Non-equilibrium and Energy Exchange Mechanisms in High Energy Flows

Eswar Josyula

Air Force Research Laboratory

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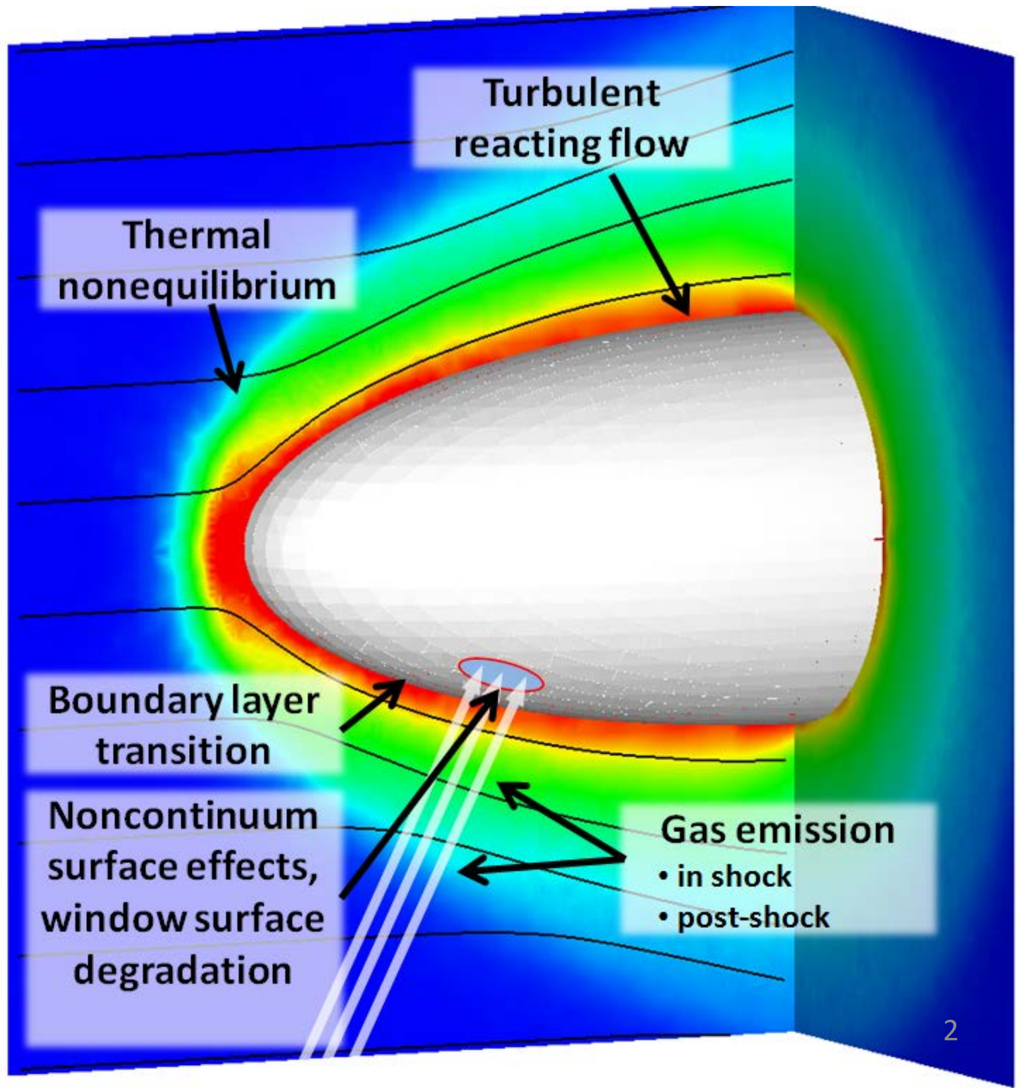
The Need

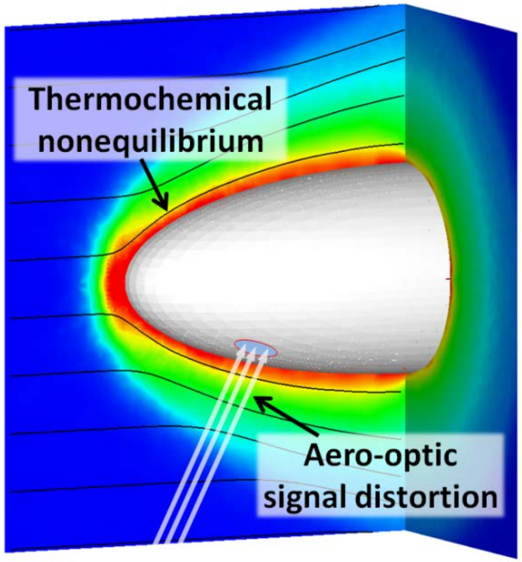
- Simulate the aerothermal environment for ISR applications
- Hand-off to RY for Sensor design analysis
- Flow-sensor interactions
  - Aero-optic effects: changes in refractivity index due to spatio-temporal density variation that may cause:
    - phase distortion
    - image lensing
    - bore-sight error
    - Jitter
  - Effect of internal energy exchanges, turbulent fluctuations, and radiation emission from shock wave on the electromagnetic signal

RQ role

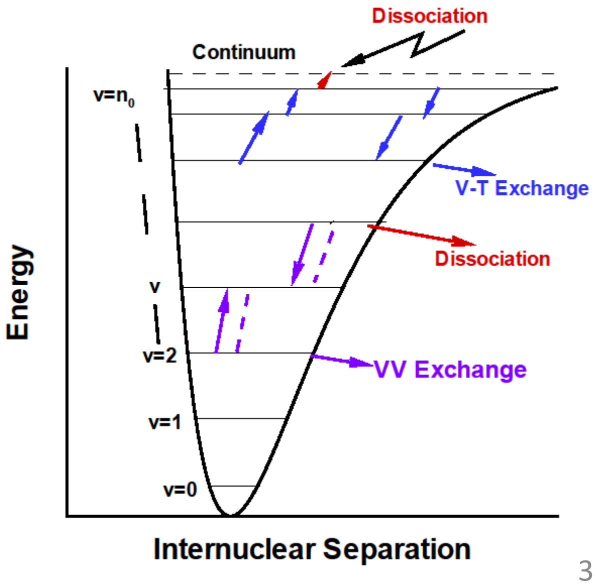


Background: Current Problem
Thermochemical nonequilibrium

- Challenge: Modeling vibrational and chemical nonequilibrium in high speed flow
  - Lack of energy equipartition between vibrational and translational/rotational degrees of freedom;
  - Deviation from equilibrium (Boltzmann) distribution in vibrational energy mode
  - Finite rate dissociation, recombination and exchange reactions in 5-species air

