Analysis of Shockwave Radiation Data in Nitrogen

Brett A. Cruden, Aaron M. Brandis
AMA Inc

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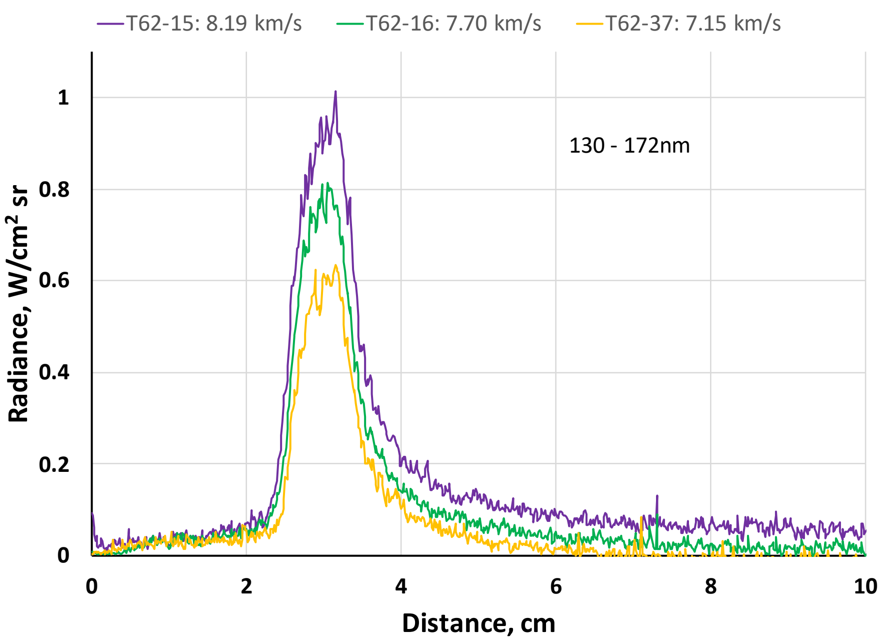
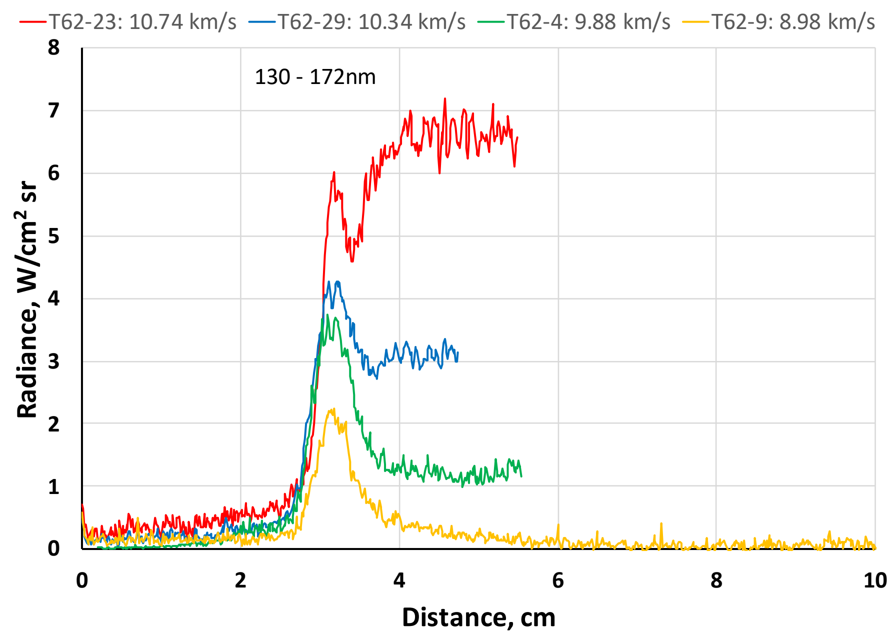
Background

- In AIAA-2018-3437 we reported a test series performed in pure N_2



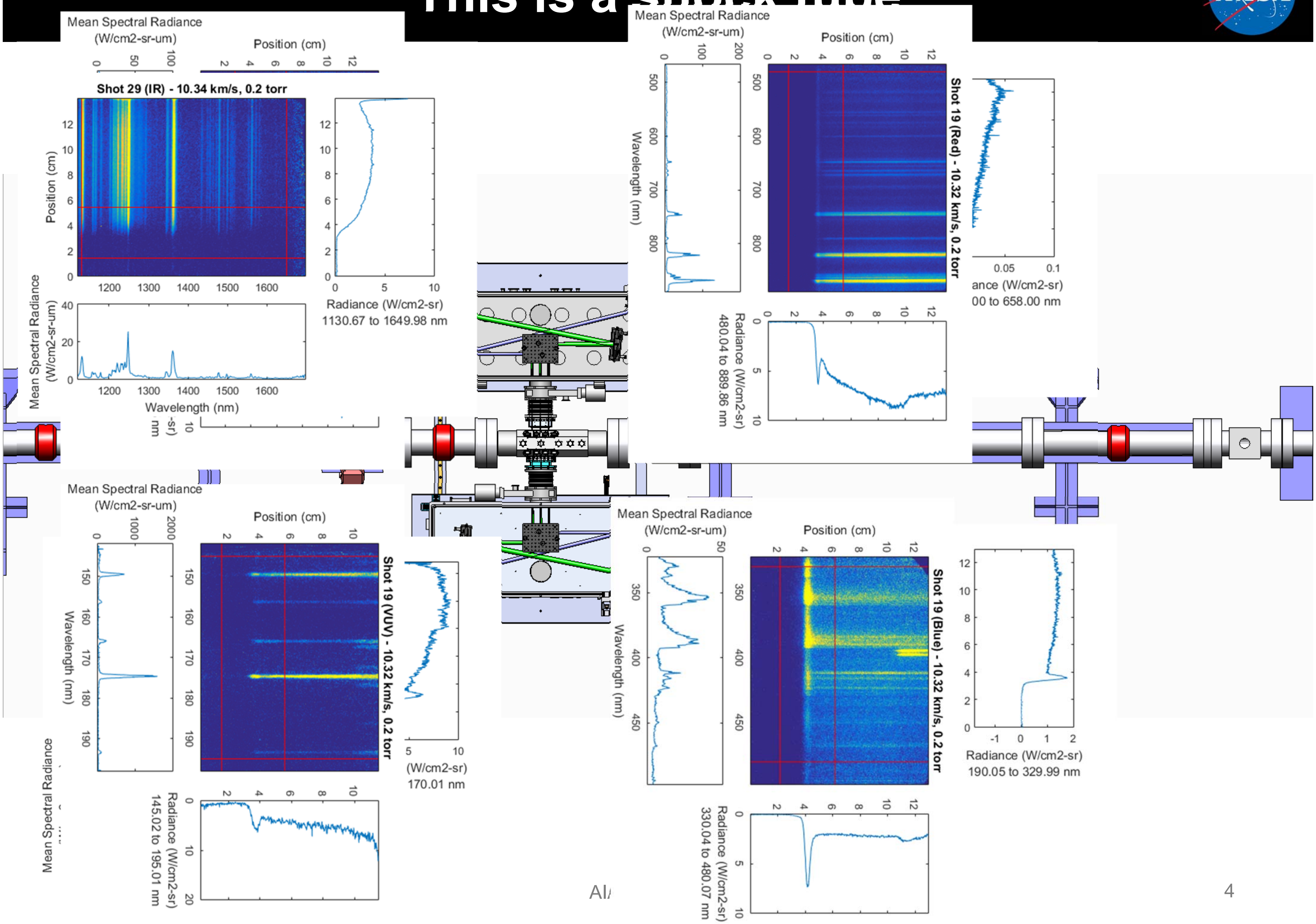


- N_2 shocks presents a simplified reaction set. Useful for model testing
- This paper presents a deeper dive into some of this data

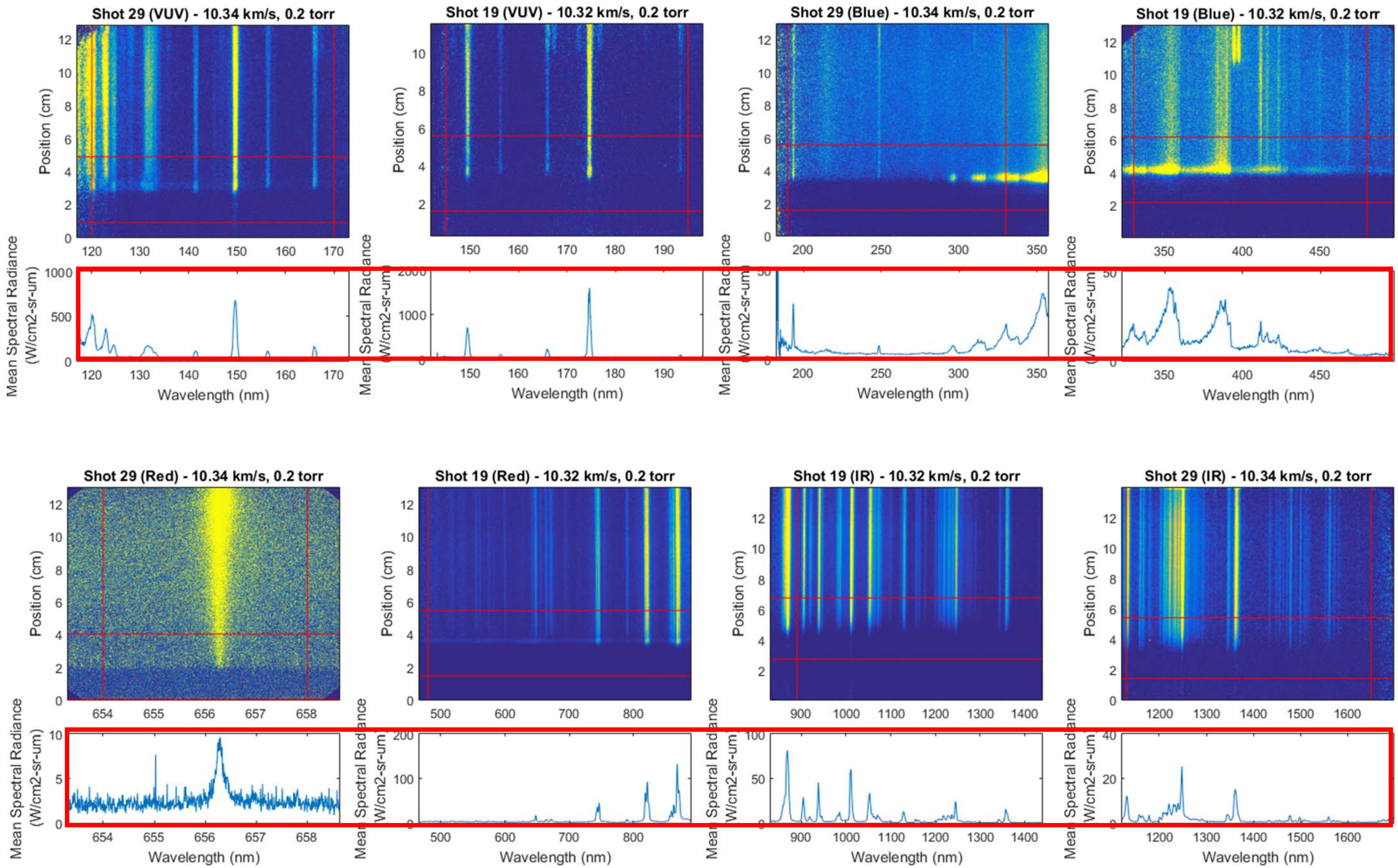
Outline

- Experimental Details
- Spectra in “Equilibrium”
  - Line identification
  - Fitting of Spectra
  - Extracting excited state data
- Spatially dependent data
- Ionization predictions

