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AFOSR MURI in FUNDAMENTAL PROCESSES IN HIGH-TEMPERATURE HYPERSONIC FLOWS

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AFOSR – MURI Review
Arlington, VA

Design and Analyses of Nonequilibrium Gas Kinetic Experiments

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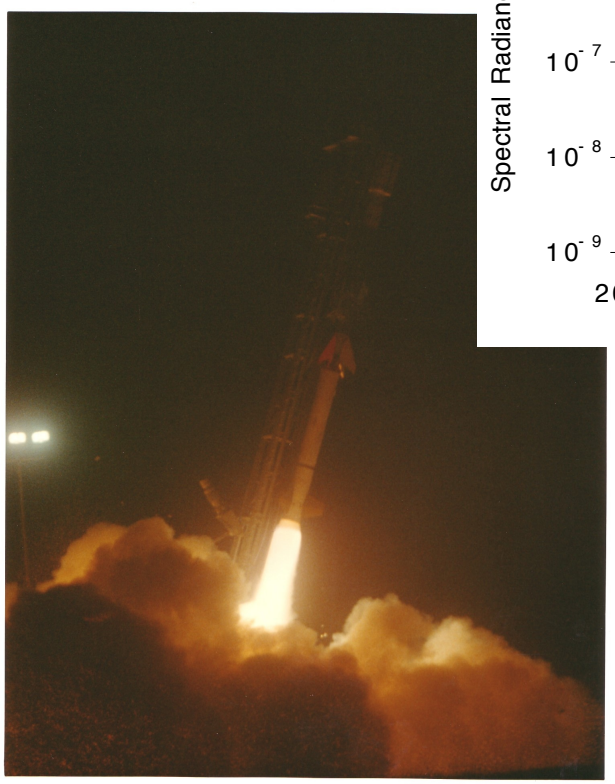
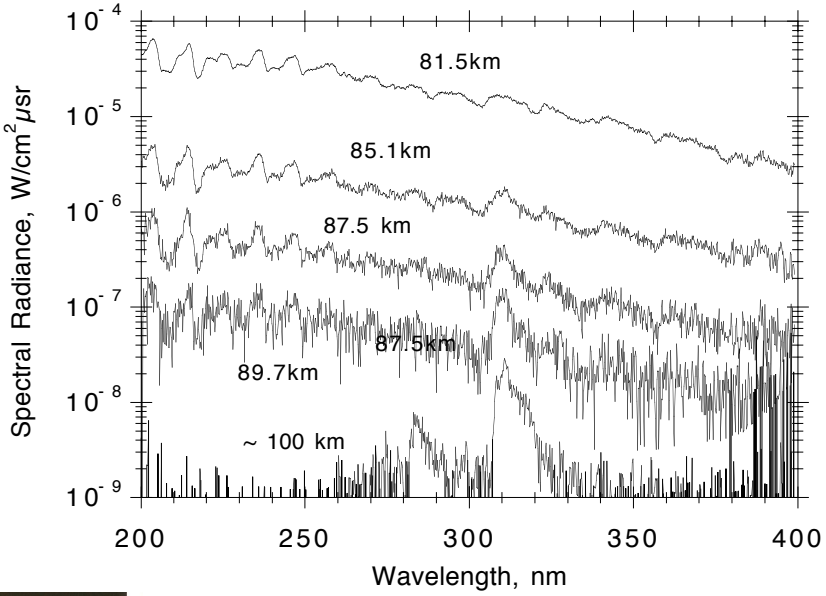
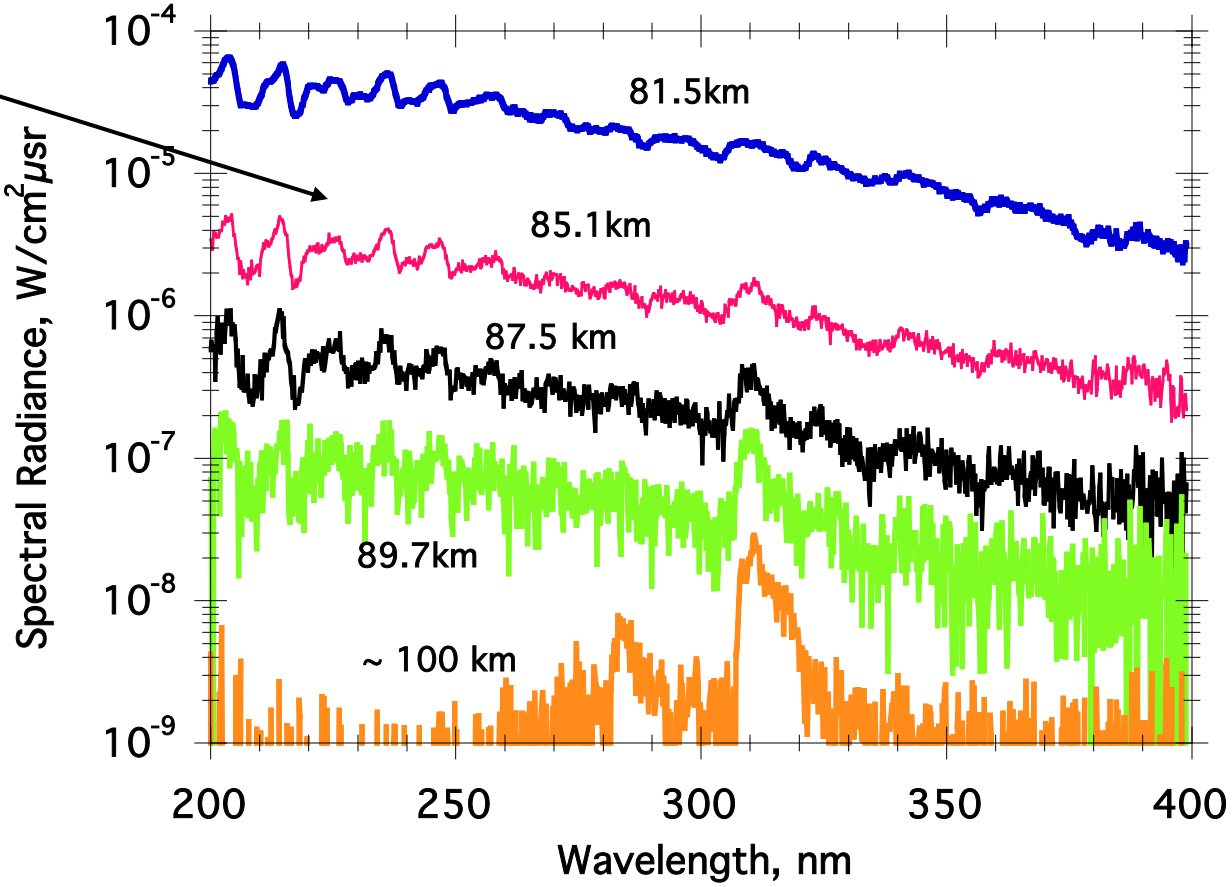




