Measurement and Prediction of Radiative Non-equilibrium for Air Shocks Between 7-9 km/s

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Outline

• Motivation
• Experimental Approach
• Sample Data
  – Comparison of Data across two shock tubes at 0.14 Torr
  – Full data Set on data.nasa.gov
• Model Adjustments
  – Nitric Oxide (NO) Radiation
  – Revisions for Atomics, N2, N2+ - in paper
• Comparison of Predictions to Data
  – 0.01 Torr and 0.70 Torr
  – 0.05, 0.14 and 0.3 Torr in paper
• Conclusions
• Outlook
Motivation

- About 8% of Lunar Return radiative heating occurs below 9 km/s
  - Based on current models
- Return from lower altitude (e.g. EFT1) is entirely in this speed regime
- Radiation phenomena not well validated in this speed regime
Radiation is measured in EAST Facility
- 24” Diameter tubes for low (<0.1 Torr) pressure
- 4” Diameter tube for higher (>0.1 Torr) pressure

Measurement by between 2-4 spectrometers covering 190-1450 nm
Conditions Measured

- 51 shots between 7-9 km/s
  - 33 (27 good) on the 24” Tube (0.01, 0.05, 0.14 Torr)
    - 15 from 190-500 nm
    - 12 from 500-1450 nm
  - 18 (17 good) on the 4” Tube (0.14, 0.30, 0.50, 0.70 Torr)
    - All from 190-1450 nm
- Subset of 10 tests selected for further analysis (1 per pressure/wavelength/tube diameter combination):

<table>
<thead>
<tr>
<th>Shot No</th>
<th>Velocity (km/s)</th>
<th>Pressure (torr)</th>
<th>Range (nm)</th>
<th>Tube Diameter (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>8.18</td>
<td>0.01</td>
<td>190-500</td>
<td>60.33</td>
</tr>
<tr>
<td>32</td>
<td>8.57</td>
<td>0.01</td>
<td>500-1450</td>
<td>60.33</td>
</tr>
<tr>
<td>8</td>
<td>8.62</td>
<td>0.05</td>
<td>190-500</td>
<td>60.33</td>
</tr>
<tr>
<td>24</td>
<td>8.87</td>
<td>0.05</td>
<td>500-1450</td>
<td>60.33</td>
</tr>
<tr>
<td>20</td>
<td>8.29</td>
<td>0.14</td>
<td>190-500</td>
<td>60.33</td>
</tr>
<tr>
<td>22</td>
<td>8.36</td>
<td>0.14</td>
<td>500-1450</td>
<td>60.33</td>
</tr>
<tr>
<td>38</td>
<td>8.33</td>
<td>0.14</td>
<td>190-1450</td>
<td>10.16</td>
</tr>
<tr>
<td>42</td>
<td>8.09</td>
<td>0.3</td>
<td>190-1450</td>
<td>10.16</td>
</tr>
<tr>
<td>46</td>
<td>7.71</td>
<td>0.5</td>
<td>190-1450</td>
<td>10.16</td>
</tr>
<tr>
<td>50</td>
<td>7.34</td>
<td>0.7</td>
<td>190-1450</td>
<td>10.16</td>
</tr>
</tbody>
</table>

Model Tests

Paper

Consistency Check
Sample Data (190-500 nm)

- Spectra are resolved in wavelength and position behind shock
Sample Data (500-1450 nm)

- Spectra are resolved in wavelength and position behind shock
(somewhat) arbitrarily assign ±2 cm of peak as “non-equilibrium zone”

Integral of this, divided by tube diameter, is the “non-equilibrium metric”

Presented as function of wavelength: “spectral non-equilibrium metric”
• **Non-equilibrium metric composite from 4 different spectrometers**
• **Spectral Non-equilibrium Metric has units of radiance**
  – It is equal to the radiance accumulated through the non-equilibrium zone if the non-equilibrium region is optically thin
0.14 Torr Tube-Tube Comparison (190-500 nm)

- Spectral metric is larger in 4” tube than 24” tube
- Overlap region of spectrometer is consistent
- CN Contamination in 4” Tube
- Velocities differ, optical thickness may differ
  - Check predictions
• Some increase in radiation predicted at 8.33 km/s
• Increase is sensitive to rate model
• Prediction does not match data
 Tube Disagreement (190-500 nm)

