Investigation of Non-Equilibrium Radiation for Earth Entry

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Overview

• Provide motivation and introduce EAST and Computational Tools
  - EAST shock tube facility
  - LAURA and DPLR for flowfield calculations
  - HARA and NEQAIR for radiation calculations

• Methodology
  - Detail the non-equilibrium metric used in analysis
  - Influence of reaction rates
  - Wavelength regions analyzed

• Results
  - Comparisons between simulations & EAST
  - Overall discrepancy

• Conclusion
  - One standard deviation scatter in non-equilibrium EAST results: 31%
  - Depending on shock speed, simulations under-predict EAST by up to 50% or over-predict up to 20%
  - At 0.2 Torr, below 9 km/s error in radiative heat flux due to non-equilibrium < 1 W/cm^2, and < 20 W/cm^2 at 11 km/s

This presentation should convey 3 main points:

1) Non-equilibrium radiance compared between EAST and NASA’s CFD & radiation simulations tools
2) Significant relative discrepancies are observed and there are compensating errors
3) The absolute level of error due to non-equilibrium is often small
Introduction

• Re-entry missions involving larger vehicles and higher entry velocities motivate improved simulation of radiative heating and associated uncertainties, e.g. EM-1

Brief Overview of Missions

**EFT-1:** First Orion flight test; entered Earth’s atmosphere from a highly elliptical orbit in December of 2014

**EM-1:** the next Orion flight will undertake a lunar return trajectory (radiation will be significant)

• Using shock tube data to validate non-equilibrium should only be attempted if equilibrium is well understood

• Previous analyses have conducted extensive comparisons between EAST and radiation calculations at equilibrium
Equilibrium Summary

- Uncertainty for model predictions of EAST was shown as a function of velocity for Earth entry up to 15.5 km/s.
- 1 Standard deviation in scatter of EAST: 17%.
- Disagreement of models w.r.t. to mean EAST result from 11 – 15.5 km/s on average [9.0%, -6.3%].
Methodology
EAST Facility

- EAST: Electric Arc Shock Tube, located at NASA Ames Research Center
- Shock is driven by an electric arc discharge.
- 10.16 cm in diameter at the test section.
- 4 spectrometers analyzing different spectral ranges in each shot. These ranges are typically:
  - VUV (≈ 120 – 215 nm)
  - UV/Vis (≈ 190 – 500 nm)
  - Vis/NIR (≈ 480 – 900 nm)
  - IR (≈ 700 – 1650 nm)
Simulation Tools

- Two sets of simulation tools are used in the analysis:
  - NEQAIR radiation calculations based on DPLR flowfields.
  - HARA radiation calculations based on LAURA flowfields.
  - Additional calculations also performed with NEQAIR and LAURA.

- Different combinations of simulations used to determine if discrepancies are due to modeling issues of the flowfield, physics or radiation.

- The latest release of DPLR has fixed the ability to run $T_e = T_v$

- NEQAIR v15.0 is used (what will become the next release)
  - The non-Boltzmann model needed to be modified for some transitions of $N_2$ and IR atomic lines
  - Previous versions of NEQAIR would have set the populations to Boltzmann

- An updated NO non-Boltzmann model has been implemented in HARA, but is not included in this presentation

- The electron impact excitation rates of Park and Huo have been also compared using NEQAIR
Computational Methodology

- DPLR used a 3m sphere with 803 grid points along the stag-line, while LAURA used a 2.5m sphere with 256 points.
- 11 species gas model, with ionization species. No ablation products.
- Two temperature model used for thermo non-equilibrium:
  - $T_{\text{trans}} = T_{\text{rot}}$
  - $T_{\text{vib}} = T_{\text{electronic}} = T_{\text{electron}}$

<table>
<thead>
<tr>
<th>Spectral Range</th>
<th>EAST Camera</th>
<th>Dominant Radiators</th>
</tr>
</thead>
<tbody>
<tr>
<td>117 – 153 nm for $V \geq 9$ km/s</td>
<td>VUV</td>
<td>N, O</td>
</tr>
<tr>
<td>123 – 153 nm for $V &lt; 9$ km/s</td>
<td>VUV</td>
<td>N, O</td>
</tr>
<tr>
<td>170 – 178 nm</td>
<td>VUV</td>
<td>N</td>
</tr>
<tr>
<td>178 – 210 nm</td>
<td>VUV/UV</td>
<td>NO</td>
</tr>
<tr>
<td>210 – 328 nm</td>
<td>UV</td>
<td>N$_2$, N$_2^+$, N</td>
</tr>
<tr>
<td>328 – 496 nm</td>
<td>UV</td>
<td>N$_2^+$, N, N$_2$</td>
</tr>
<tr>
<td>496 – 888 nm</td>
<td>Vis/NIR</td>
<td>N, O, N$_2$</td>
</tr>
<tr>
<td>888 – 1445 nm</td>
<td>IR</td>
<td>N, O</td>
</tr>
</tbody>
</table>
Differences Between Reaction Sets

- The main difference between Park 90 and Park 93 chemistry is that Park 90 does not contain the nitrogen electron exchange reaction:
  \[ \text{N}^+ + \text{N}_2 \leftrightarrow \text{N}_2^+ + \text{N} \]
  
- LAURA chemistry uses a combination of newer rates from various sources, rates tuned to match EAST and some of the heritage rates from Park 90 and Park 93.