Expansion of High-Altitude Portion of BSUV2 Trajectory

NO spectral radiation



Spectra as a Diagnostic in Thermochemical Nonequilibrium Flows

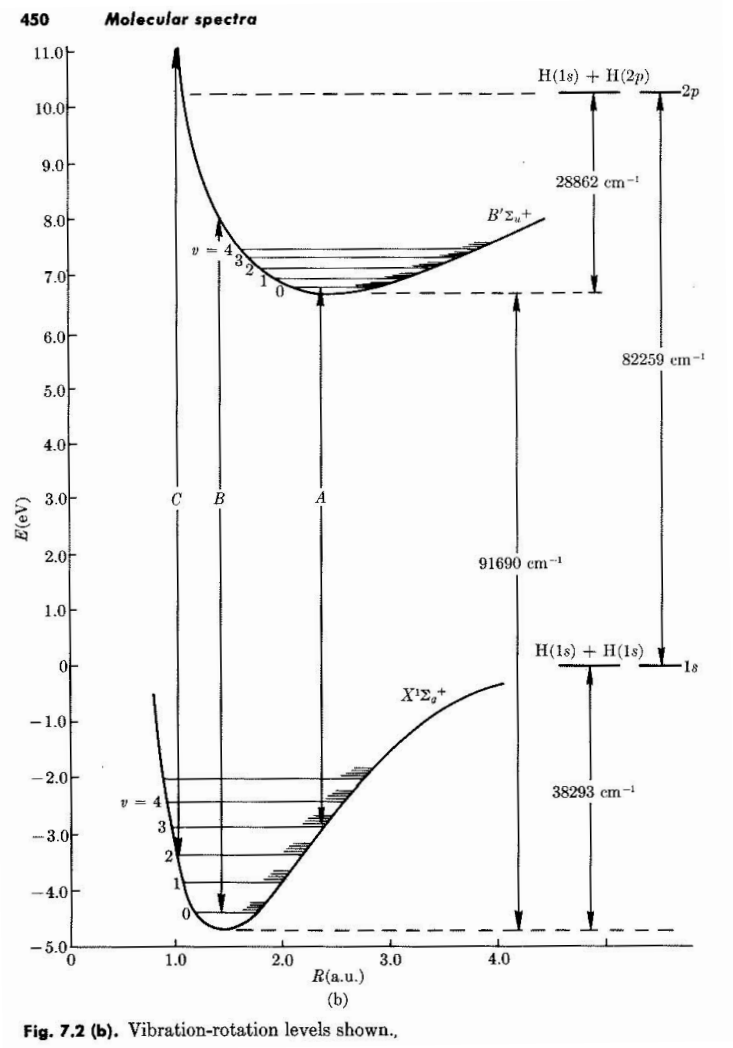
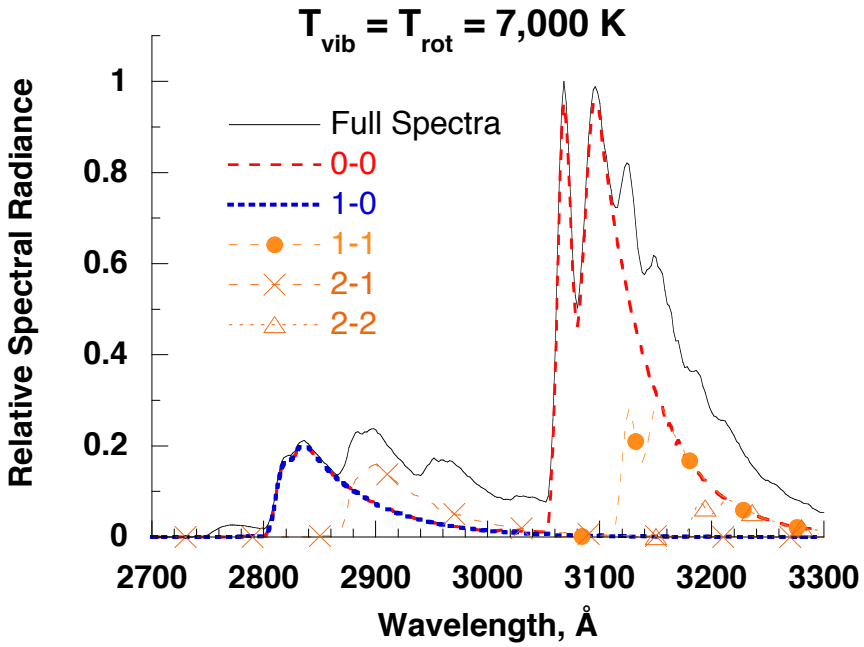


Fig. 7.2 (b). Vibration-rotation levels shown.,

- Ro-vibronic spectra is the simultaneous change of electronic, vibrational, and rotational quantum states.
- Determine shocklayer temperatures and chemical species.

Vibrational State Components



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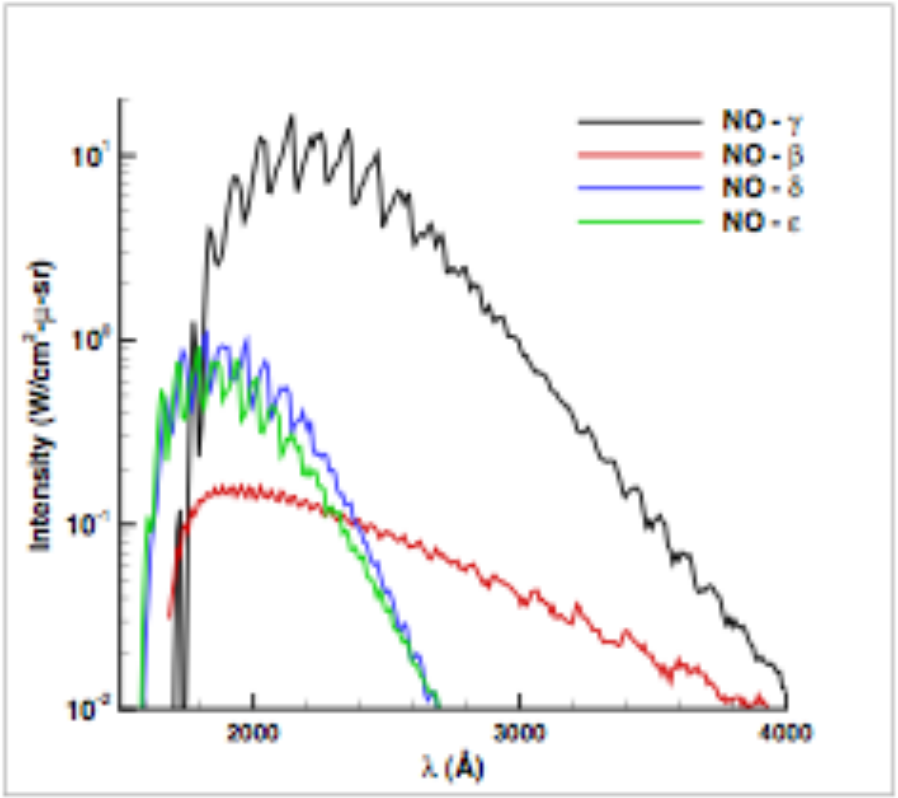
Theory of Molecular Emission

