SAND2024-11774C

Formulation of a General Collisional-Radiative Model for NO to Study Non-Equilibrium, Hypersonic Flows

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2024 AFOSR/ONR/HVSI Portfolio Review

Computational resources were provided through the NSF ACCESS program and the TACC Stampede2, Stampede3 and Frontera supercomputers with project codes TG-PHY210065, PHY220158 and CTS23002.

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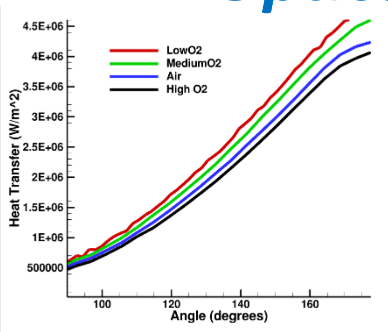
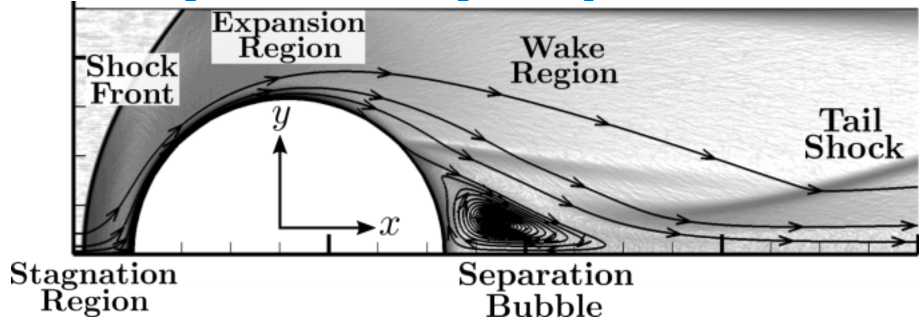
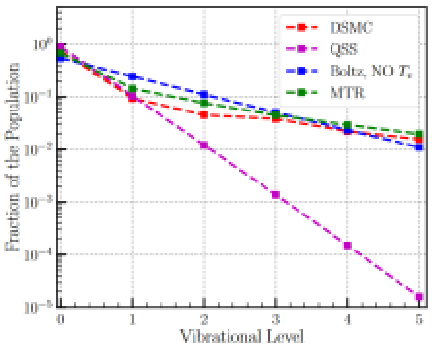
Optical Measurements - why are they important?

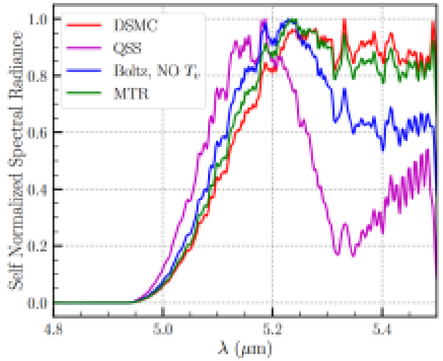


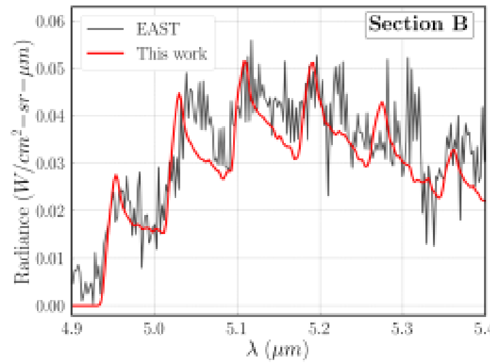
- Good agreement of surface pressure and temperature distributions with experiments
- But little sensitivity to thermochemistry.



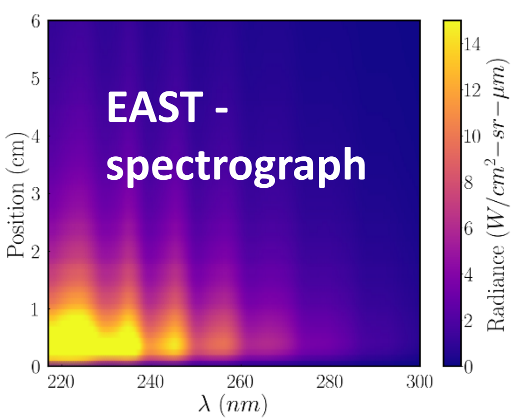
NO Collisional-Radiative (CR) models account for non-Boltzmann behavior and flow transport!