This is a shock tube

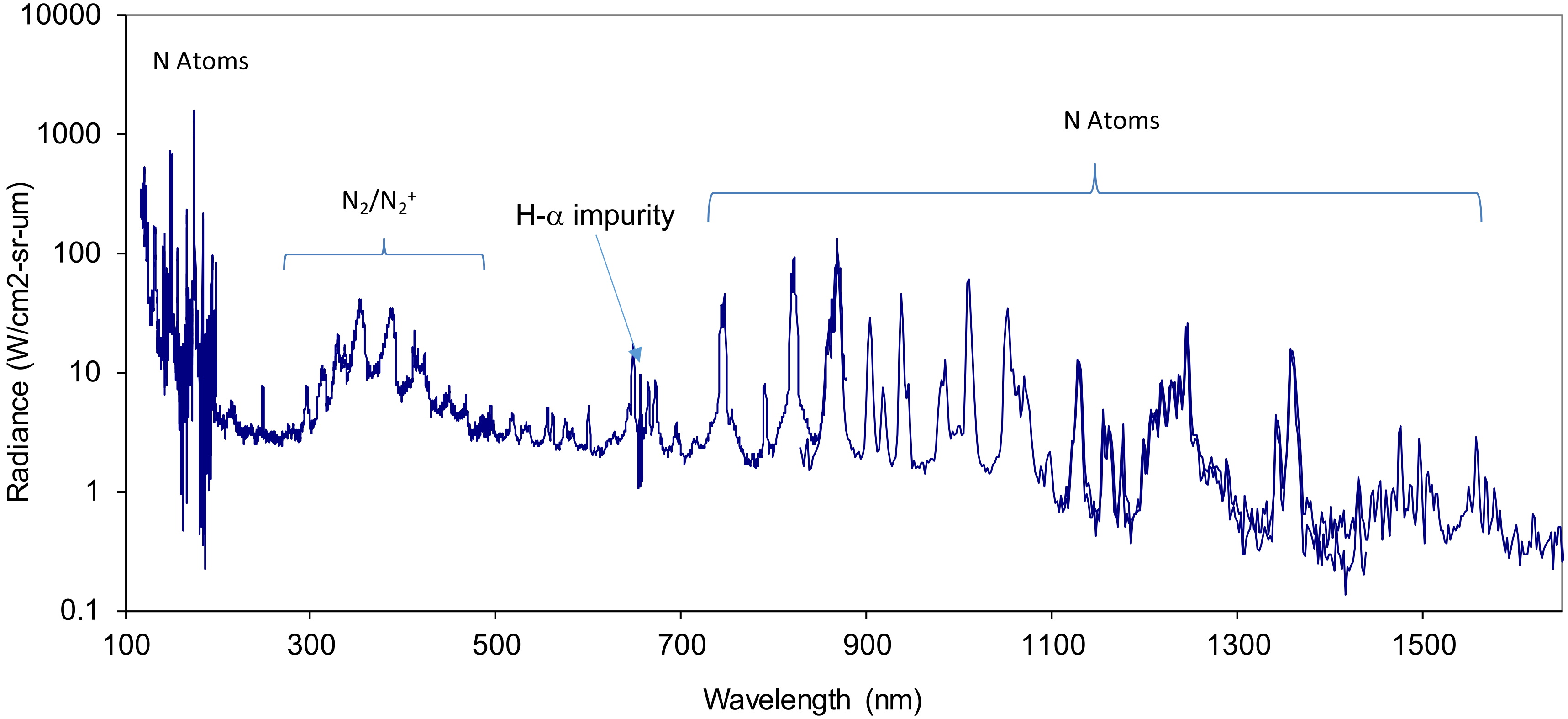


Composite Spectra



Composite non-equilibrium spectrum

- Composite spectrum generated from the 8 images
- Will look at four of the regions individually

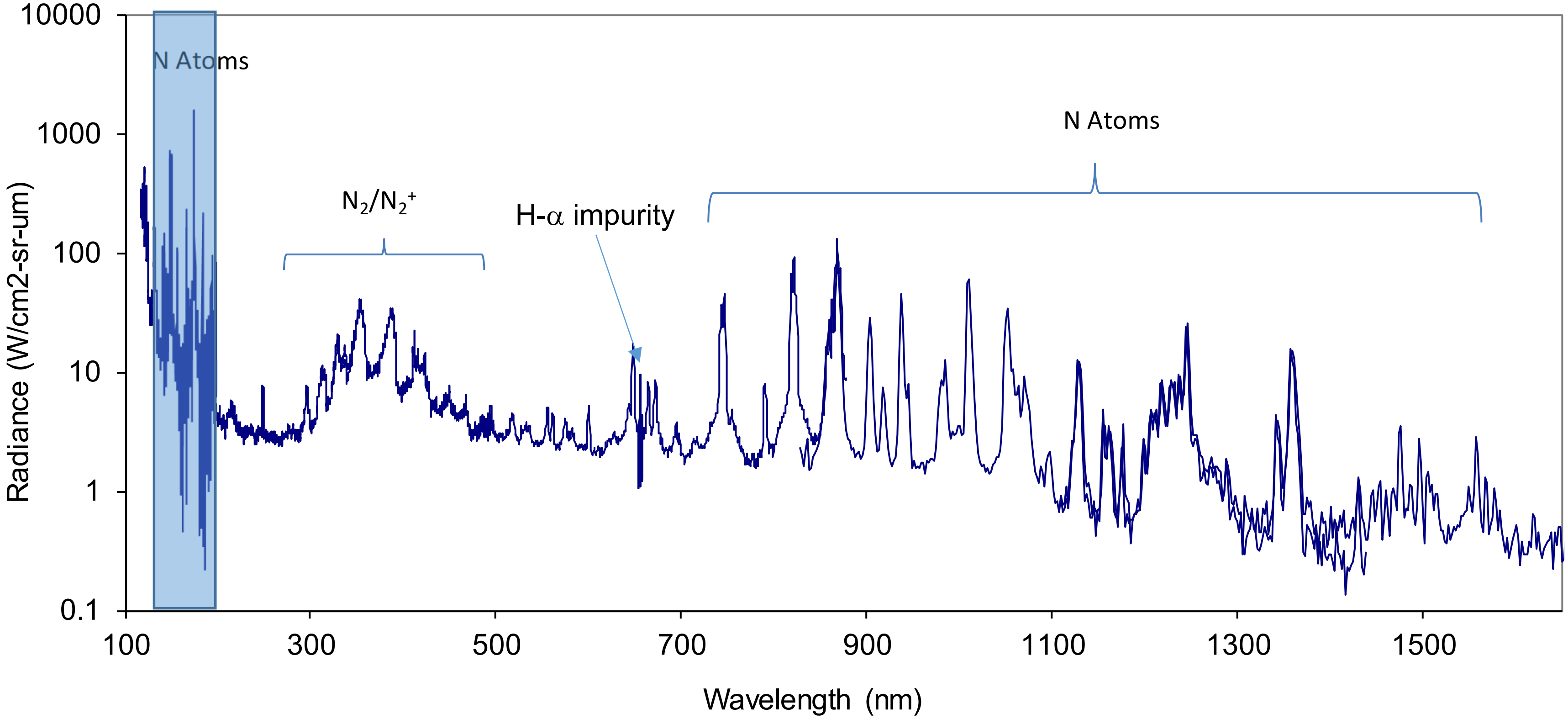


Notes on Spectral Analysis

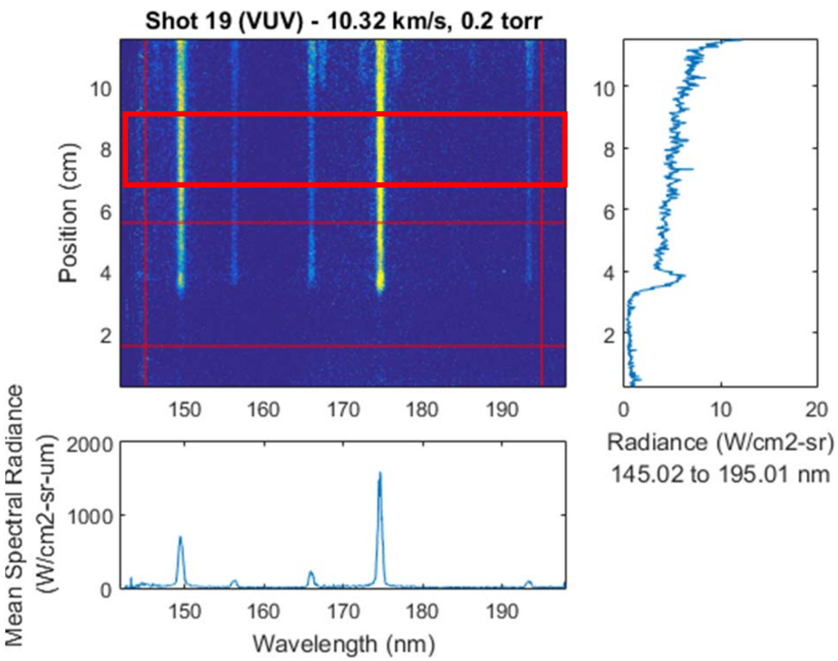
- We will use NEQAIR v15.1β to fit the spectra
- Fit parameters will include temperatures, species number densities
- Excited state densities may be:
  - Assumed Boltzmann distributed
  - Solved using NEQAIR's non-Boltzmann (QSS) Model
  - Fit individually
- The resultant analysis would represent the state of the flow *assuming the model to be correct*
- Error-bars reported:
  - Are the error in the fit parameters (e.g. aleatory)
  - Does not account for error/bias in experimental data
  - Does not include the error in the model construction (i.e. epistemic)
    - This might be the most important source of error in this analysis

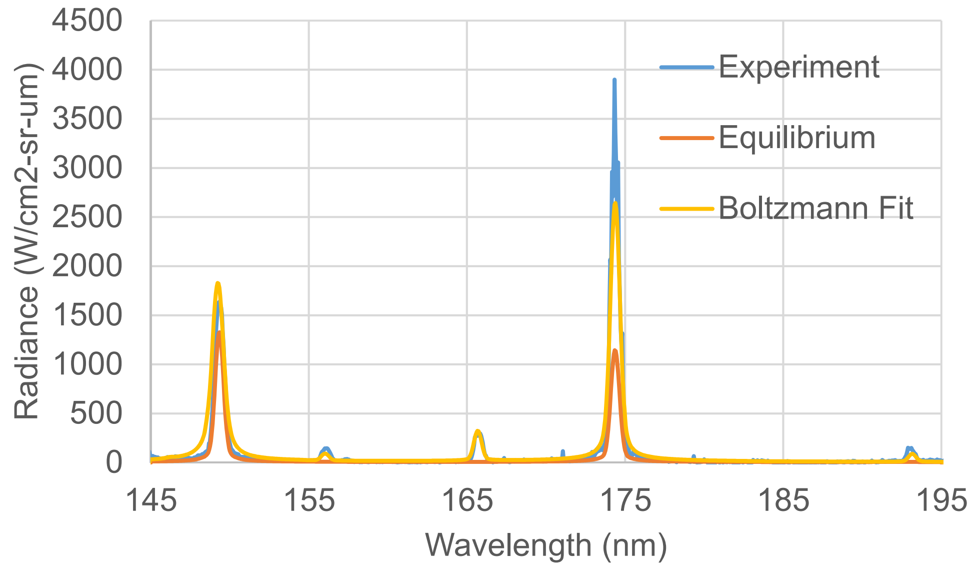
Composite non-equilibrium spectrum

- Composite spectrum generated from the 8 images
- Will look at four of the regions individually



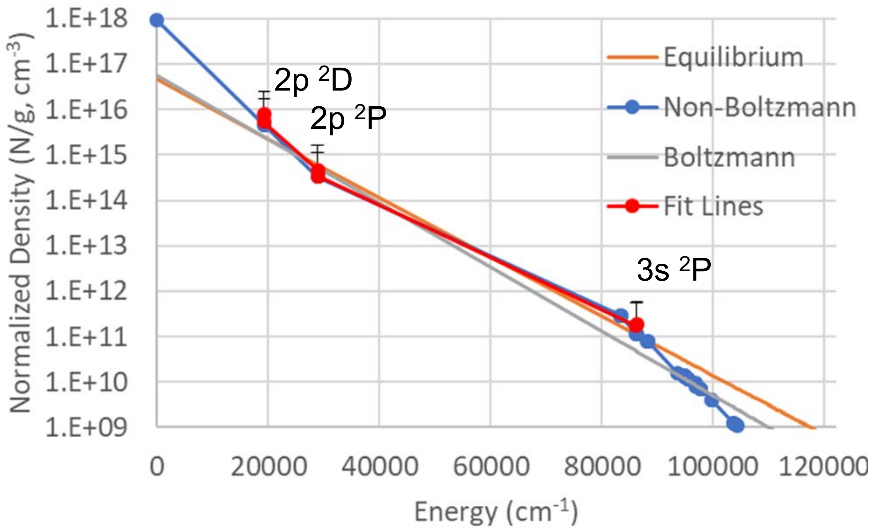
VUV Spectrum

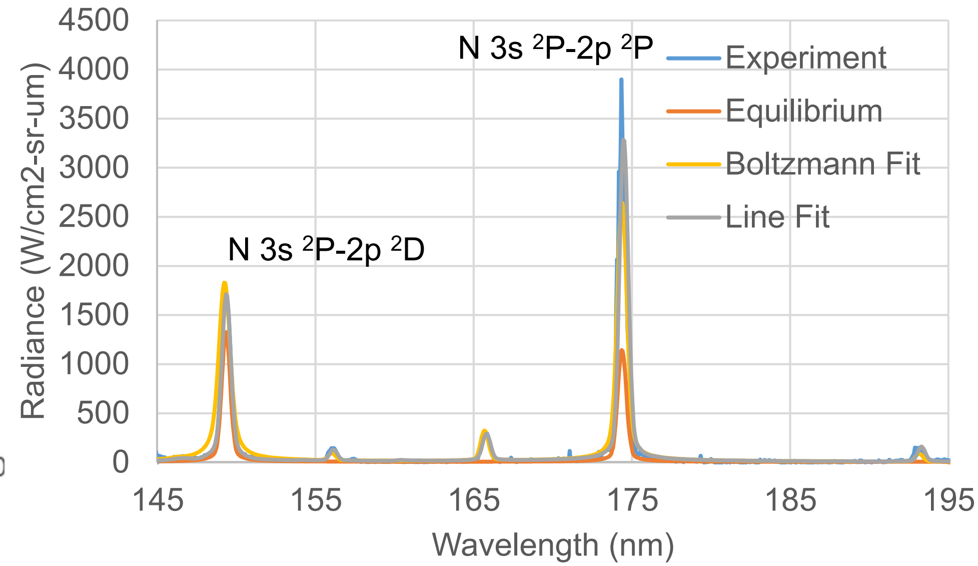




- Intensity of N 174 nm line exceeds equilibrium prediction
- Can perform a “best fit” of the spectrum
  - Obtains 8850K, 2 x 10^{17} cm^{-3} N, 3 x 10^{17} e-, 40 ppm C
  - Equilibrium : 9570K, 2 x 10^{17} cm^{-3} N, 7 x 10^{15} e-
  - Not a great agreement spectrally