$$E \propto \frac{16\pi^3 c\bar{\nu}^4}{3(2J'+1)} N_u \left\{ \left| R_e\left(\bar{r}_{v',v''}\right) \right|^2 q_{v',v''} \right\} \left\{ S^{J'\Lambda'}_{J''\Lambda''} \right\}$$



- **Most of above constants and physical parameters are well known for systems of interest in our flight regime.**
- **N_u = number of molecules in excited electronic state that radiate. It can be related back to flow simulations.**

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Advances in Modeling and Simulation Since "BSUV1 and 2"

Particle - Methods

- Capture correct fundamental behavior in shocks
- Molecular Dynamics/Quasi-classical trajectory (MD/QCT) chemistry models
- State specific particle methods
  - N_2 state specific vibrational and dissociation models in a shock,
  - State specific chemical models, NO formation,
  - Electronic state specificity
- Improve radiation predictive modeling as a tool to study fundamental nonequilibrium.

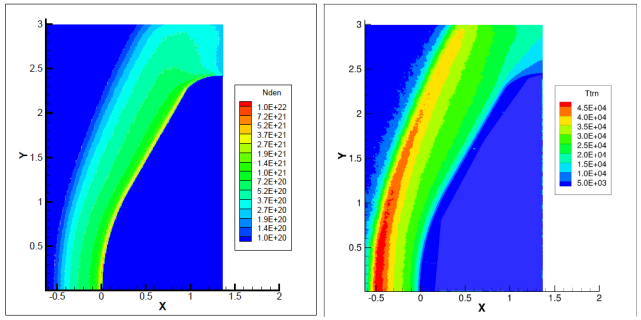
Direct Simulation Monte Carlo

1. DSMC follows the motions of many virtual particles on a grid over a series of time steps, tracking their collisions.
2. Particle-surface collisions are calculated.
3. Reactions and changes in internal energies and velocities of the components are also tracked.
4. Particles are indexed within cells.
5. Particle collision outcomes (i.e., relaxation and chemistry) are calculated using Monte Carlo techniques.
6. Post-collision velocities are determined, observing conservation of energy and momentum.
7. Provides multi-scale approach to modeling thermochemical nonequilibrum in hypersonic shock layers.

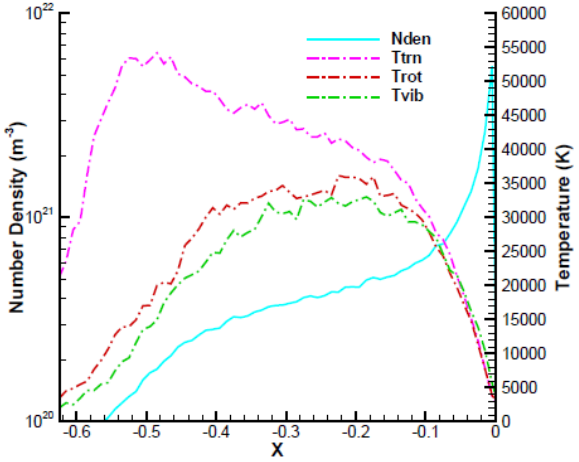
Objectives and Approach of Thermochemical Modelling

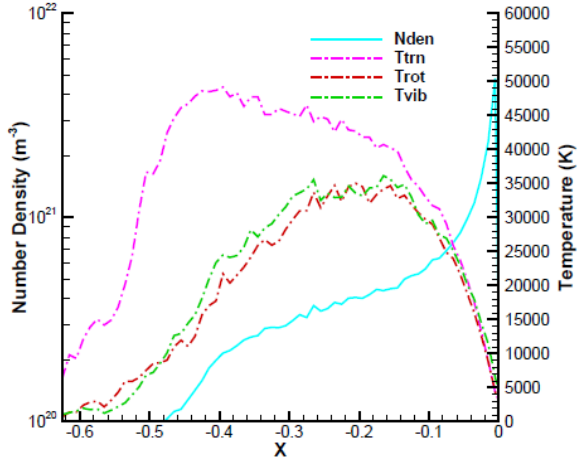
- **The transitions between the vibrationally excited states of the N_2, its dissociation, and formation of NO from different N_2 vibrational excited states are modeled.**
- **Collisions that cause translational to vibrational energy exchange with better representation of physics have been tested:**
  - **the discrete Larson-Bernakke (baseline),**
  - **Schwartz-Slawsky-Herzfeld (SSH),**
  - **Forced Harmonic Oscillator (FHO).**
- **The chemistry models include: (1) TCE, (2) QCT - Bose, and (3) QCT - Jaffe and Magin (N_2 dissociation).**
- **Collaborate with D. Truhlar, S. Doraiswamy and G. Candler to use new N3 and N4 potential energy surfaces.**
- ***Explore sensitivity of NO spectral radiation using soon to have data from CUBRIC/R. Parker.***

