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Physics of Coupled, Multi-Scale Nonequilibrium Flows

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Challenges of Multi-scale Nonequilibrium Flows

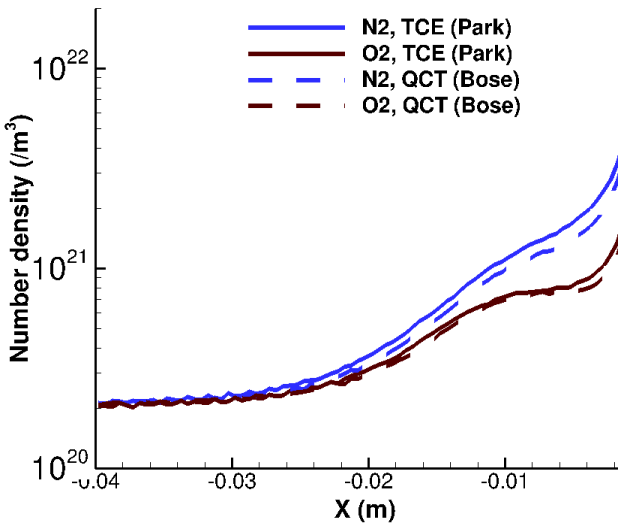
- Multiscale flows include regions of equilibrium and non-equilibrium.
- Understand sensitivity of flows to physical models such as thermal relaxation and chemistry.
- Use experiments to validate approach:
  - Data from HET to validate gas dynamic- shock interactions,
  - Spectral emissions to validate thermochemical models (especially NO emissions.)
- Want to treat these using non-continuum, particle approaches:
  - Severe numerical constraints,
  - Employ hybrid, particle methods → quest for breakdown criteria.

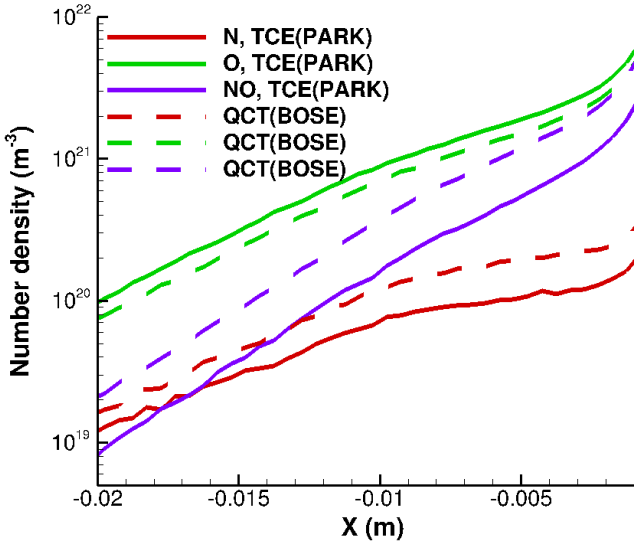
Objectives and Approach of Thermochemical Modelling

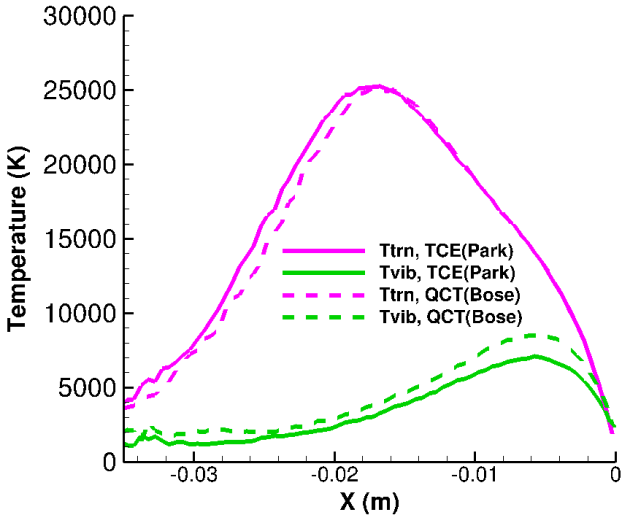
- **The transitions between the vibrationally excited states of the nitrogen molecule, as well as its dissociation, and formation of NO from different vibrational excited states are being modeled.**
- **The relaxation models that will be assessed include the discrete LB VT rate model, Schwartz-Slawsky-Herzfeld (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.)**
- ***Electronic excitation of NO molecules using quenching rate data from recent experiments are modeled for accurate calculation of spectral radiation.***

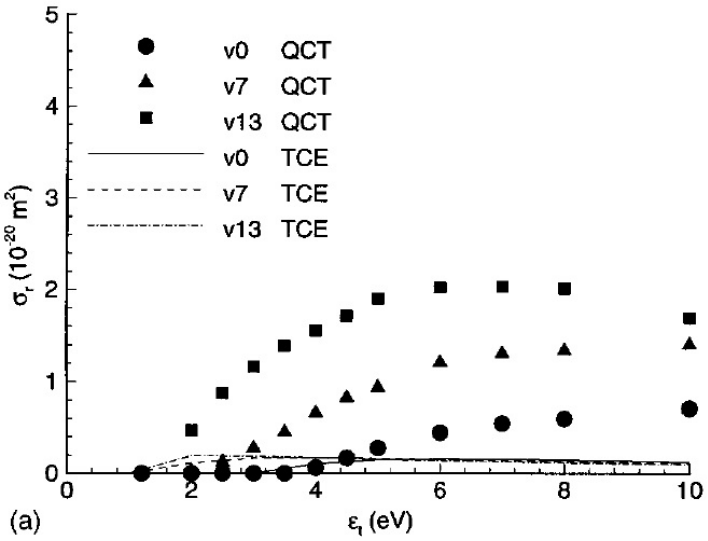
Sensitivity of NO Formation to Chemistry Model
TCE vs. QCT/Bose $N_2 + O \rightarrow NO + N$

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





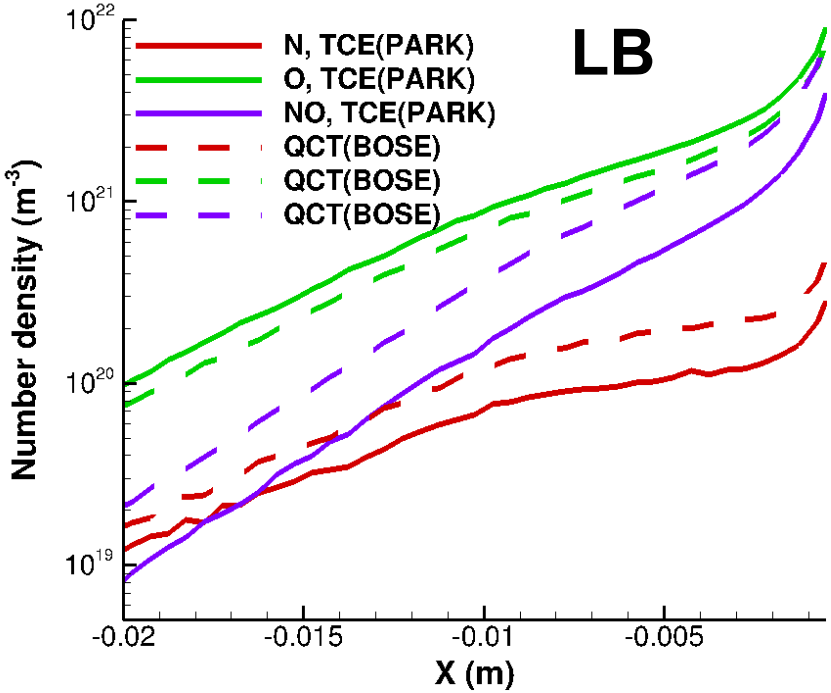


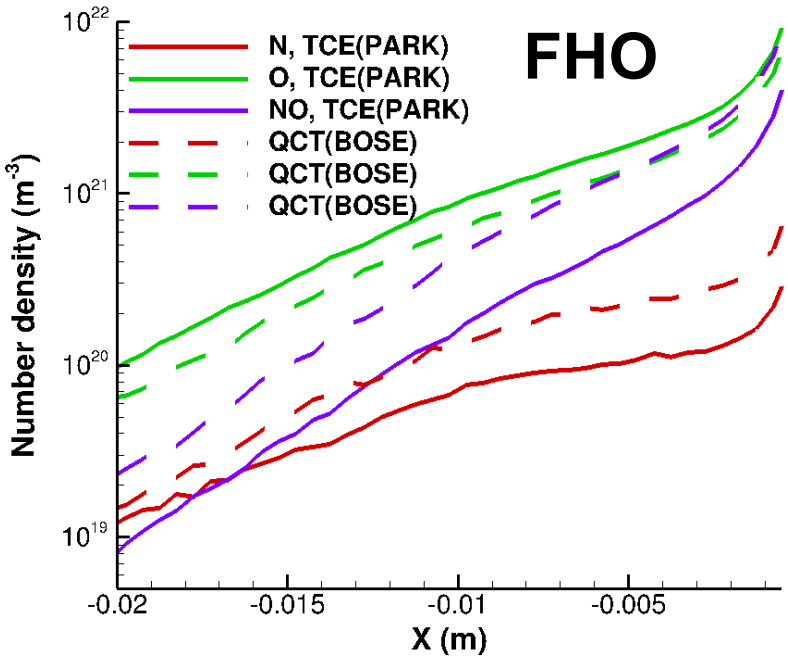


- In the "QCT(Bose)" calculation, discrete N_2 vibrational levels used and LB model is used for VT transition, state-specific cross section data for each N_2 vibration level and collision energy is used for NO formation.
- TCE uses Park, JTHT, 1994 rates.
- NO concentration from Bose model about 50% higher due to higher cross sections.
- T_{vib} is higher for QCT than TCE due to higher NO concentration.