Fitting Individual Lines

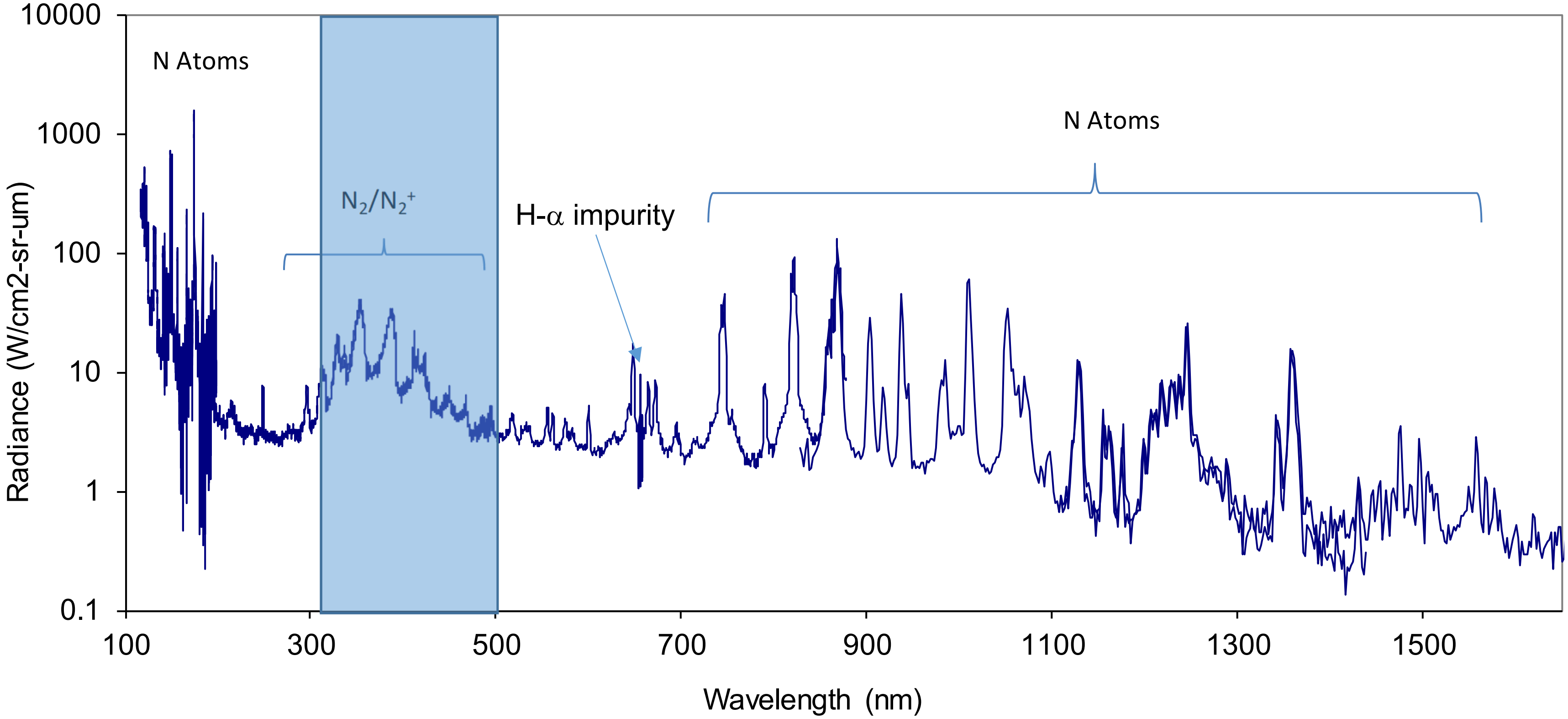




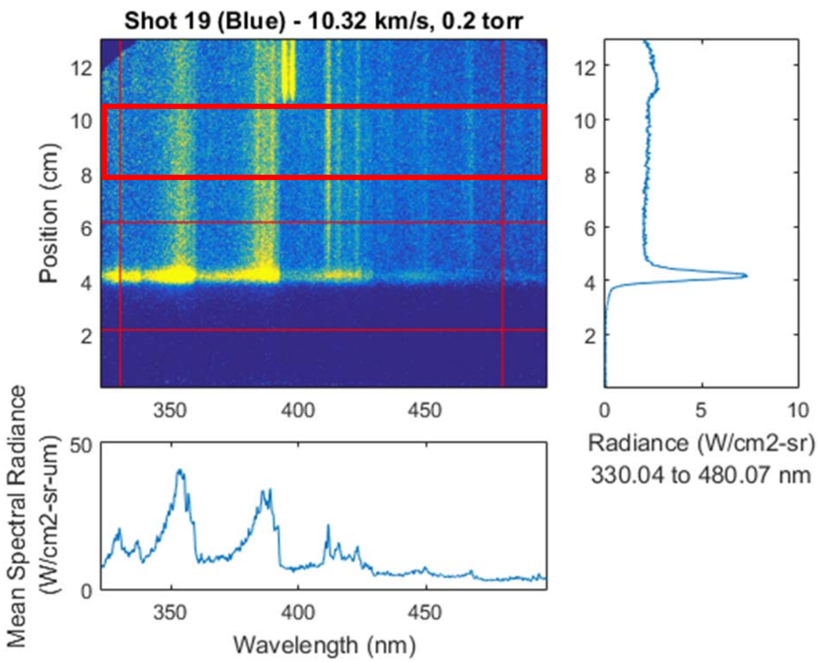
- A better fit is obtained by adjusting density of individual levels
- Result shows a deviation from equilibrium, with ^{2}P states being overpopulated
- Best non-Boltzmann fit obtains unrealistic ground state and ion densities
- Note that optically thick line intensity strongly sensitive to broadening mechanism
  - Stark broadening coefficient or electron density plays a role

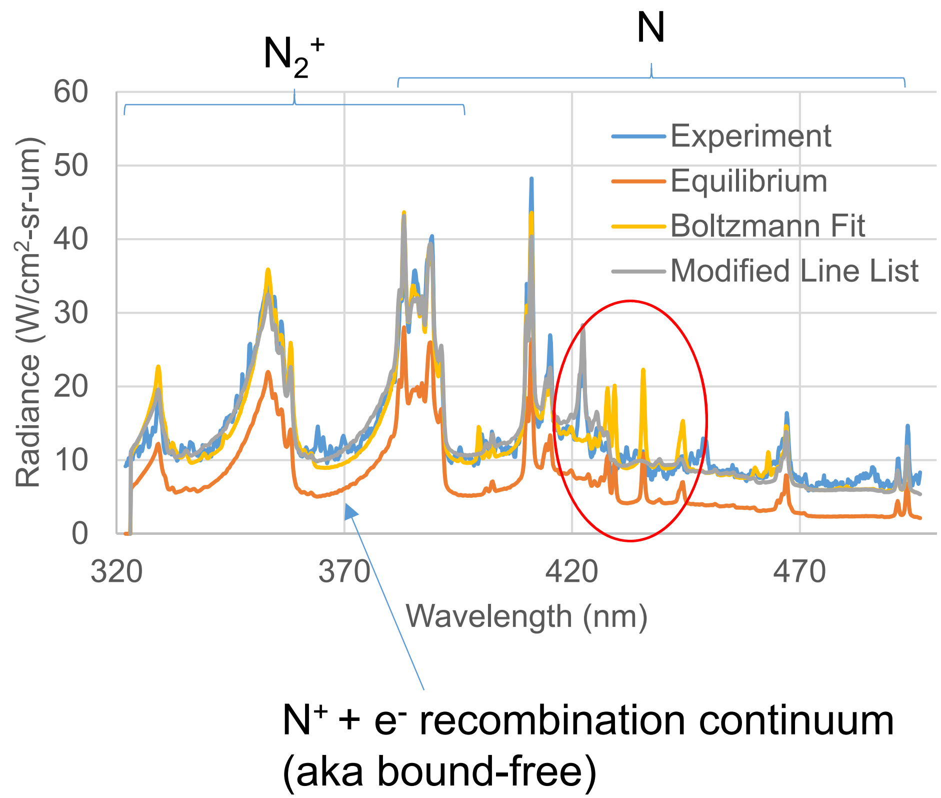
Next Region

- Next, examine UV region (330-500 nm)



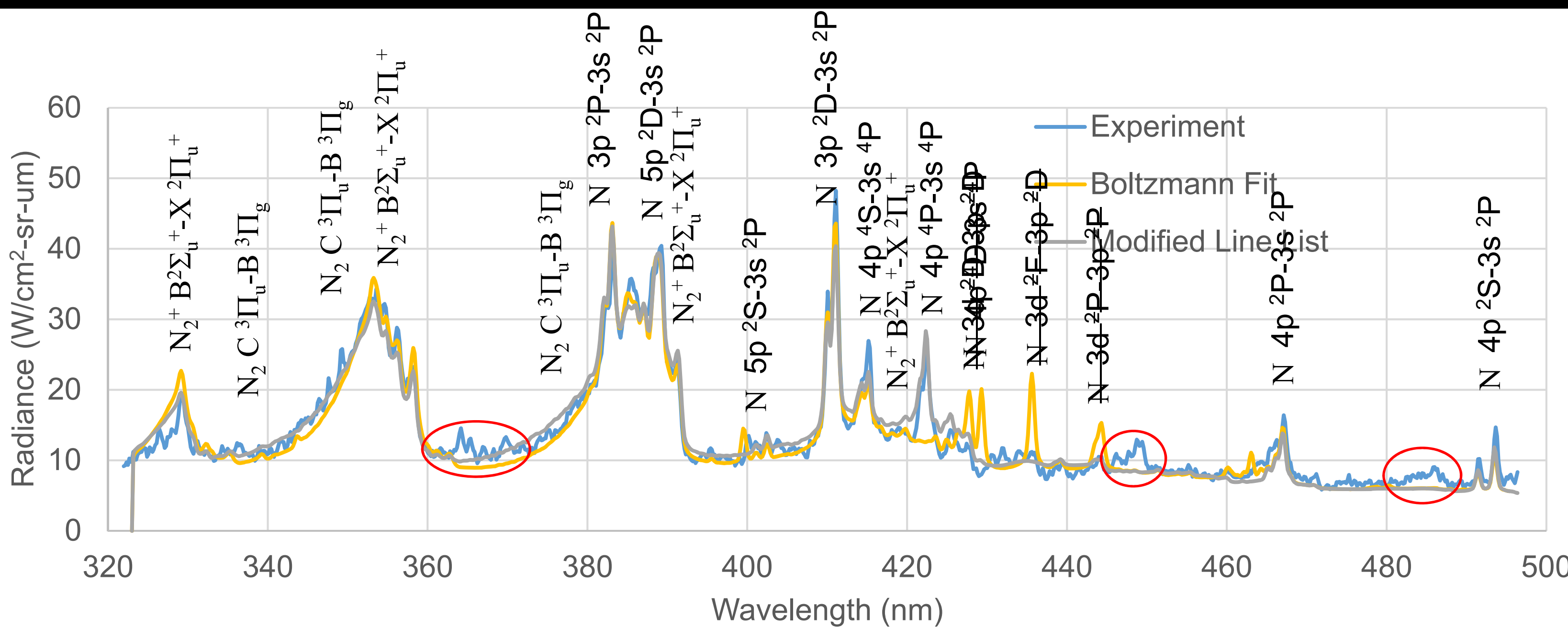
UV Spectrum





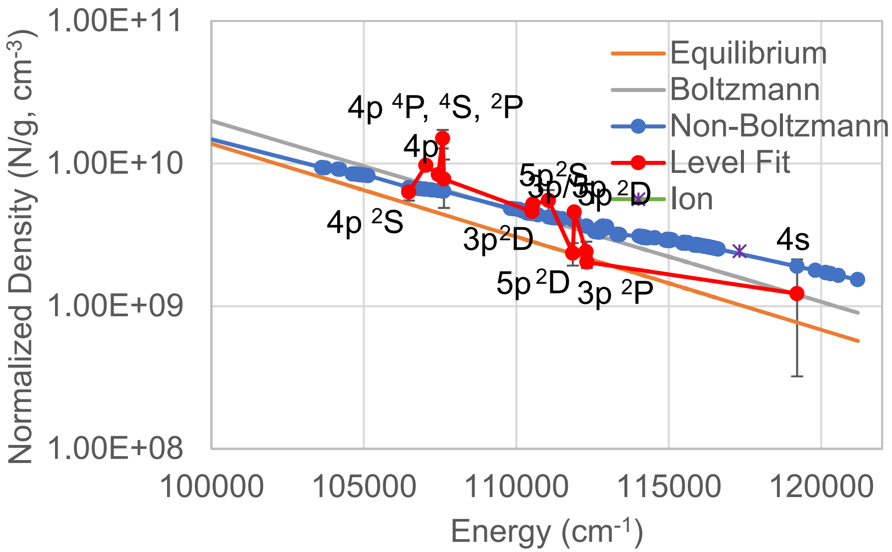
- Equilibrium prediction does not match continuum
- Best Boltzmann fit of the spectrum
  - Requires 2x the N^+ (e^-) density, 10 ppm of CN
- Errors in atomic line prediction
- Improve the atomic line list