Pure N_2/N Flow over a Blunt Body, Importance of T-V Relaxation Kn_∞~0.3

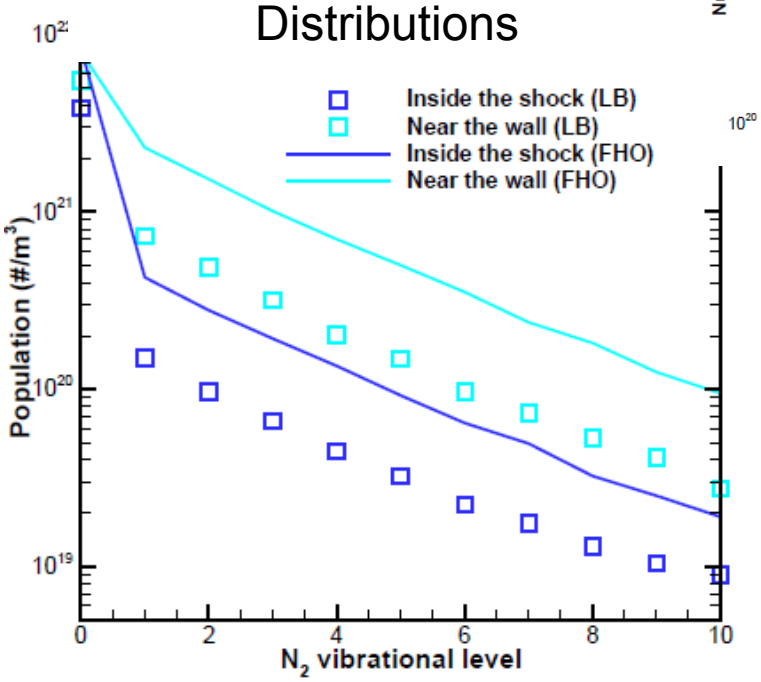


LB-baseline vs Advanced FHO



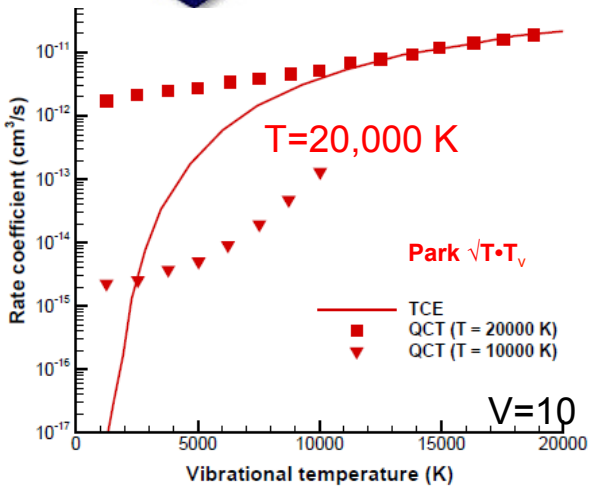


Nonequilibrium Vibrational Distributions



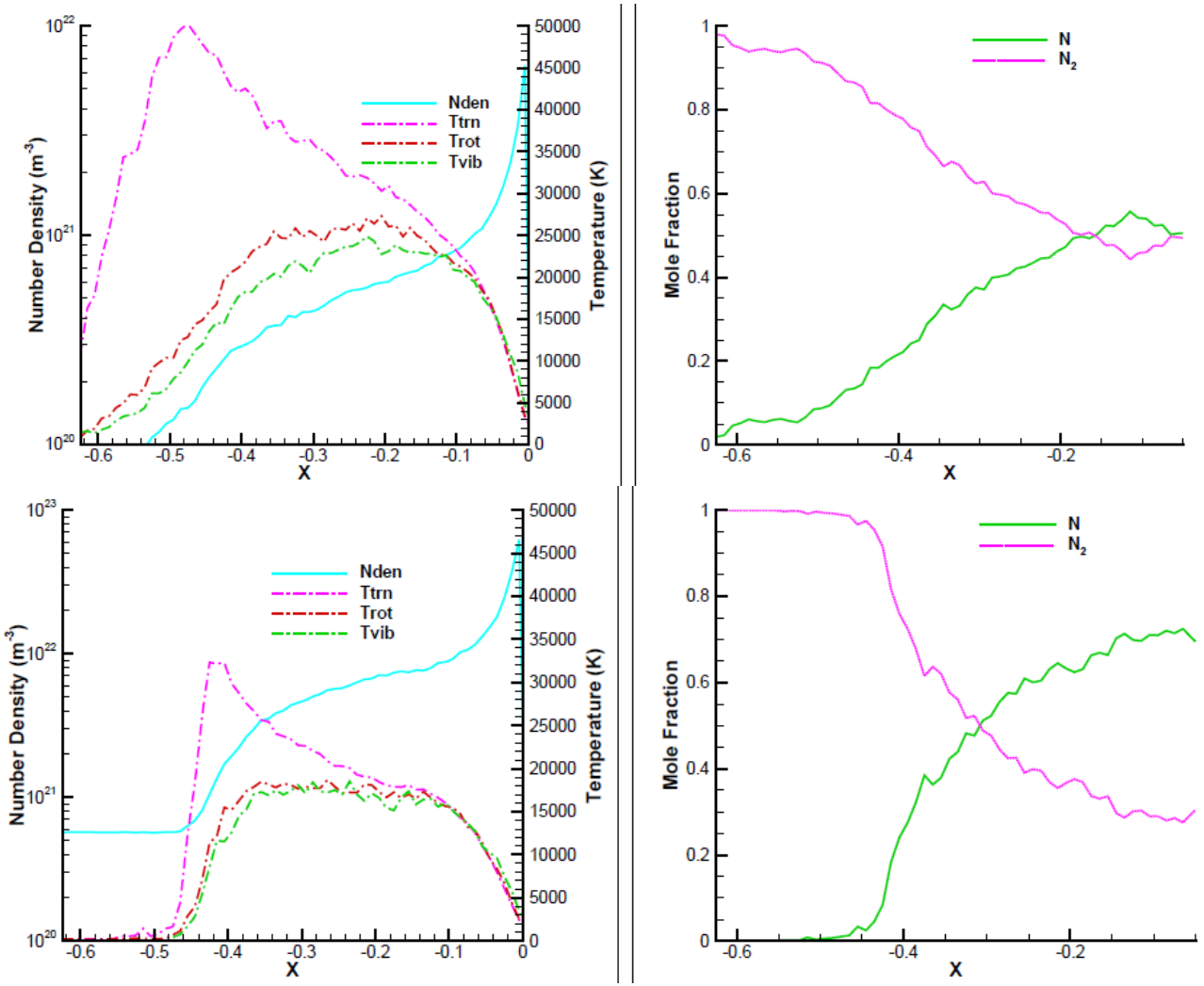
- FHO V-T transition rate > LB rate gives,
  - higher FHO vibrational populations
  - higher vibrational temperatures
- The shock width is reduced when using the FHO model ~ 15% difference

Sensitivity of N_2 Dissociation to Chemistry Model - Kn_∞~0.3



- QCT rates are high for low vibrational levels – crucial in ladder climbing in a shock.
- QCT gives higher degree of dissociation due high rate at low vibrational levels