Sensitivity of NO formation to Chemistry and VT Transition Models

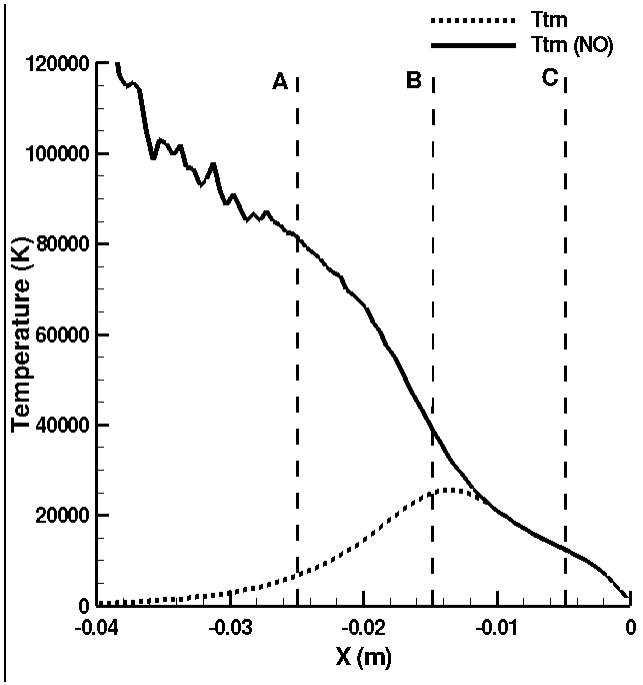
7km/s, 81 km, free stream, 50% N_2 and 50% O_2



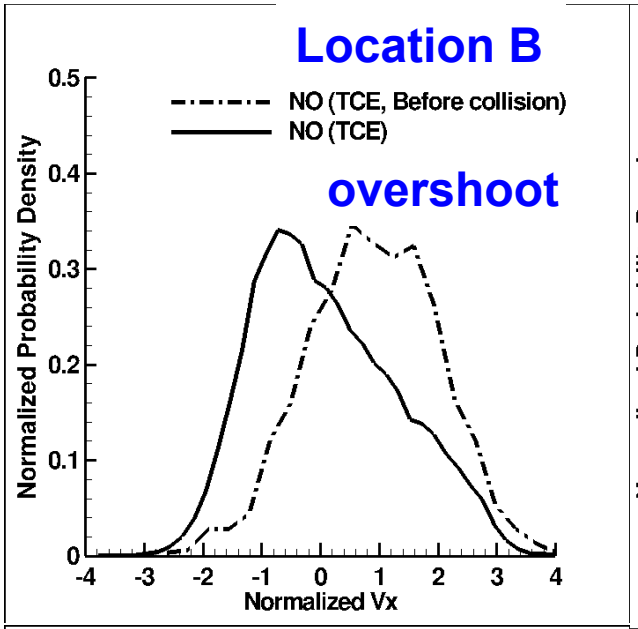


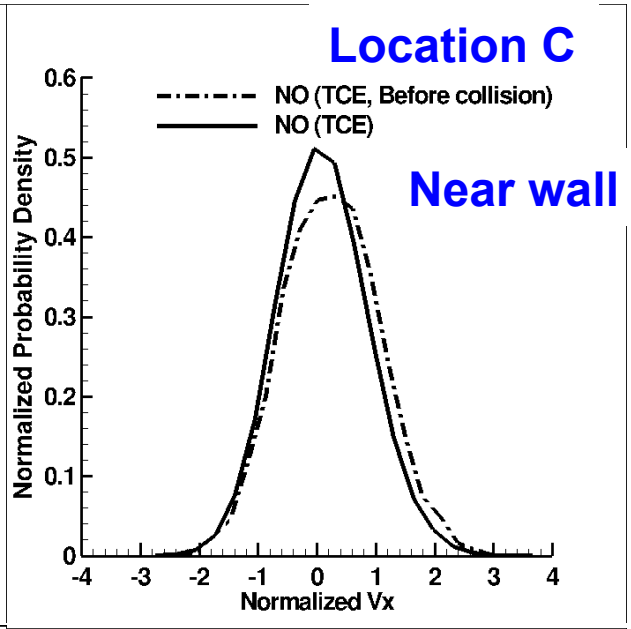
- **When QCT chemistry is applied, the NO number density from FHO case is about 20% higher than the LB case.**
- **Using FHO for VT and QCT for chemistry significantly increases the NO formation in the 81 km and 7km/s case.**

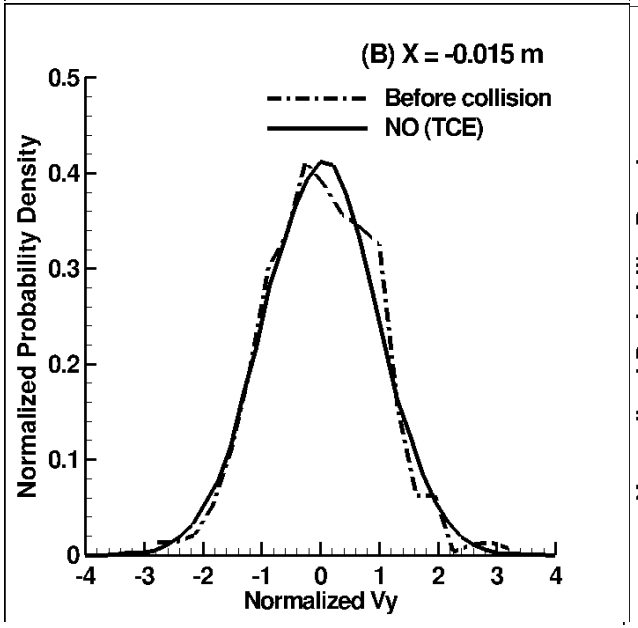
Velocity Distributions of NO Molecules

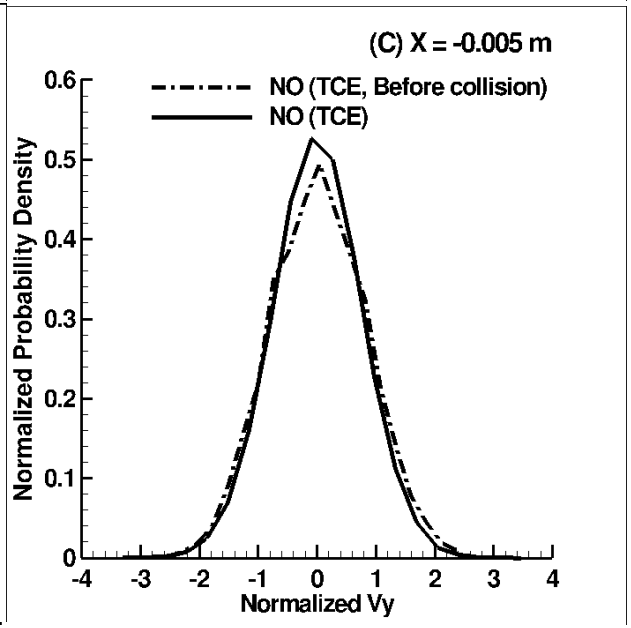


7 km/s, 81 km, TCE free stream, 50% N_2 and 50% O_2, Kn=0.03,
N_2+O→NO*+N
NO*+M→NO+M