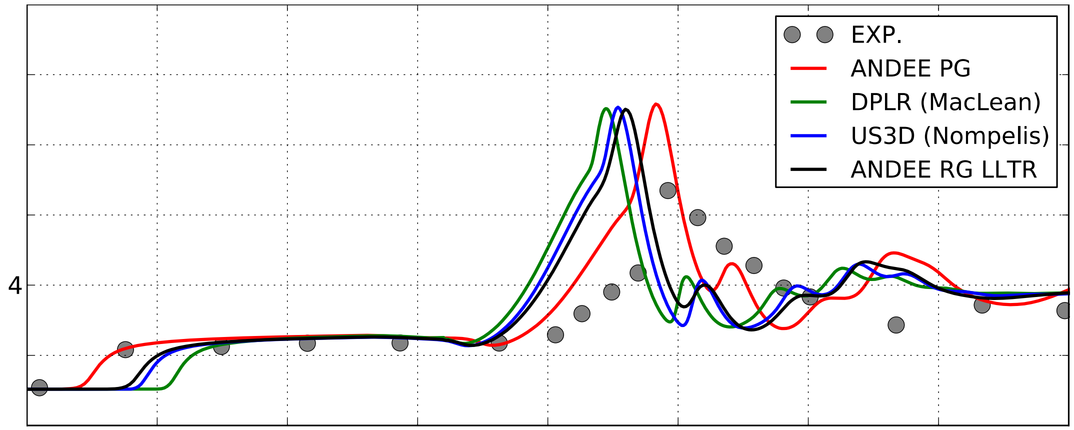


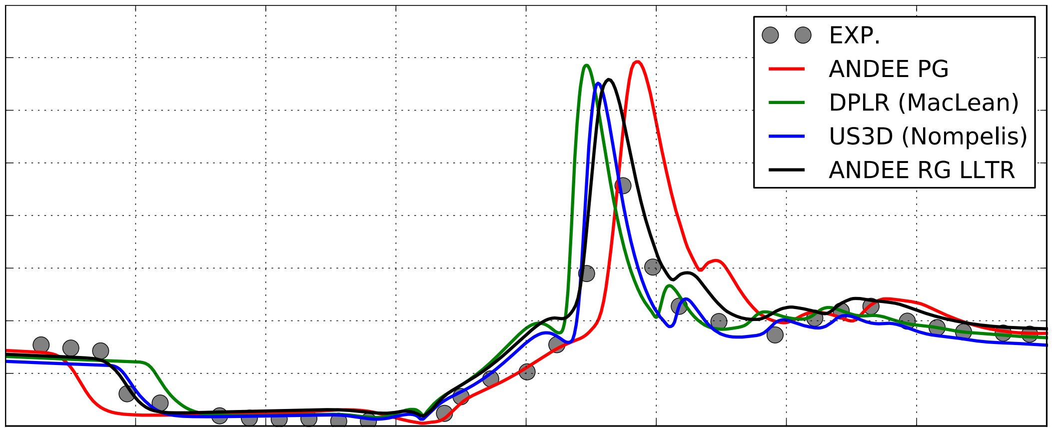
- Multi-dimensional Nonequilibrium Flow Solver Development
  - Influence of multiquantum jumps
  - Comparison with experiments



Motivation

CFD vs. Experiment (Lens-XX RUN1 - Laminar)





From AIAA 2017-0664

Approach
Governing Equations

- 2D flow solver coupled to master equation with VT and dissociation: Aerothermal Nonequilibrium Detailed Energy Exchange (ANDEE) code

$$\frac{\partial}{\partial t}(\rho_n) + \nabla.(\rho\,\vec{u}) = \omega_n \qquad\qquad n = 0,1,2....,48$$

$$\omega_n = \frac{1}{M}\{\sum_n [k_{VT}(n' \to n)\rho_{n'}\rho - k_{VT}(n \to n')\rho_n\rho$$
$$- k_{nD}(n \to Continuum)\rho_n\rho_{O2} - \tilde{k}_{nD}(Continuum \to n)\rho_n\rho_O]\}$$

Molecule-Molecule Reactions

V-T Process

$$O_2 + O_2(n) \leftrightarrow O_2 + O_2(n')$$
$$N_2 + N_2(n) \leftrightarrow N_2 + N_2(n')$$

V-D Process

$$O_2 + O_2(n) \leftrightarrow O_2 + 2O$$
$$N_2 + N_2(n) \leftrightarrow N_2 + 2N$$

Atom-Molecule Reactions

V-T Process

$$O + O_2(n) \leftrightarrow O + O_2(n')$$
$$N + N_2(n) \leftrightarrow N + N_2(n')$$

V-D Process

$$O + O_2(n) \leftrightarrow 3O$$
$$N + N_2(n) \leftrightarrow 3N$$

Compatibility: STS and LT in Single Solver

STS formulation for some of the air species N_2, O_2, NO, N, O

$$\frac{\partial \rho_{ci}}{\partial t} + \nabla \bullet \left[\rho_{ci}\left(v + V_c + \tilde{V}_{ci}\right)\right] = \dot{\omega}_{ci} \;;\; \rho = \sum_{i=1}^{N} \rho_i \qquad \rho e_{vib-c} = \rho \sum_{i=1}^{N} \varepsilon_i$$

Anharmonic Oscillator

LT collision of remaining species with species treated as STS

$$\frac{\partial \rho_c}{\partial t} + \nabla \bullet \left[\rho_c\left(v + V_c\right)\right] = \dot{\omega}_c \qquad c\text{: STS } N_2 \text{ or } O_2\text{; LT: } NO, N, O$$

$$\frac{\partial(\rho e_{vib-c})}{\partial t} + \nabla \bullet \left[\rho e_{vib-c}\left(v + \tilde{V}_c\right) + \dot{q}_{vib-c}\right] = \rho\,\dot{\omega}_{vib-c} + e_{vib-c} + Q_{VT}$$

Harmonic Oscillator

Problem: Conservation of mass and vibrational energy

Reason: Energy input to collisions is inconsistent between LT and STS models due to different energy distributions

Methods to conserve vibrational energy

- Update Energy
  - Set new energy and distribute populations according to Boltzmann
- Mapping the Solutions
  - From anharmonic ⟺ harmonic
- Energy Reconciliation
  - Compare and adjust energies in STS and LT

Update Energy Method

Consistent update of state population of species treated with STS, $\rho_{k\,c}$ such that

$$\sum_k \rho_{kc} = \rho_{new\,c} \quad (LT) \qquad k = 1,2,3,\dots \max L; \;\; c = \mathrm{O}_2 \text{ or } \mathrm{N}_2$$

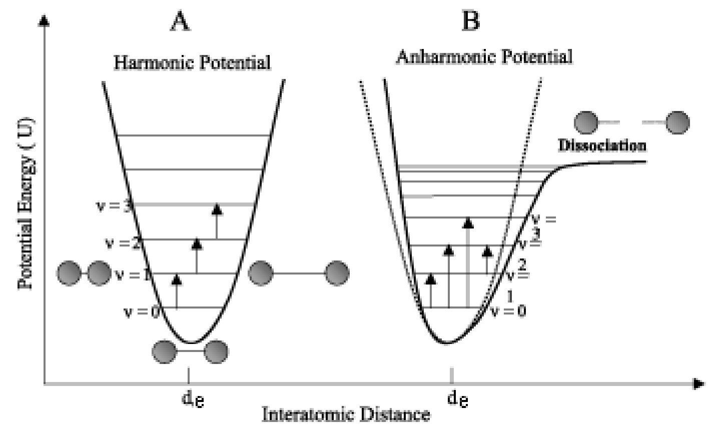
$$\sum_k \rho_{kc}\, E_k = \rho_{new\,c} E_{vib\;\;new\;\;c} \quad (LT)$$