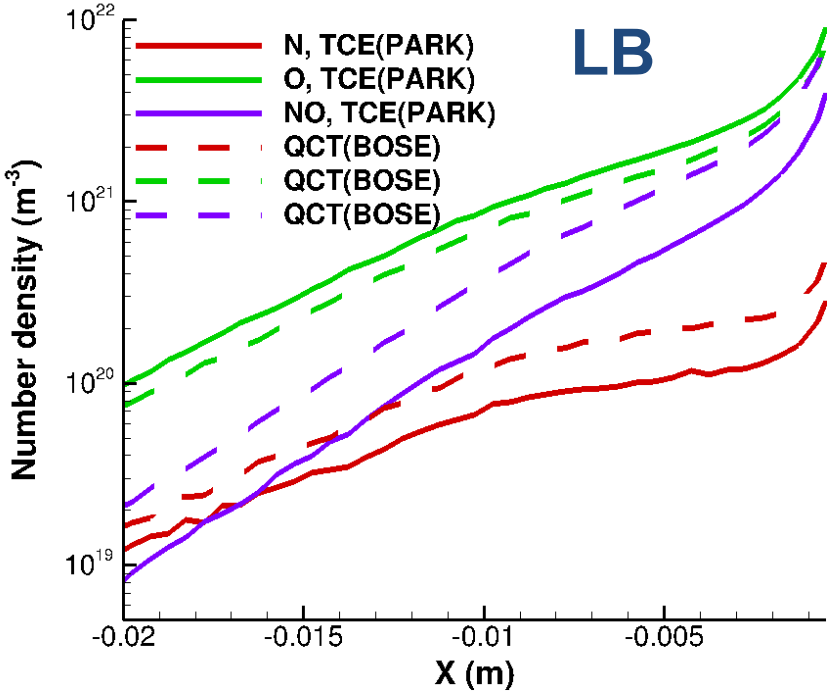
Baseline TCE

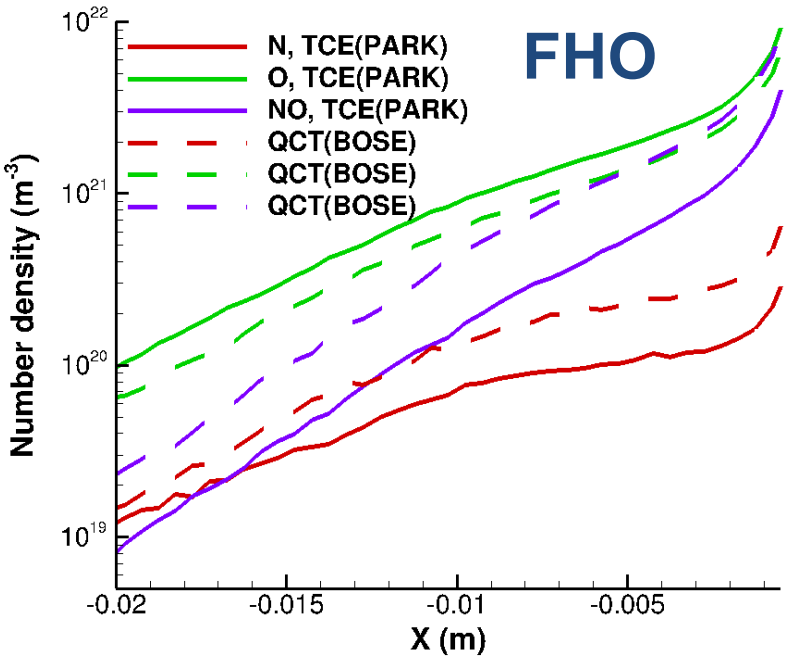


vs New QCT

Sensitivity of NO Formation to Chemistry Model

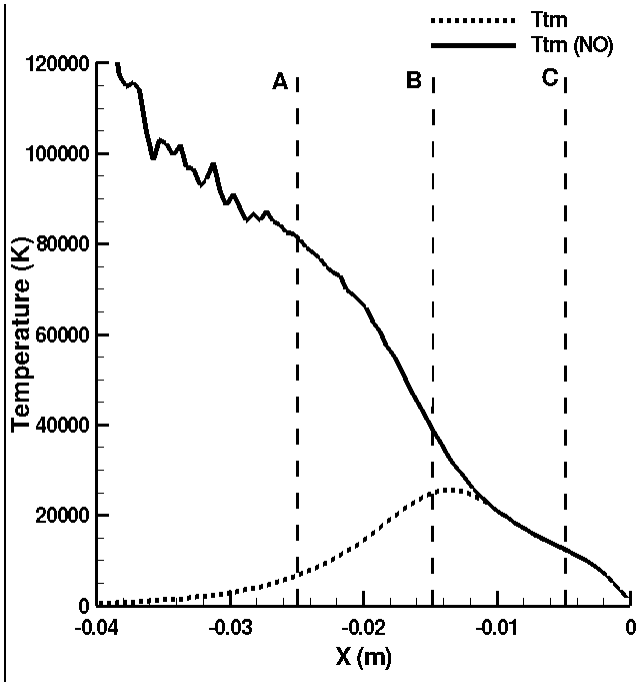
7km/s, 81 km, free stream, 50% N_2 and 50% O_2