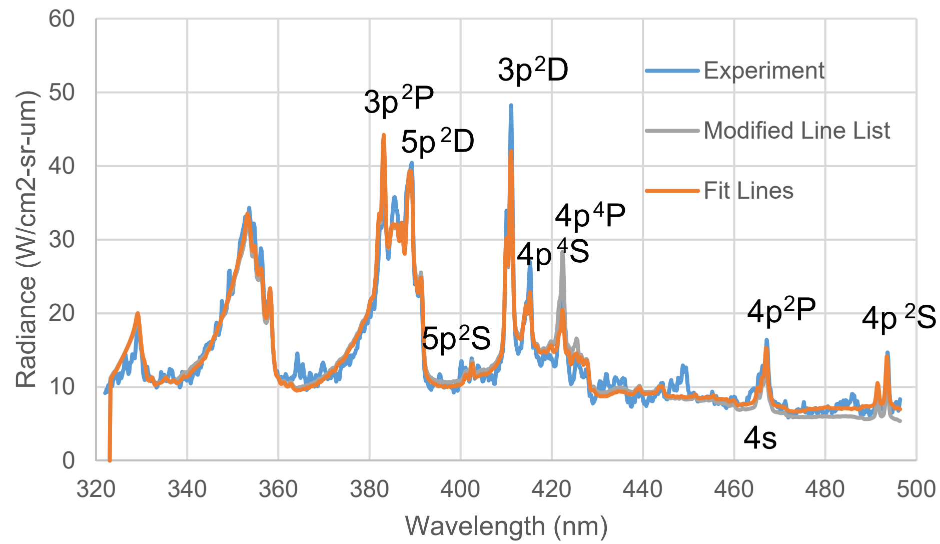
Feature Identification



- Molecular Contributions:
  - N_2^+ 1st Negative
  - N_2 2nd Positive obscured by N_2^+ in "equilibrium"
- Atomic N Lines
  - Transitions from 3p, 4p, 5p to 3s positively Identified from NIST
  - Transitions from 3d to 3p predicted incorrectly
    - These states have energy above the ionization limit
  - Some 4p-3s transitions missing from NIST, identified through other databases
  - Still additional missing features. Many states of N in this range with transitions not evaluated

UV Spectrum Level Fit

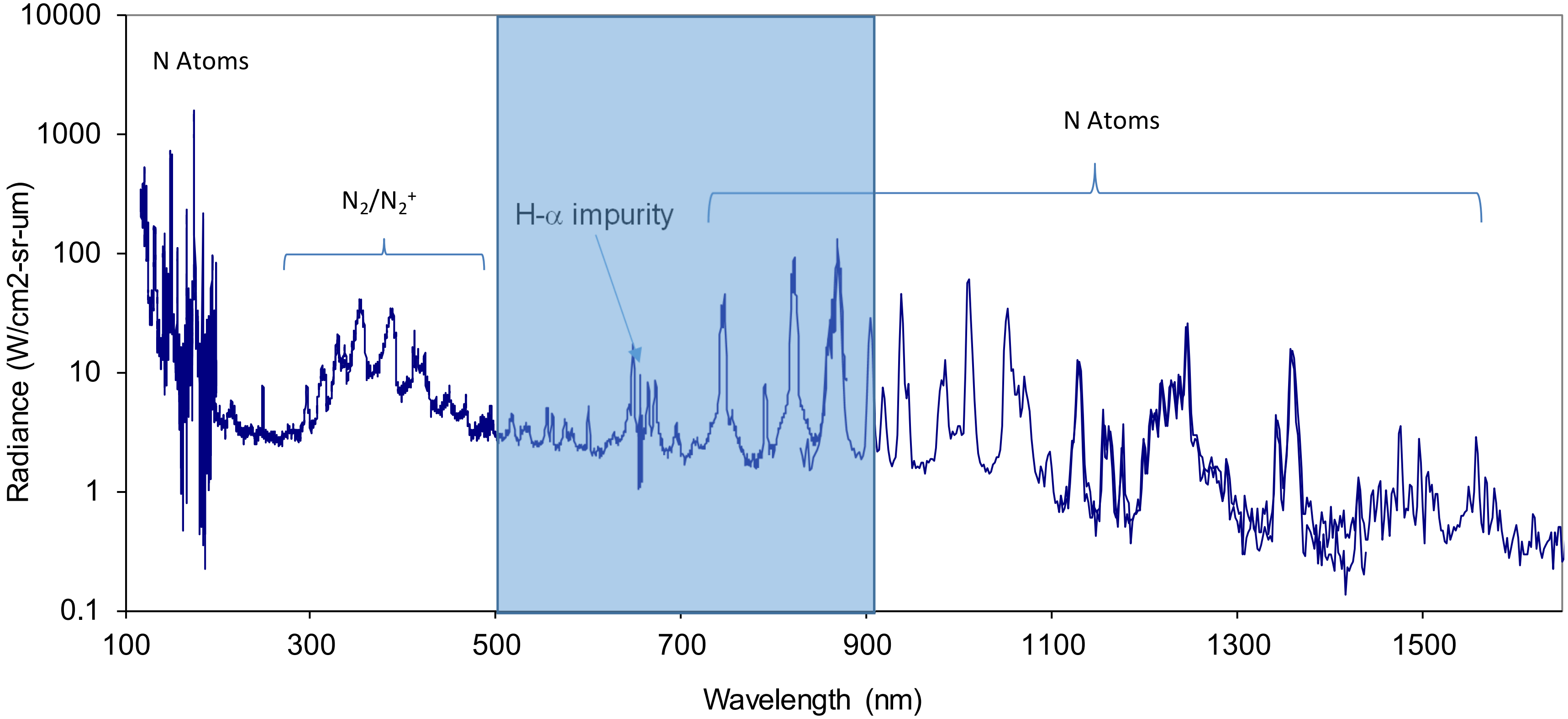




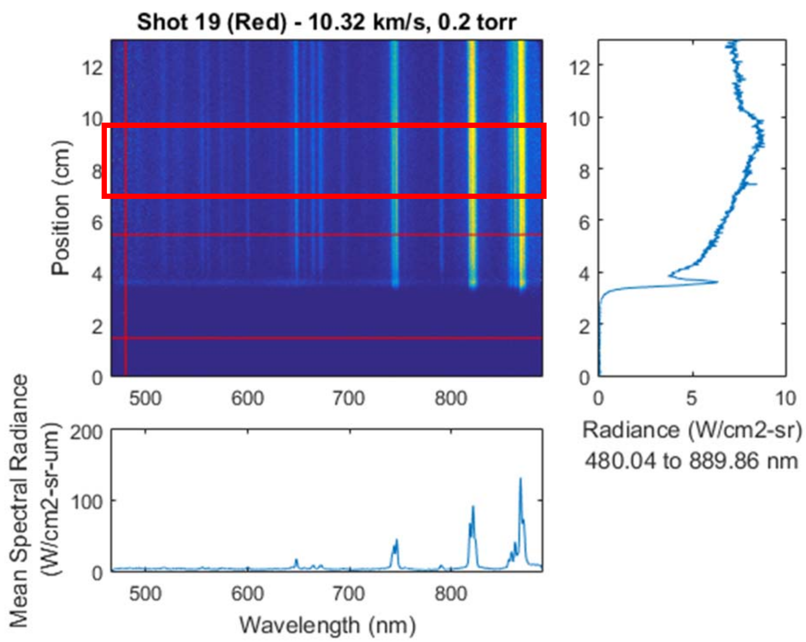
- Boltzmann fit requires elevated T, n_e
- Non-Boltzmann – slope differs
  - Similar populations in 3p,4p,5p range
- Level Fit
  - Some states agree with Equilibrium distribution
  - Some states overpopulated

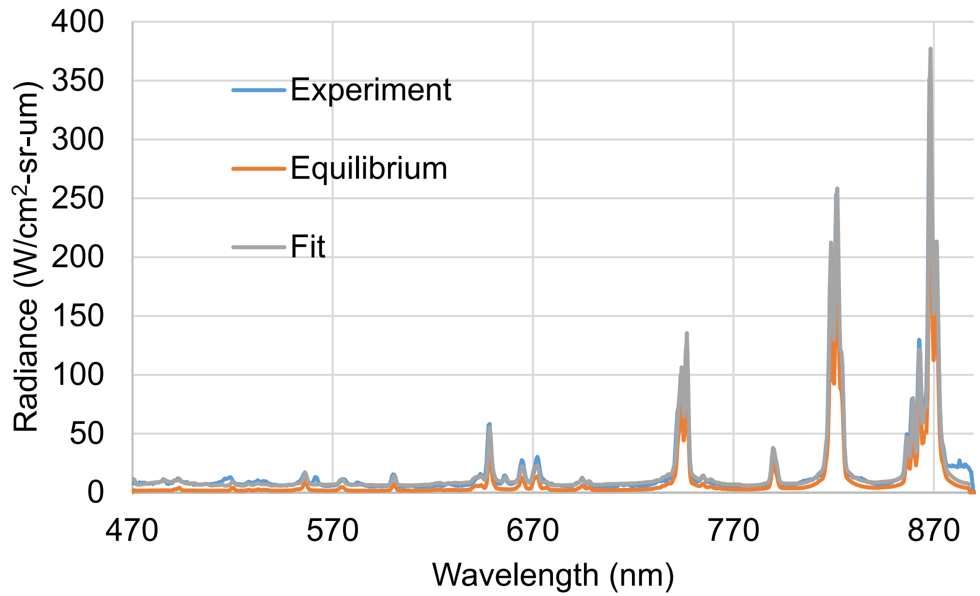
Next Region

- Next, examine Visible region (500-890 nm)