Distribute energies according to

$$\rho_{kc}^{new} = \rho_{new\,c} \frac{e^{-(E_k / E_{vib\;\;new\;\;c})}}{\sum_q e^{-(E_q / E_{vib\;\;new\;\;c})}}$$

Mapping the Solutions

- Mapping the solution from anharmonic => harmonic oscillator => anharmonic
  - Molecule-Molecule/Atom collision as STS
    - Map the solution to harmonic oscillator
  - Molecule-Molecule/Atom collision as LT
    - Map the solution to anharmonic



- Mapping from anharmonic ↔ harmonic
  - requires formulation of a matrix of weighted energies
  - each energy depends on the densities of all the states
  - and its eventual inversion

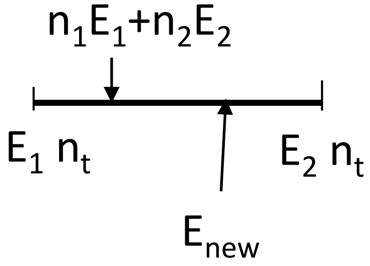
Energy Reconciliation Method

$\Delta E = Evib_{LT} \;\; and \;\; Evib_{STS}$

If $\Delta E \sim 0$, neglect difference between LT and STS energies

If $\Delta E \neq 0$, then :

Set $E_{new} = n_1 E_1 + n_2 E_2 + \Delta E$, Then sum of first two levels, $n_t = n_1 + n_2$



If $n_t E_1 < E_{new} < n_t E_2$, then (Condition 1)

$$n_1' = \frac{n_t E_2 - E_{new}}{E_2 - E_1} \qquad n_2' = n_t - n_1'$$

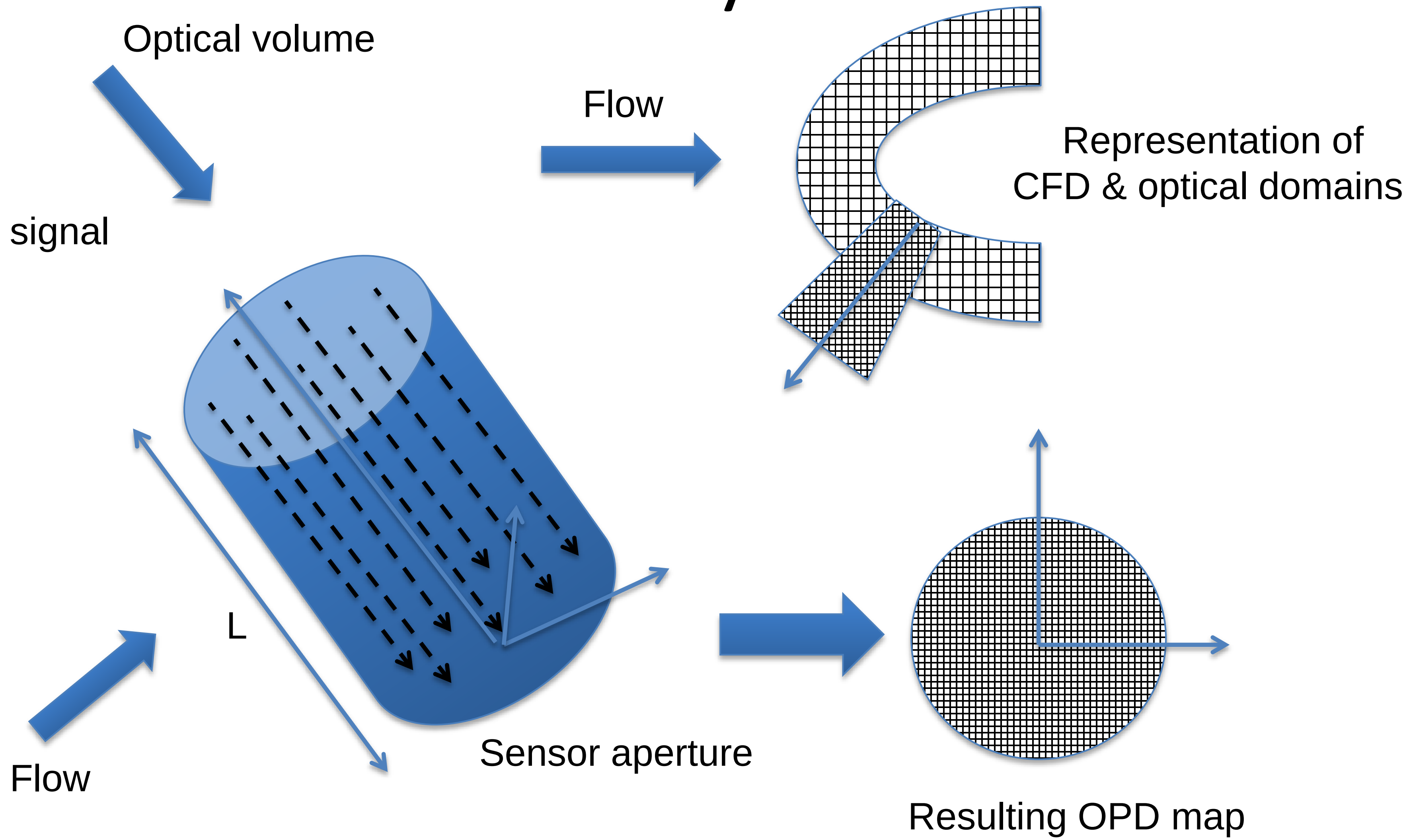
If $n_t E_1 > E_{new}$ then

increase n_t and E_{new} at the expense of higher states so that E_{new} satisfies condition 1

If $n_t E_2 < E_{new}$, then

decrease n_t and E_{new} by modifying higher states so that E_{new} satisfies condition 1

Optical Path Difference Grid System



Optical Path Difference
Aerodynamics Effects => Optical Effects

- Extract density field from CFD simulation $\rho(X,Y,Z,t)$
- **Dry Air** refractive index $N - 1 = \rho\ (K_{GD})$
  - K_{GD} mass averaged Gladstone-Dale constant
- Interpolate to optical volume mesh (x,y,z); refractive index is defined at center of cell
- The Optical Path Length (OPL) for a given cell [i,j,k] of thickness dz[k] at location (x,y,z) is
  - $OPL[i,j,k,t] = N[i,j,k,t]\ dz[k]$
- We integrate to get the OPL at every (x,y) location and then the Optical Path Difference (OPD) map
  - $OPL[i,j,t] = \Sigma_k\ OPL[i,j,k,t]$
  - $OPD[i,j,t] = OPL[i,j,t] - OPL_{ref} = OPL[i,j,t] - \langle OPD \rangle$