- Median disagreement: 46% (cf. 16% predicted)
  - Not clear how much of remaining 30% is due to errors in prediction or experiment
- Divergence at low wavelength
  - 24” Tube calibration suspect based on S/N
- CN contamination radiance
0.14 Torr Tube-Tube Comparison (500-890 nm)

- **Molecular emission (500-700 nm)**
  - 4” Tube 30% larger than 24” Tube

- **Atomic radiation significantly higher in 4” Tube**
  - Lines may be optically thick
Predicted Non-equilibrium metric

- DPLR/NEQAIR prediction shows larger metric in 4” Tube
  - Indicates atomic lines are optically thick
- Molecular radiation not predicted by NEQAIR
Ratio of Tube measurements (500-890 nm)

- Ratio observed in EAST matches predicted ratio for atoms
Predictive Modeling

- DPLR/NEQAIR are used to produce 1D (stag. line) profiles for comparison to shock tube data
- Three “heritage” modeling options discussed
  - Park90 with \( Te = T_t \) (DPLR Default)
  - Park93 with \( Te = T_v \)
  - Johnston14 with \( Te = T_v \) (LAURA default)
- Revisions to Model will be discussed
  - Use data to guide reasonable modeling assumptions
  - Use third party measurements of input parameters
  - Do not “tune to fit”
  - Maintains some level of independence between model and data set
Spectral Non-equilibrium Metric

- Analysis will be divided by spectral features for discussion
NO Radiance

- **NO Radiance from (primarily) γ, ε bands**
  - Originate from $A^2\Sigma$ and $D^2\Sigma$ states
- **Also δ band ($C^2\Pi$)**
Underpredicted at all conditions, by all models
Boltzmann Radiance is typically an upper bound for non-equilibrium radiation (in compression)
Park models cannot match Boltzmann radiance at 0.7 Torr
   Must check reaction rates
Boltzmann radiation too high at 0.01 Torr
   Non-Boltzmann model needs examination
NO Reaction Kinetics

- NO Formation is driven by so-called Zel’dovich exchange Reactions:
  \[ \text{N}_2 + \text{O} \leftrightarrow \text{NO} + \text{N} \]
  \[ \text{O}_2 + \text{N} \leftrightarrow \text{NO} + \text{O} \]

- NO Destruction depends on direct dissociation:
  \[ \text{NO} + \text{M} \leftrightarrow \text{N} + \text{O} + \text{M} \]

We opt to carry rates from combustion literature (Tsang/Baulch)
Impact on NO concentration (0.7 Torr)

- Updating Exchange Reactions increases peak NO density
- Reducing dissociation rate reduces decay
- Changing the ratio of dissociation by atoms vs. molecules further increases NO density
  - Johnston follows Park: ratio is 22
  - Figure shows ratio of 1.0
  - Tsang recommended ratio of <1
NO Non-Boltzmann modeling

- For these conditions, NO non-Boltzmann is dominated by heavy particle processes
  - Internal excitation:
    \[ \text{NO}(X) + M \leftrightarrow \text{NO}(A,C,D) + M \]
  - Heavy particle impact Dissociation:
    \[ \text{NO}(A,C,D) + M \leftrightarrow N + O + M \]

- Internal excitation rates in NEQAIR are only approximate, fundamental data is not available

- The reverse of internal excitation is quenching: rates are available at 300K. Assume:
  \[ k_q = k_{q,0} \sqrt{\frac{T_i (K)}{300}} \]

- Heavy particle impact dissociation is updated to be consistent with rate chemistry
- Ratio of atomic to molecular driven dissociation is still undetermined
Adjust Atom/Molecule Rates

- Rates adjusted consistently in DPLR and NEQAIR
- Ratio of 5 matches 0.7 Torr data
- Also matches NO $\gamma$ at 0.01 Torr
- NO $\delta$ is overpredicted at 0.01 Torr
  - Possibly experimental error due to lower sensitivity in this region
Summary of Model Revisions

- **Flowfield model**
  - Update NO dissociation and exchange rates to be consistent with combustion literature
  - Alter ratio of NO dissociation by atoms vs. molecules to 5
  - Electron impact dissociation rate from radiation model used for flowfield
  - Associative Ionization controlled by T_e
  - Update selected charge exchange rates