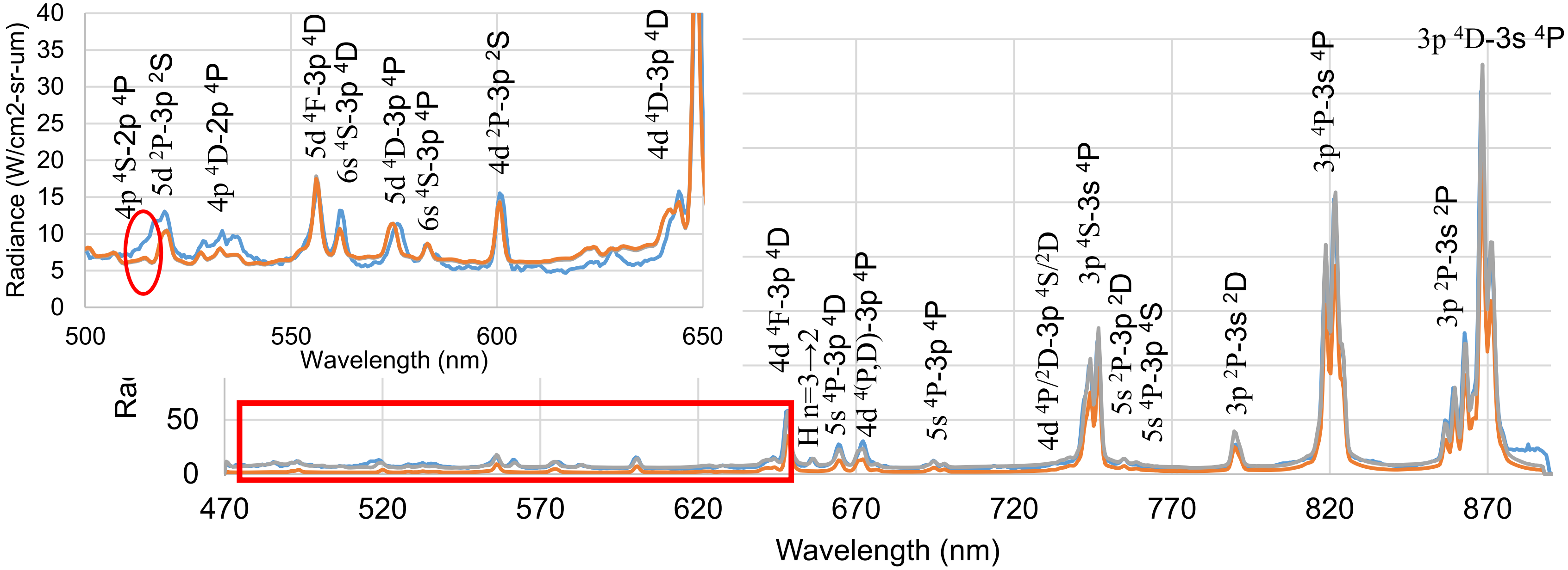
Vis Spectrum





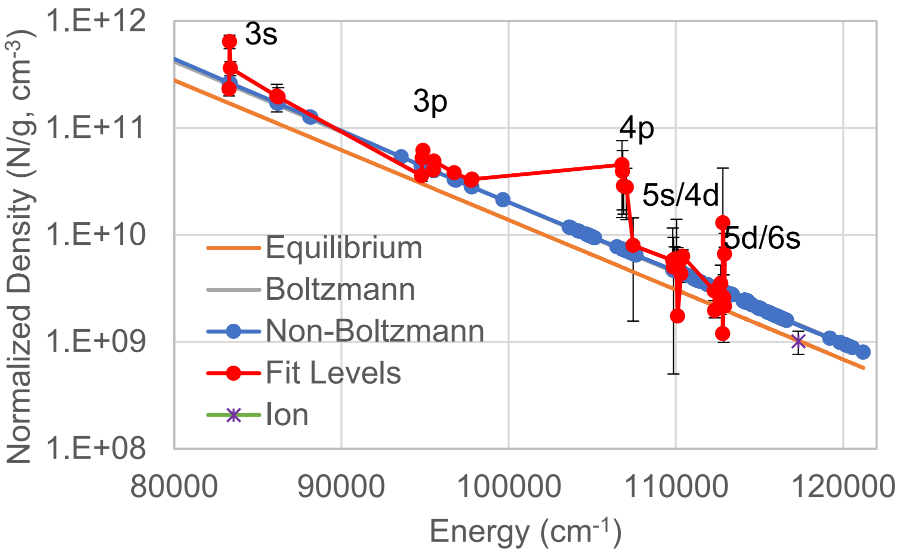
- Equilibrium prediction does not match continuum
- Best Boltzmann fit of the spectrum
  - Requires 50x the N_2 density, 2x the N density, 0.1% of H

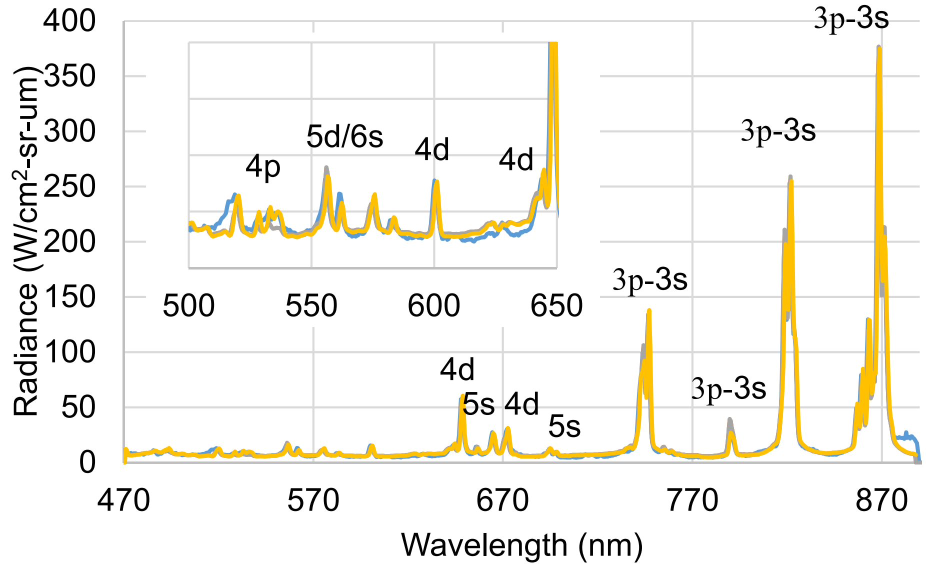
Feature Identification



- Strong (optically thick) lines from 3p state of N
- Several weaker lines from 4d and 5s states
- Hydrogen as impurity
- Weaker lines still from 4p, 4d, 5d
- Missing lines from 6s, 4p identified
- Additional missing features not identified

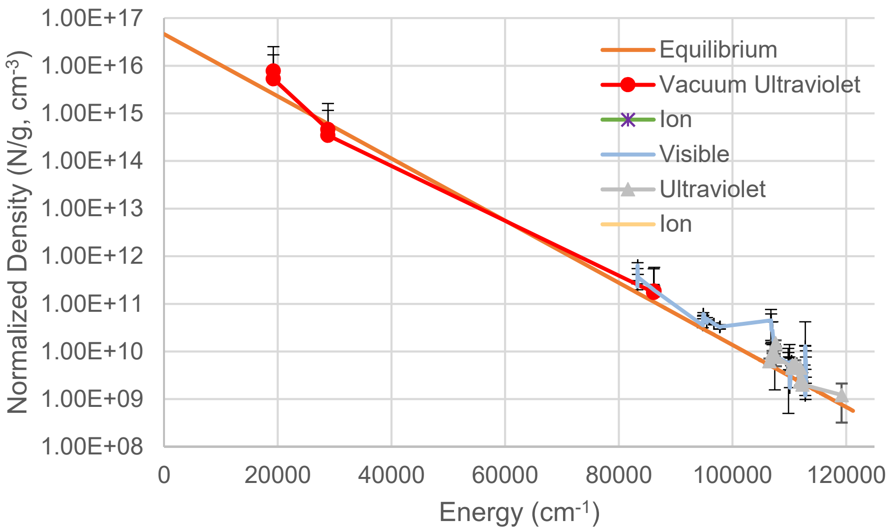
Level Fit





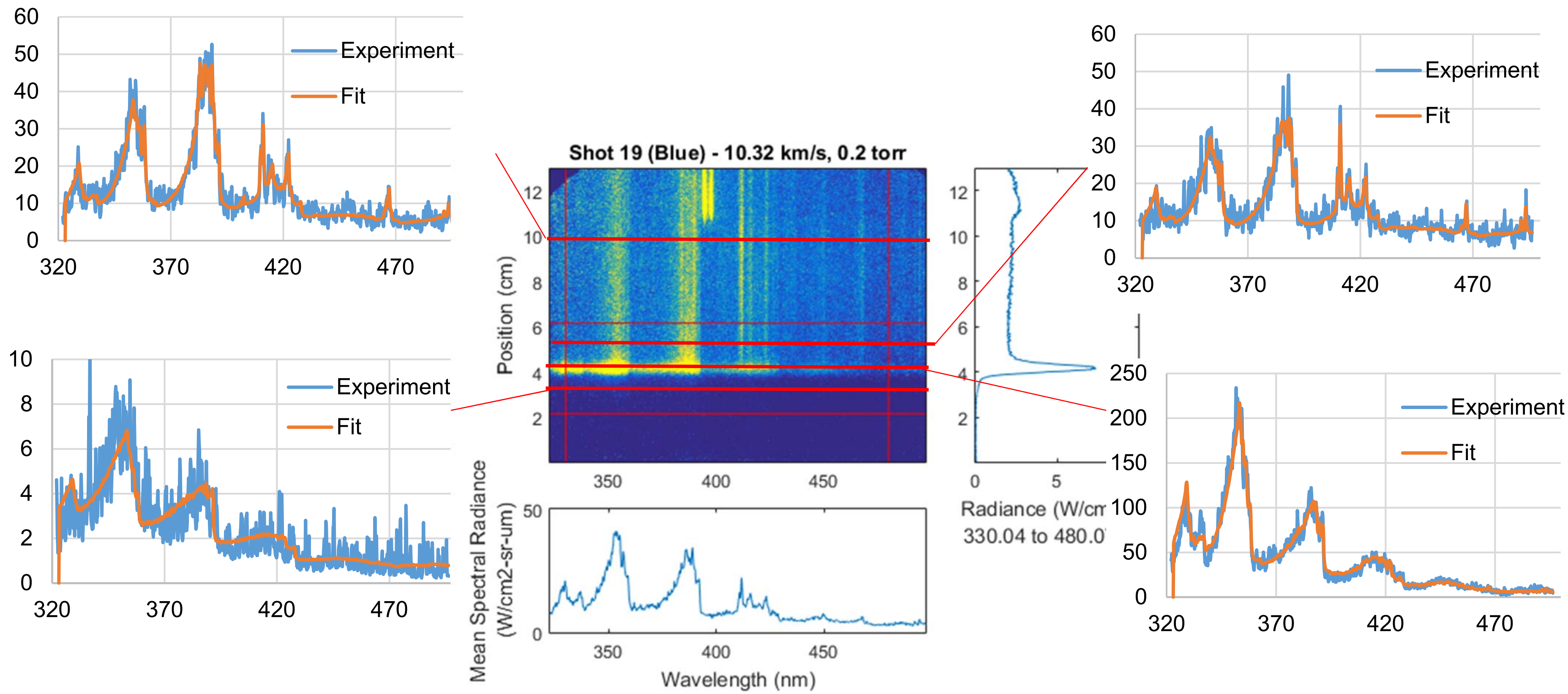
- Boltzmann Fit – elevated n_e, N. Slope (T) is same
- Non-Boltzmann Fit – Mirrors Boltzmann Fit
- Level Fit – Relatively consistent with Non-Boltzmann fit
  - 4p Levels significant overpopulation – probably issue with linelist

Combined Boltzmann Plot



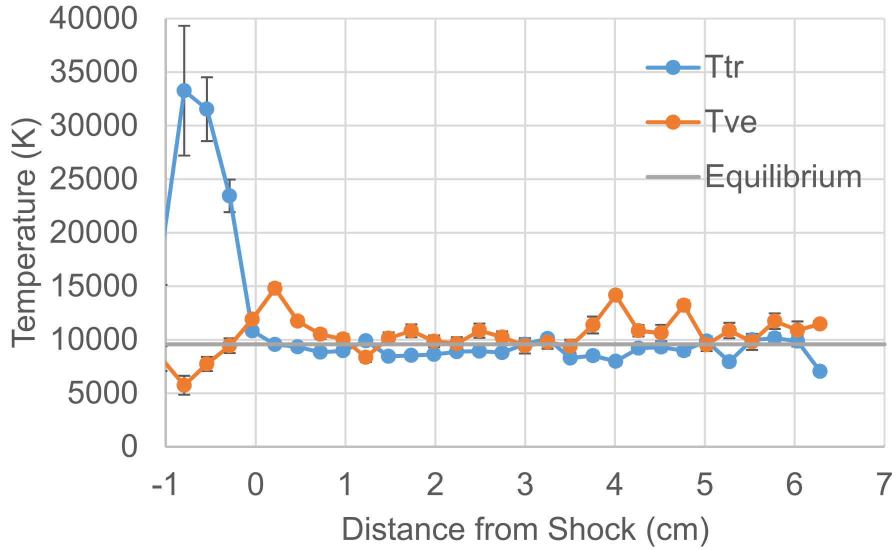
- Taking level populations from all three spectra, Boltzmann plot is relatively consistent

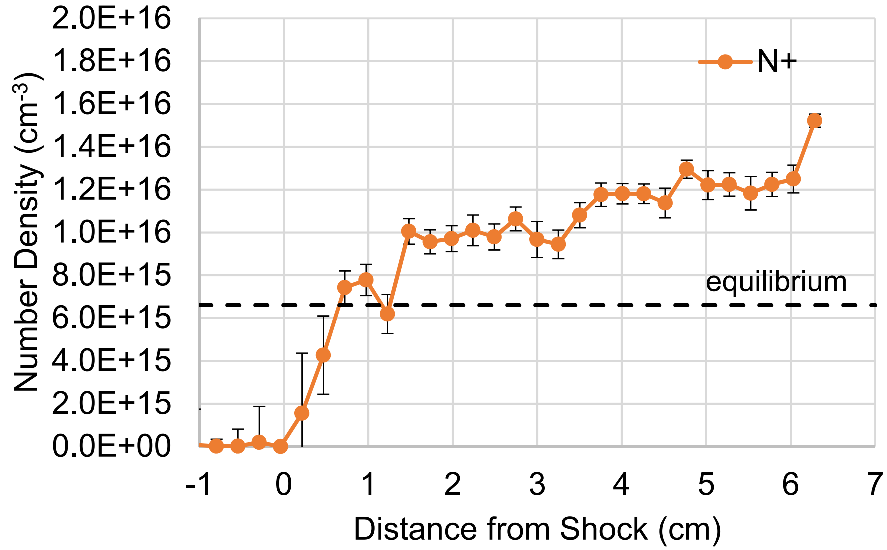
Transient Data Fits - Ultraviolet



- From spectrum, grab different spatial regions
  - Early/pre-shock: Weak radiance from N_2^+
  - Just post-shock: Strong N_2^+ radiance, some N_2, no atoms
  - Behind shock: N_2^+ decreases, atomics apparent
  - Much further behind shock: radiance is steady