Planned Results and Benefits

- Quantities of interest: population distributions at select locations, density variation in the flow field, translational and internal energy temperatures
- Benefit this past year: Comparison with experiments: accuracy gains using STS approach
- Desired outcomes, impact on related fields:
  - Inputs to evaluate signal distortion and deflection
  - Extend STS approach to large scale hypersonic flow simulation
  - Influence of nonequilibrium on turbulent flows
  - Prediction of onset of boundary layer transition

If the Work were Not to Get Done

- Increased uncertainties in EO/IR signal corrections
- Overly large TPS tolerances, increased vehicle weight
- Increased errors in aero database for controls algorithms and control surface sizing
- Improper inputs on thermal loading for analysis of aero-structure interactions

Where we left off last year

- Simulation of Mach 7-15 oxygen flow past sphere-cone
  - Level-specific dissociation rate shows competing effect of depletion and thermal excitation at Mach 11, unlike at 7 and 15
- Compared several different measures of vibrational nonequilibrium using state-resolved simulation of hypersonic flow
  - Qualitative agreement among the different measures
  - Significant differences in locations influence by both compression and expansion
- Developed techniques for spatially adaptive state-resolved modeling of vibrational nonequilibrium. Viz. Normalized temperature difference, Damkohler number, and Entropy cut-off
  - Need for improved treatment of upper levels in near-equilibrium regions
  - Need physics-based cut-off criterion to automate in CFD codes

