R6)
  \]

- Konnov model also lacks
  The formation & destruction of Nitro-Alkyl
  (Particularly, CH\textsubscript{3}NO\textsubscript{2})
  \[
  \text{CH}_3 + \text{NO}_2 \rightleftharpoons \text{CH}_3\text{NO}_2 \quad (R7)
  \]
  HONO Reaction
  \[
  \text{CH}_4 + \text{NO}_2 \rightleftharpoons \text{CH}_3 + \text{HONO} \quad (R8)
  \]
Kinetic Analysis # Mathieu and Gersen Model

Flux Analysis of Unperturbed Case ($\phi = 1.0$)

1. Qualitatively similar $C_0-C_2+NO_x$ coupling pathways.
2. Predict similar profiles of NO, NO$_2$, and CH$_3$NO$_2$ evolution.

- Exists discrepancy, particularly at longer residence time.
- At longer residence time, NO$_x$ species equilibrates.
- Continuing need to study the coupling of NOx chemistry to the chemistry of small reactive species generated from methane/natural gas oxidation.

3. Unclear whether the predicted net sequestration of NOx into CH3NO2 is due to chemistry directly linked to CH$_3$NO$_2$, or
   - An imbalanced NO$_x$ flux through other reactions (such as R5 & R6)
Trace NO$_x$ Perturbed Case (φ = 1.0): Present Model
Kinetic Modeling of NO$_x$
Proposed \( \text{H}_2/\text{CO}/\text{NO}_x \) Model

- 77 species, 442 reactions
- \( \text{H}_2/\text{C}_1-\text{C}_4/\text{NO}_x \) Model
  - 302 species, 1952 reactions


**Prompt-NO Route Updates**

HCN $\rightarrow$ one of the major intermediates in prompt-NO kinetics

12 additional reactions and 9 rate updates are proposed based on the path flux comparisons of the NO$_x$ model of Dagaut et al. (2008) and the proposed model

Table I  Reactions and forward rate parameters for the modified Fenimore reaction pathways

<table>
<thead>
<tr>
<th>Reactions</th>
<th>A</th>
<th>b</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. CN + HNO = HCN + NO</td>
<td>1.80E+13</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>2. CN + CH$_2$O = HCN + HCO</td>
<td>4.20E+13</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>3. HCN + N$_2$ = H + CN + N$_2$</td>
<td>3.60E+26</td>
<td>-2.60</td>
<td>124890</td>
</tr>
<tr>
<td>4. HCN + M = HNC + M [\text{AR/0.7/ H$_2$O/7.0/ CO$_2$/2.0}]</td>
<td>1.60E+26</td>
<td>-3.23</td>
<td>54600</td>
</tr>
<tr>
<td>5. HCN + OH = HNCO + H</td>
<td>2.80E+13</td>
<td>0.0</td>
<td>3700</td>
</tr>
<tr>
<td>6. HNCO + O$_2$ = HNO + CO$_2$</td>
<td>1.0E+12</td>
<td>0.0</td>
<td>35000</td>
</tr>
<tr>
<td>7. NCO + NO = N$_2$O + CO</td>
<td>4.00E+19</td>
<td>-2.16</td>
<td>1743</td>
</tr>
<tr>
<td>8. NCO + NO = N$_2$ + CO$_2$</td>
<td>1.50E+21</td>
<td>-2.74</td>
<td>1824</td>
</tr>
<tr>
<td>9. HCNO + OH = NCO + H + OH</td>
<td>4.5E+12</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>10. HCNO + OH = NCO + H$_2$O</td>
<td>3.50E+12</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>11. HNCO + OH = HCO + HNO</td>
<td>4.50E+12</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>12. HCNO + OH = NO + CO + H$_2$</td>
<td>1.42E-07</td>
<td>5.64</td>
<td>9220</td>
</tr>
<tr>
<td>13. NO$_2$ + HCO = HONO + CO [\text{N$_2$/0.0/ O$_2$/1.5/ H$_2$O/10.0}]</td>
<td>6.50E+12</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>14. HOCN + O = NCO + OH</td>
<td>1.70E+08</td>
<td>1.50</td>
<td>4133</td>
</tr>
<tr>
<td>15. HOCN + OH = HCO + H$_2$O</td>
<td>1.20E+06</td>
<td>2.0</td>
<td>-248</td>
</tr>
<tr>
<td>16. H$_2$CN + OH = HCN + H$_2$O</td>
<td>1.50E+19</td>
<td>-2.18</td>
<td>2166</td>
</tr>
<tr>
<td>17. HOCN + OH = HCH + OH</td>
<td>7.20E+10</td>
<td>0.841</td>
<td>8612.0</td>
</tr>
<tr>
<td>18. CN + H$_2$O = HCN + OH</td>
<td>3.90E+06</td>
<td>1.83</td>
<td>10300</td>
</tr>
<tr>
<td>19. OH + HCN = HOCN + H</td>
<td>5.90E+04</td>
<td>2.40</td>
<td>12500</td>
</tr>
<tr>
<td>20. OH + HCN = HNCO + H</td>
<td>2.00E-03</td>
<td>4.0</td>
<td>1000</td>
</tr>
<tr>
<td>21. HOCN + H = HNCO + H</td>
<td>3.10E+08</td>
<td>0.84</td>
<td>1917</td>
</tr>
</tbody>
</table>
Prompt-NO Route Updates