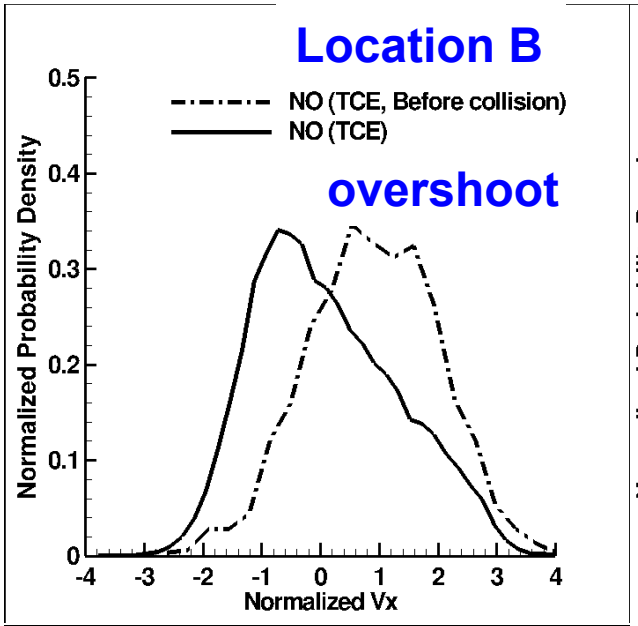


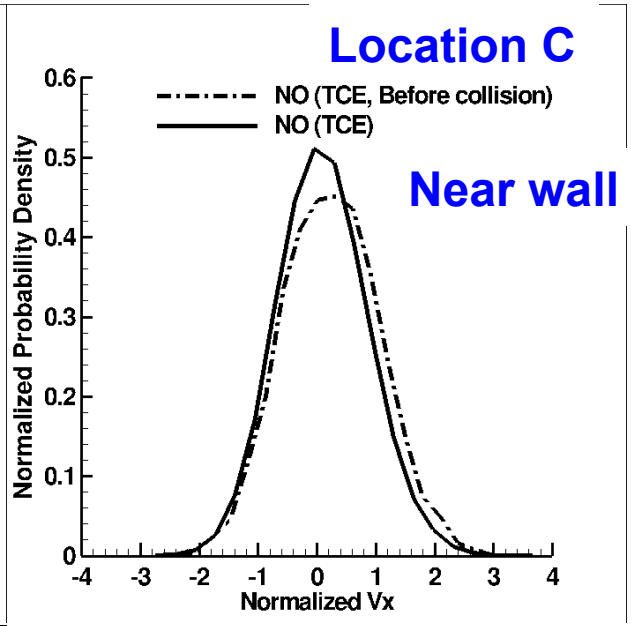
- **When QCT chemistry is applied, the NO number density from FHO case is about 20% higher than the LB case.**
- **Using FHO for VT and QCT for chemistry significantly increases the NO formation in the 81 km and 7km/s case.**

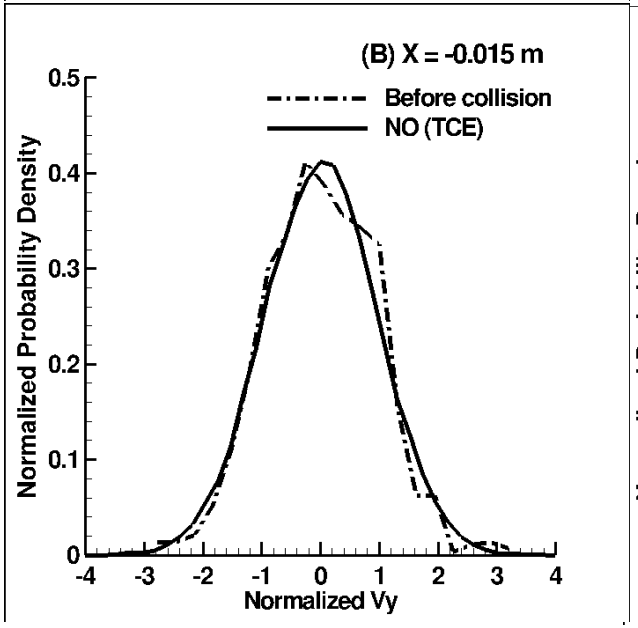
Velocity Distributions of NO Molecules

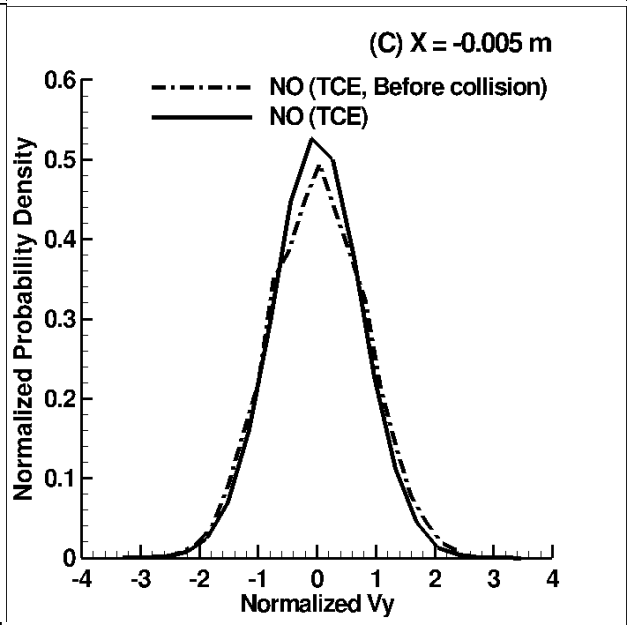


7 km/s, 81 km, TCE free stream, 50% N_2 and 50% O_2, Kn=0.03,
N_2+O→NO*+N
NO*+M→NO+M