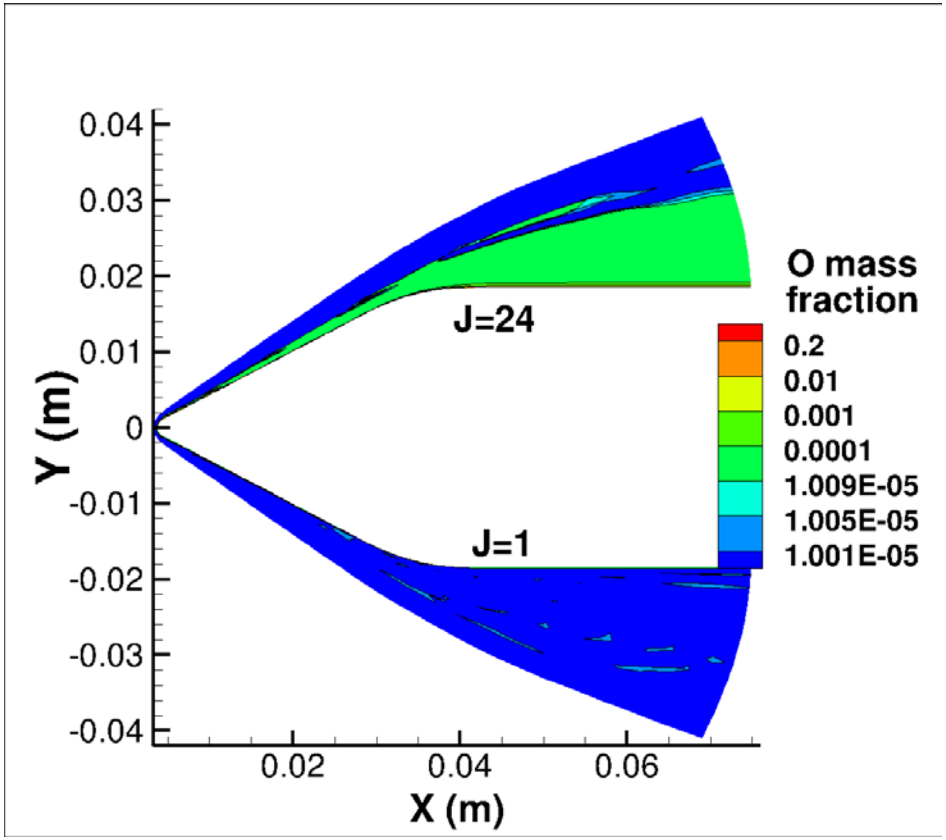
NEW RESULTS

Atomic Mass Fraction Contours

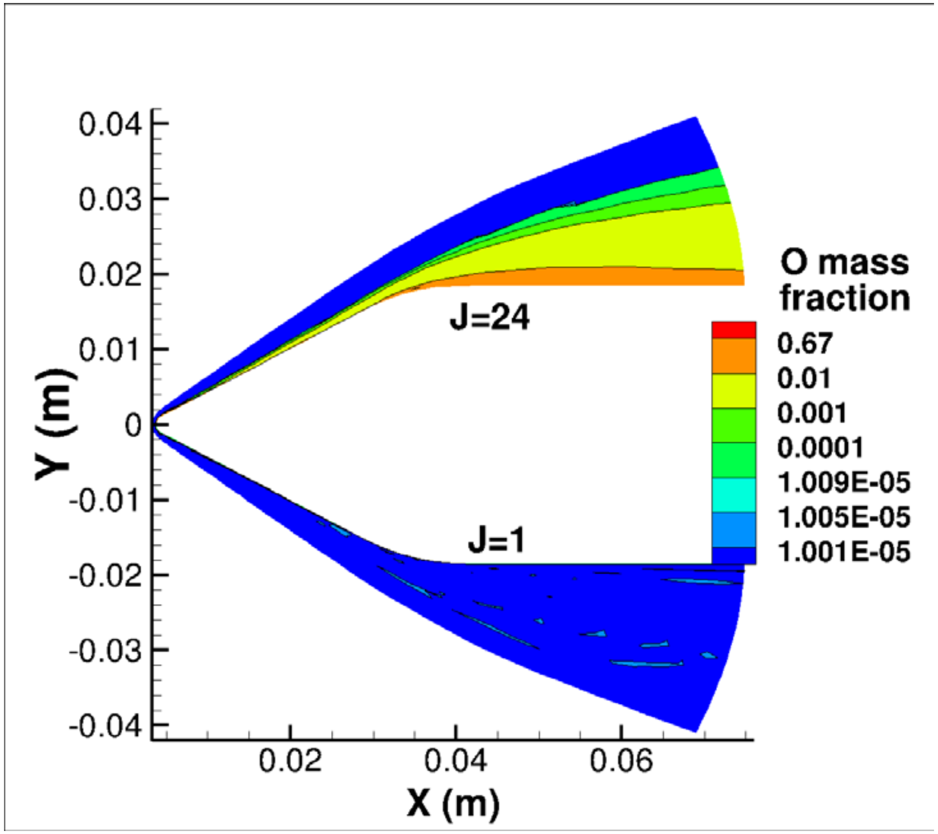
Comparison of J=1 and 24

J=Max Quantum Jump

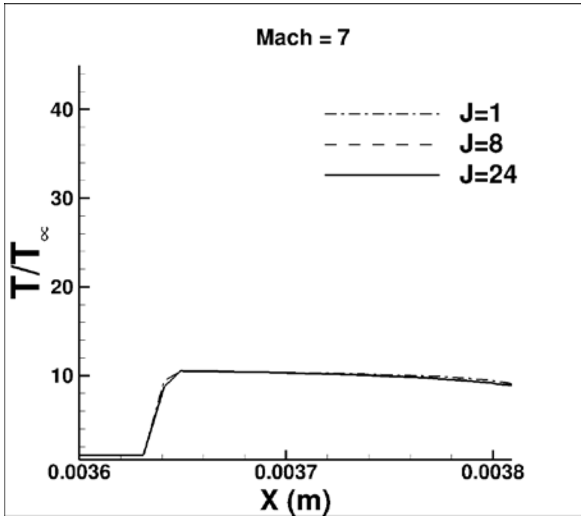
Mach 11 Oxygen Flow

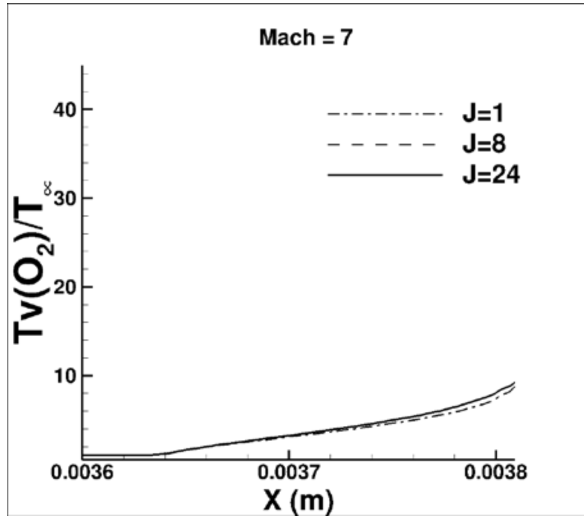


Mach 15 Oxygen Flow



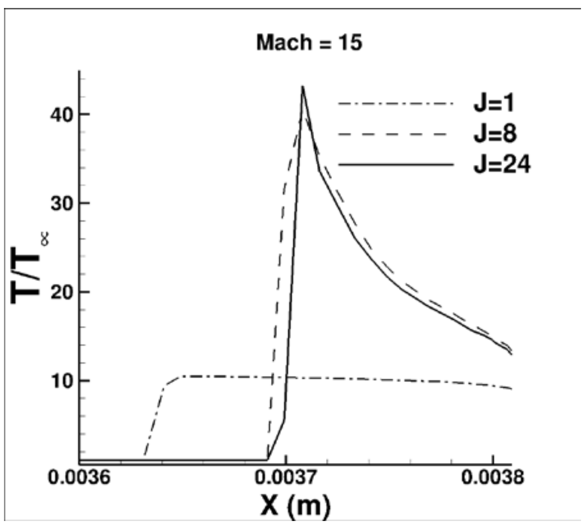
Effect of J on T and Tv along Stagnation Streamline

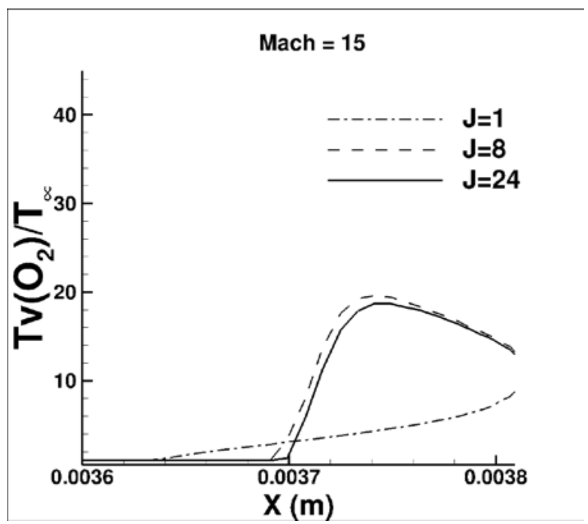




J=1
J=8
J=24

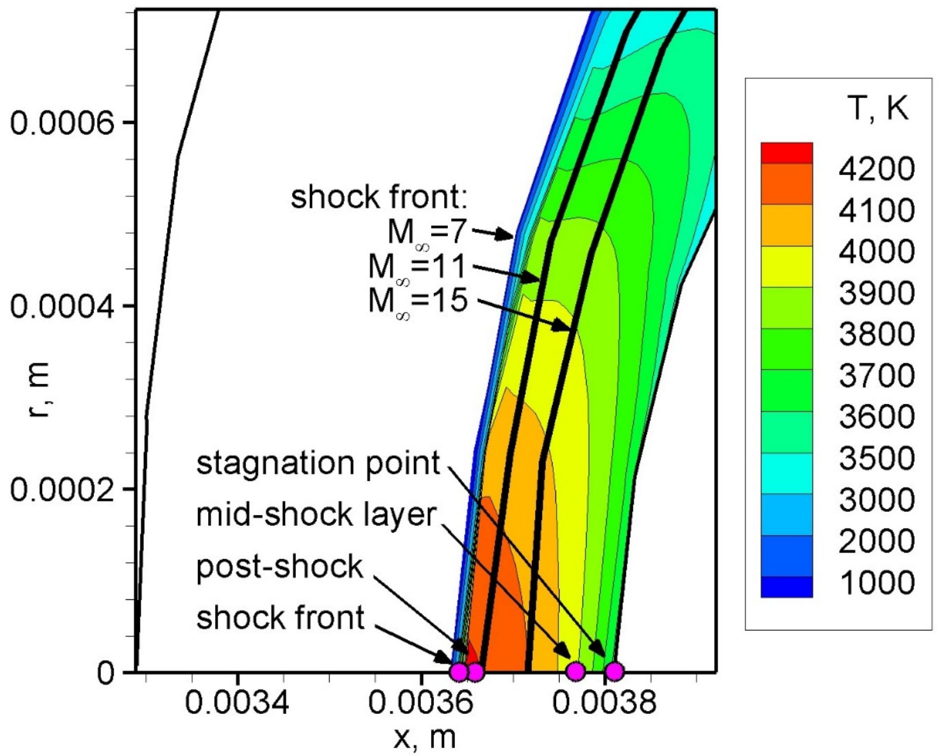
Tv for Mach 7 increases monotonically towards the wall but decreases for Mach 15 near wall due to endothermic process in dissociation