- **Non-Boltzmann Radiation Model - Molecules**
  - Heavy particle dissociation rate consistent with flowfield dissociation rate
  - Use quenching rates from literature to calculate heavy particle excitation rates for molecules
  - Electron impact dissociation calculation corrected
    - Estimate and include contributions from excited states

- **Non-Boltzmann Radiation Model – Atoms**
  - Excitation rates updated to hybrid of Huo (dipole allowed) and Park (unallowed)
  - Include Associative Ionization process
Results – 0.7 Torr, 7.34 km/s (190-500 nm)

- NO and N\textsubscript{2}\textsuperscript{+} underpredictions rectified (mostly)
- N\textsubscript{2} 2\textsuperscript{nd} Positive Somewhat Overpredicted
- Reasonable match to temporal trend
Results – 0.01 Torr, 8.18 km/s (190-500 nm)

- $N_2^+$ still overpredicted
- $N_2$ 2nd Positive overpredicted
- NO matched 240-290nm (Gamma bands)
- NO overpredicted < 240 nm (Epsilon bands)
Results – 0.7 Torr, 7.34 km/s (500-890 nm)

- N₂ 1ˢᵗ Positive Matched
- Atomic lines nearly matched
- Reasonable match to temporal trend
Results – 0.01 Torr, 8.58 km/s (500-890 nm)

- Underprediction N₂ 1ˢᵗ Positive Matched
- Extra atomic lines eliminated
- Other atomic lines underpredicted
- Temporal trend shows spike at shock front
Results – 0.7 Torr, 7.34 km/s (890-1450 nm)

- Atomic overprediction eliminated, lines that are present are reasonably close
- Missing molecular radiation source (TBD)
- Temporal trend looks ok
Results – 0.01 Torr, 8.58 km/s (890-1450 nm)

- Atomic overprediction eliminated
- Integral matches data
- Spike observed at shock front, trend otherwise ok
Summary

- Non-equilibrium Radiation Data Measured from 7-9 km/s at 6 freestream pressures from 0.01-0.70 Torr
  - Comparison across two tubes with different diameter, calibration source indicate confidence in data of ~30% (in UV) or better (Vis/NIR)
  - Presentation focuses on highest and lowest pressure ranges

- Agreement to Predictive (DPLR/NEQAIR) Model has been improved
  - Underprediction of N₂/NO resolved by changes to rate chemistry, heavy particle excitation rates
  - N₂⁺ overpredicted at low pressure, revised rate/excitation model fixes underprediction at high pressure
  - Prediction of atomic radiation improved by
    - Changing excitation model (high energy states)
    - Including associative ionization in non-Boltzmann model (3p states)

- How does your model do?
  [https://data.nasa.gov/docs/datasets/aerothermodynamics/EAST/index.html](https://data.nasa.gov/docs/datasets/aerothermodynamics/EAST/index.html)
Work to go

- Low pressure overpredictions of
  - $\text{N}_2^+$: State specific associative ionization?
  - NO, $\text{N}_2$: Pre-dissociation rates?

- Missing molecular features in infrared (high pressure)

- Spike in shock front at low pressure

- Underpredicted atomic lines at low pressure

- non-Boltzmann associative ionization model: needs realistic statewise rates
Backup
Spectral Non-equilibrium Metric

- Identification of features suggests regions for further analysis

- 190-500 nm
  NO, N₂, N₂⁺

- 500-890 nm
  N₂, N, O (3p-3s)

- 900-1450 nm
  N, O (3d-3s)
### Reaction Rates

- There are between up to 23 reactions rates across the 3 models, 11 of which have some differences:

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Source/Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{NO} + \text{M} \leftrightarrow \text{N} + \text{O} + \text{M} )</td>
<td>Increased by Johnston</td>
</tr>
<tr>
<td>( \text{N}_2 + \text{O} \leftrightarrow \text{NO} + \text{N} )</td>
<td>Johnston used rate from Fujita, 2006</td>
</tr>
<tr>
<td>( \text{NO} + \text{O} \leftrightarrow \text{O}_2 + \text{N} )</td>
<td>Johnston uses rate from Bose, 1997</td>
</tr>
<tr>
<td>( \text{N} + \text{O} \leftrightarrow \text{NO}^+ + \text{e}^- )</td>
<td>Updated Park93, Johnston/Park90 same</td>
</tr>
<tr>
<td>( \text{N} + \text{N} \leftrightarrow \text{N}_2^+ + \text{e} ^- )</td>
<td>Updated Park93, Johnston/Park93 same</td>
</tr>
<tr>
<td>( \text{O} + \text{O} \leftrightarrow \text{O}_2^+ + \text{e} )</td>
<td>Updated Park93, Johnston/Park93 same</td>
</tr>
<tr>
<td>( \text{O}^+ + \text{NO} \leftrightarrow \text{N}^+ + \text{O}_2 )</td>
<td>Activation energies differ</td>
</tr>
<tr>
<td>( \text{N}^+ + \text{N}_2 \leftrightarrow \text{N}_2^+ + \text{N} )</td>
<td>Missing from Park90, Johnston/Park93 same</td>
</tr>
<tr>
<td>( \text{O}_2^+ + \text{O} \leftrightarrow \text{O}^+ + \text{O}_2 )</td>
<td>Missing from Park90*, Johnston/Park93 same</td>
</tr>
<tr>
<td>( \text{N}_2 + \text{e} \leftrightarrow \text{N} + \text{N} + \text{e} )</td>
<td>Differs across all three chemistries</td>
</tr>
<tr>
<td>( \text{O}_2 + \text{e} \leftrightarrow \text{O}_2^+ + \text{e} )</td>
<td>Missing from Park90/Park93</td>
</tr>
</tbody>
</table>

*As implemented in DPLR
## Reaction Molar Product (cm³/mol·s) n Ea (K) Controlling Temperature Ref

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Molecule/Atom</th>
<th>A</th>
<th>n</th>
<th>Ea (K)</th>
<th>(\sqrt{TT_{ev}})</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO + M → N + O + M</td>
<td>Molecule</td>
<td>1.5 × 10¹⁵</td>
<td>0</td>
<td>74,570</td>
<td>(\sqrt{TT_{ev}})</td>
<td>[21]</td>
</tr>
<tr>
<td>NO + M → N + O + M</td>
<td>Atom</td>
<td>7.3 × 10¹⁵</td>
<td>0</td>
<td>74,570</td>
<td>(\sqrt{TT_{ev}})</td>
<td>This work</td>
</tr>
<tr>
<td>N + e⁻ → N⁺ + 2e⁻</td>
<td></td>
<td>2.5 × 10³⁴</td>
<td>-3.82</td>
<td>168,600</td>
<td>(T_e)</td>
<td>[6]</td>
</tr>
<tr>
<td>O + e⁻ → O⁺ + 2e⁻</td>
<td></td>
<td>3.9 × 10³³</td>
<td>-3.78</td>
<td>158,500</td>
<td>(T_e)</td>
<td>[5]</td>
</tr>
<tr>
<td>N₂ + O → NO + N</td>
<td>Atom</td>
<td>9.0 × 10⁹</td>
<td>1.0</td>
<td>3,270</td>
<td>(T_t)</td>
<td>[24]</td>
</tr>
<tr>
<td>N + O → NO⁺ + e⁻</td>
<td></td>
<td>8.8 × 10⁸</td>
<td>1.0</td>
<td>31,900</td>
<td>(T_e)</td>
<td>[6]</td>
</tr>
<tr>
<td>N + N → N₂⁺ + e⁻</td>
<td></td>
<td>4.4 × 10⁷</td>
<td>1.5</td>
<td>67,500</td>
<td>(T_e)</td>
<td>[6]</td>
</tr>
<tr>
<td>O + O → O₂⁺ + e⁻</td>
<td></td>
<td>7.1 × 10²</td>
<td>2.7</td>
<td>80,600</td>
<td>(T_e)</td>
<td>[6]</td>
</tr>
<tr>
<td>N⁺ + N₂ → N₂⁺ + N</td>
<td></td>
<td>7.0 × 10⁶</td>
<td>1.47</td>
<td>13,130</td>
<td>(T_t)</td>
<td>This work</td>
</tr>
<tr>
<td>O⁺ + N₂ → N₂⁺ + O</td>
<td></td>
<td>9.1 × 10¹¹</td>
<td>0.36</td>
<td>22,800</td>
<td>(T_t)</td>
<td>[5]</td>
</tr>
<tr>
<td>O₂⁺ + O → O⁺ + O₂</td>
<td></td>
<td>4.0 × 10¹²</td>
<td>-0.09</td>
<td>18,000</td>
<td>(T_t)</td>
<td>[6]</td>
</tr>
<tr>
<td>O⁺ + NO → N⁺ + O₂</td>
<td></td>
<td>1.4 × 10⁵</td>
<td>1.9</td>
<td>26,600</td>
<td>(T_t)</td>
<td>[6]</td>
</tr>
<tr>
<td>NO⁺ + O₂ → O₂⁺ + NO</td>
<td></td>
<td>2.4 × 10¹³</td>
<td>0.41</td>
<td>32,600</td>
<td>(T_t)</td>
<td>[5]</td>
</tr>
<tr>
<td>NO⁺ + N → N₂⁺ + O</td>
<td></td>
<td>7.2 × 10¹³</td>
<td>0</td>
<td>35,500</td>
<td>(T_t)</td>
<td>[5]</td>
</tr>
<tr>
<td>NO⁺ + O → N⁺ + O₂</td>
<td></td>
<td>1.0 × 10¹²</td>
<td>0.5</td>
<td>77,200</td>
<td>(T_t)</td>
<td>[5]</td>
</tr>
<tr>
<td>O₂⁺ + N → N⁺ + O₂</td>
<td></td>
<td>8.7 × 10¹³</td>
<td>0.14</td>
<td>28,600</td>
<td>(T_t)</td>
<td>[5]</td>
</tr>
<tr>
<td>O₂⁺ + N₂ → N₂⁺ + O₂</td>
<td></td>
<td>9.9 × 10¹²</td>
<td>0</td>
<td>40,700</td>
<td>(T_t)</td>
<td>[5]</td>
</tr>
<tr>
<td>NO⁺ + N → O⁺ + N₂</td>
<td></td>
<td>3.4 × 10¹³</td>
<td>-1.08</td>
<td>12,800</td>
<td>(T_t)</td>
<td>[5]</td>
</tr>
<tr>
<td>NO⁺ + O → O₂⁺ + N</td>
<td></td>
<td>7.2 × 10¹²</td>
<td>0.29</td>
<td>48,600</td>
<td>(T_t)</td>
<td>[5]</td>
</tr>
<tr>
<td>NO + N⁺ → NO⁺ + N</td>
<td></td>
<td>1.8 × 10¹²</td>
<td>0.57</td>
<td>0</td>
<td>(T_t)</td>
<td>This work</td>
</tr>
</tbody>
</table>