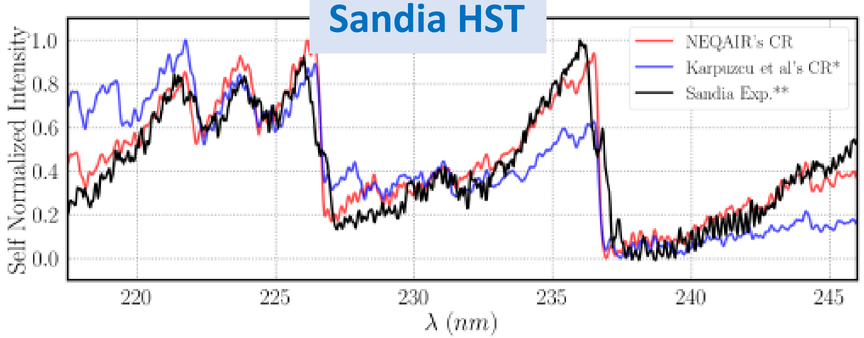




Modeling UV emission spectra



Sandia HST



NO potential energy states

> Mach 20

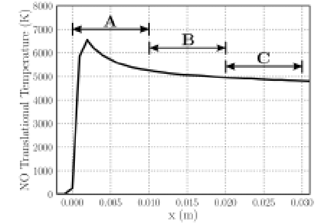
Mach 7

UV

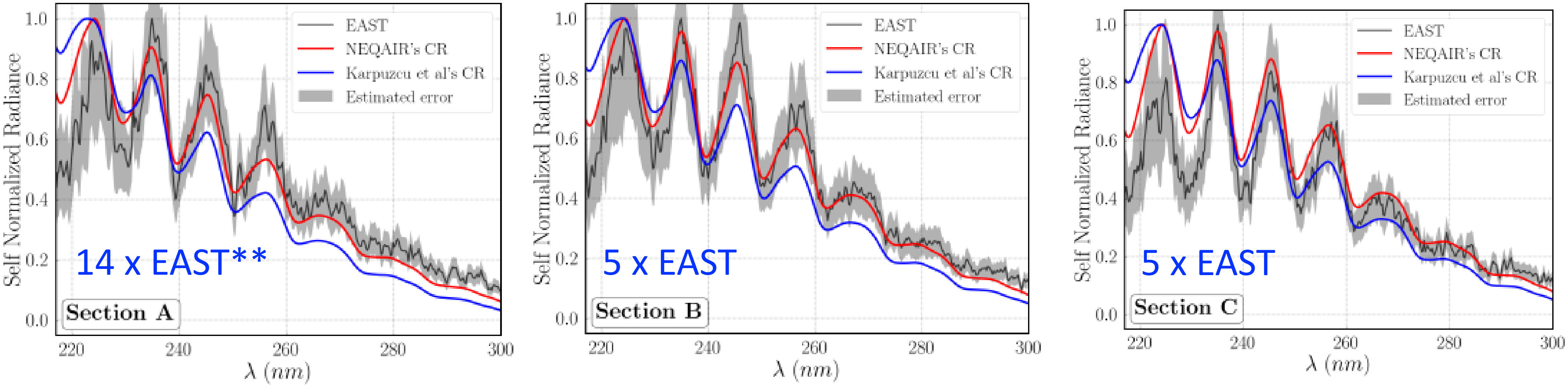
IR

NO – centric – key species in Mach 7 thermochemistry

Comparison of EAST UV Spectra vs. Simulations*

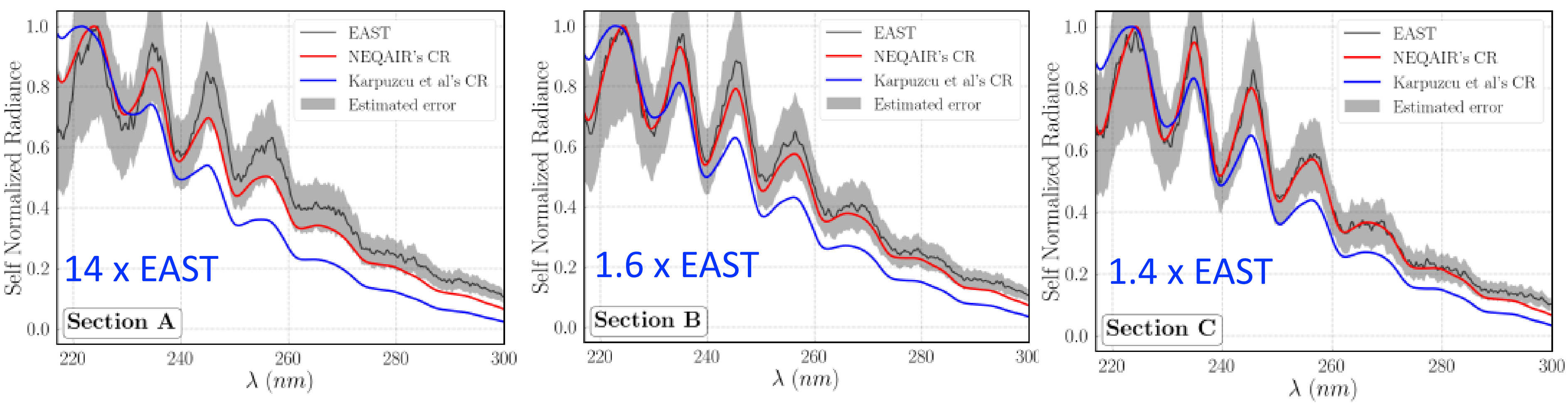


Shot 26 (3.81km/s): UV emission spectra



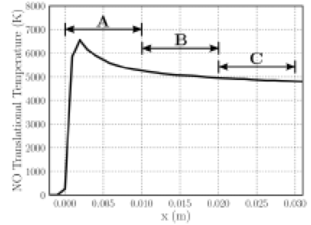
**Ratio of Karpuzcu CR to EAST Data

Shot 27 (4.51km/s): UV emission spectra

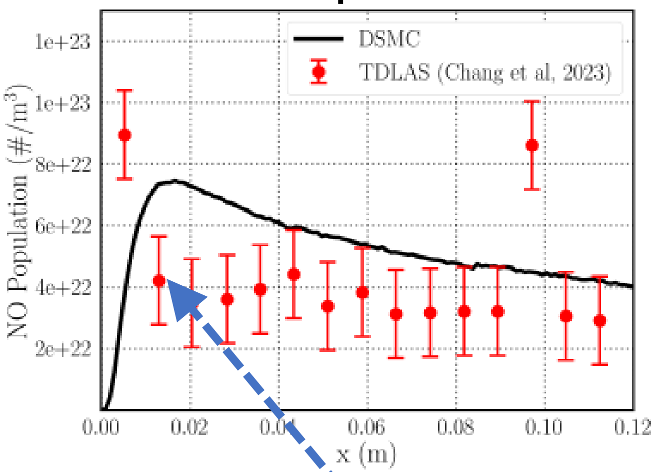


* Karpuzcu, I. T., Jouffray, M.P., and Levin, D. A., "*Collisional Radiative Modeling of Electronically Excited States in a Hypersonic Flow*", Journal of Thermophysics and Heat Transfer, Vol. 36, No. 4, 2022, pp. 982–1002.

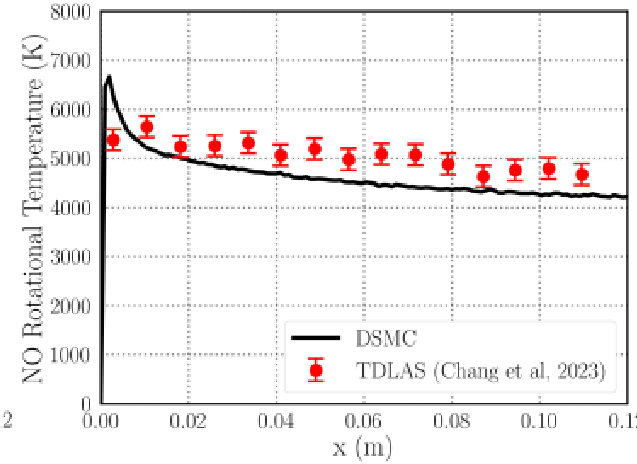
Shot 26 (3.81km/s): Comparison with TDLAS Data*



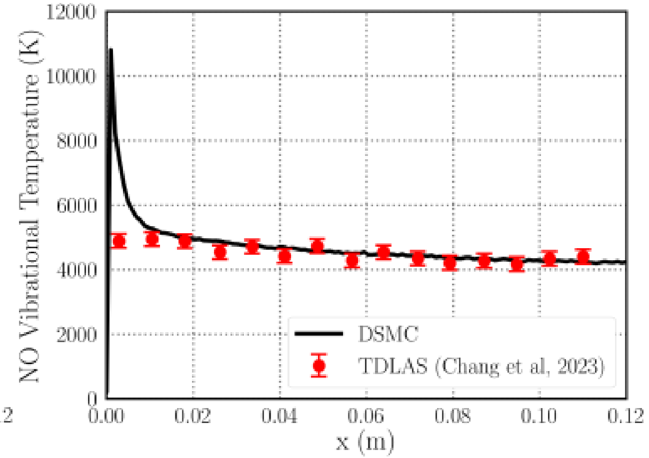
NO Population

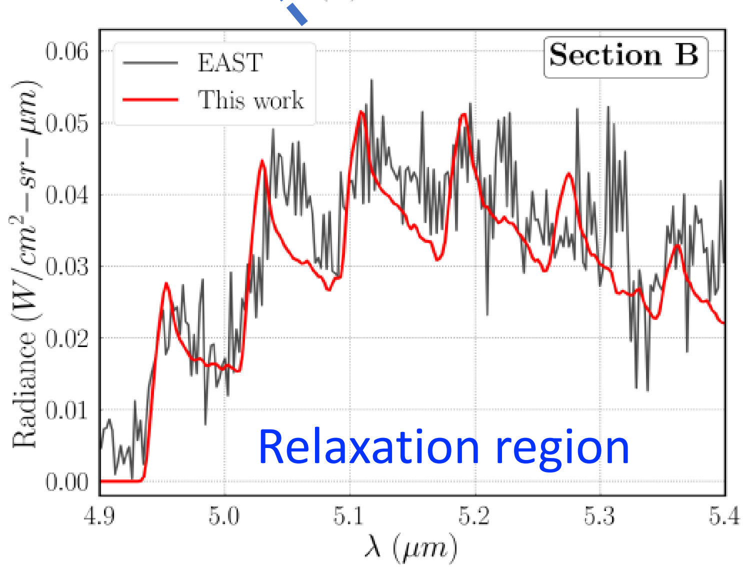


NO Rotational Temperature



NO Vibrational Temperature





- Rapid-Scanning Tunable Diode Laser Absorption (TDLAS) measurements were made by Chang et. al* during EAST Test Series 66.
- *NO populations are within 1.5 times of DSMC estimates and temperatures also show a good match – ANCHOR SIMULATIONS – Need more.*
- Discrepancy near the shock might be a result of TDLAS scan rates and/or reaction rates used in the DSMC solver – not resolved.