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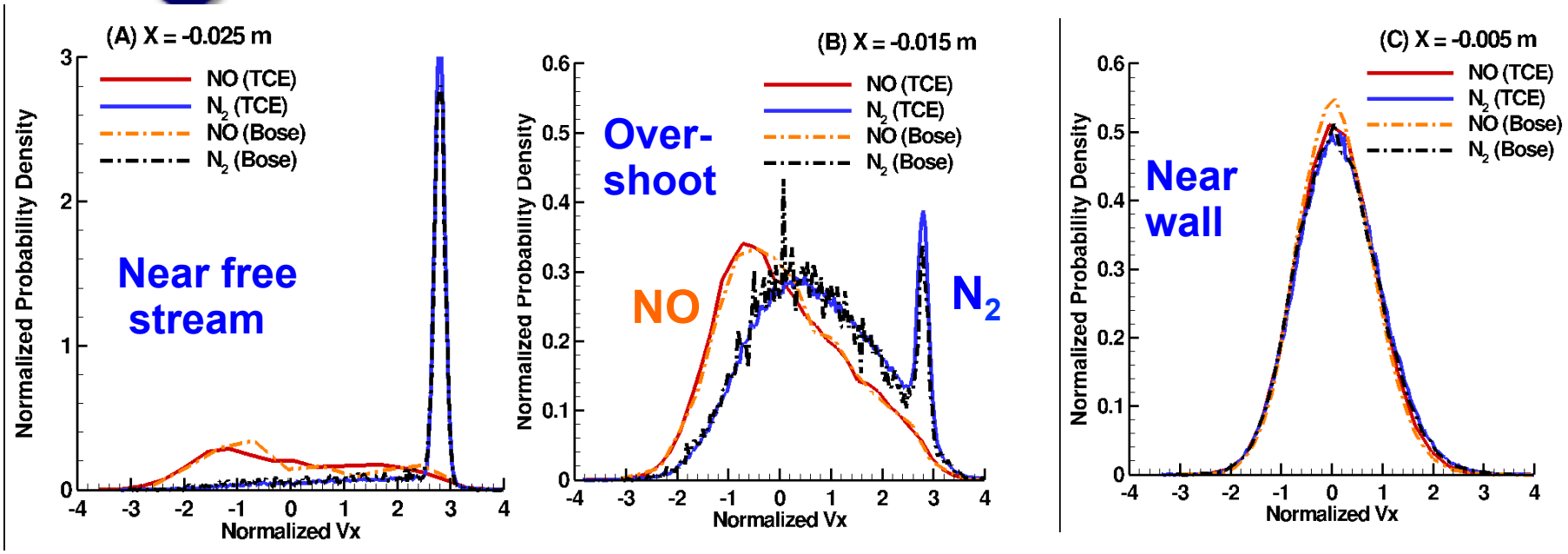
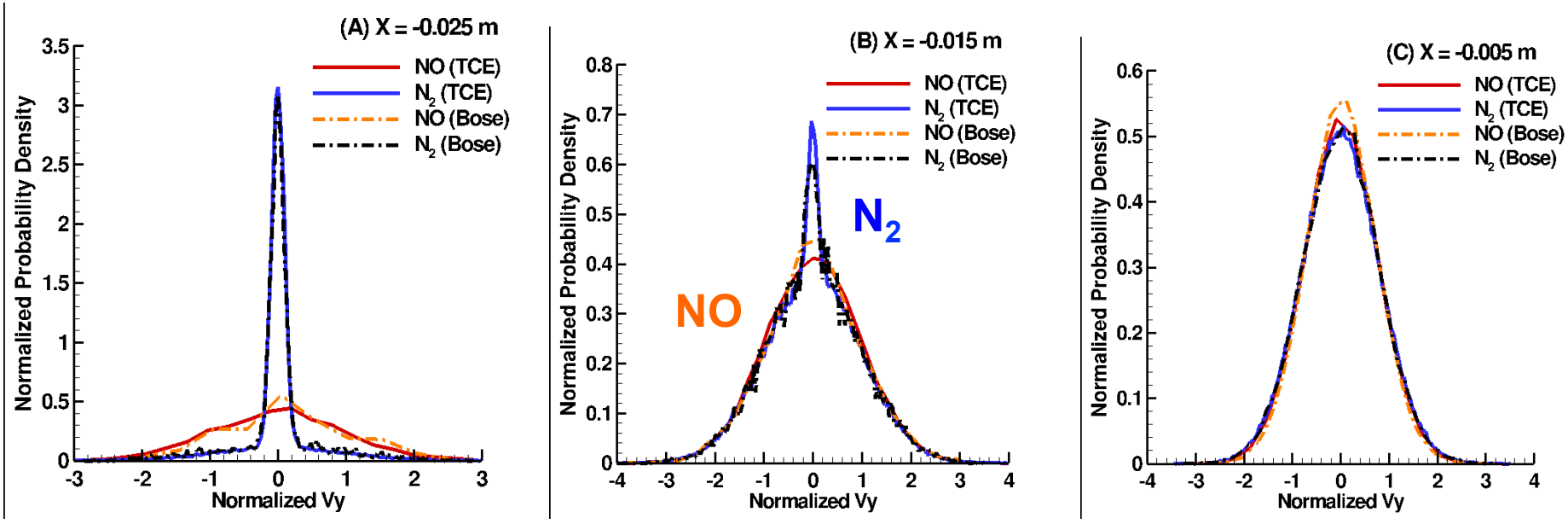
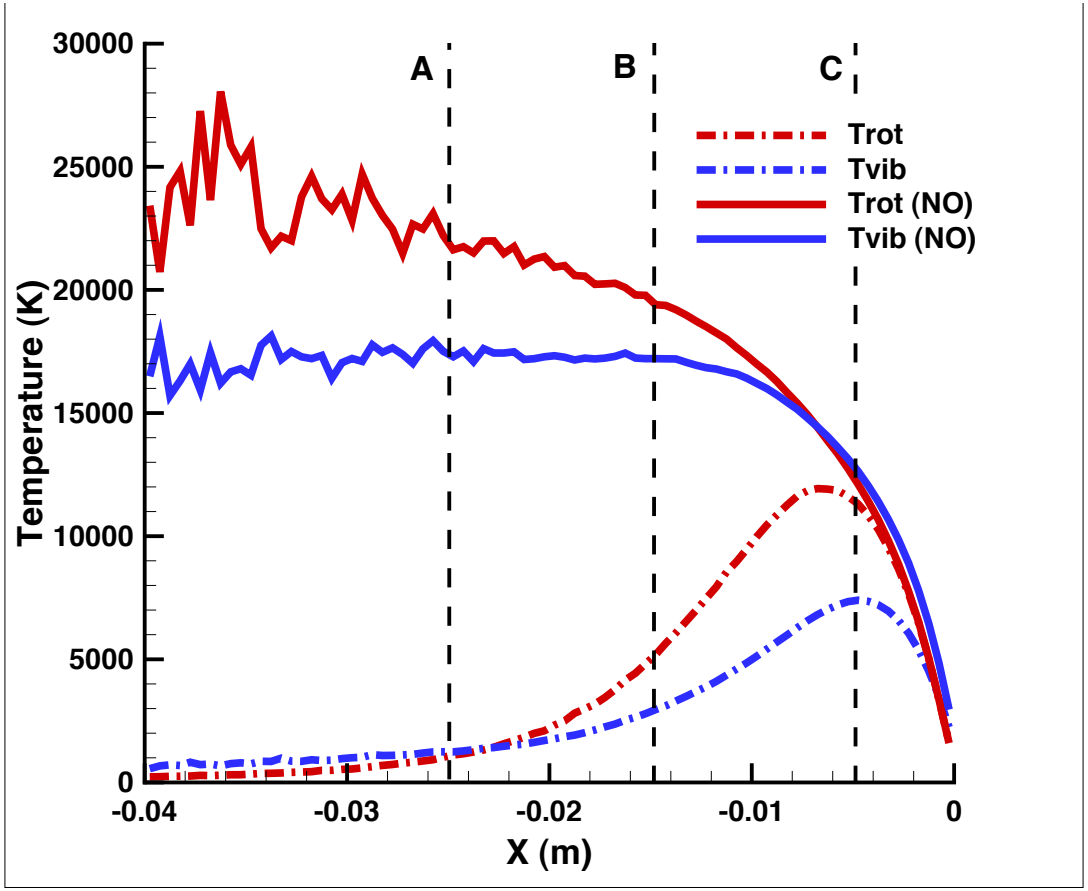
Comparison of Velocity Distributions of NO vs N_2



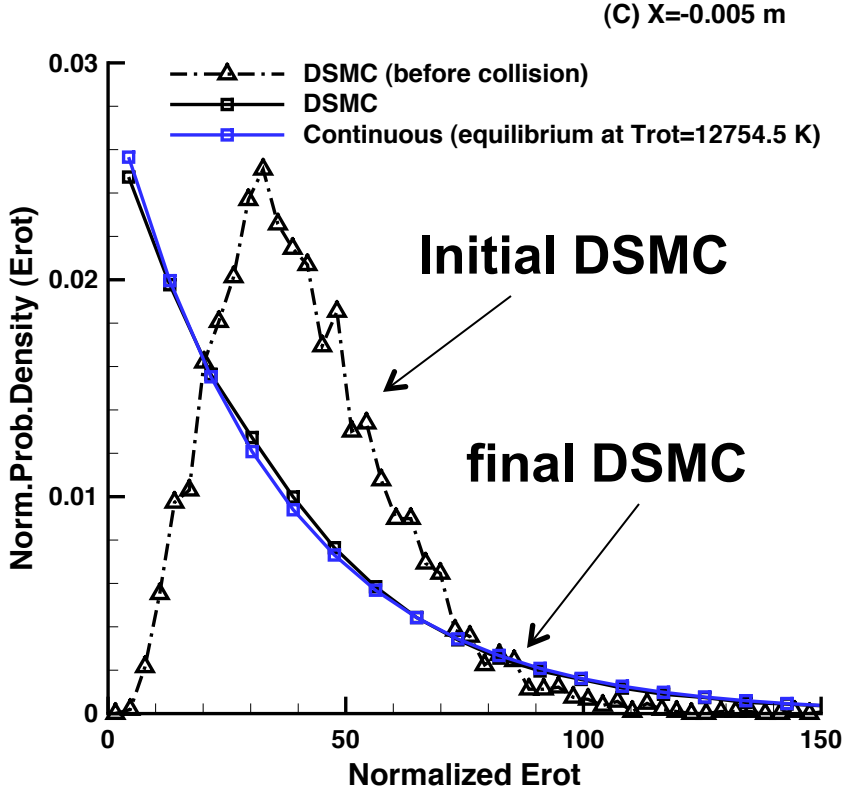


Comparison of Bulk vs NO Internal Temperatures along Stagnation Streamline

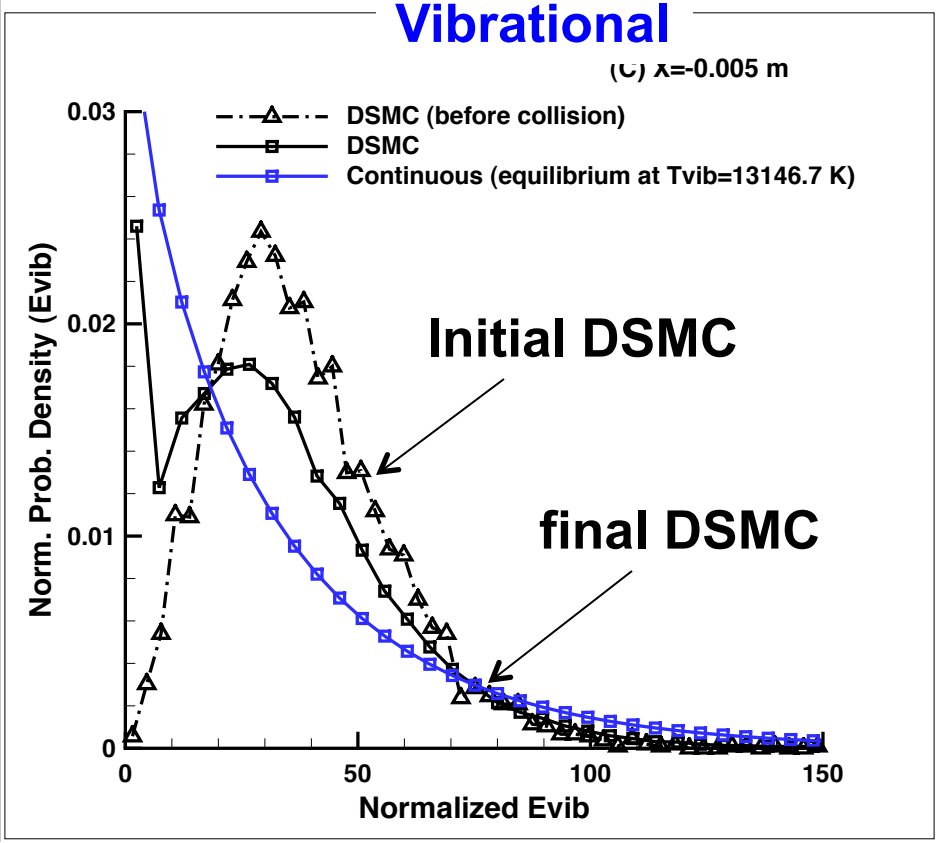


Near-wall Nascent and Final NO Rotational and Vibrational Energy Distributions in a Shock