### Notes

- **Park 90**
- **Park 93**
- **Combustion Literature**

**Evaluated from ion collision cross-section data**

**From electron-impact cross-sections**

**Adjusted to match data**
N₂ Model
**N₂ Radiance**

- **N₂ Features from**
  - 1\textsuperscript{st} Positive System \((B^3\Pi \rightarrow A^3\Pi)\)  \(500-750\) nm
  - 2\textsuperscript{nd} Positive System \((C^3\Pi \rightarrow B^3\Pi)\)  \(280-390\) nm
N$_2$ 1$^{\text{st}}$ Positive

- Underpredicted at all conditions
- Bonus Atomic Lines!
**N_2 2^{nd} Positive**

8.18 km/s, 0.01 Torr

- Underpredicted at all conditions

- Partly obscured by N_2^+ radiation at 0.01 Torr

7.34 km/s, 0.70 Torr

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**Entry Systems and Technology Division**
7.34 km/s, 0.70 Torr

- Changing NO rates reduced underprediction @ 0.7 Torr
- Introducing N₂ Quenching rates brought data into overprediction
- Updating electron impact processes obtains near-agreement
  - Slight underprediction of N₂ 1ˢᵗ Positive, overprediction of 2ⁿᵈ Positive

- 0.01 Torr data (not shown) now overpredicted in UV, matched in Visible
N$_2^+$ Model
**N$_2^+$ Radiance**

- **N$_2^+$ Radiation from**
  - 1$^{st}$ Negative System ($B^2\Sigma \rightarrow X^2\Sigma$) 320-500 nm
**N$_2^+$ Comparison to Heritage**

8.18 km/s, 0.01 Torr

7.34 km/s, 0.70 Torr

- Underpredicted at high pressure
- Overpredicted at low pressure
  - Park90 gets right magnitude, but transient (not shown) is incorrect
**N$_2^+$ after updates**