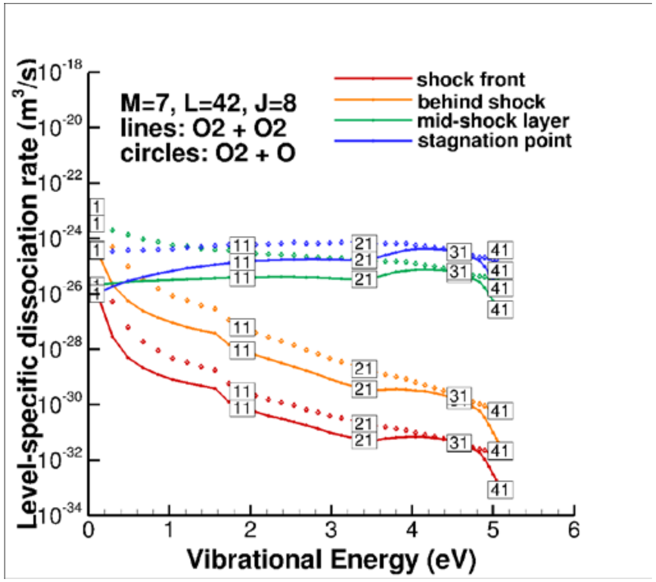


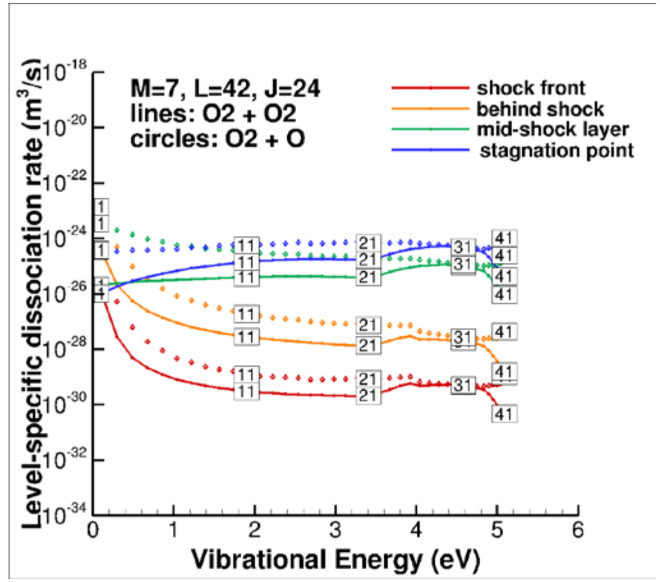
Higher degree of dissociation for higher J resulting in reduced shock-standoff distance

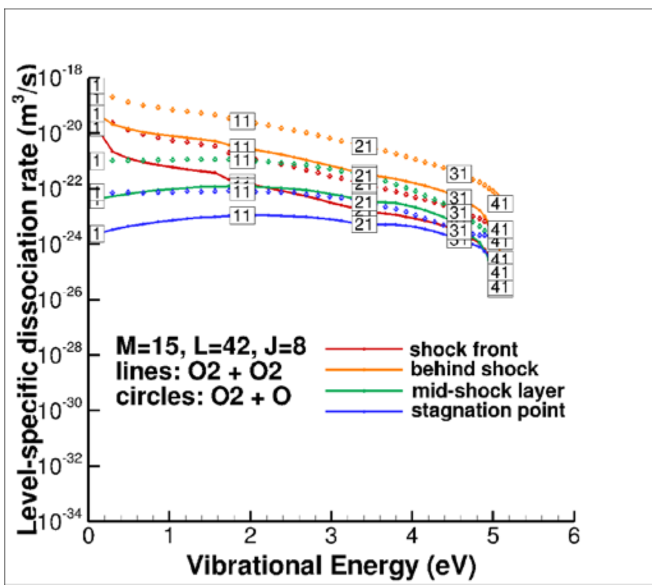
Locations for Showing Results

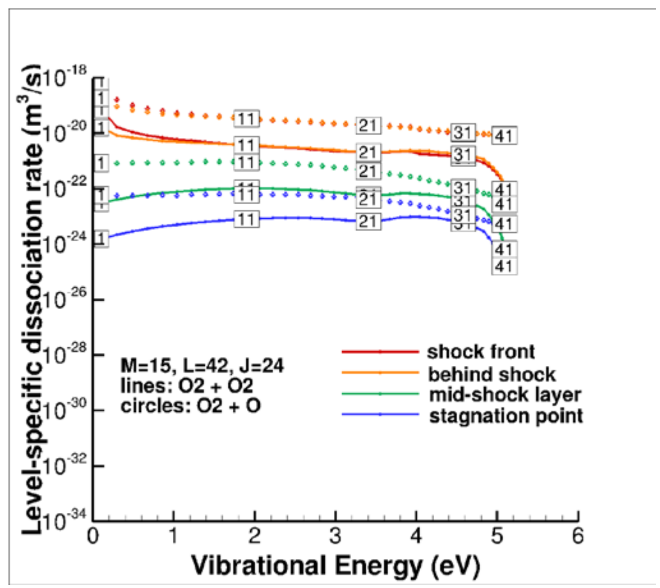


Dissociation rate Along Stagnation Streamline









Dissociation rate shows varying influence in shock layer:

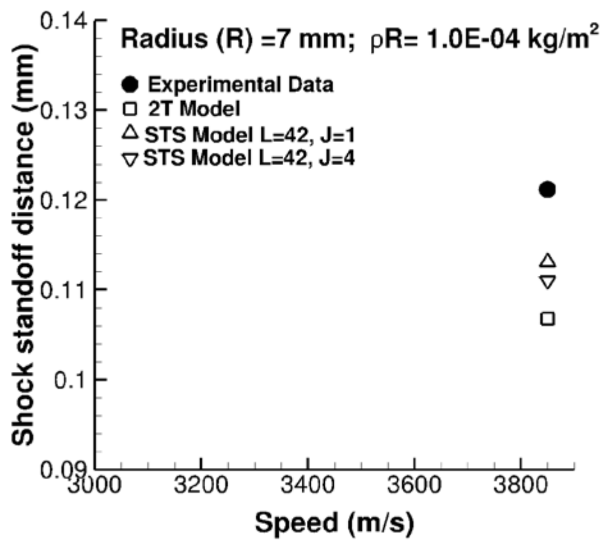
- decrease in population with increase in quantum number (behind shock)
- higher dissociation probability for molecules with higher vibrational energy (stagnation point)

Higher J increases population in upper states due to more efficient energy exchanges

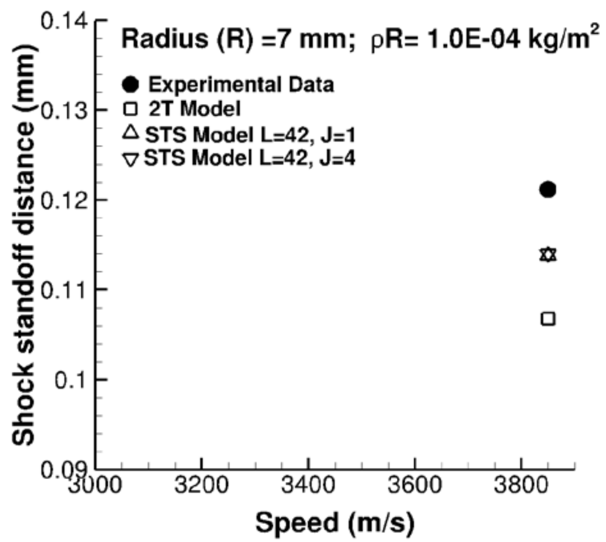
Higher dissociation rates for higher Mach number