* Chang, E., Streicher, J.W., Strand, C.L., Hanson, R.K., Tibere-Inglesse, A.C. and Cruden, B. A., "*Rapid-Scanning Tunable Laser Absorption Measurements of Shock-Heated Nonequilibrium Air Species in the NASA Electric Arc Shock Tube*", International Symp. on Shock Waves, July 2023

0D Thermal Bath: Development of a New Relaxation Model for NO(v)+O →NO(v')+O

- The **vibrational relaxation number:** $Z_v^C := \tau_v/\tau_c$ = vibrational relaxation time constant/mean time between collisions.

- Track evolution of T_v and relaxation parameter, Λ,

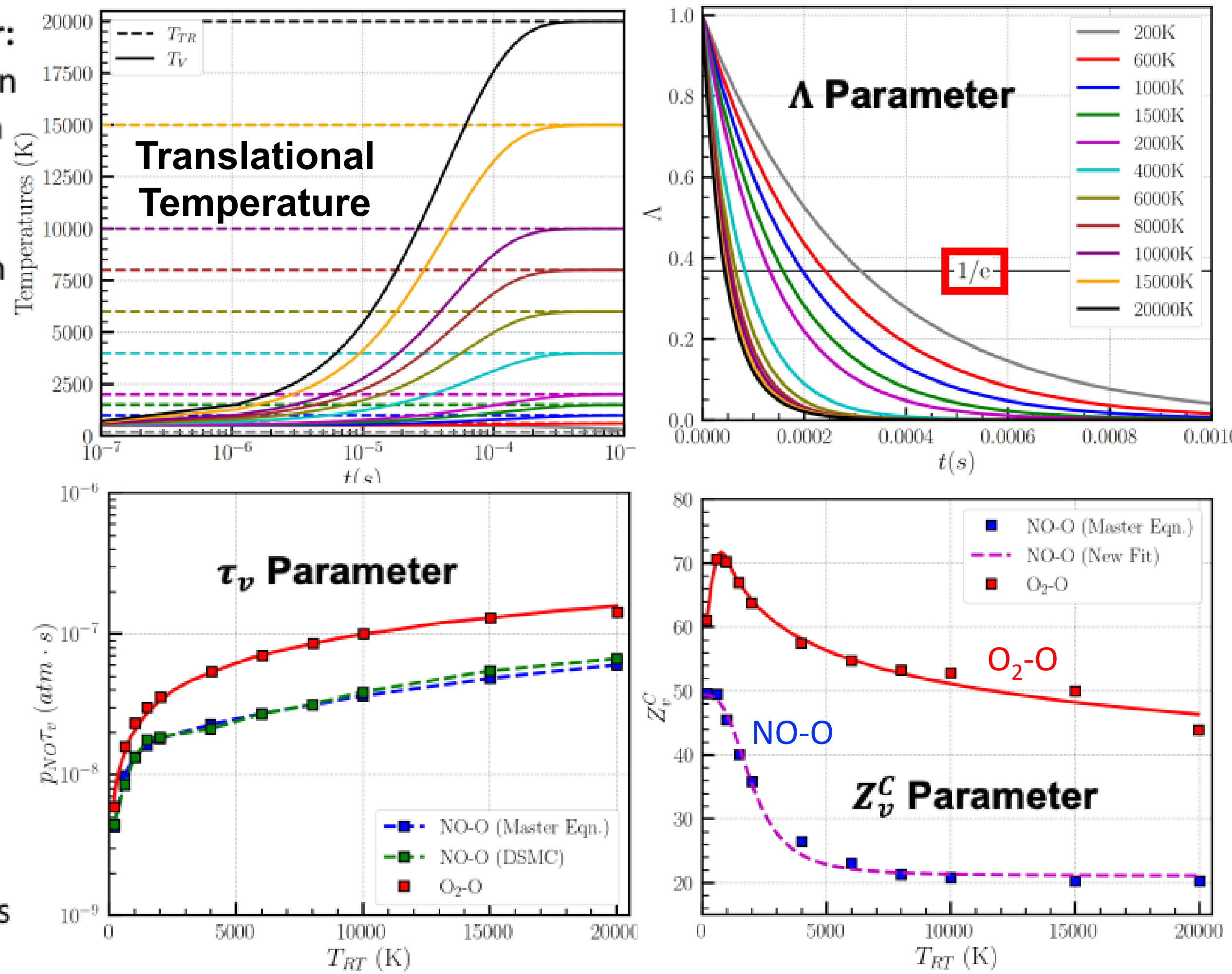
$$\Lambda(t, T_{RT}) = \exp\left(-\frac{1}{\tau_v}\right) = \frac{\overline{E_v(t)} - E_{eq,v}(T_{RT})}{E_v^0 - E_{eq,v}(T_{RT})}$$

where $\overline{E_v(t)}$ is instantaneous T_v calculated as:

$$\overline{E_v(t)} = \frac{\sum_v E_v(v) \exp\left(-\frac{E_v(v)}{kT_V}\right)}{\sum_v \exp\left(-\frac{E_v(v)}{kT_V}\right)}.$$

- τ_v is evaluated for $\Lambda = 1/e$.
- Mean collision time is calculated as

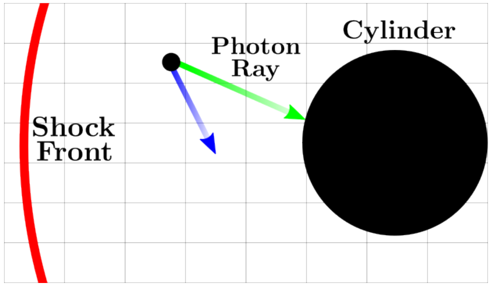
$$\tau_c = \frac{1}{2\sqrt{\pi} d^2 \sqrt{2kT_{RT}/m_R} (T_{ref}/T_{RT})^{\omega-0.5}}$$

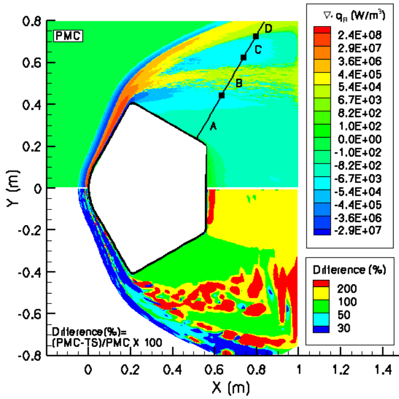


- NO-O relaxation is faster than O_2-O
- Agreement between Master Eq and DSMC demonstrates correct implementation for flow over cylinder.

In Progress and Future Directions

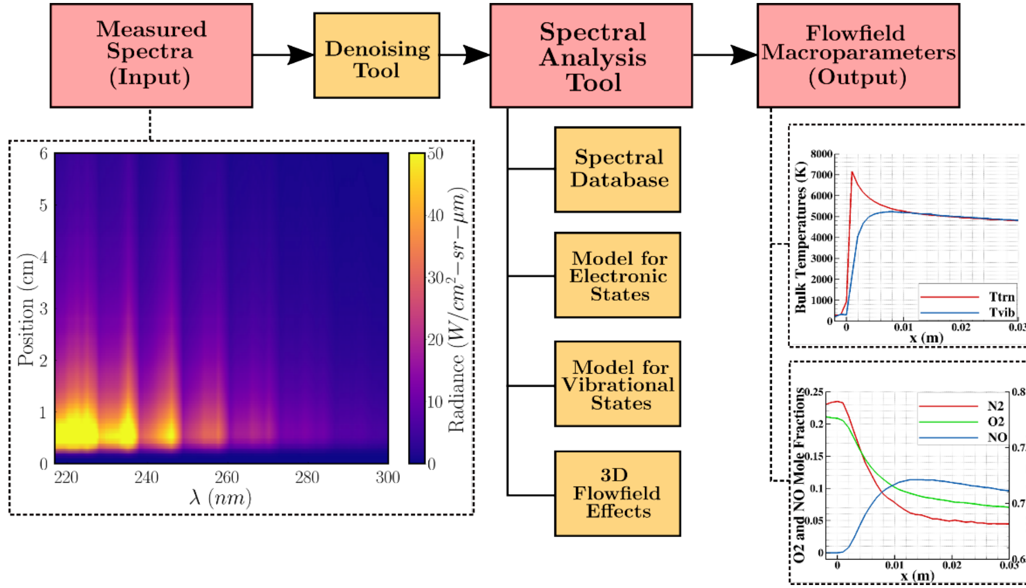
(1) Photon Monte Carlo – most general approach to calculating optical thickness for arbitrary viewing geometries*





*** I. Sohn, Z. Li, and D. Levin , "Effect of Nonlocal Vacuum Ultraviolet Radiation on Hypersonic Nonequilibrium Flow,", Journal of Thermophysics and Heat Transfer, 2012.**

(2) Artificial Neural network (ANN) to extract flowfield information from spectral data



- ANN trained on spectral databases, thermochemical models and line-of-sights effects
- Denoising tool to extract relevant features from noisy experimental data.
- ANN will extract flowfield information given spectral data.
- Enable comparison of data across different facilities.