- Discrepancy at higher pressure mostly solved by revisions to rate model
- Low pressure discrepancy remains

8.18 km/s, 0.01 Torr

![Graph 1](image1.png)

7.34 km/s, 0.70 Torr

![Graph 2](image2.png)
Low Pressure $N_2^+$ : Controlling Reaction

- $N_2^+$ primarily formed by associative ionization:

\[
N + N \leftrightarrow N_2^+ + e^- \]

- This rate typically controlled by $T_t$ : becomes rapid when thermal non-equilibrium is significant

- However, ground state N does not cross $N_2^+$ states

- Reactions proceed through metastable (and possibly excited) N atoms

- This creates dependence on $T_e$
• Experimental Radiation profile matches $N_2^+$ density when $T_e$ controlling

• The predicted radiance (and profile) does not match, however
Atomic Radiance

- **Atomic Radiation**
  - 3p states 700-900 nm
  - 3d states 900-1450 nm
O atom:
- 777 nm underpredicted at all cases
- 845 nm underpredicted high pressure, matched low pressure

N atom:
- Low pressure: Fair agreement
- High pressure: adjusting for baseline, matched by Park93/Johnston, overpredicted by Park90
N, O 3d Comparison to Heritage

- Significant overprediction, all lines/pressures

8.18 km/s, 0.01 Torr

7.34 km/s, 0.70 Torr
Internal Excitation Rates

- Park rates place 3d states at Boltzmann level (overpredicted)
- Huo rates equilibrate all states closer to ionization level
- Zatsarinny rates place highest states near ionization limit, lower states progress toward Boltzmann
- Hybrid Huo/Park equilibrates between Boltzman/Saha

Peak Radiance
7.34 km/s, 0.7 Torr
\( T_t = 10,598 \text{K} \)
\( T_e = 10,645 \text{K} \)
\( N = 1.27 \times 10^{17} \text{ cm}^{-3} \)
\( N^+ = 2.42 \times 10^{14} \text{ cm}^{-3} \)
Impact of Excitation Rate on Radiance

7.34 km/s, 0.70 Torr

- Revised rates underpredict 3p atomic lines
- Three alternatives eliminate 3d overprediction
- Huo/Park slightly higher than Huo or Zatsarinnny
• Traditionally, QSS balances internal excitation with ionization
• But, Ionization accounts for 0.15% of N atom chemistry
• N atom mass derivative is:
  – 81% exchange reactions
  – 10% molecular dissociation
  – 9% associative ionization

Peak Radiance
7.34 km/s, 0.7 Torr
\( T_t = 10,598 \text{K} \)
\( T_e = 10,645 \text{K} \)
\( N = 1.27 \times 10^{17} \text{ cm}^{-3} \)
\( N^+ = 2.42 \times 10^{14} \text{ cm}^{-3} \)
Including Dissociative Recombination in QSS

- State-wise associative ionization rates assumed proportional to overall associative ionization rates
- Preference factors dictate which atomic states are formed from a given ion state
- Best agreement uses literature data for ground state preference, no preference for other states of $N_2^+$
Flip-through of Non-equilibrium Metric Comparisons
Non-equilibrium – 190-500 nm (0.01 Torr, 8.2 km/s)

- All models underpredict NO
- \( \text{N}_2^+ \) overpredicted by \( T_e = T_v \) options, Heritage does ok
- \( \text{N}_2 \) 2\(^{\text{nd}} \) Positive underpredicted

60 cm tube

\[ \text{Spectral Non-eq Metric (W/cm}^2\text{-sr-um)} \]

- EAST
- Park93
- Johnston14
- Park90 (\( T_e = T_v \))
Non-equilibrium – 190-500 nm (0.05 Torr, 8.6 km/s)

- NO still underpredicted
- N$_2^+$ improving for T$_e$=T$_v$ options, Heritage now too low
- N$_2$ 2$^\text{nd}$ Positive still underpredicted
Non-equilibrium – 190-500 nm (0.14 Torr, 8.3 km/s)

60 cm tube

- NO still underpredicted
- N₂⁺ slightly over for Te=Tᵥ options, Heritage underpredicts
- N₂ 2nd Positive underpredicted
Non-equilibrium – 190-500 nm (0.14 Torr, 8.3 km/s)