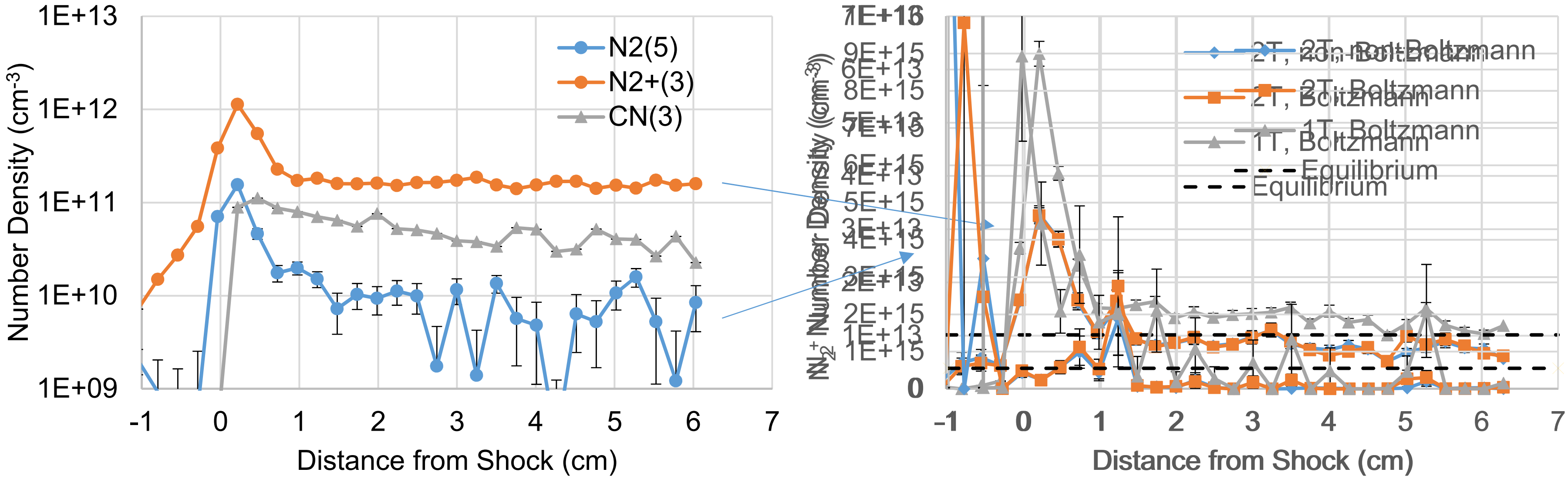
Temperature, Electron Density Trend





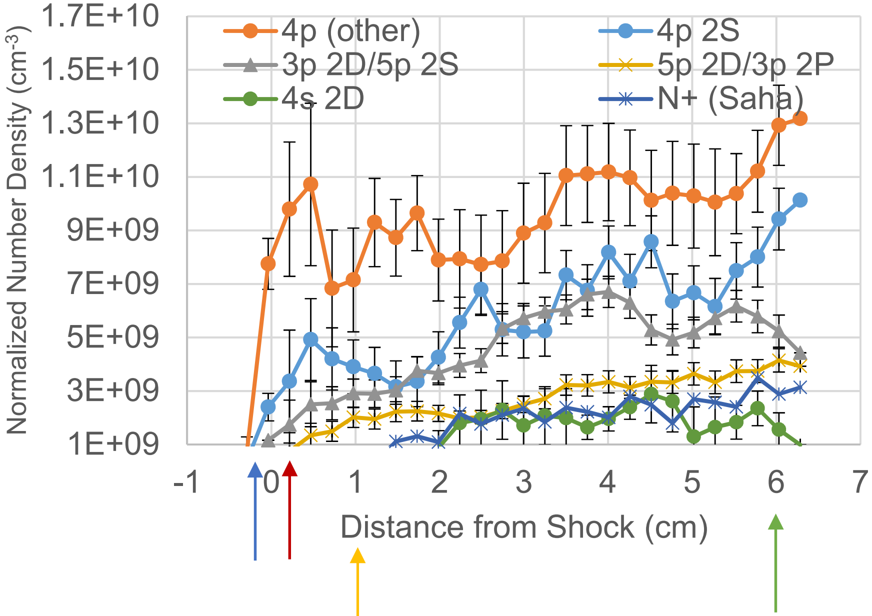
- From fit, obtain temperature trend
  - Translational temperature peaks before shock front determined by pressure sensors
    - Note: accuracy of shock front determination ~0.5 cm
  - Some overshoot of Tv from Tt observed at shock front
  - Temperature relatively constant following
- N^+ (electron) density trend
  - Rises to slightly above equilibrium level within 1 cm
  - Continues rising further away from shock front

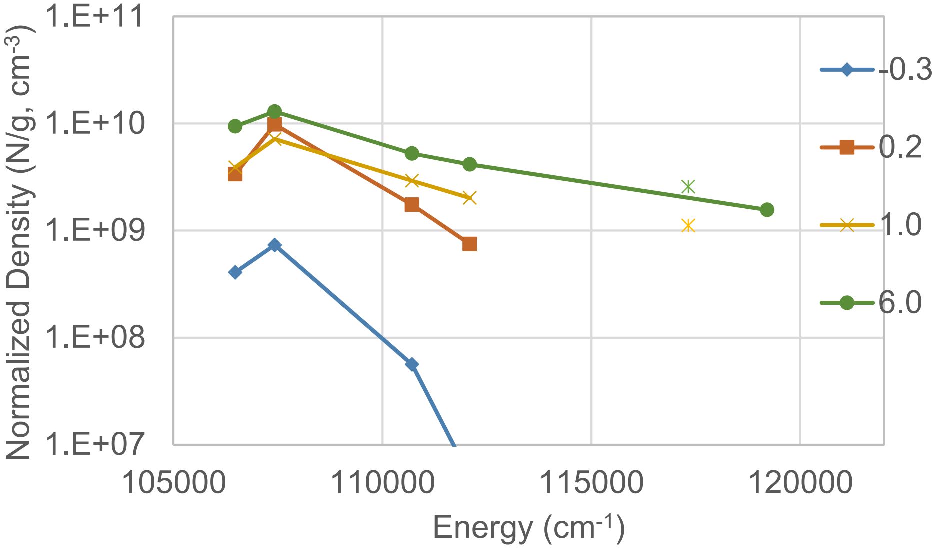
Transient behavior of Molecular Features



- Fit density of excited levels:
  - N_2 (C $^3\Pi_u$) state peaks just after shock front, drops near detection limit at ~1 cm
    - Density at single temperature is inferred to drop from 10^{16} cm^{-3} (lower than frozen concentration) to detection limit
    - Difficult to infer density with multi-temperature model
  - N_2^+ (B $^2\Pi_u^+$) state peak similarly, relaxes to steady levels in 1 cm
    - Inferred N_2^+ density, assuming 2-T, peaks at 3×10^{13} cm-3, drops to equilibrium
    - Single temperature inference more sharply peaked, remains above equilibrium

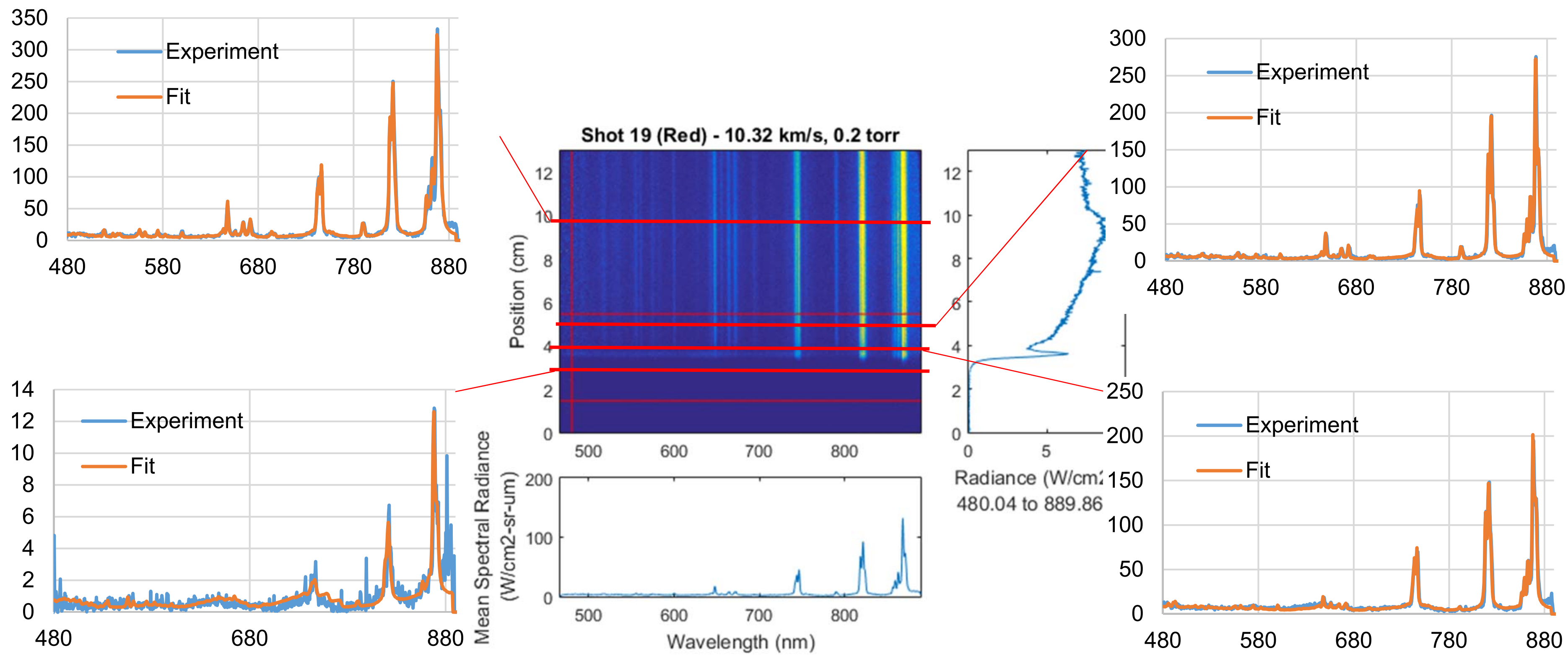
Atomic Feature Transient





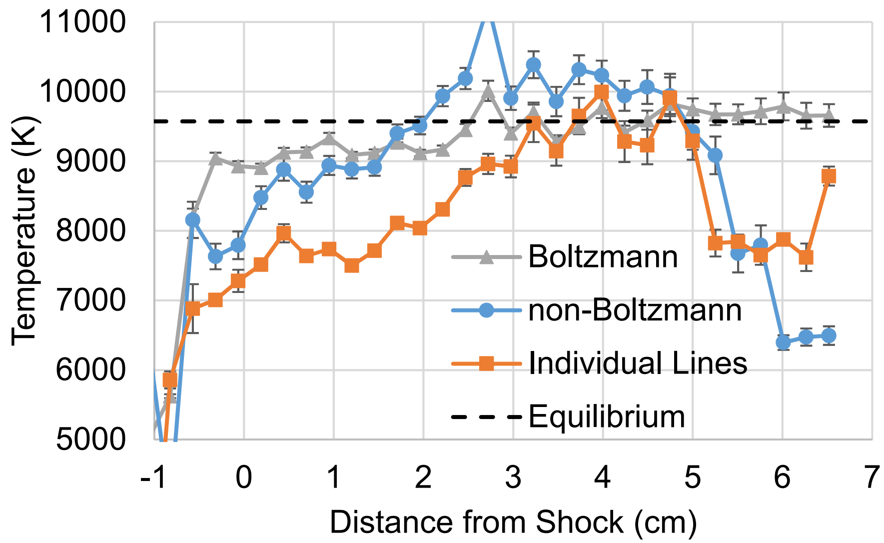
- Atomic state populations noisy, needed averaging and grouping
- Observe near steady behavior of most 4p states
- Gradual rise in higher energy states
- N^+ density (Saha normalized) tracks the 4s ^{2}D state
- Boltzmann plot shows
  - Rising slope (T) in 1 cm
  - Increasing density at later distances