(3) Develop IR CR model to simulate non-Boltzmann populations in laser adsorption measurements

(4) Simulate optical signatures of time-accurate, unsteady flows

Present collaborations:

- Daniil Andrienko and Alexander Fangman for providing the QCT rates for NO-O vibrational relaxation
- Drs. Brett Cruden and Dr. Augustin C Tibère-Inglesse, NASA/Ames EAST shock tube facility data.
- Dr. Kyle Lynch Sandia Hypersonic Shock Tunnel (HST) spectroscopic emission data.

Publications 2024

- **Conference papers/presentations:**
  - **Shubham Thirani, Irmak Karpuzcu, and Deborah Levin, "Experimental Validation of Modeling Efforts to Estimate Nitric Oxide Emission in High Mach Number Flows, Scitech 2024, AIAA 2024-2089, https://doi.org/10.2514/6.2024-0228**
  - **D. Levin, "Multiscale Modeling of Nonequilibrium Plasma Flows using Particle-kinetic Methods," University of New South Wales, Canberra, AU, February 26, 2024.**
  - **D. Levin, "Thermo-physical Insights into Nonequilibrium Plasma Flows using Particle-kinetic Methods," School of Engineering, College of Engineering, Computing and Cybernetics, Australian National University, Canberra, AU, February 22, 2024.**
  - **D. Levin, "A Tale of Two non-Maxwellians," Invited talk at the Direct Simulation Monte Carlo 2023: Theory, Methods, and Applications Conference, Santa Fe, New Mexico, September 24-27, 2023.**
  - **Shubham Thirani, Deborah A. Levin and Ingrid J. Wysong, "Calibration of the Larsen-Borgnakke Model for NO-O Vibrational Relaxation," 33rd International Symposium on Rarefied Gas Dynamics, Gottingen, Germany, July 15, 2024.**
  - **Shubham Thirani, Irmak Karpuzcu, Deborah Levin Elijah Jans, Kyle Daniel, and Kyle Lynch, "Modeling of Hypersonic Flow Over a Cylinder in a Reflected Shock Tunnel Facility," 10th International Workshop on Radiation of High Temperature Gases for Space Missions, Sept 9 – 12, 2024, Oxford University.**
- **Journal papers**
  - **Shubham Thirani, Irmak T. Karpuzcu, and Deborah A. Levin, "Modeling of Nitric Oxide Vibrational Level Populations in the Ground Electronic State for High Mach Number Flows," in preparation for Journal of Thermophysics and Heat Transfer.**

Thank you for your attention

EAST Shock Tube Work

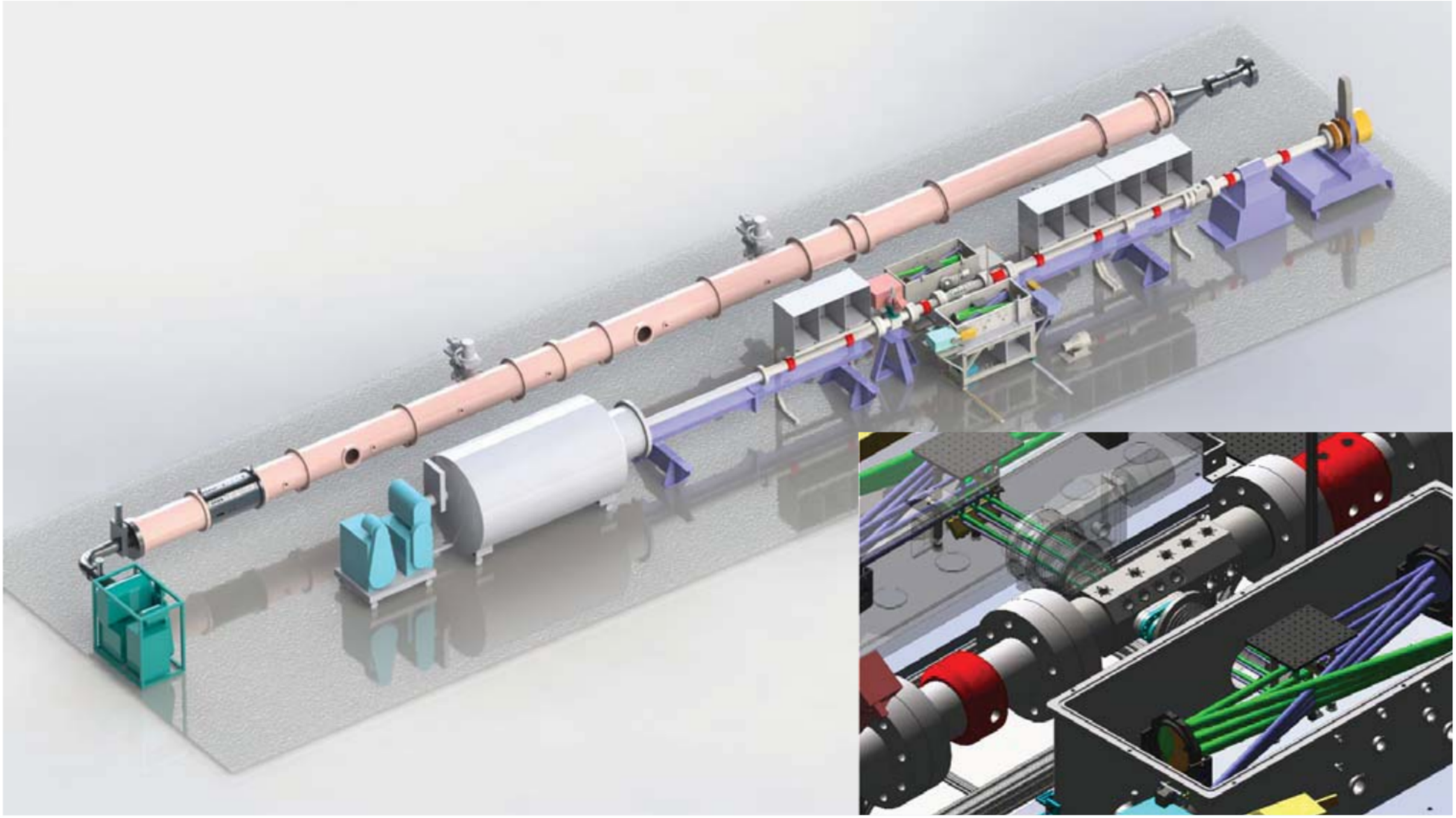


Figure 1. Rendering of the EAST Facility showing both shock tubes. (upper inset) cross-section of driver assembly, (lower inset) close-up of test section and optical boxes.