10 cm tube

- **NO** underpredicted
- **N\textsubscript{2}\textsuperscript{+}** matched for \(T\textsubscript{e}=T\textsubscript{v}\) options, Heritage underpredicts
  - CN contamination accounts for disagreement at 388 nm
- **N\textsubscript{2} 2\textsuperscript{nd} Positive** underpredicted
Non-equilibrium – 190-500 nm (0.30 Torr, 8.1 km/s)

10 cm tube

- **NO** underpredicted
- **N₂⁺** matched for \( T_e = T_v \) options, Heritage underpredicts
  - CN contamination accounts for disagreement at 388 nm
- **N₂** 2\(^{\text{nd}}\) Positive underpredicted
Non-equilibrium – 190-500 nm (0.50 Torr, 7.7 km/s)

10 cm tube

- **NO** still underpredicted
- **N$_2^+$** being underpredicted
  - Worse for Heritage
- **N$_2$** 2$^{nd}$ Positive underpredicted
Non-equilibrium – 190-500 nm (0.70 Torr, 7.3 km/s)

10 cm tube

- **NO** still underpredicted
- **$\text{N}_2^+$** more underpredicted
  - Heritage and newer models becoming more similar
- **$\text{N}_2$ 2$^{\text{nd}}$ Positive underpredicted**
Non-equilibrium – 190-500 nm (0.70 Torr, 7.3 km/s)

10 cm tube – with Boltzmann state populations

- NO matched with Boltzmann distribution for Johnston rates
- \( \text{N}_2^+ \) and \( \text{N}_2 \) are overpredicted by Boltzmann model
Summary 190-500 nm

- NO is always underpredicted
- N2 $2^{nd}$ Positive always underpredicted
- N2+ $1^{st}$ Negative underpredicted at high pressure, overpredicted at low pressure
Non-equilibrium – 500-890 nm (0.01 Torr, 8.6 km/s)

60 cm tube

- Broad features due to $N_2$ 1$^{st}$ Positive absent from prediction
- High level (4d,5s) N and O lines absent from data
- O 3p: 777 underpredicted, 845 underpredicted
- N 3p: overpredicted
- Errors cancel out when integrated – radiance appears well matched
Non-equilibrium – 500-890 nm (0.05 Torr, 8.9 km/s)

60 cm tube

- Broad features due to N$_2$ 1$^{st}$ Positive still absent
- High level (4d,5s) N and O lines still overpredicted
- O 3p : underpredicted, but closer than before
- N 3p : matched by Park90/Park93, overpredicted Johnston
- Errors cancel out when integrated – Johnston appears to matched
Non-equilibrium – 500-890 nm (0.14 Torr, 8.4 km/s)

60 cm tube

- Broad features due to $N_2$ 1$^{\text{st}}$ Positive still absent
- High level (4d,5s) N and O lines still overpredicted
- O 3p : matched by heritage model, underpredicted other models
- N 3p : overpredicted by heritage, matched other models
Non-equilibrium – 500-890 nm (0.14 Torr, 8.3 km/s)

10 cm tube

- Broad features due to N$_2$ 1$^{\text{st}}$ Positive still absent
- High level (4d,5s) N and O lines overpredicted
- O 3p: matched by heritage model, underpredicted other models
- N 3p: overpredicted by heritage, matched other models
Non-equilibrium – 500-890 nm (0.30 Torr, 8.1 km/s)

10 cm tube

- Broad features due to $N_2$ 1st Positive still absent
- High level (4d,5s) N and O lines overpredicted, but less significantly
- O 3p : matched by heritage model, underpredicted other models
- N 3p : further overpredicted by heritage, matched other models
Non-equilibrium – 500-890 nm (0.50 Torr, 7.7 km/s)

10 cm tube

- Broad features due to N$_2$ 1$^{st}$ Positive still absent
- High level (4d,5s) N and O lines overpredicted
- O 3p : matched by heritage model, underpredicted other models
- N 3p : overpredicted by heritage, matched other models
Non-equilibrium – 500-890 nm (0.70 Torr, 7.3 km/s)

10 cm tube

N₂ 1ˢᵗ Positive
(B³Π→A³Π)