Rotational

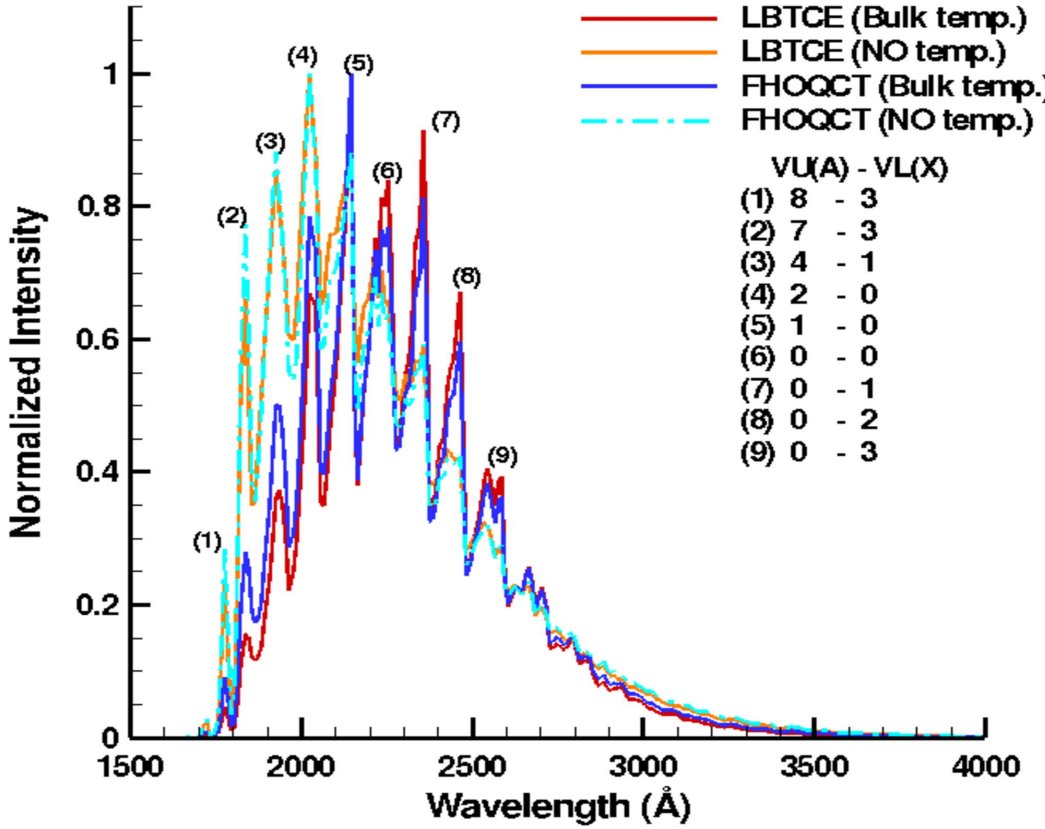


Vibrational



- Nascent rotational and vibrational distributions are similar,
- Since $T\text{-}T_{rot} >> T\text{-}T_{vib}$, vibrational distribution never equilibrates,
- Consistent with usual temperature profiles across shock.

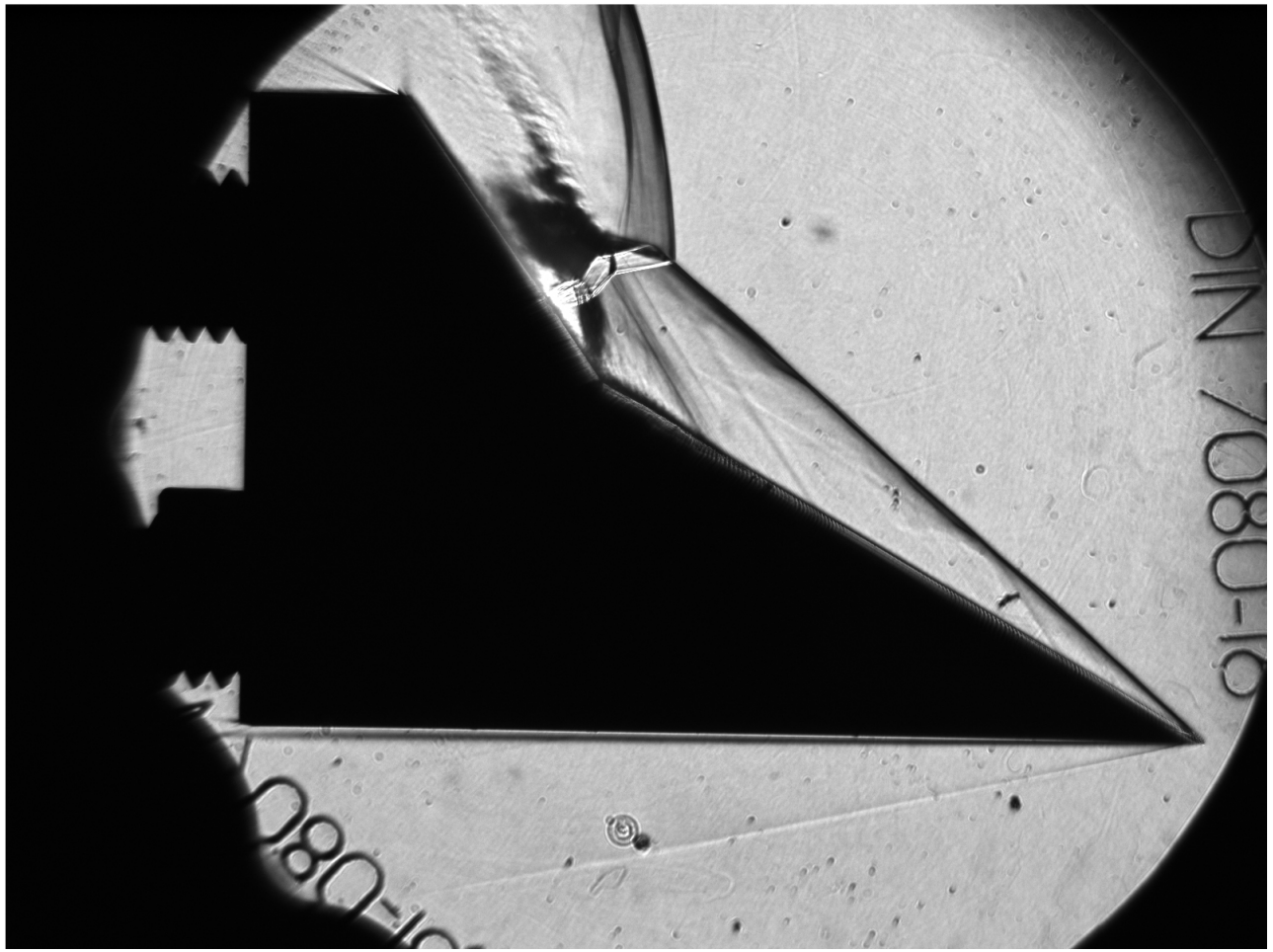
Effect of T-V Relaxation Rates, Chemistry Models, and Temperatures on NO Vibronic Spectra



- Use of NO vs bulk temperatures most important in determining spectral shape.
- Measured spectra necessary to validate nonequilibrium thermochemical models.