HCN $\rightarrow$ one of the major intermediates in prompt-NO kinetics

Dagaut et al. (2000) JSR data for HCN/H\textsubscript{2}O/N\textsubscript{2} oxidation used to compare performance of the proposed model

Solid line: \textit{w/o updates}  
Dashed line: \textit{w updates}  

\textit{Dagaut et al., Combust. Sci Tech 155 (2000)}  
\textit{Dagaut et al., Prog Energy Combust Sci 34 (2008)}
Prompt-NO Route Updates

HNCO → a significant intermediate in fuel-nitrogen oxidation

Flow tube experiments of Glaborg et al. (1994) on the effects of NO and CO on HNCO oxidation used to check the updated model performances

Reasonable agreements with the experimental findings are observed with the updated model

Glarborg et al., Combust. Flame 98 (1994)
Multi-dimensional Laminar Reacting Flow Modeling

- Experiments were simulated using an in-house multi-dimensional laminar reacting flow model which solves the conservation equations.
- Two-dimensional axi-symmetric analysis of syngas/NO\textsubscript{x} oxidation in the McKenna burner and its associated tube arrangement was performed adopting the open-source OpenFOAM® framework.
- Detailed syngas/NO\textsubscript{x} oxidation chemistry of Ahmed et al.\textsuperscript{1} was employed in the simulation which includes 77 species and 442 elementary reactions.

**POST FLAME MODEL - REACTIVITY**

- The McKenna burner itself is not computationally resolved instead the post flame reactivity is modeled.
- The post flame combustion products obtained from the CHEMKIN PRO burner stabilized module were provided as the inlet boundary conditions for this model.
- The wall temperature was prescribed to be room temperature (300 K).
- The experimental measurements of the centerline temperature and NO\textsubscript{x} speciation were compared with the post flame modeling results.

Multi-dimensional Laminar Reacting Flow Modeling: Post Flame Model

100 ppm initial NO doping

Recirculation bubbles formed at the dead zone

NO & NO\textsubscript{2} concentration contours

H\textsubscript{2}:CO = 1, \(\varphi = 0.5\), flow rate 4 slpm, 100 ppm NO feed, Air = 0.0713 kg/s, Fuel = 0.00858 kg/s
100 ppm initial NO doping

H$_2$:CO = 1, $\varphi$ = 0.5, flow rate 4 slpm, 100 ppm NO feed, Air = 0.0713 kg/s, Fuel = 0.00858 kg/s
Multi-dimensional simulations show an initial NO to NO$_2$ conversion very close to the inlet.
Summary

• Influence of trace impurities on combustion characteristics.

• Trace NO\textsubscript{x} – emittents can alter the combustion behavior, global/optimized models can not capture intricate features. Performance of existing model has been analyzed and inclusions are proposed.

• The validated H\textsubscript{2}/CO/NO\textsubscript{x} model has been updated to included HCN routes – prompt NO routes.

• Multi-dimensional CFD+Kinetic model/simulations conducted to investigate the NO\textsubscript{x} speciation experiments.
Experiments for Speciation Measurements
Schematic of Experimental Setup

**Experimental Conditions**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Phi$</td>
<td>0.5-1</td>
</tr>
<tr>
<td>$\text{H}_2/\text{CO}$</td>
<td>0.25-1</td>
</tr>
<tr>
<td>Total Flow Rate</td>
<td>3-6 SLPM</td>
</tr>
</tbody>
</table>
Flame Temperature Measurement / Simulation

Temperature predictions with CHEMKIN PRO burner stabilized module simulations compared against experimental measurements

**H₂/CO: 1 and 4LPM**

**Φ: 0.5 and 4LPM**
Multi-dimensional Temperature Measurements/Predictions

H₂/CO:1  Φ: 0.5

2-D Temperature Profile

Radial Temperature Profile

Centerline Temperature Profile

Experiment (525 points)
Multi-dimensional Temperature Measurements/Predictions

Experiment

Simulation
H$_2$/CO:1 and 100 ppm initial NO doping

As $\Phi$ increases, NO concentration ↑
NO$_2$ concentration ↓

One of the dominant NO formation paths contributes more for $\Phi = 1.0$ (34%) than for $\Phi = 0.5$ (20%)