O 3p→3s

N 3p→3s

• Broad features due to N₂ 1ˢᵗ Positive still absent
• High level (4d,5s) N and O lines overpredicted
• O 3p : underpredicted all models
• N 3p : overpredicted by heritage, matched other models
  – Apparent disagreement due to missing underlying N₂ radiation
Non-equilibrium – 500-890 nm (0.70 Torr, 7.3 km/s)

10 cm tube (Boltzmann Model)

- Boltzmann matches N$_2$ 1$^\text{st}$ Positive (Heritage slightly over)
- High level (4d,5s) N and O lines overpredicted by Boltzmann
- O 3p matched by Boltzmann (all models)
- N 3p : slightly overpredicted at Boltzmann
Impact of Alternate N Atom Excitation Cross-sections

- **Huo excitation cross-sections**
  - Eliminate spurious radiation from N 4d, 5s
  - Underpredict N 3p features
Summary 500-890 nm

- $N_2$ is always underpredicted
- Spurious N and O lines originating from 4d, 5s states
- N 3p lines
  - Matched by Park90 ($Te=Tu$) at 0.05 Torr, overpredicted elsewhere
  - Matched by Johnston at 0.14-0.7 Torr, overpredicted at lower pressure
  - Matched by Park93 at 0.05-0.7 Torr, overpredicted at lower pressure
- O 3p lines
  - Underpredicted by Park93/Johnston, except at 0.01 Torr
    - 845 nm line overpredicted at 0.01 Torr
  - Heritage approach
    - Nearly matches 845 nm line from 0.01-0.50 Torr
    - Underpredicts 777 nm line, but not badly
Non-equilibrium – 890-1450 nm (0.01 Torr, 8.6 km/s)

60 cm tube

- All lines in this range overpredicted
Non-equilibrium – 890-1450 nm (0.05 Torr, 8.9 km/s)

60 cm tube

- Most lines overpredicted
  - Park90 matches 1362 nm line
  - N 3p line (939 nm) less overpredicted than others
Non-equilibrium – 890-1450 nm (0.14 Torr, 8.4 km/s)

60 cm tube

- All lines overpredicted
Non-equilibrium – 890-1450 nm (0.14 Torr, 8.4 km/s)

10 cm tube

• All lines overpredicted
10 cm tube

- All lines overpredicted
- N 3p line (939 nm) near match by Park93/Johnston
Non-equilibrium – 890-1450 nm (0.50 Torr, 7.7 km/s)

10 cm tube

- Most lines overpredicted
- N 3p line (939 nm) matched by Park93/Johnston
Non-equilibrium – 890-1450 nm (0.70 Torr, 7.3 km/s)

10 cm tube

- Most lines overpredicted
- N 3p line (939 nm) matched by Park93/Johnston
- Continuum (N₂ Band) not predicted
Alternate N Excitation Cross Sections

60 cm tube

- Alternate cross-sections underpredict N 3p line
- Other lines near noise limit
- O atoms unchanged
Non-equilibrium – 890-1450 nm (0.70 Torr, 7.3 km/s)

10 cm tube (Boltzmann)

- Boltzmann improves background agreement, lines still too intense
Summary 890-1450 nm

- Atomic Lines originating from higher states generally over predicted
- One N 3p line is matched well by Park/Johnston from 0.3-0.7 Torr
- Molecular radiation at 0.7 Torr mostly matched under Boltzmann
Predictive Summary

- Agreement to Predictive (DPLR/NEQAIR) Model is mixed
  - Molecular radiation from $N_2/NO$ is underpredicted
    - Boltzmann distribution takes up underprediction for $N_2$ B state and NO radiation
    - $N_2$ C state is overpredicted by Boltzmann
  - $N_2^+$ radiation prediction varies with pressure
    - At low pressure: overpredicted for $T_e=T_v$, matched by heritage model
    - Reasonably matched for intermediate pressure range
    - Underpredicted at high pressure
  - High lying N, O state radiation overpredicted
  - Radiation from 3p states of N predicted well, except at lowest pressure
  - Radiation from 3p states of O mostly underpredicted

- How does your model do?
  
  [https://data.nasa.gov/docs/datasets/aerothermodynamics/EAST/index.html](https://data.nasa.gov/docs/datasets/aerothermodynamics/EAST/index.html)

  (Test 59 - available soon)