Gas Dynamic Modeling

Hypervelocity Expansion Tube (HET) at the University of Illinois- Prof. Joanna Austin



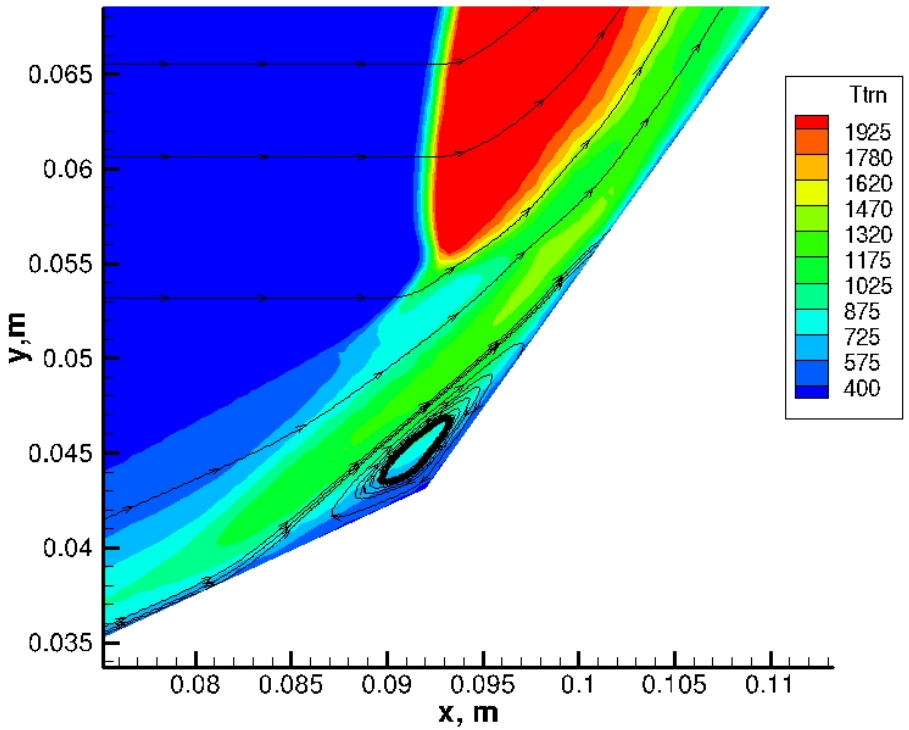
(1) Double Cone Studies of Moss and Bird*

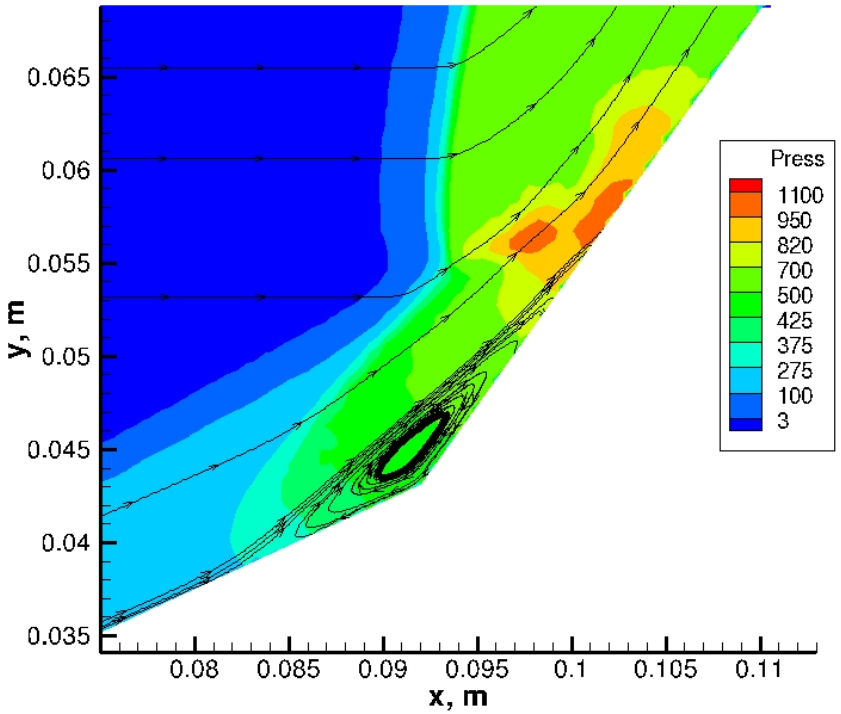
Experimental conditions performed for Mach 15.6 nitrogen flow about a 25-/55-deg bi-conic model

Freestream Parameters :	
Temperature, *K*	42.6
Number Density, m^3	3.779×10^{21}
Speed, m/s	2073
Density, kg/m^3	1.757×10^{-4}
Pressure, Pa	2.23
Mach number	15.6
Reynolds number	1.37467×10^{5}
Knudsen number	1.7×10^{-4}

***Moss, J. N. and Bird, G. A., "Direct Simulation Monte Carlo of Hypersonic Flows with Shock Interactions," *AIAA Journal*, Vol. 43, No. 12, 2005, pp. 2565-2573.**

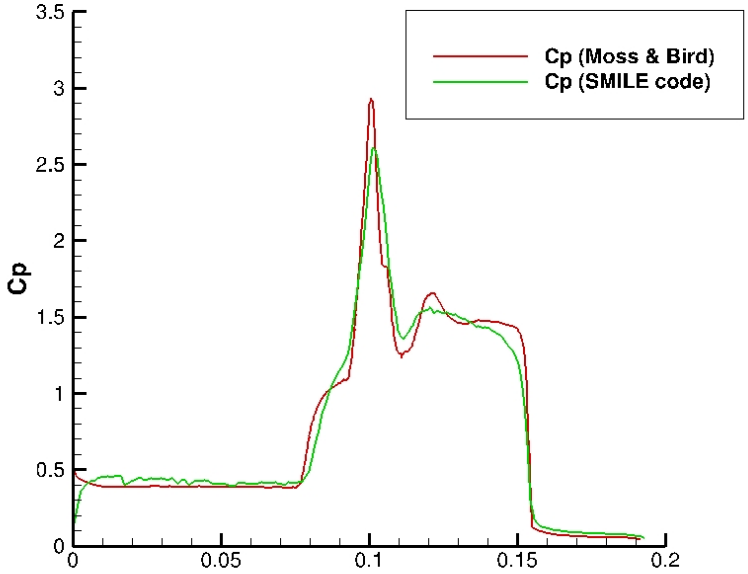
Double Cone Temperature and Pressure Contours

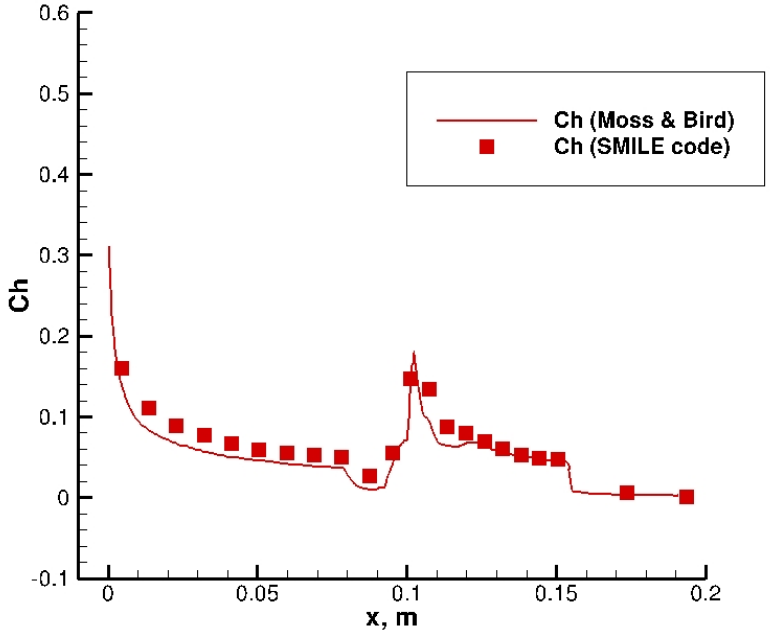


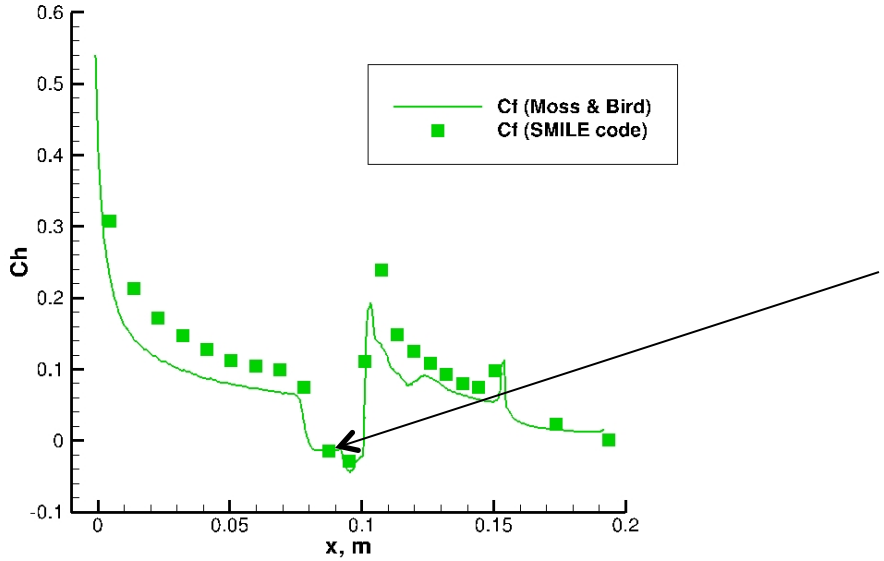


- **Physics is dominated by presence of separation zone and**
- **Sharp leading edge.**

Comparison of Surface Profiles – Double Cone Configuration







- **Separation zone well modeled.**

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(2) HET Mach 7 Nitrogen Flows

- Computational study of the complex shock interactions resulting from the hypersonic flow about a double wedge configuration presented in the paper AIAA 2012-0284 by A.B. Swantek and J. M. Austin.
- Stagnation enthalpies from 2-8 MJ/kg, about a 30-/55-deg double wedge model.
- Computations are carried using two-dimensional/axisymmetric Direct Simulation Monte Carlo simulations.