N + OH = NO + H (R1)

More dominant NO to HNO path through NO + H(+M) = HNO(+M) for $\Phi = 1.0$ (33%) than for $\Phi = 0.5$ (12%)

Less dominant NO to NO$_2$ path through NO + O(+M) = NO$_2$(+M) for $\Phi = 1.0$ (43%) than for $\Phi = 0.5$ (73%)

• No N$_2$O was observed.
Experiments were repeated with uncooled probe to see if there is any NO$_2$ formation in the sampling probe.

Consistent results were obtained for both cooled and uncooled probes.
NO$_x$ Speciation Measurement/Prediction by Flame Simulation

$\Phi =$0.5 and 100 ppm initial NO doping

HNO Source

$\text{NH} + \text{OH} = \text{HNO} + \text{H}$ \hspace{1cm} (R4)

15\% ($\text{H}_2/\text{CO}:0.25$), 45\% ($\text{H}_2/\text{CO}:1$)

$\text{NH} + \text{O}_2 = \text{HNO} + \text{O}$ \hspace{1cm} (R5)

6\% ($\text{H}_2/\text{CO}:0.25$), 12\% ($\text{H}_2/\text{CO}:1$)

More dominant for $\text{H}_2/\text{CO}:1$

Lower NO production for $\text{H}_2/\text{CO} = 1$

$\text{NH} + \text{O} = \text{NO} + \text{H}$ \hspace{1cm} (R6)

67\% ($\text{H}_2/\text{CO}:0.25$), 55\% ($\text{H}_2/\text{CO}:1$)

As $\text{H}_2/\text{CO}$ increases \hspace{1cm} NO concentration $\downarrow$
NO\textsubscript{x} Speciation Measurement/Prediction by Flame Simulation

$\Phi = 0.5$ and 75 ppm initial NO\textsubscript{2} doping

- Overall contribution of NO to HNO formation:
  - $\text{NO} + \text{H}(+\text{M}) = \text{HNO}(+\text{M})$ (R7) 11%
  - Small percentage of NO comes from NO\textsubscript{2}:
    - $\text{NO}_2 + \text{H} = \text{NO} + \text{OH}$ (R8) 3%
  - Other HNO Sources are more dominant:
    - $\text{NH} + \text{OH} = \text{HNO} + \text{H}$ (R4) 47%
    - $\text{NH} + \text{O}_2 = \text{HNO} + \text{O}$ (R5) 13%

As $\text{H}_2/\text{CO}$ increases, NO concentration decreases.

More dominant for $\text{H}_2/\text{CO}: 1$
Lower NO
**NO\textsubscript{x} Speciation Measurement/Prediction by Flame Simulation**

**H\textsubscript{2}/CO:1 and 75 ppm initial NO\textsubscript{2} doping**

One of the dominant NO formation paths contributes more for $\phi = 1.0$ (33%) than for $\phi = 0.5$ (18%)

\[ \text{N + OH = NO + H (R1)} \]

More dominant NO to HNO path through $\text{NO + H(+M) = HNO(+M)}$ for $\phi = 1.0$ (33%) than for $\phi = 0.5$ (11%)

Less dominant NO to NO\textsubscript{2} path through $\text{NO + O(+M) = NO\textsubscript{2}(+M)}$ for $\phi = 1.0$ (48%) than for $\phi = 0.5$ (75%)

As $\phi$ increases

- NO concentration $\uparrow$
- NO\textsubscript{2} concentration $\downarrow$

Qualitative trends are captured for speciation predictions but they are not in quantitative agreement due to possible multi-dimensional transport - possible axial and radial variation not captured in the model.
H₂/CO=1, Φ=0.5 and 100 ppm initial NO doping

**NO₂-NO interconversion paths**
- \( \text{NO}_2 + H = \text{NO} + \text{OH} \) (R8) 86%
- \( \text{NO} + O(+M) = \text{NO}_2(+M) \) (R9) 100%
- \( \text{NO}_2 + O = \text{NO} + \text{O}_2 \) (R10) 9%
- \( \text{NO}_2 + \text{OH} = \text{NO} + \text{HO}_2 \) (R11) 5%