<table>
<thead>
<tr>
<th>Rate</th>
<th>Comment</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO + M $\leftrightarrow$ N + O + M</td>
<td>Adjusted by Johnston to match EAST CO$_2$/N$_2$ data</td>
<td>Johnston et al.</td>
</tr>
<tr>
<td>N$_2$ + e $\leftrightarrow$ N + N + e</td>
<td>Updated rate for electron dissociated impact</td>
<td>Bourdon et al.</td>
</tr>
<tr>
<td>O$_2$ + e $\leftrightarrow$ O$_2^+$ + e + e</td>
<td>Updated rate</td>
<td>Teulet et al.</td>
</tr>
<tr>
<td>N$_2$ + O $\leftrightarrow$ NO + N</td>
<td>Updated rate</td>
<td>Fujita et al.</td>
</tr>
<tr>
<td>O$_2$ + N $\leftrightarrow$ NO + O</td>
<td>Updated rate</td>
<td>Bose and Candler</td>
</tr>
</tbody>
</table>
Increased level of ionization with Park 90
Many insights gained by comparing equilibrium radiance vs velocity trends between simulations and experiments.

For non-equilibrium, it is not clear that 1 metric can represent all aspects of the flow. Ideally, the metric would be:

- Independent of experimental parameters (such as gate width and spatial resolution).
- Applicable to a wide range of conditions.
- Easily comparable to simulation results.
- Consistent with limitations of test time in the facility.
- Accommodate a shot dominated by equilibrium.
Non-equilibrium Metric

Absolute Non-Equilibrium Radiance

Integrated +/- 2cm either side of shock front. Normalized by shock tube diameter
Radiation Emitted From Different Wavelengths

Low shock speeds dominated by molecular emission in VUV->UV

High shock speeds dominated by atomic emission in deep VUV, Red -> IR
Results

Simulations vs EAST
Simulations vs EAST

• Simulations vs EAST are shown for 4 spectral regions:
  - VUV, UV, Vis/NIR and IR
  - Constant free-stream pressure: 0.2 Torr

• Each slide will show 4 plots:
  - Comparison between EAST and simulations on a linear and log scale
  - The scatter of the EAST data around the line of best fit
  - The weighted difference between the simulations and EAST

• A prominent conclusion (or 2) will be highlighted for each spectral region.
Simulations vs EAST: VUV

Under-prediction in the VUV

Large relative differences in the VUV at low speed
Overall, good agreement in the UV
Very large relative differences in the Vis/NIR at low speed.
Certain modeling choices can create a significant over-prediction in the IR at low speed.
Overall Summation

- The summation of the weighted discrepancies (overall difference) is shown below.

- Lower speeds, where non-equilibrium is more significant, there are large differences.

- Improving agreement between the codes as shock speed is increased.

![Graph showing summation of weighted discrepancies](image)

- Large under-prediction for DPLR/NEQAIR (with Huo electron impact)

- Good agreement between LAURA/HARA and DPLR/NEQAIR (with Park electron impact)
Overall Summation

• Even though the differences between 2 simulations and EAST might be similar, it can be due to compensating errors.

• Both plots below sum to similar values, but show different characteristics.

The over-prediction in the IR is counter acted by the under-predictions of the VUV/UV

![Graphs showing weighted difference vs. shock speed for LAURA/HARA dd and DPLR/NEQAIR (Park N).]
Overall Summation

• Even though the relative differences can be high, the absolute differences tend to be small.

- The root sum square differences of the non-equilibrium metric was multiplied by 2, to give an upper bound estimate for the radiative head flux of a 2cm optically thin shock layer.

- < 9 km/s, the difference is less than 1 W/cm², ~ 11 km/s, less than 20 W/cm².

For $\rho = 3\times10^{-4}$ kg/m³, $R_n = 5$m, $V = 9$ km/s:
$Q_{\text{conv}} \approx 111$ W/cm², $Q_{\text{rad}} \approx 23$ W/cm²

For $\rho = 3\times10^{-4}$ kg/m³, $R_n = 0.5$m, $V = 9$ km/s:
$Q_{\text{conv}} \approx 355$ W/cm², $Q_{\text{rad}} \approx 8$ W/cm²

For $\rho = 3\times10^{-4}$ kg/m³, $R_n = 5$m, $V = 11$ km/s:
$Q_{\text{conv}} \approx 180$ W/cm², $Q_{\text{rad}} \approx 725$ W/cm²

For $\rho = 3\times10^{-4}$ kg/m³, $R_n = 0.5$m, $V = 11$ km/s:
$Q_{\text{conv}} \approx 610$ W/cm², $Q_{\text{rad}} \approx 255$ W/cm²
Summary

• A metric has been used to compare non-equilibrium radiation measurements and NASA’s simulation tools.

• The scatter of the EAST experiments was calculated to have a 1 standard deviation of 31%.

• Depending on the shock speed, simulations were shown to under-predict by up to 50% or over-predict by up to 20%.

• The level of ionization calculated using Park 90 chemistry is very high, and should not be used in simulations to predict radiative heating.

• LAURA/HARA and DPLR/NEQAIR (using excitation rates from Park) agree well
Summary

• Using the excitation rates from Huo in NEQAIR results in an under-prediction
  - For a back shell case, this would become an over-prediction (as its expanding flow)

• Future work should focus on N₂, N₂⁺, NO and under-prediction of VUV

• Even with significant relative differences, the absolute magnitude of the error for non-equilibrium is fairly small
  - N.B. At much lower pressures, non-equilibrium will become more significant and the uncertainty will likely be much higher

• Framework for running radiation calculations for flight cases should be re-visited.
Questions?