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Summary of 2 HET Freestream Conditions

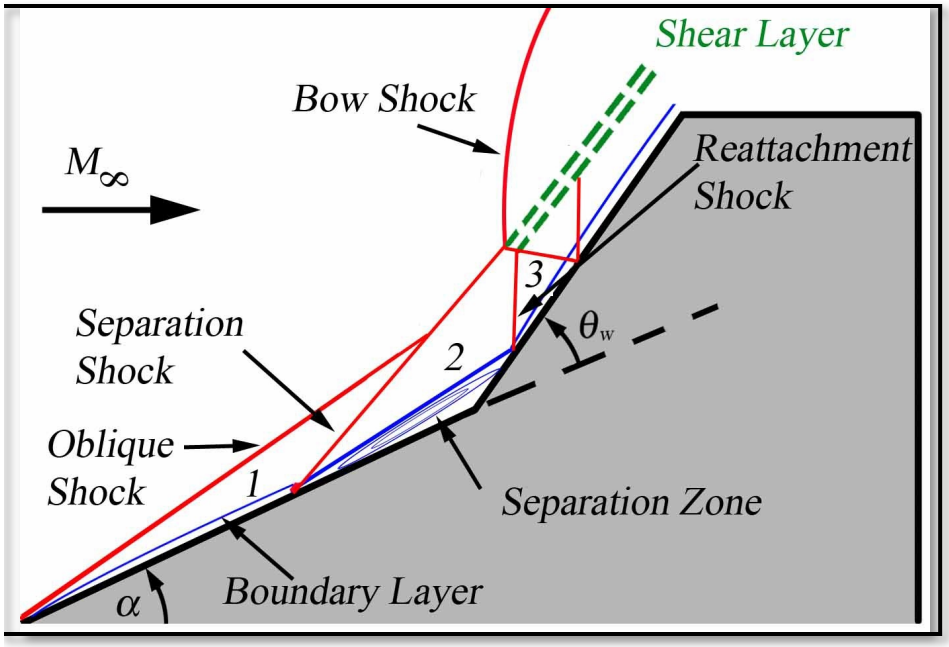
Freestream Parameters	M 7_8 (High Enthalpy)	M 7_2 (Low Enthalpy)
Mach number	7.14	7.11
Static Temperature, K	710	191
Static Pressure, kPA	0.78	0.39
Velocity, m/s	3812	1972
Density, kg/m^3	0.0037	0.0069
Number Density, $/m^3$	7.96×10^{22}	1.48×10^{23}
Stagnation Enthalpy, MJ/kg	8.0	2.1
Unit Reynolds number, /m	0.4156×10^{6}	1.0653×10^{6}
Knudsen number	4.0256×10^{-4}	1.5742×10^{-4}

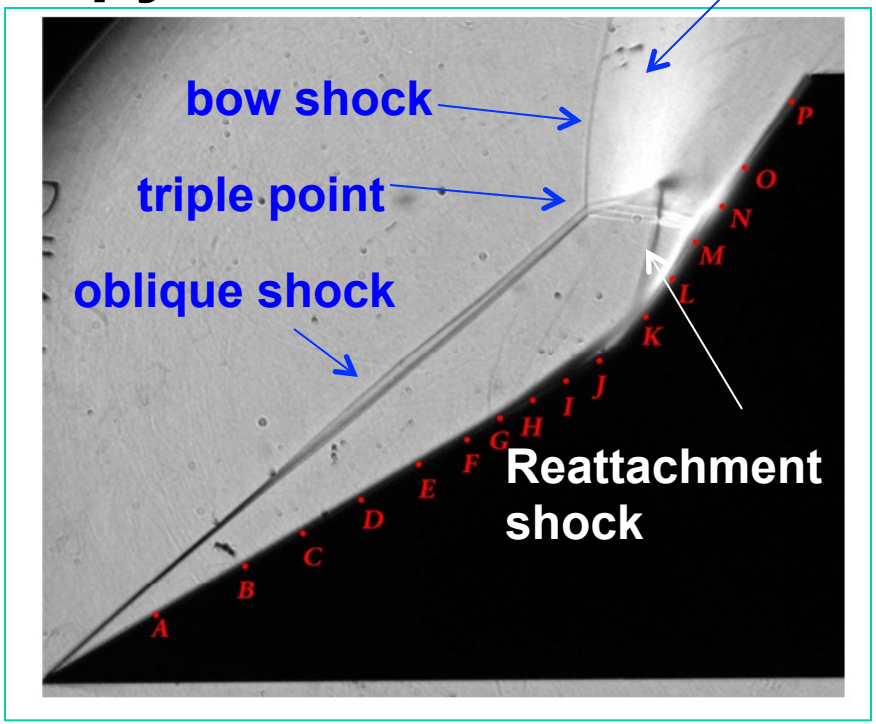
Summary of Numerical Parameters Used in the DSMC Calculations

	Case	Number of Processors used	Time Step (s)	PFnum	Number of Collisional Cells
High Enthalpy	1	32	2.0×10^{-7}	1.0×10^{14}	450x350
	2	32	2.0×10^{-8}	3.0×10^{13}	1800x1600
	3	32	1.0×10^{-9}	3.0×10^{13}	1800x1600
Low Enthalpy	1	32	1.0×10^{-9}	3.0×10^{13}	1800x1600
	2	32	1.0×10^{-9}	1.0×10^{13}	3600x3200

The computational domain from -20 to 70 mm along the x direction and from 0 to 80 mm in the y direction.

Strong Shock Interactions – High Enthalpy Case

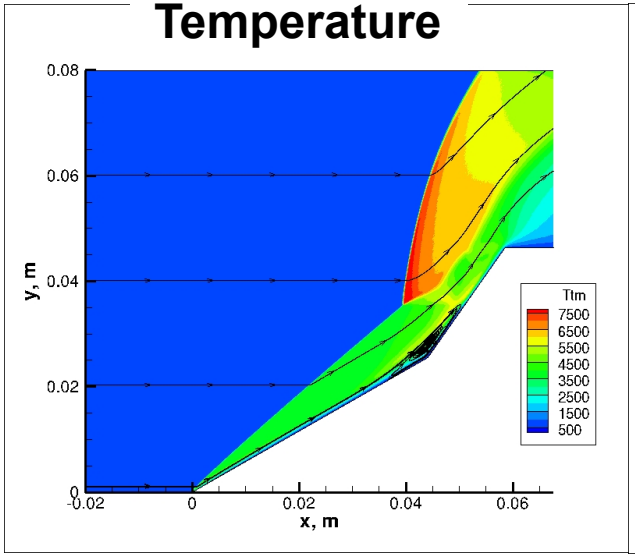




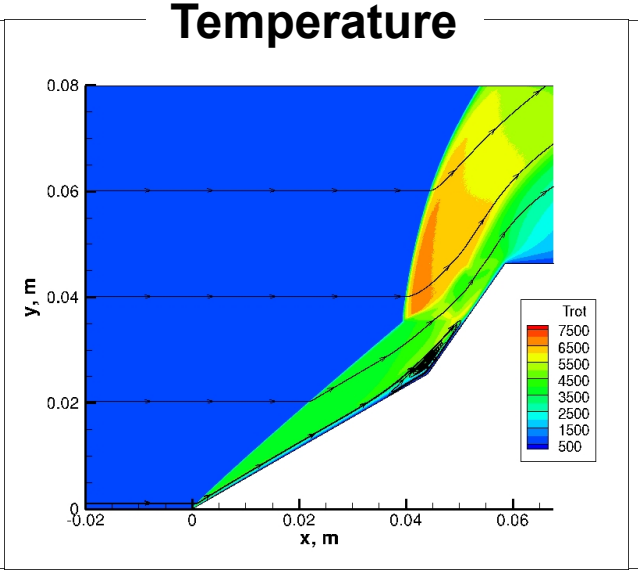
- separation and reattachment shocks
- triple point
- shear layers
- boundary layer interactions
- attached shock from the first cone/wedge interacts with the detached bow shock from the second cone/wedge.