**NO-HNO interconversion**
- \( \text{NO} + \text{H}(+M) = \text{HNO}(+M) \) (R7) 39%
- \( \text{HNO} + H = \text{NO} + \text{H}_2 \) (R12) 32%
- \( \text{HNO} + \text{OH} = \text{NO} + \text{H}_2\text{O} \) (R13) 55%
- \( \text{HNO} + O = \text{NO} + \text{OH} \) (R14) 13%
Centreline NO\textsubscript{x} Speciation Profile with Multi-dimensional Laminar Reacting Flow Modeling

\( \frac{H_2}{CO}=1, \ \Phi=0.5 \) and 75 ppm initial NO\textsubscript{2} doping

\[ \text{NO}_2-\text{NO interconversion paths} \]
- \( \text{NO}_2 + H = \text{NO} + \text{OH} \) (86%)
- \( \text{NO} + \text{O}(+\text{M}) = \text{NO}_2(+\text{M}) \) (100%)
- \( \text{NO}_2 + \text{O} = \text{NO} + \text{O}_2 \) (9%)
- \( \text{NO}_2 + \text{OH} = \text{NO} + \text{HO}_2 \) (5%)

\[ \text{NO-HNO interconversion} \]
- \( \text{NO} + \text{H}(+\text{M}) = \text{HNO}(+\text{M}) \) (39%)
- \( \text{HNO} + \text{H} = \text{NO} + \text{H}_2 \) (32%)
- \( \text{HNO} + \text{OH} = \text{NO} + \text{H}_2\text{O} \) (55%)
- \( \text{HNO} + \text{O} = \text{NO} + \text{OH} \) (13%)
High Pressure System

- Sampling Probe
- Thermocouple
- Electrical feed through igniter
- Quartz Diffuser
  - Length = 35"
- Optical Windows
- Exhaust
- Pressure Transducer
- Back-pressure Regulator
- Pressure Gauge
- Ignitor feed through
- Exhaust port for ¼" SS Tubing
- Probe Sealing (Hex size: 1.25")
- Rupture Disk
- Shielding gas
- Tube size ½"
- Flange Center
- Cooling water In/Out
- Nitrogen
- Syngas/Air
- Back-pressure Regulator
- Water trap
- Relief valve
- Stainless steel chimney
- Stainless steel tubing
- Electrical feed throughs & Igniter
- Port (Sealing) Close to probe
- Exhaust port for ¼" SS Tubing
- 3.8125"
- Thermocouple Port (Sealing)
- 0.75" OD for 0.5" OD ¼" SS Tubing
High Pressure System

- Sampling Probe
- Thermocouple
- Electrical feed & igniter
- Optical Windows
- Exhaust
- Pressure Transducer
- Back-pressure Regulator
- Stainless steel chimney
- Quartz Diffuser
- Length = 35"
- Nitrogen
- Syngas/Air
- Burner
- Stainless steel tubing
- Electrical feed-throughs & Igniter
- Back-pressure Regulator
- Sampling Probe
- Optical Windows
Overall Summary

• NO\textsubscript{x} model for high hydrogen content fuel; model has been validated against a wide range of targets. Prompt pathways have been revised and updated.
• NO\textsubscript{x} perturbed natural gas oxidation experiments conducted in a flow reactor configuration. Presence of trace NO\textsubscript{x} significantly alters the oxidation behavior.
• The performance of different models are compared and analyzed against the experimental data.
• Multi-dimensional post flame CFD simulations conducted. The model captures the post flame reactivity with the coupled transport and detailed kinetics.
• Flame needs to be resolved numerically to obtain the NO-NO\textsubscript{2} conversion occurring prior to the flame.
• Axial and radial temperature profiles were obtained
• NO\textsubscript{x} speciation data at atmospheric pressure was collected at different conditions.
• There was a reasonable agreement between experimental data and simulations.

Future Work

• NO\textsubscript{x}-CO speciation data will be collected at higher pressures considering the effect of different parameters such as hydrocarbons and diluents.
• Effect of exhaust gas recirculation will be investigated.
Publications


• Ahmed, S., Santner, J., Padak, B., Dryer, F., Farouk, T., “Computational study of NO\textsubscript{x} formations at conditions relevant to gas turbine operation part II: NO\textsubscript{x} in high hydrogen content fuel combustion at elevated pressure” *Energy and Fuel* (2016), 30, 7691 - 7703.


• Santner, J., Ahmed, S., Farouk, T., Dryer, F., “Computational study of NO\textsubscript{x} formation at conditions relevant to gas turbine operating conditions” 9\textsuperscript{th} *U.S. National Combustion Meeting*, Cincinnati, Ohio, May 17 – 20, 2015.
Thank You
Temperature Measurements

**Flame T measurements**  **Radial and axial T profile measurements**

- Radiation correction was applied to T measurements
- Using the R-type thermocouple, the radiation loss was % 8

![Thermocouple diagram](image)