Shock-Standoff distance for Mach 11.2 air flow past a sphere

2T and STS models without adjusting energies



2T and STS models after adjusting energies

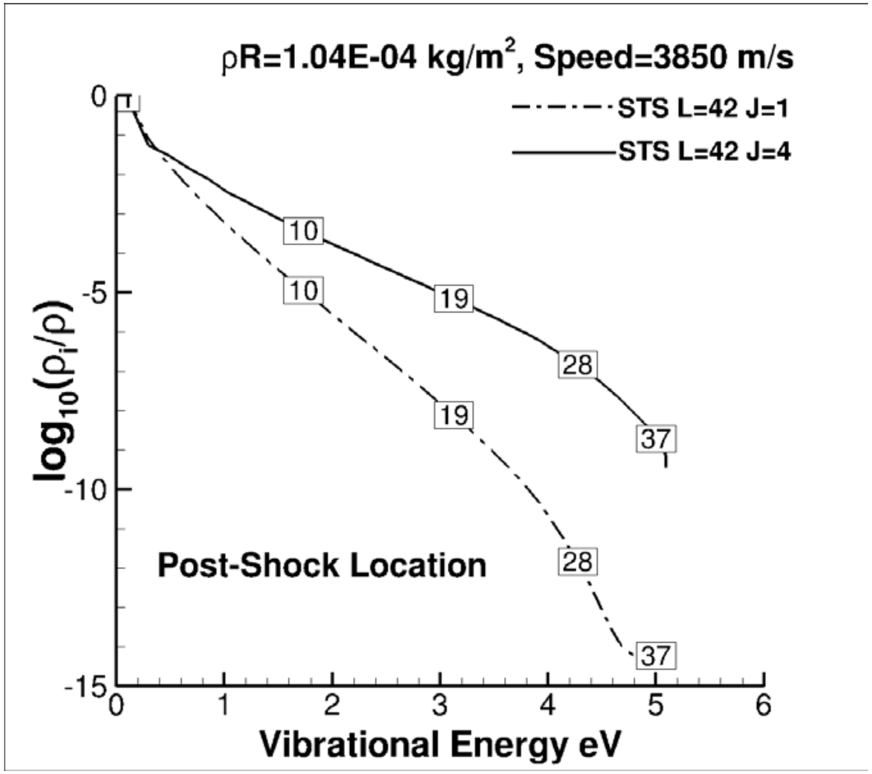


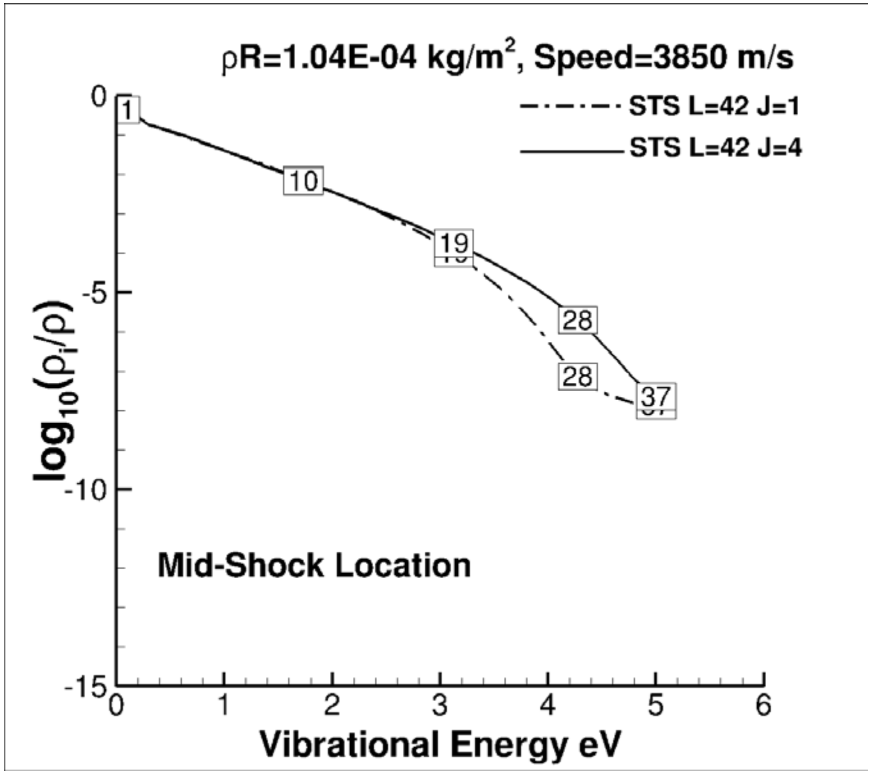
Verification of conservation of mass and vibrational energy using experimental data

STS Model more accurate than 2T Model

Multiquantum transitions have minor effect on shock-standoff distance

Population Distribution Along Stagnation Streamline In Post-Shock and Mid-Shock Layer