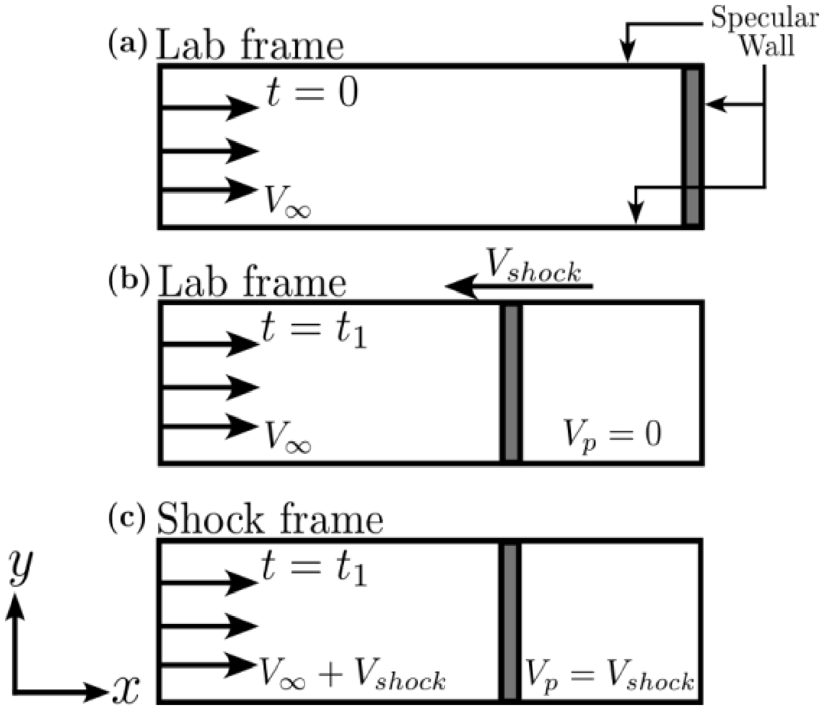
* Figure from Brett A. Cruden, *"Absolute Radiation Measurements in Earth and Mars Entry Conditions", 2014*

*Modeling Approach of NASA EAST Shock-tube Data**

- Unsteady flowfield results generated by Direct Simulation Monte Carlo (DSMC) using "reflected shock approach on right"**
  - Multiple samples in time are averaged to obtain a statistically converged 1D shock solution.
  - 2D simulation with specular top, end and bottom walls
- Non-equilibrium thermochemistry modeling using
  - Bias Model** for dissociation
  - Forced Harmonic Oscillator for N_2 and O_2 V-T relaxation
  - Larsen-Borgnakke model for NO relaxation
  - Discrete Internal Modes
- Optical emissions of 1D shocks simulated to compare with EAST data.

	Shot 26	Shot 27
Upstream velocity, V_∞ (m/s)	3450	4000
Upstream Mach number	9.915	11.495
Total enthalpy (MJ/kg)	6.25	8.30
Temperature (K)	300	300
Pressure (Pa)	300	300
Number Density (#/m3)	7.243 x 10^{22}	7.243 x 10^{22}

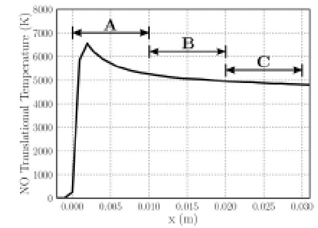
Schematic of the shock tube domain



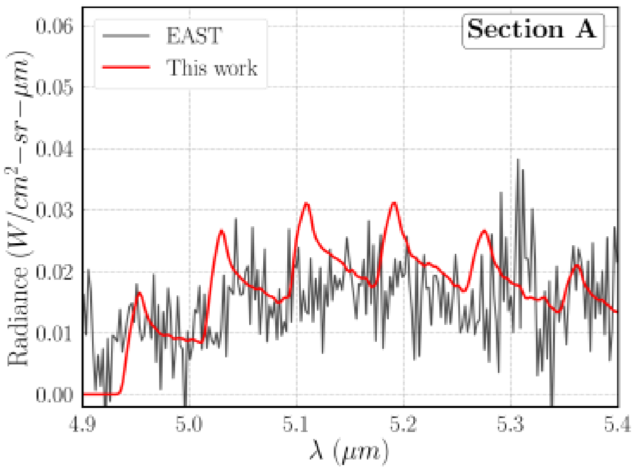
Analogous to shock tube

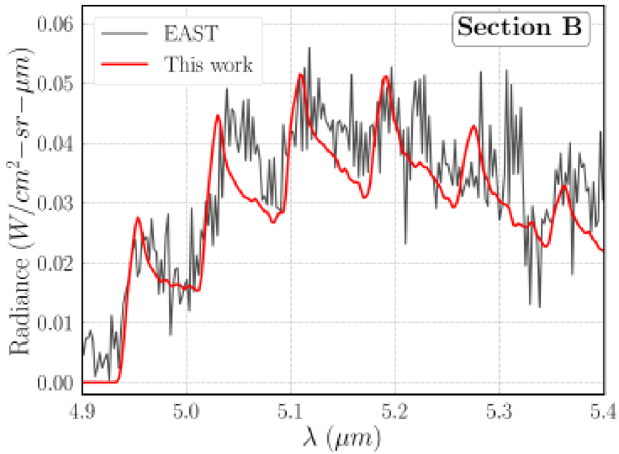
- 'Test series 66' air test series, conducted October through November 2022.
- **Shubham Thirani, Irmak Karpuzcu, and Deborah Levin, "Experimental Validation of Modeling Efforts to Estimate Nitric Oxide Emission in High Mach Number Flows, Scitech 2024, AIAA 2024-2089, https://doi.org/10.2514/6.2024-0228 .

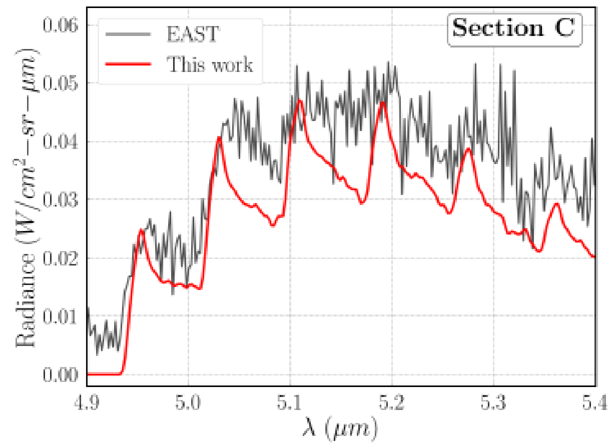
Comparison of EAST IR Spectra vs. Simulations*