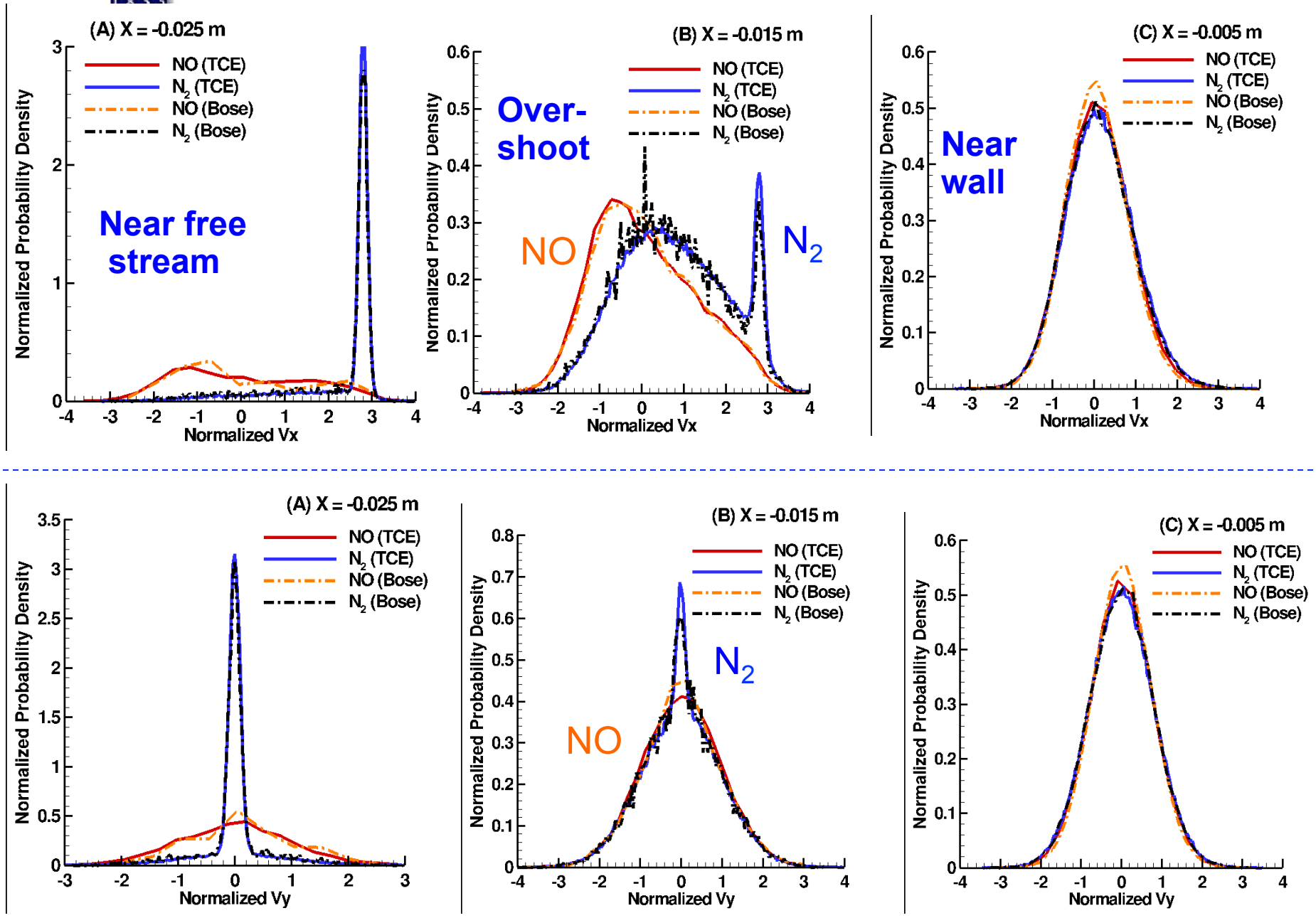




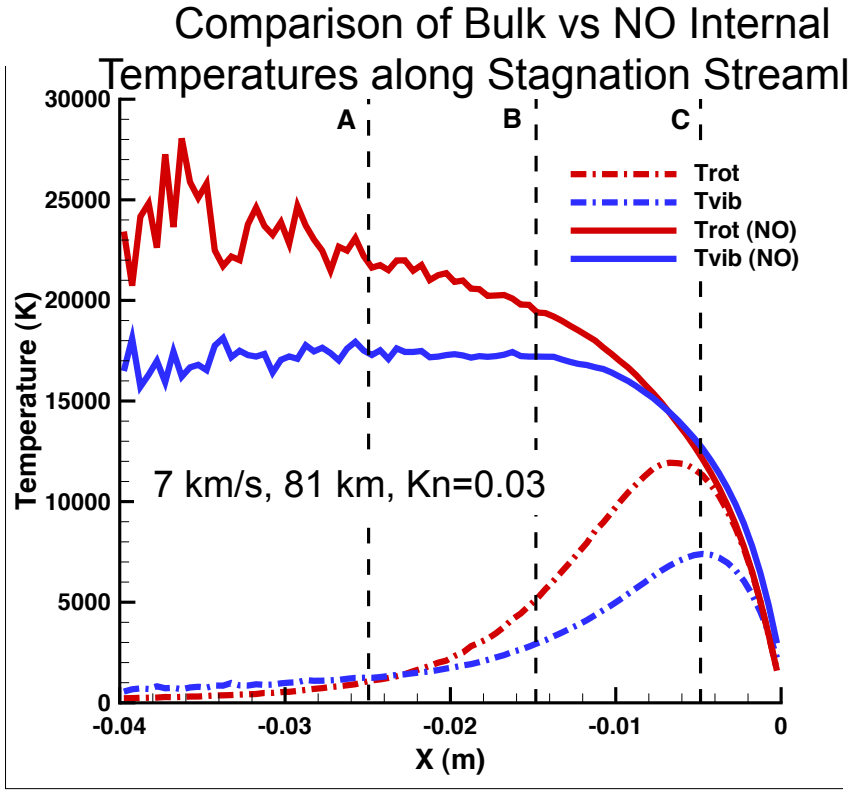


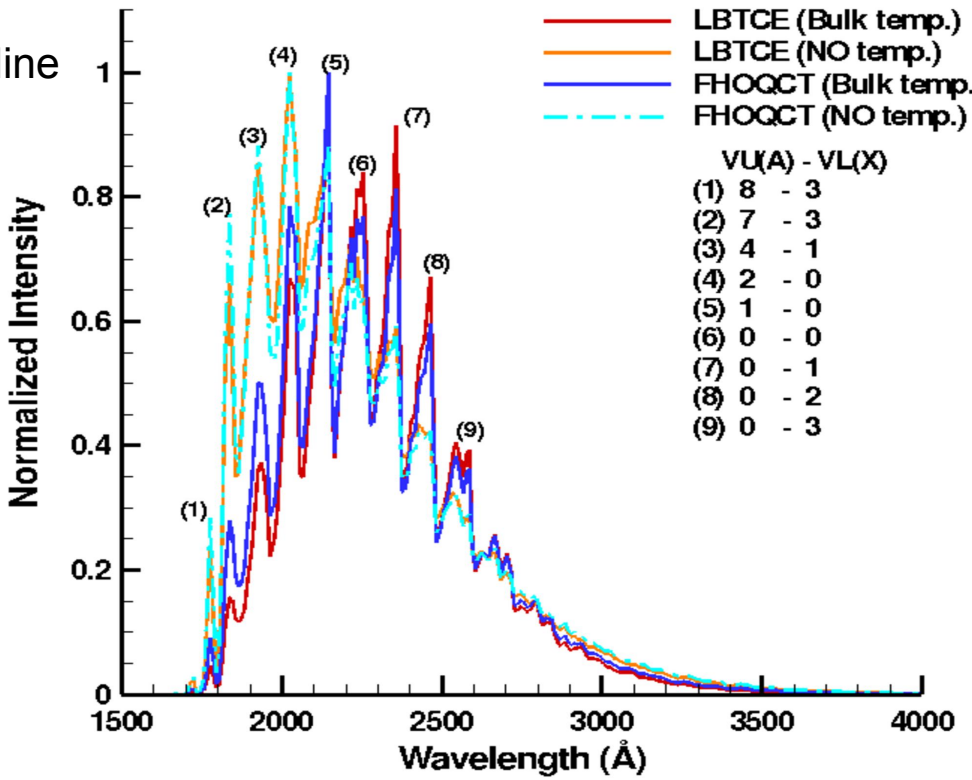


Comparison of Velocity Distributions of NO vs N_2



Sensitivity of Spectral Simulations to Nonequilibrium





- 8 ➔ 3, 7 ➔ 3, and 4 ➔ 1 transitions as a result of high NO T_{vib} for both FHO-QCT and LB-TCE cases.
- Use of NO vs bulk temperatures most important in determining spectral shape.
- Measured spectra necessary to validate nonequilibrium thermochemical models.