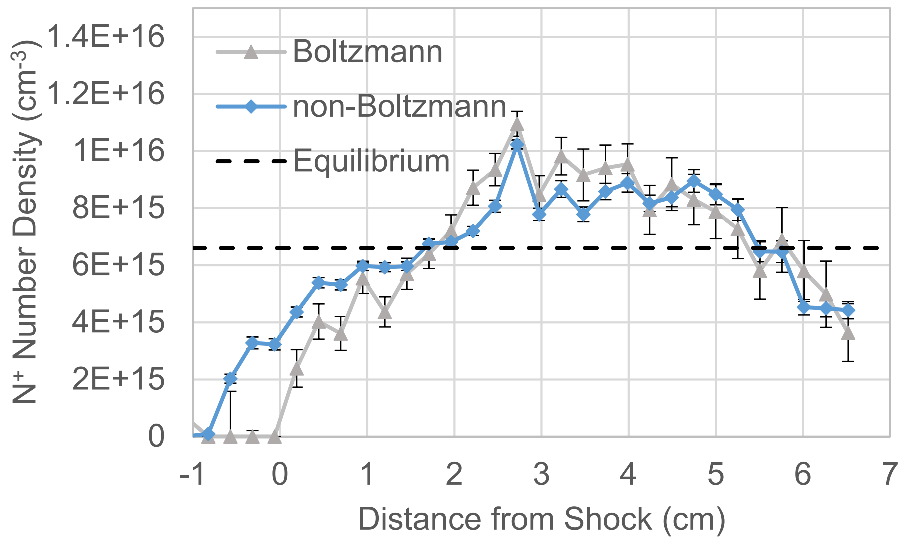
Transient Data Fits - Visible



- From spectrum, grab different spatial regions
  - Early/pre-shock: Weak molecular radiance from N_2 and N
  - Still(?) pre-shock: Still N_2 radiation, peak in atomic radiation
  - Behind shock: N_2 hard to distinguish, strong atomic radiation
  - Much further behind shock: atomic radiation continues to increase

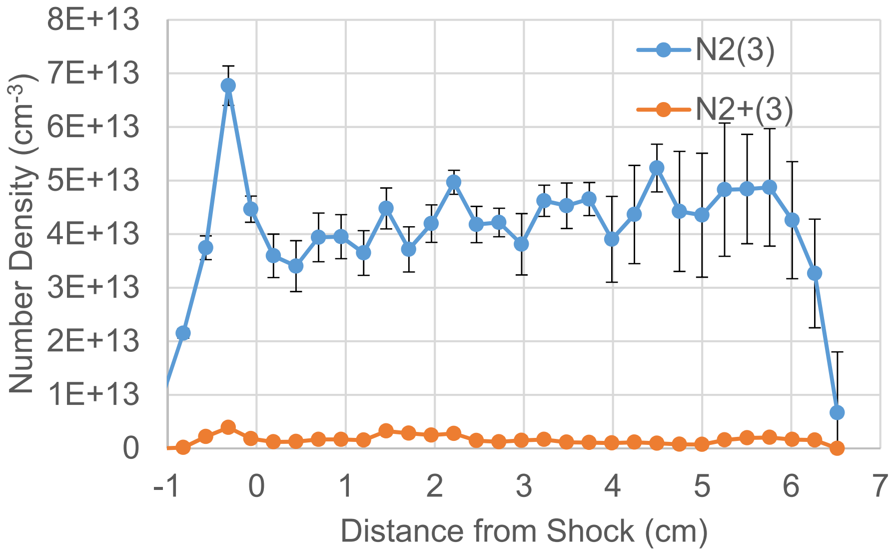
Temperature and Ionization Trend

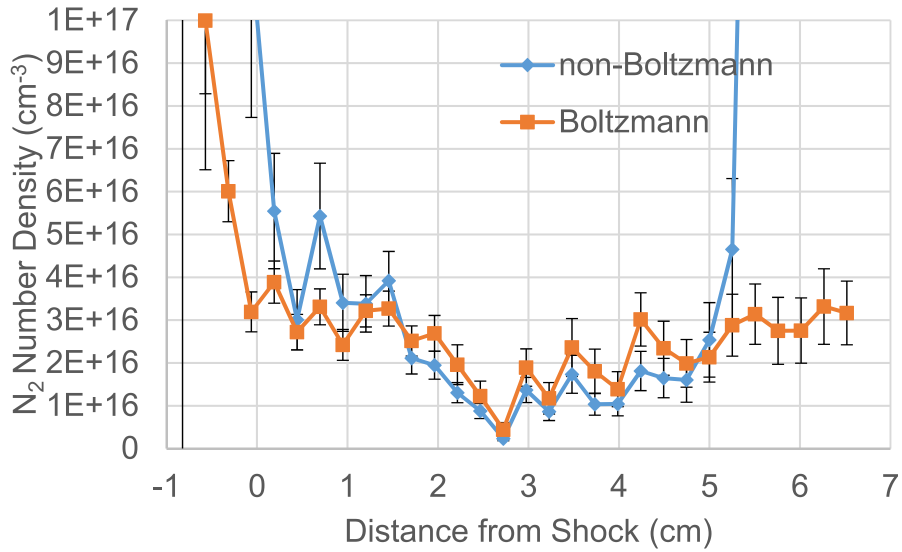




- Temperature trend inferred from infrared data
  - Multi-temperature fits give non-sensible results
    - Fit is dominated by electron(ic) temperature
  - Takes several cm to reach equilibrium
  - Temperature is lower when lines are fit independently
- Electron number density
  - Could not be inferred from independent line fit
  - Non-Boltzmann infers earlier rise time than Boltzmann
  - Trend overshoots equilibrium

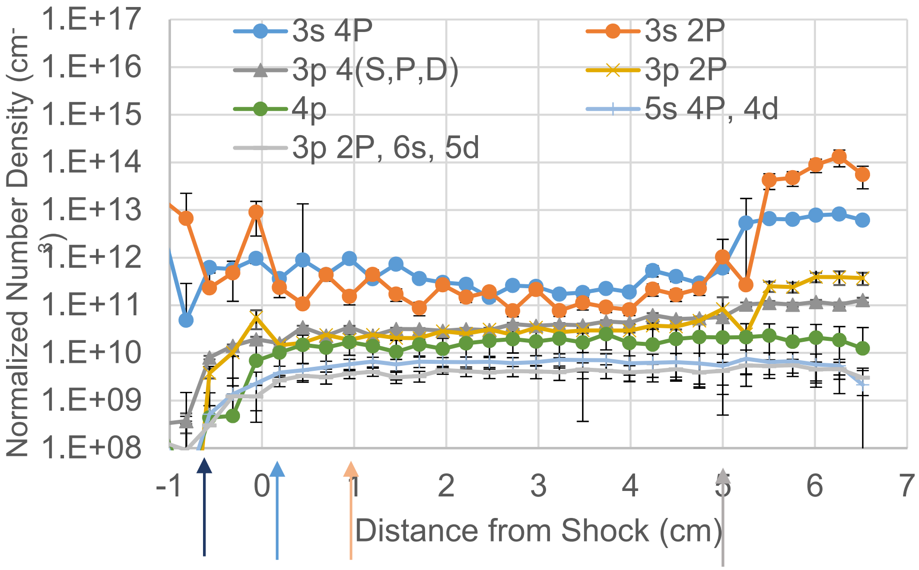
Molecular State Density

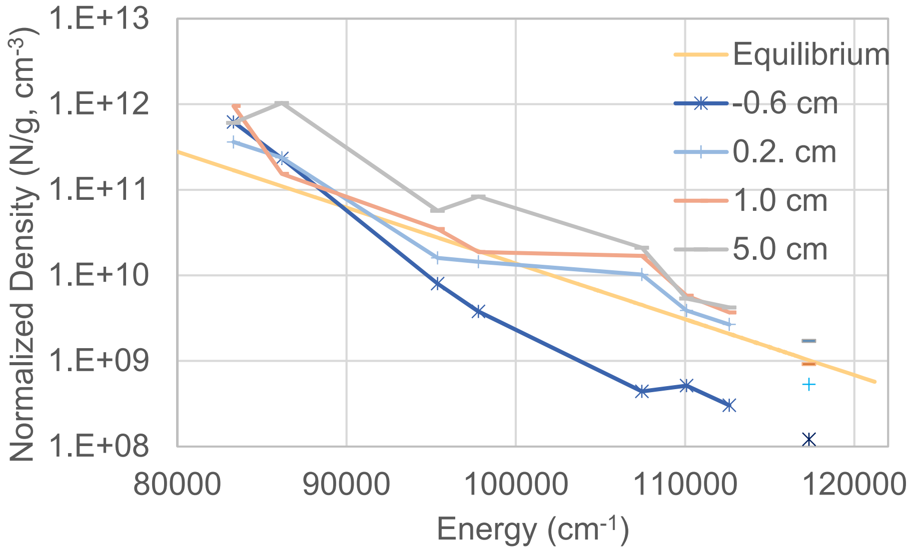




- Fit density of excited levels:
  - N_2 (B $^3\Pi_g$) displays sharp peak, then is steady at 4×10^{13} cm^{-3}
- N_2 density inferred by Boltzmann or non-Boltzmann model
  - Shows decay from large values (greater than frozen density)
  - Settles at 10^{16} cm^{-3} (50x higher than equilibrium)

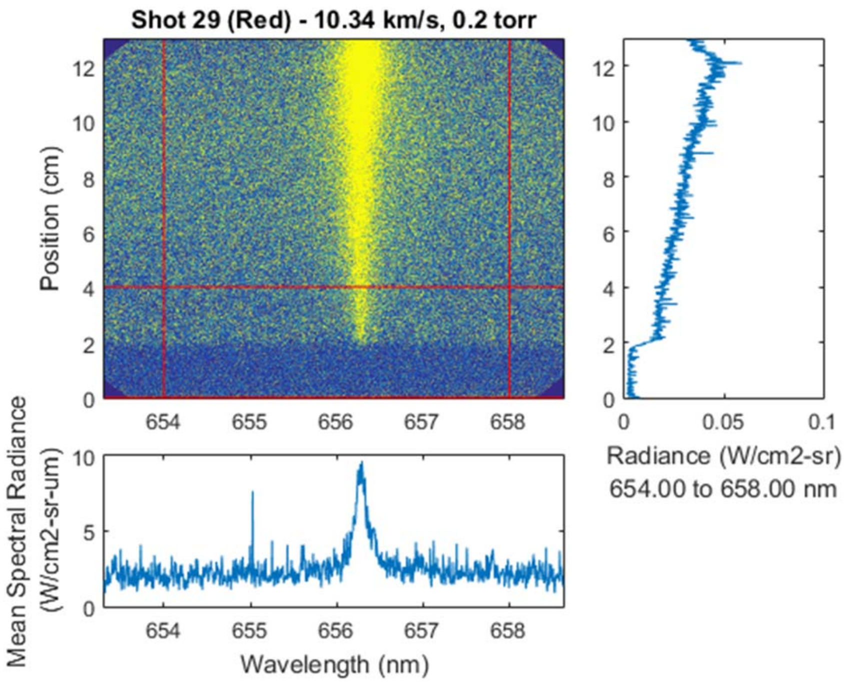
Atomic Feature Transient

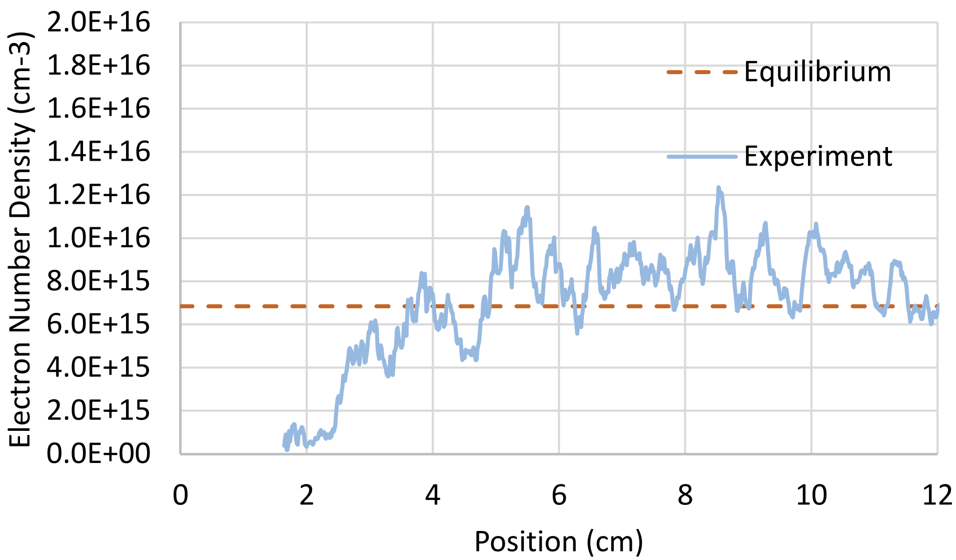




- Atomic states grouped by configuration, term for plotting purposes
- 3s states are at fairly steady concentration throughout
- Other states rise to steady level over ~1 cm
- Boltzmann plot shows
  - Rising slope (T) in 1 cm
  - Increasing density at later distances

Electron Number Density





- From Stark Broadening of the Hydrogen-α line, electron number density trend was obtained
- Different shock from previous analysis, but similar velocity

Ionization Models

- There are only 5 reactions:

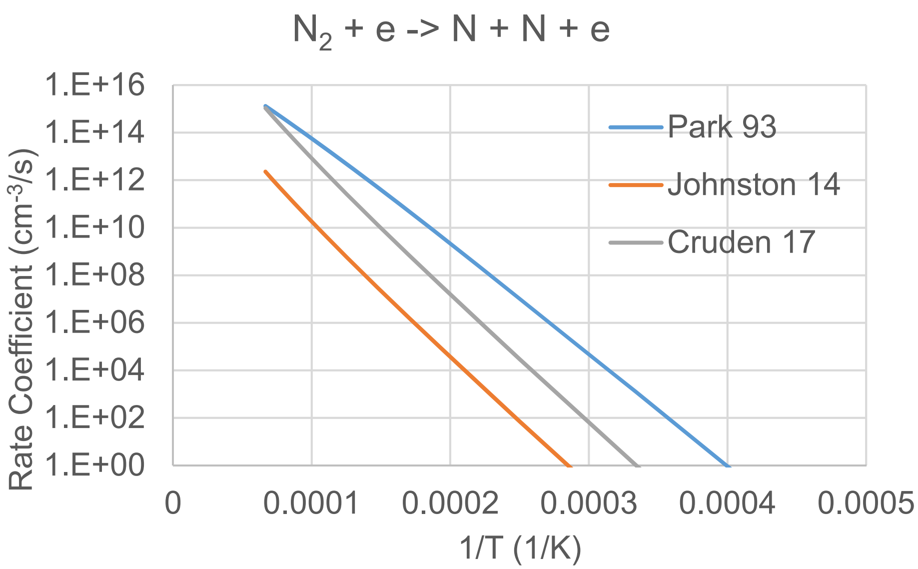
$$N_2 + M \leftrightarrow N + N + M \qquad (1)$$

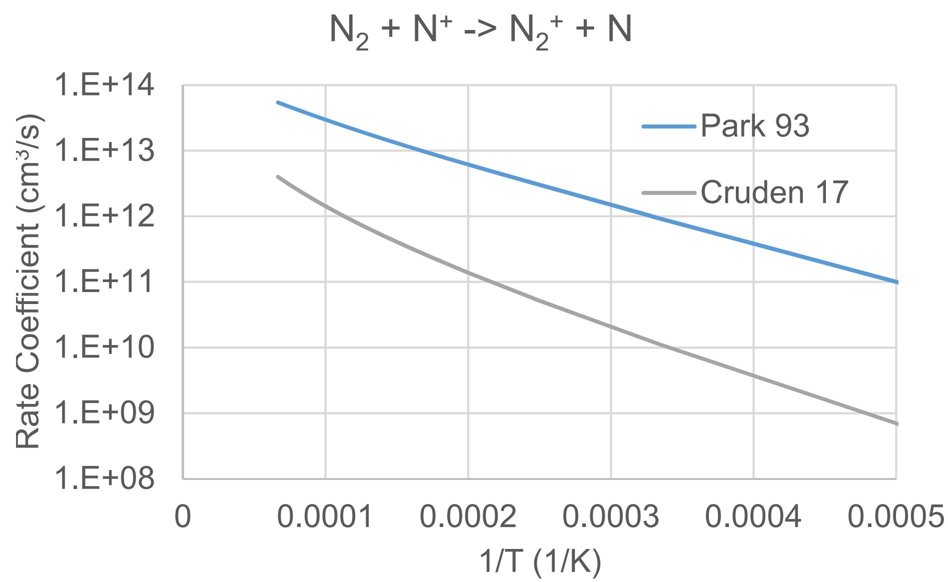
$$N_2 + e^- \leftrightarrow N + N + e^- \qquad (2)$$

$$N + e^- \leftrightarrow N + e^- + e^- \qquad (3)$$

$$N + N \leftrightarrow N_2^+ + e^- \qquad (4)$$

$$N^+ + N_2 \leftrightarrow N_2^+ + N \qquad (5)$$





- Multiple order of magnitude variation has been reported for reactions (2) and (5)

Comparison of Ionization Models

- All 3 models predict an overshoot in ionization
- Mechanism:
  - $N + N \rightarrow N_2^+ + e^-$

    produces first electrons
  - $N_2 + e^- \rightarrow N + N + e^-$

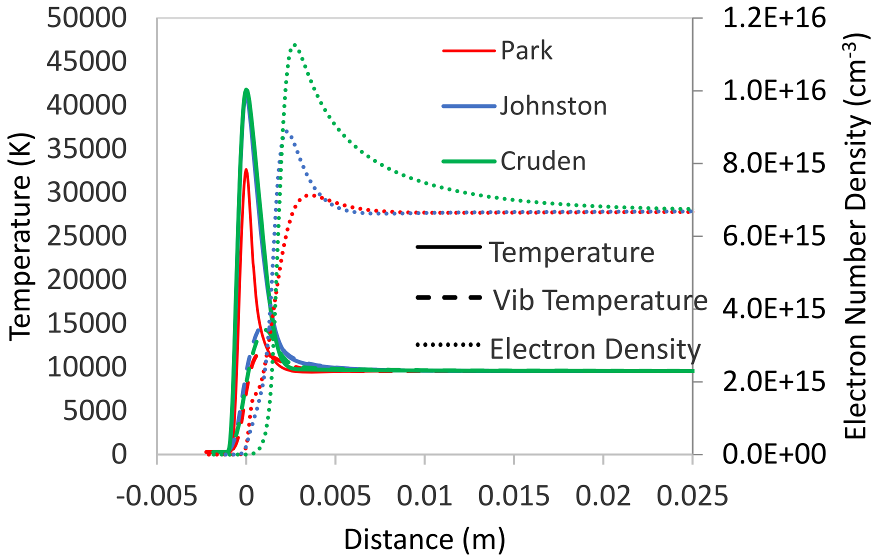
    Exothermic, temperature falls

    Fast in Park Model

    → Reduces temperature
  - $N + e^- \rightarrow N^+ + e^- + e^-$

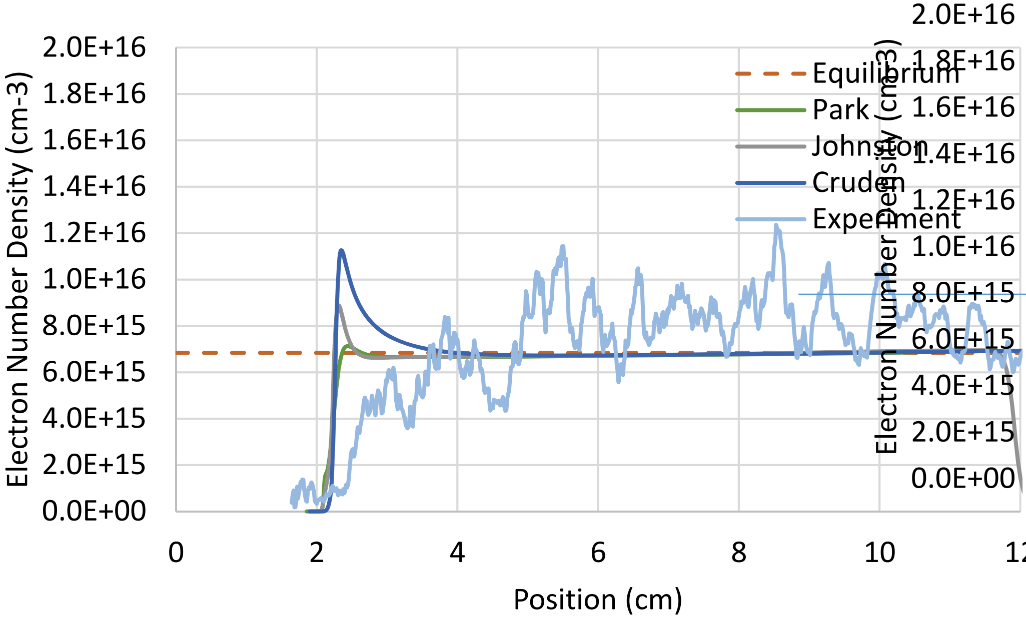
    proceeds at T_e

    Ionization overshoot follows temperature overshoot
  - Relaxation of Ionization overshoot proceeds through
    - $N^+ + N_2 \leftrightarrow N_2^+ + N$ slow in Cruden 17
    - $N_2^+ + e^- \rightarrow N + N$ fast

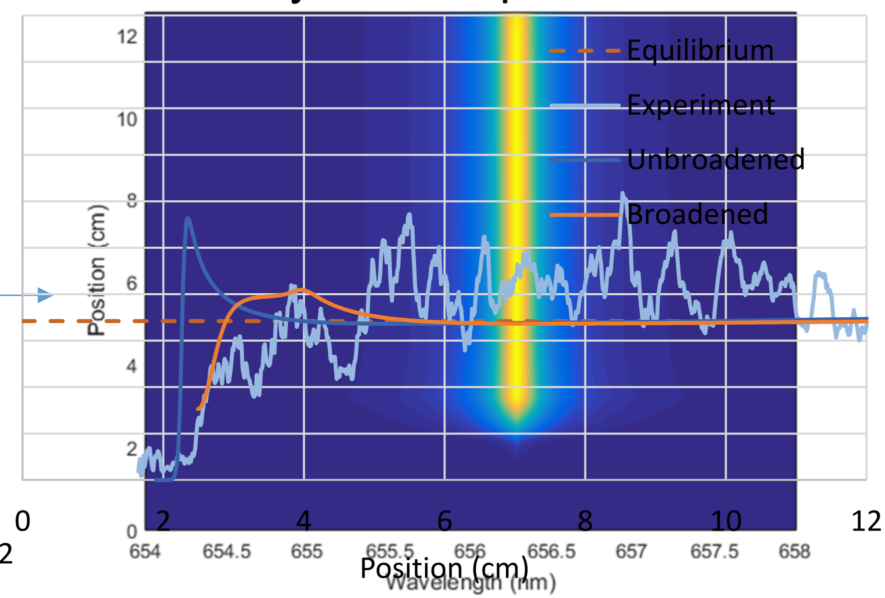


Account for Experimental Resolution

Predicted trend

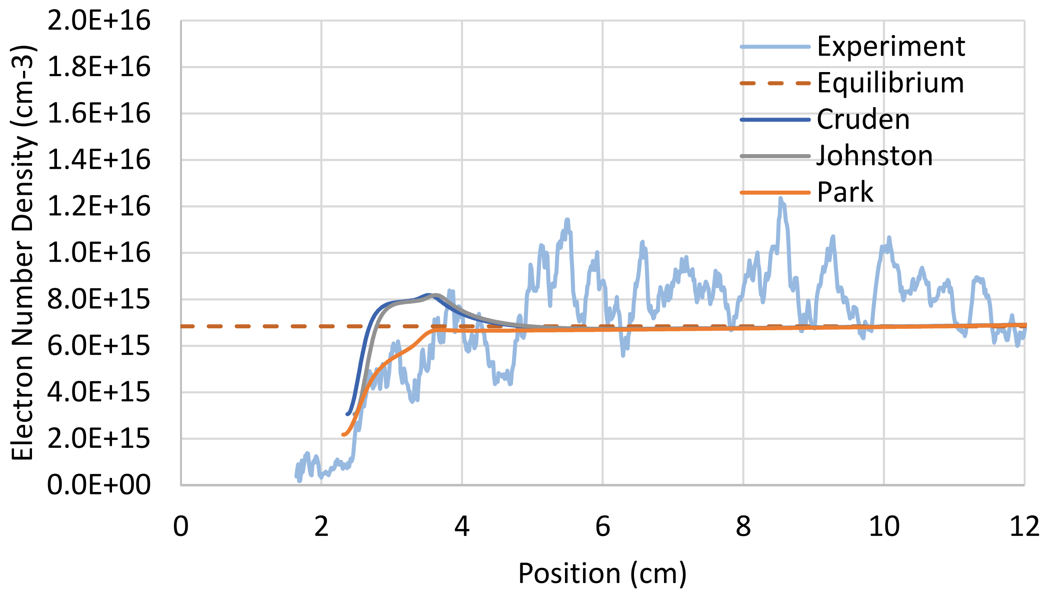


Broadened Synthetic Spectrum



- 1D Profiles used as input to radiation code
- Synthetic Spectrum Broadened with experimental functions
- Synthetic Broadened Spectrum fit with voigt function
  - Electron density extracted
  - Overshoot greatly reduced due to experimental resolution

Comparison of Ionization Models



- Park Model Follows data closely
- Based on traditional energy transfer mechanism
  - 28% of ionization energy comes electro-vibrational modes
  - Ions and electrons created/destroyed at energy of mixture

Conclusions

- Analysis of N2 shock wave at 10.3 km/s (Nominal)
- Concentration and temperature profiles extracted from spectral data
- Equilibrium Analyses
  - Temperatures generally from 1-3% of equilibrium
  - Some concentrations inferred to exceed equilibrium
    - Electron density must be 2x higher than equilibrium to explain continuum
    - Visible region infers 2x the N atom density, 50x the N_2 density
- Review of Atomic N Lines
  - Some high energy lines (3d) above ionization threshold not observed
  - Other lines (4p, 6s) missing from NIST database
  - Still additional features not predicted – likely additional lines
- Transient Analysis
  - Obtained transient concentrations of excited species
- Ionization – Park93 still the best
- Quality of fit dependent upon models assumed