Shot 26 (3.81km/s): IR emission spectra







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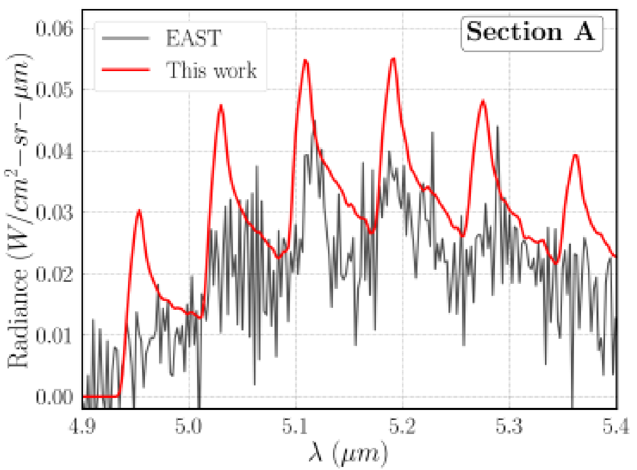
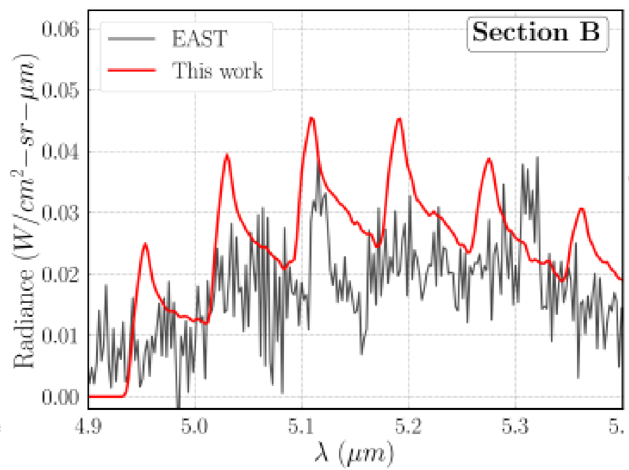
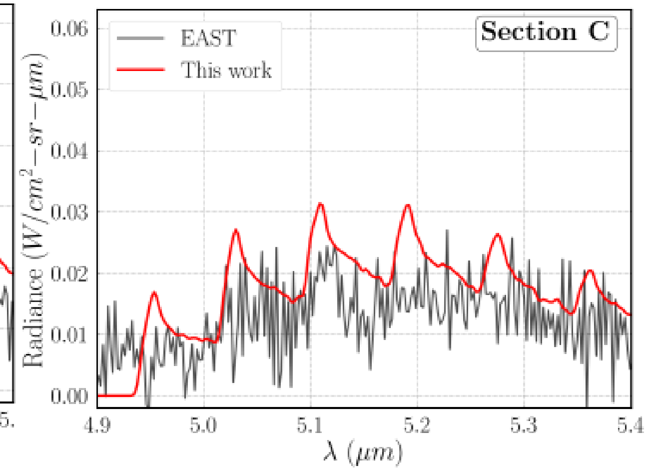




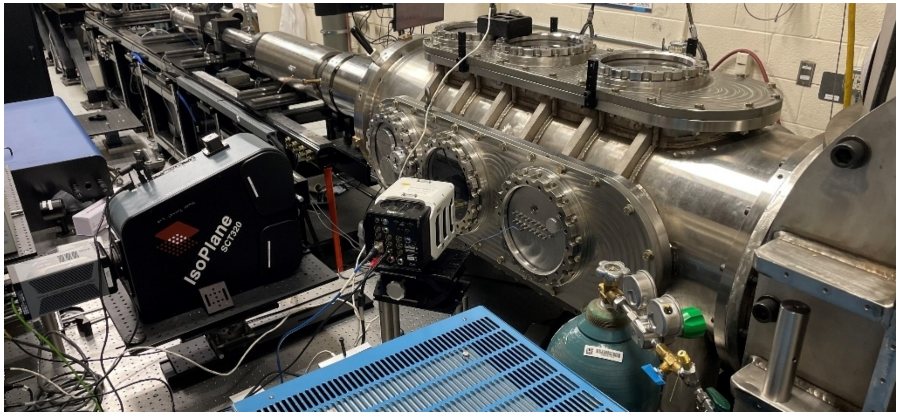


*** Shubham Thirani, Irmak T. Karpuzcu, and Deborah A. Levin, "Modeling of Nitric Oxide Vibrational Level Populations in the Ground Electronic State for High Mach Number Flows," in preparation for Journal of Thermophysics and Heat Transfer.**

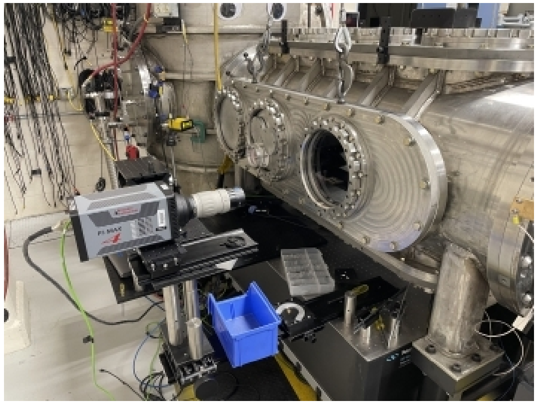
Sandia Reflected Shock Tunnel Measurements - Setup

Test Object in Wind Tunnel

Imaging Spectrometer

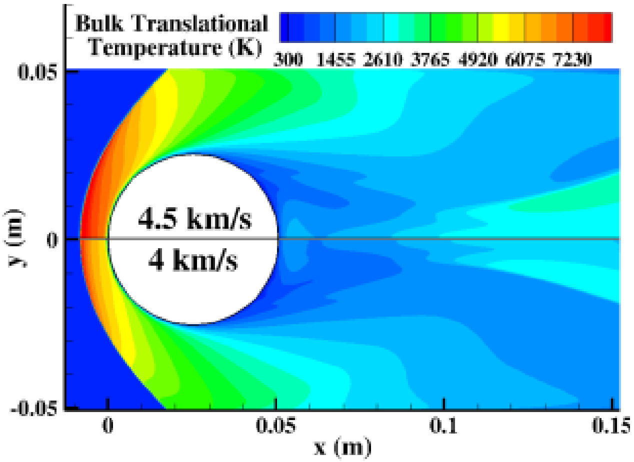


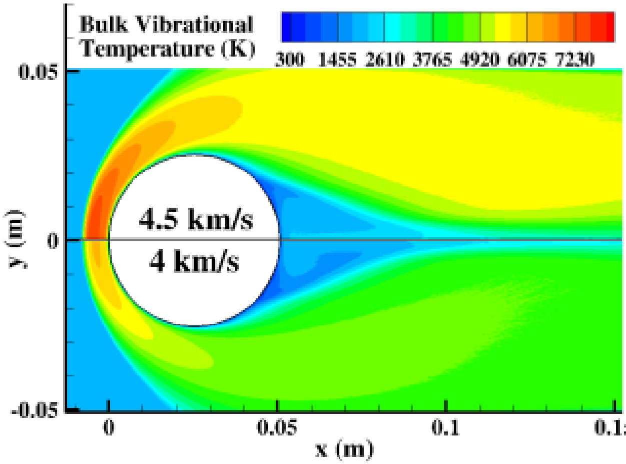
UV Imaging Camera

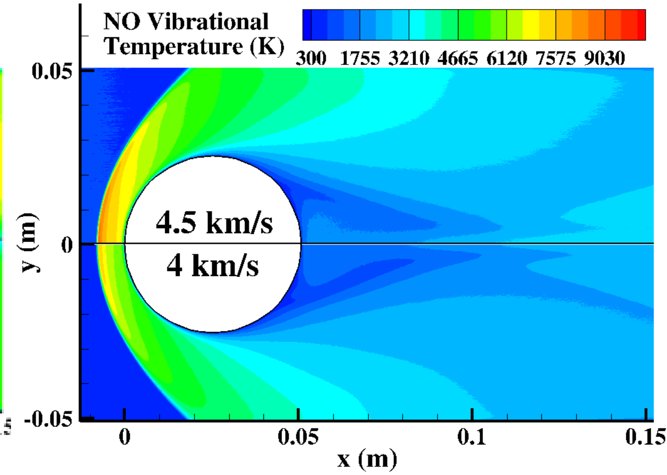


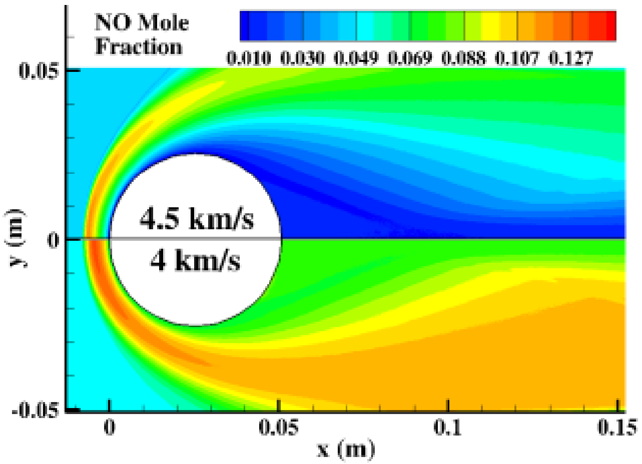
- High enthalpy flow conditions being tested in Sandia's Hypersonic Shock Tunnel (HST).
- Two different geometries are being tested: Cylinder (2" diameter) – 4km/s, 4.5km/s and Wedge (2" square) – 4.5km/s.
- A total of 15 shots across all conditions.
- Measurements include spectrally resolved UV emission measurements, spectrally banded imaging measurements in 2-dimensional physical space and estimates of internal temperatures based on spectral data.