Limitations of BSUV Flight Data - Questions still Unanswered (1/2)

1. No spectral data from the UV *through* IR at any free stream velocity. Therefore missing independent measurements of T_{vib} and T_{rot}, especially for species that do not strongly radiate in the UV.
2. UV spectra have a spectral resolution of only 1 nm, a choice dictated by instrument type, anticipated S/N, and measurement time. This spectral resolution is adequate for modeling of electronic and vibrational temperatures averaged over the shocklayer, but, does not provide enough sensitivity to validate flow rotational temperatures.
3. Measurements taken at fixed views of the shocklayer and do not provide *any* estimate of range resolution along the line of sight to the vehicle.

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Limitations of BSUV Flight Data - Questions still Unanswered (2/2)

4. By design, the BSUV data was taken for "clean", non-ablating flows, but, for Air Force reusable vehicle concepts the creation of ablating species and their role in modifying the shock layer thermochemical nonequilibrium is important.
5. PAET suggests that importance of ionization for Earth reentry flows occurs even at ~6 km/s. What is the true velocity threshold?
6. Finally, 15 years later we still do not have UV spectral data taken under flight conditions that would confirm the major thermochemical and radiation mechanisms for speeds on the order of 7 km/s!
7. Cubric/Lens XX data can answer many of these important, remaining questions.

Acknowledgments

- This research performed at the Pennsylvania State University was supported by AFOSR Grant No A001650203

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Numerical Flow Modelling in DSMC:

Simulation Approach

❑ Numerical Approach

- Majorant frequency scheme for pair selections
- VHS model for collisions.
- Borgnakke-Larsen (BL) model for internal energy exchange.
- Total collision energy (TCE) model is used for chemical reactions, also Bose model for NO formation

❑ Numerical parameters:

- 180 k simulated particles, 32 k collisional cells, 32 k macro parameter Cells
- Time step: 2×10^{-7} s, 1000 steps before sampling and 9000 sampling steps.

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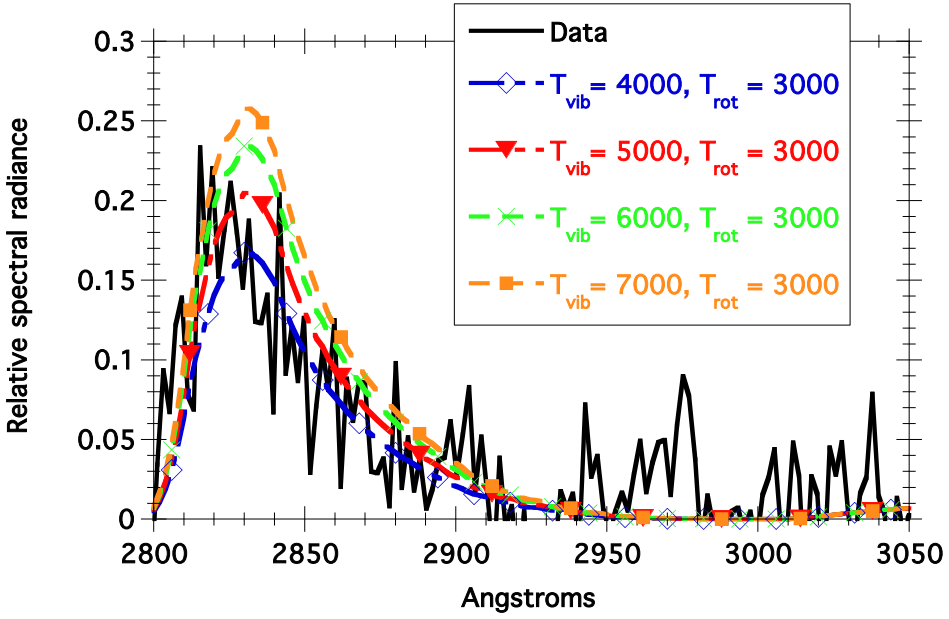
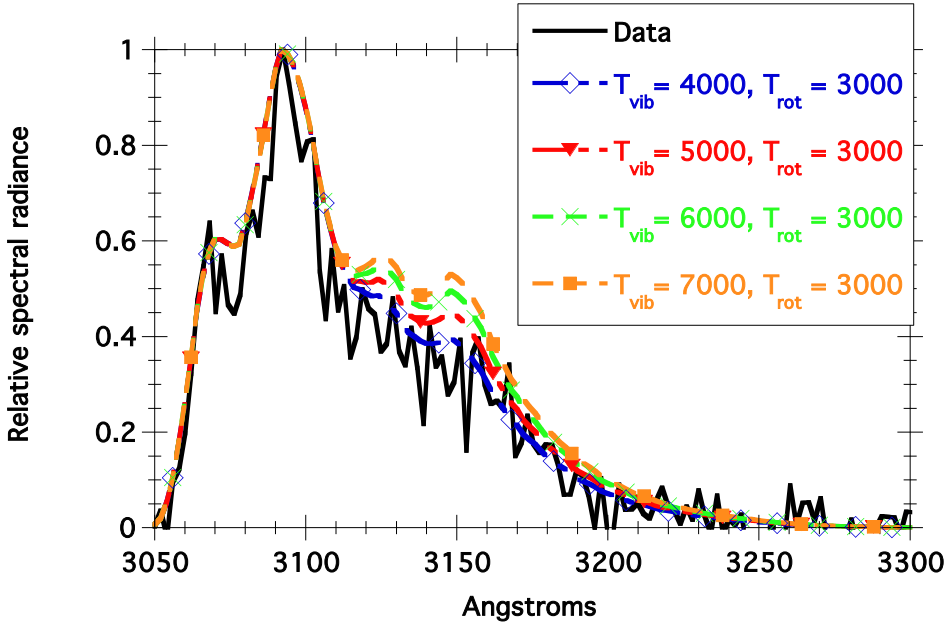
Assessment of OH ro-vibronic Temperatures by Comparison with BSUV2 Data

1-0 spectral region



0-0 spectral region



- **"The uncertainty in the temperature assignment remains high because of the noise in the data, but the most likely temperature assignment of the spectral data are vibrational and rotational temperatures of 5,000-6,000 and 3,000-4,000 K, respectively."**
- **No relationship to N_2 shocklayer temperatures.**

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- **The transitions between the vibrationally excited states of the N_2, its dissociation, and formation of NO from different N_2 vibrational excited states are modeled.**
- **The relaxation models/assessed include the discrete LB VT rate model, Schwartz-Slawsky-Herzfeld (SSH) V-T model, and Forced Harmonic Oscillator (FHO) V-T model.**
- **The chemistry models include: (1) TCE, (2) QCT - Bose, and (3) QCT - Jaffe and Magin (N_2 dissociation).**
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