High Enthalpy Case 3 – DSMC Temperatures

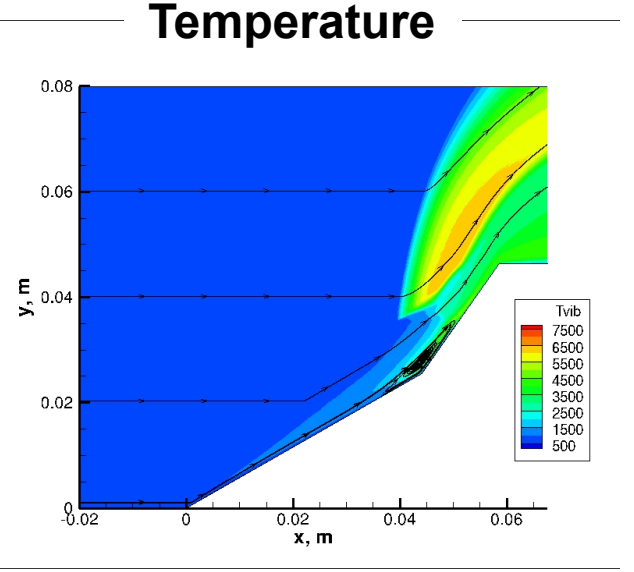
Translational Temperature



Rotational Temperature

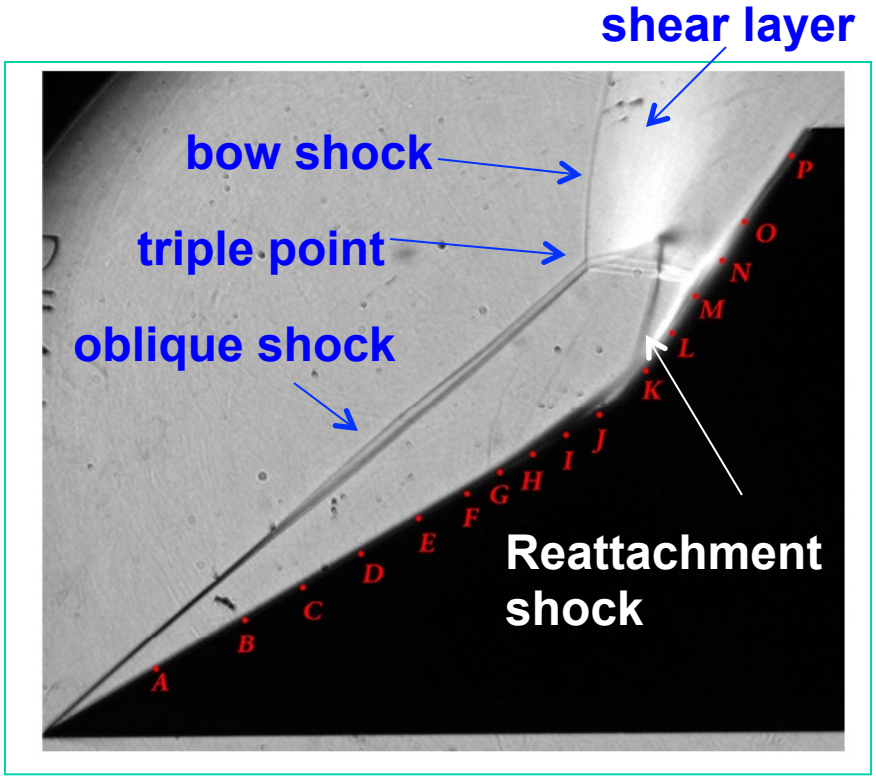


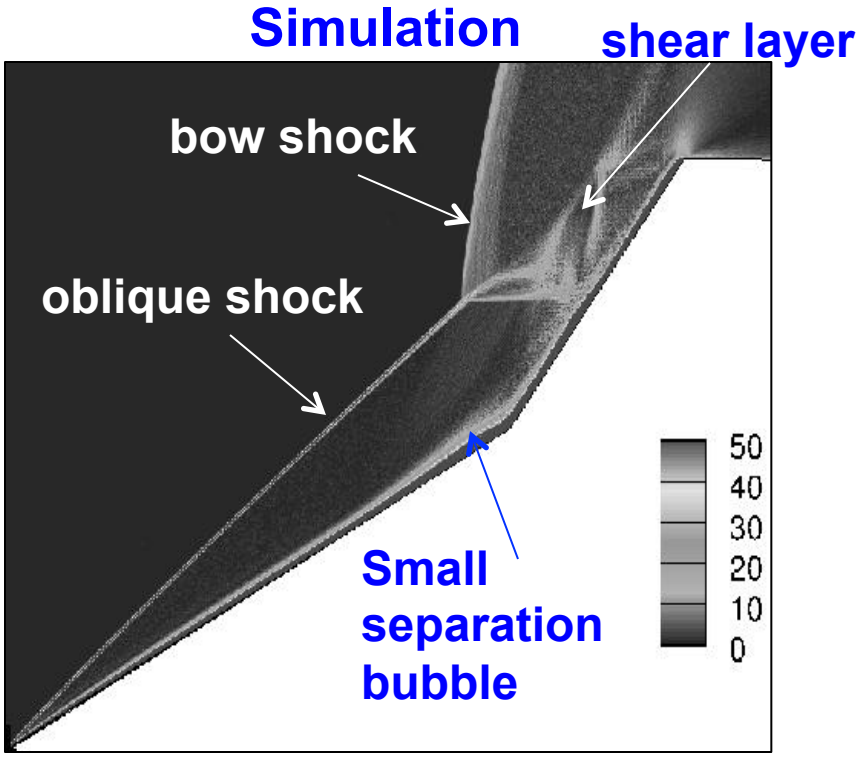
Vibrational Temperature



- **Characteristic separation bubble seen,**
- **$T \sim T_{rot}$, T_{vib} out of equilibrium even for continuum-like flow,**
- **Need to assess separation bubble structure on T-V relaxation models.**

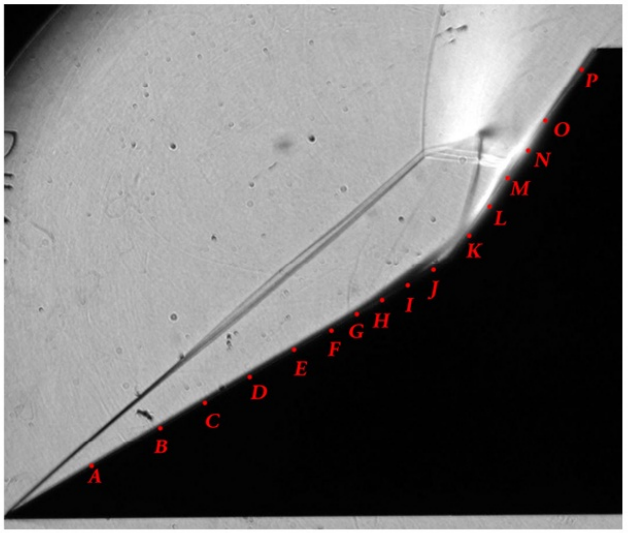
Comparison of Shock Structure - High Enthalpy Case

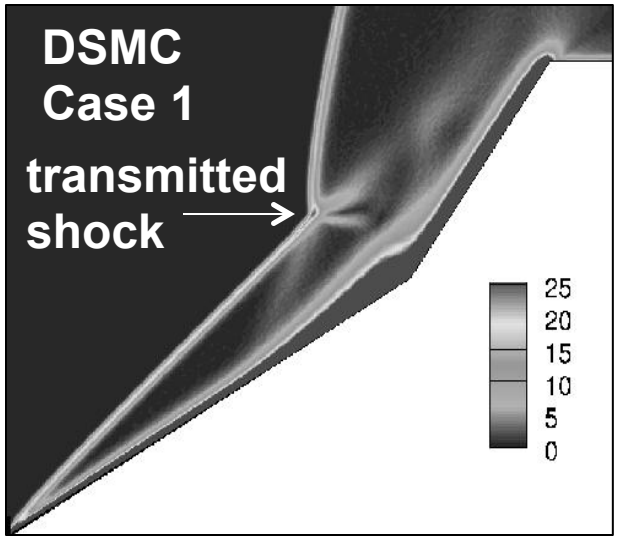


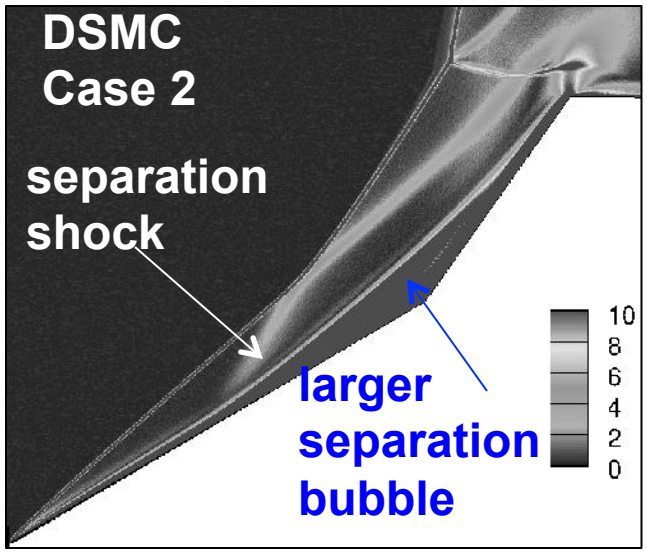


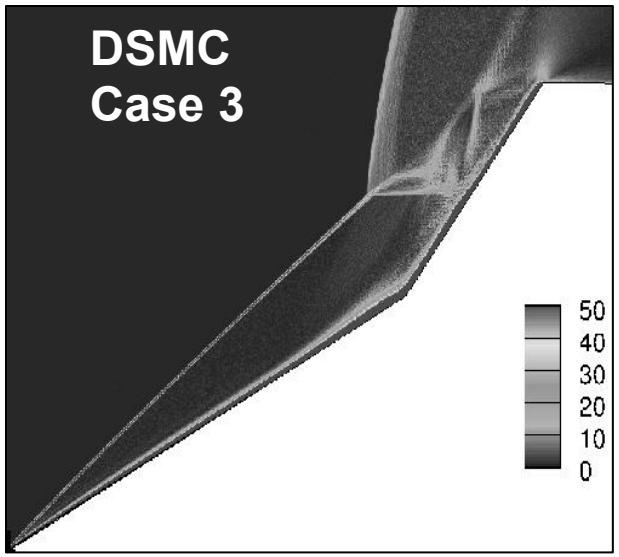
- Reasonable, but, not perfect structure agreement.
- Affect of razor-sharp leading edge on downstream structure?