*Modeling of measurements in Sandia Reflected Shock Tunnel – Preliminary Results for Cylinder**





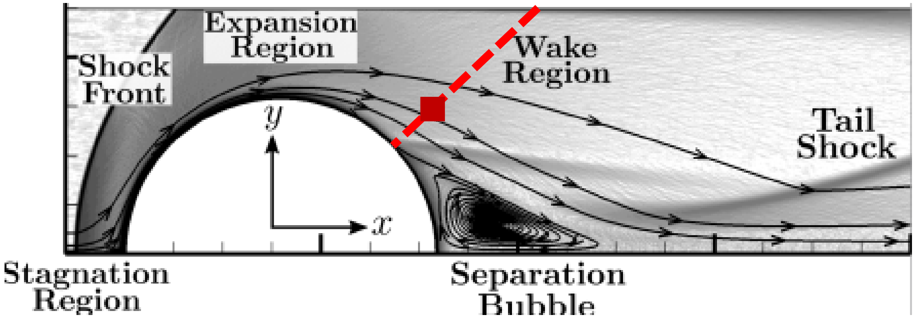


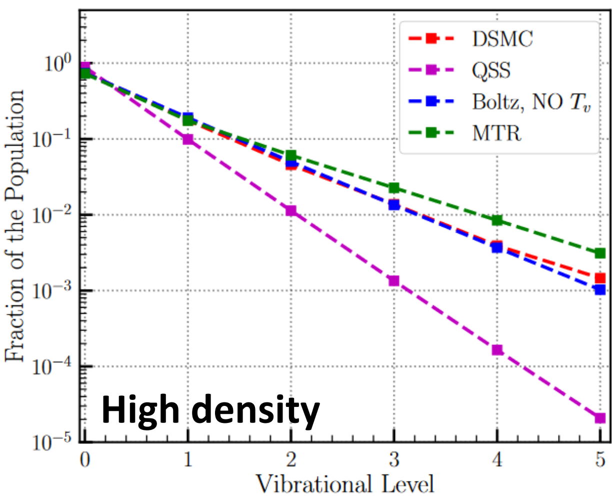


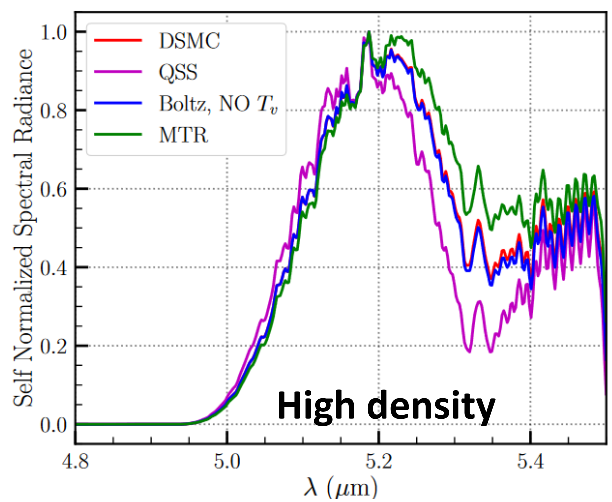
- Hypersonic flow over the cylinder geometry with freestream at 4km/s and 4.5km/s in a state of thermal non-equilibrium simulated using DSMC.
- Sandia freestream values validated using laser-based characterization of freestream.*
- The 4km/s case is similar to Caltech/HET conditions but freestream properties in nonequilibrium
- Spectrally resolved UV emission measurements made along stagnation line and 30^{o} and 60^{o} lines from the front.
- Currently working on generating numerical estimates of spectra and spectrally banded image of the flowfield.
- Sandia working on absolute calibration.

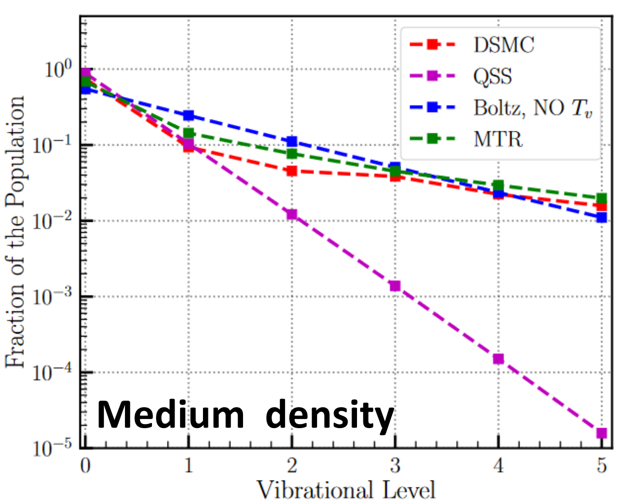
* Elijah R. Jans et al, "*Laser-Based Characterization of Reflected Shock Tunnel Freestream Velocity and Multi-Species Thermal Nonequilibrium with Comparison to Modeling*," *AIAA SciTech 2024*, AIAA 2024-1753.

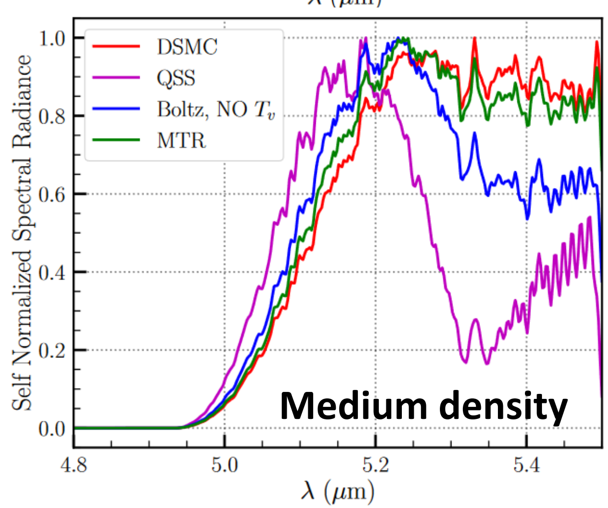
Predicted IR Spectra for Hypersonic Flow over a Cylinder











degree of equilibrium

- NO vibrational state distributions sampled from DSMC, overlay solution, QSS, and Boltzmann distribution at NO T_v.
- High density:
  - Boltzmann distribution at NO T_v can capture the vibrational state distribution
  - QSS solution underpredicts population fractions of higher vibrational states and absolute intensity.
- Medium density:
  - Overlay approach is essential for capturing non-Boltzmann distribution of vibrational states
  - Estimating NO vibrational temperature using LAS with Boltzmann approx. can lead to incorrect estimates when probing v less than or equal to 3.

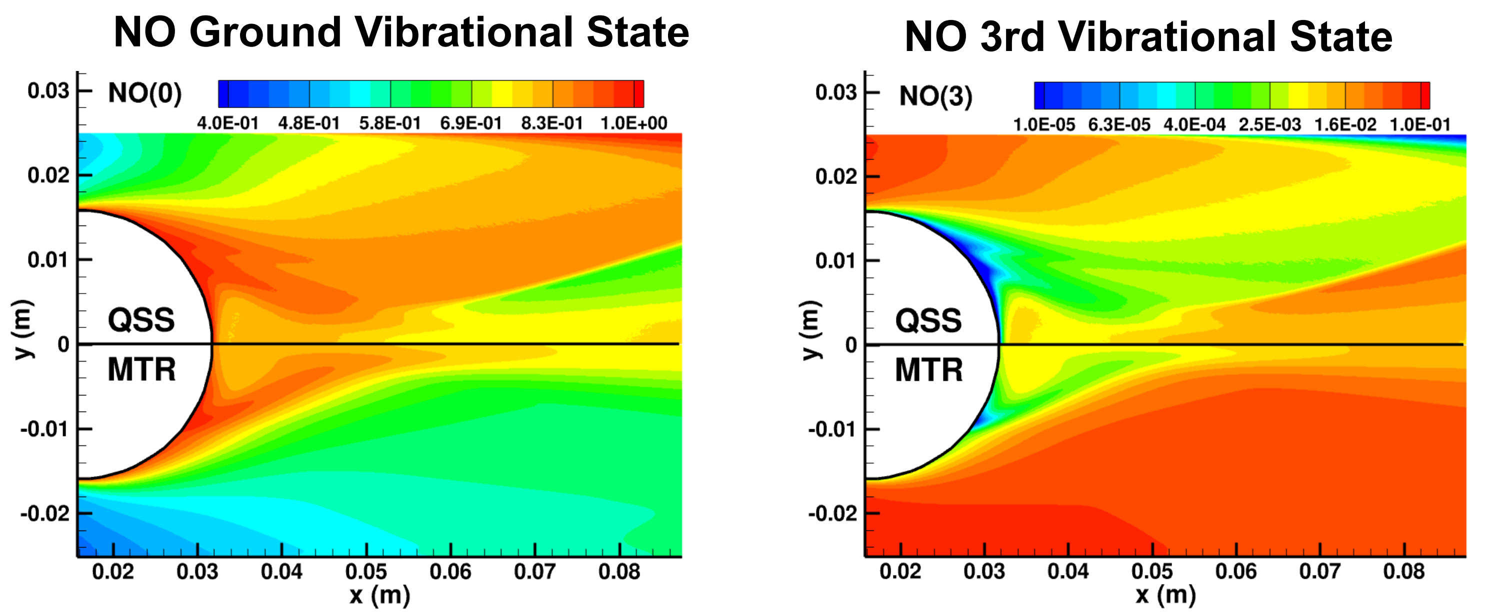
An Overlay Approach to Implement Infrared CR Model

- **Objective:** Couple transport processes with infrared CR modeling efforts.
- **Assumption:** Changes in distributions of NO vibrational states does not affect base flowfield macro-parameters
- **Approach:**
  - Use DSMC flowfield solutions and mass transport equations to estimate NO vibrational state distributions.
  - 2-D mass transport (MTR) equations for each vibrational state defined as

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial \rho_i u_x}{\partial x} + \frac{\partial \rho_i u_y}{\partial y} = D_i\left(\frac{\partial^2 \rho_i}{\partial x^2} + \frac{\partial^2 \rho_i}{\partial y^2}\right) + S_i \text{ where } i \in [0,6]$$

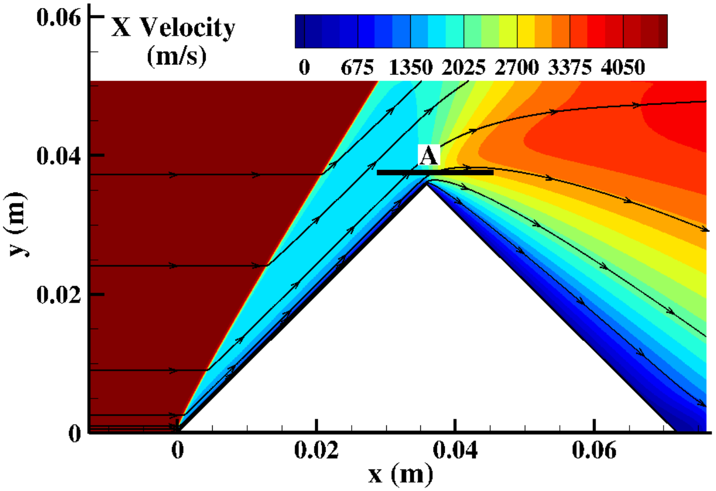
$$\mathrm{NO}(v) + \mathrm{O} \leftrightarrow \mathrm{NO}(v') + \mathrm{O} \text{ where } v, v' \in [0,48], v \neq v'$$

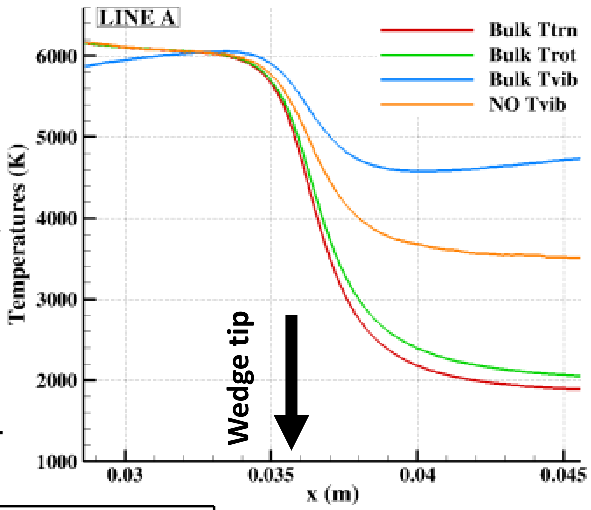
  - Source term, S_i, is rate of change described by IR CR model and couples system of equations.

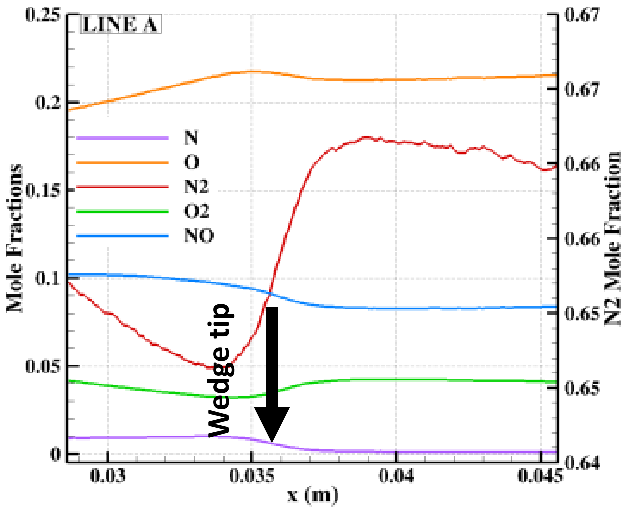


- MTR equation solver predicts distributions significantly different from QSS solutions because it accounts for low residence times in flow regions with strong expansions.

*Modeling of Measurements in Sandia Reflected Shock Tunnel – Preliminary Results for Flow over a Wedge**







	4.5km/s
Rotational Temp. (K)	650.14
N_2, O_2, and NO Vibrational Temps. (K)	2081.42, 902.18, 794.56
Mach Number	8.43
Pressure (Pa)	295.09
N_2, O_2, NO and O Mole Fractions	0.702, 0.091, 0.043, 0.164

- Rapid expansion over wedge tip drives thermal non-equilibrium in flow.
- Plot of temperatures along Line A illustrates increase in thermal non-equilibrium as the flow rapidly expands over the wedge tip.
- Wavelength resolved spectra has been collected along Line A.
- Little variation observed for specie mole fractions along Line A implies that flow is chemically frozen.

***Shubham Thirani, Irmak Karpuzcu, Deborah Levin Elijah Jans, Kyle Daniel, and Kyle Lynch, "Modeling of Hypersonic Flow Over a Cylinder in a Reflected Shock Tunnel Facility," 10th International Workshop on Radiation of High Temperature Gases for Space Missions, Sept 9 – 12, 2024, Oxford University.**