Shock Structure Dependence on Numerical Parameters – High Enthalpy Case

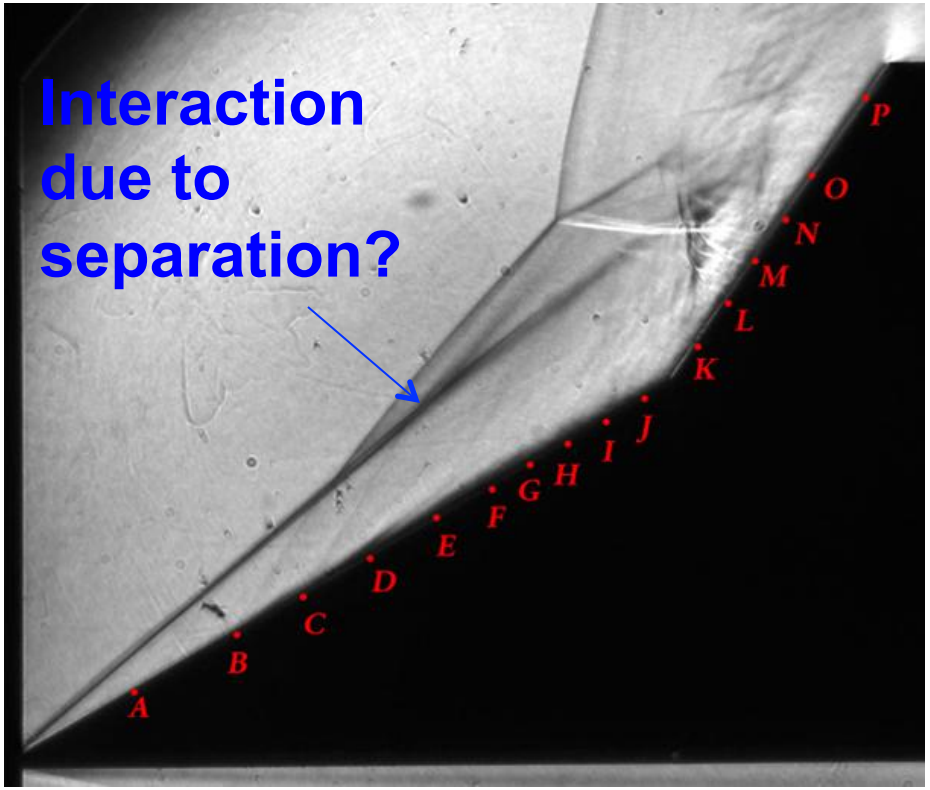


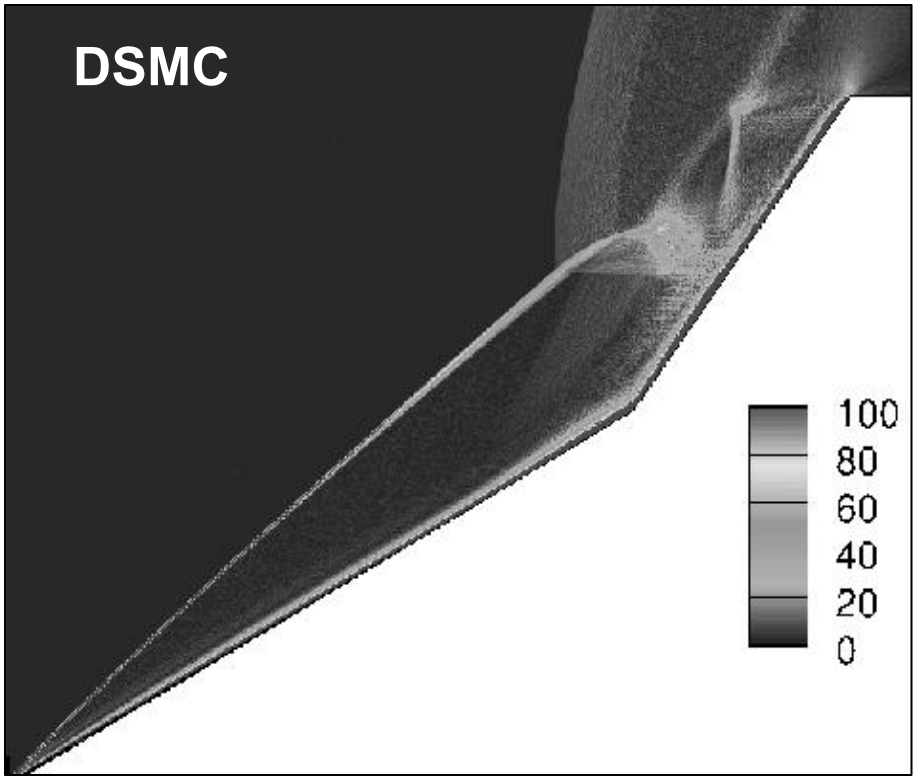






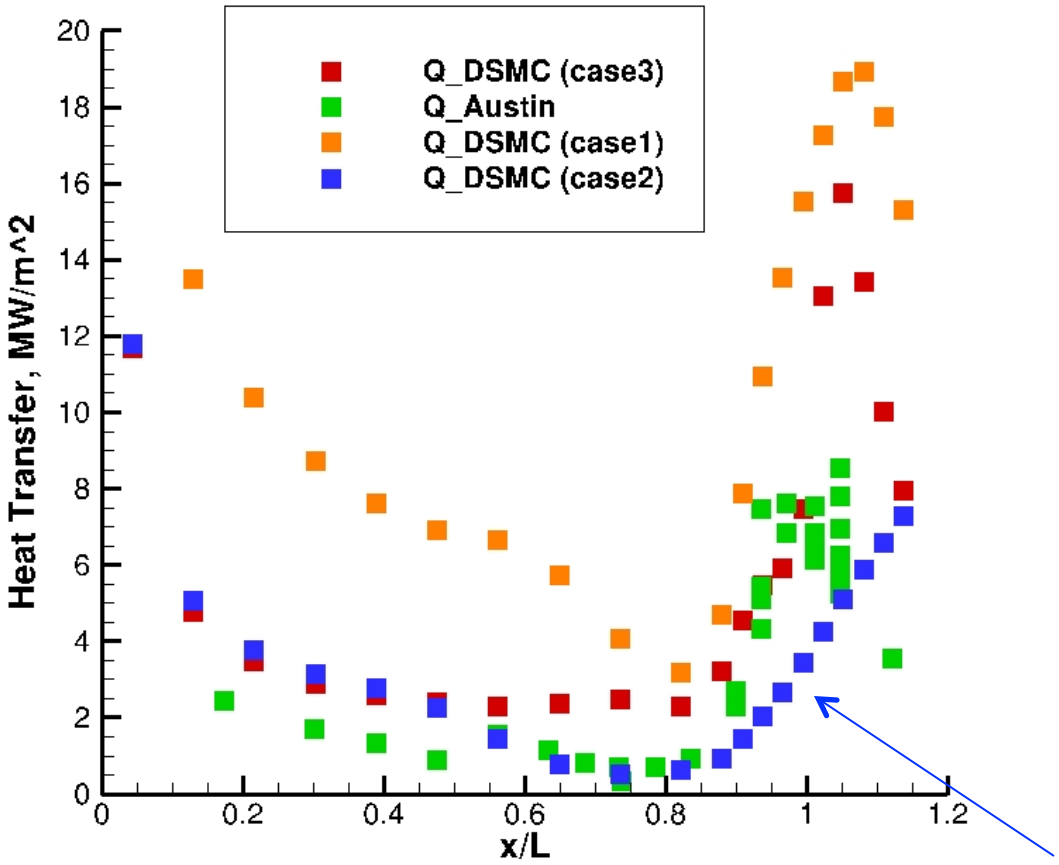
Comparison of Shock Structure - Low Enthalpy Case





- **Different flow features such as the oblique-bow shock interaction, separation shock, separation region, and triple point.**
- **The experiment seems to have a larger separation region resulting in different flow features.**
- **Not as confident yet in convergence of numerical parameters.**

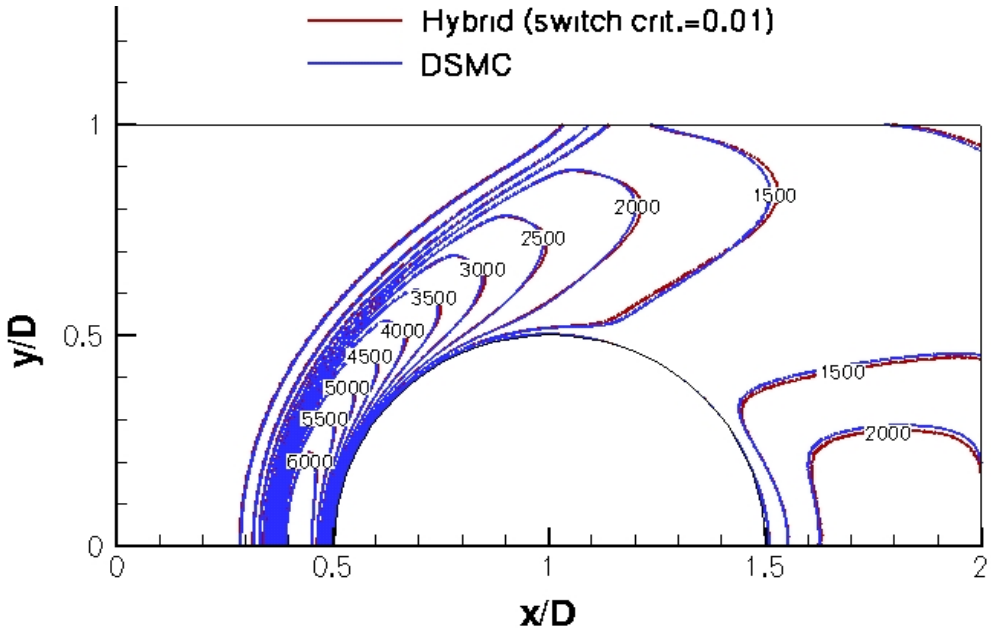
Comparison of Heat Transfer – High Enthalpy Case



- **DSMC Case 2 seems to capture similar trends, ie., jump at the hing (x/L = 0.8).**
- **But DSMC Case 2 had "wrong" shock structure.**
- **Separation bubble too large.**

Outstanding Scientific Issues

- **Nonequilibrium thermochemical models still are incomplete and unvalidated (in both particle and continuum approaches). Need more data and less code-to-code comparisons.**
- **Need to characterize and quantify facilities for non-equilibrium gas dynamic calculations.**
- ***Particle-particle* hybrid schemes:**
  - **What is our criteria for detecting equilibrium break down?**
  - **Will the ES-BGK approach be sufficiently general to include internal energy?**
  - **Can we apply it to shock-shock interactions?**
  - **Can we handle unsteady flows?**



Acknowledgments

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