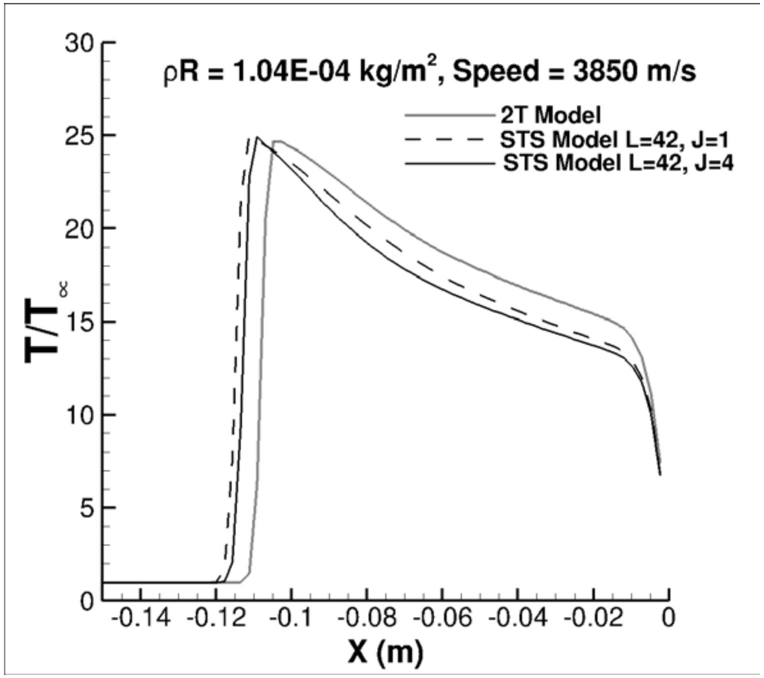


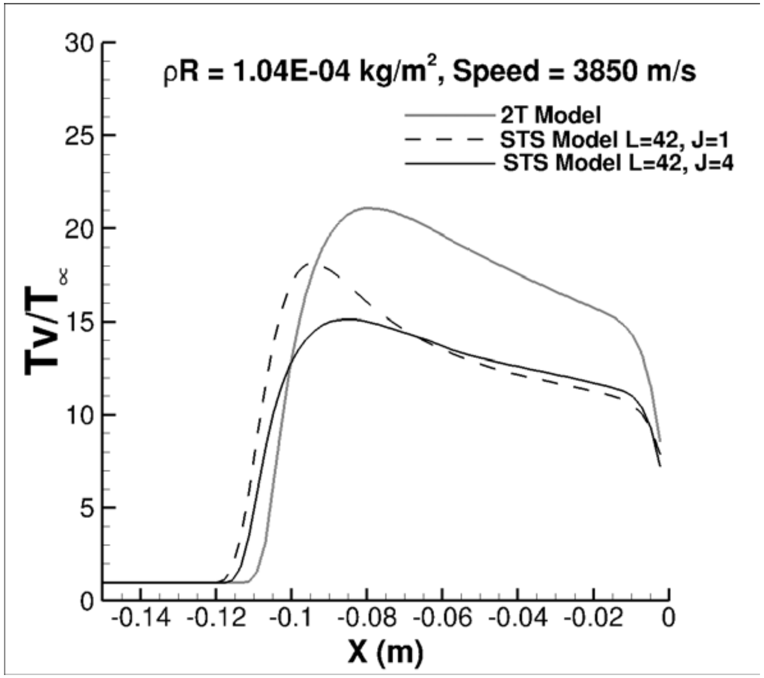
Greater non-Boltzmann distributions in the post-shock location

High J causes lower population depletion due to more efficient energy exchanges in the upper energy states

As flow velocity decreases, populations are closer to Boltzmann distributions

Temperature Distribution Along Stagnation Streamline

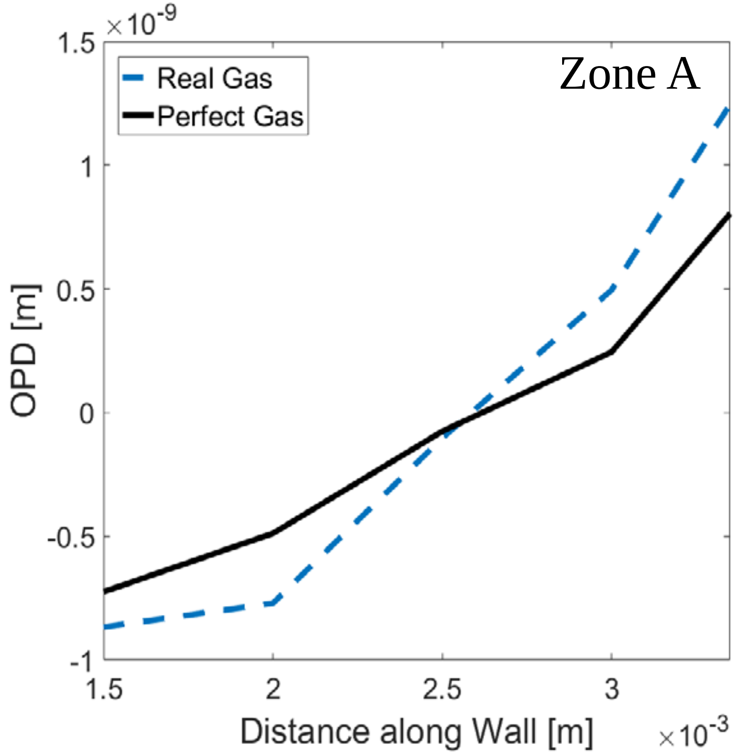


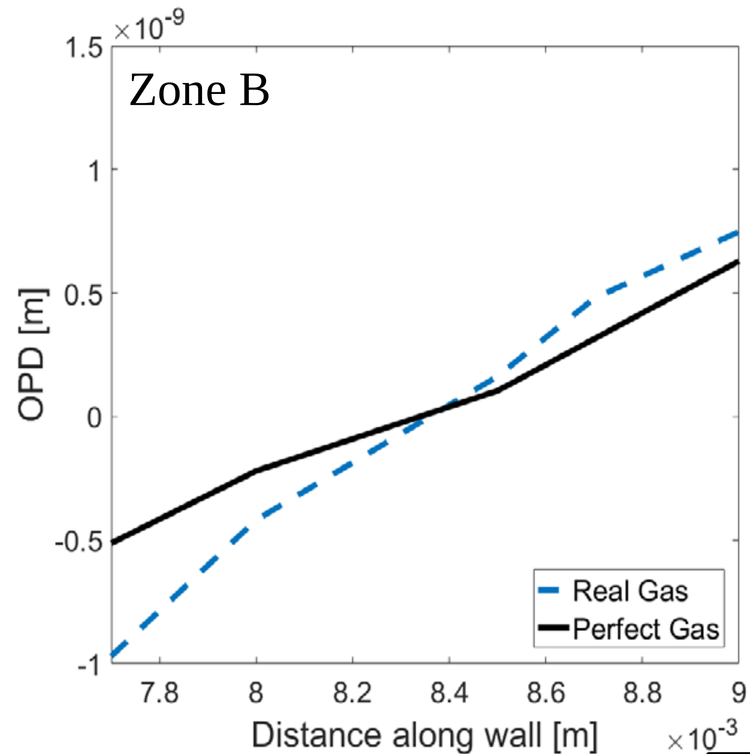


STS model has more rapid relaxation in the shock layer compared to the 2T model

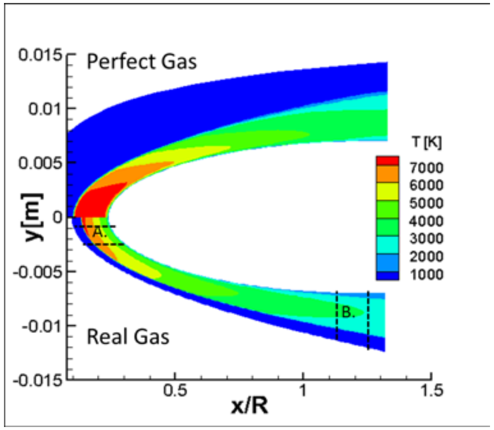
2T model has greater discrepancy with STS model in the temperature prediction in the shock layer

Effect of Non-equilibrium on OPD





Lauren Mackey



Freestream Conditions

Mach No.=11.2
P = 1200 Pa
T = 293 K
λ=500 nm

- ZONE A Real Gas OPD_{rms} 65% larger than perfect gas
- ZONE B Real Gas OPD_{rms} 44% larger than perfect gas
- Including real gas effects increases the OPD
  - More varied density profiles
  - Varied Gladstone-Dale constants

Summary

- Multiquantum transitions cause:
  - increase in population in upper energy states due to more efficient energy exchanges
  - greater dissociation results in reduced shock-stand off distance
- Monoquantum (J=1) transitions:
  - dissociation is lower as it underestimates population in intermediate and upper levels
- Dissociation rate shows opposing influence in shock layer
  - Behind shock: decrease in population with increase in quantum number
  - Stagnation point: higher dissociation probability for molecules with higher vibrational energy
- Energy reconciliation method of conserving mass and energy with STS and LT verified by comparing shock-standoff distance with experiment
- OPD predictions are dependent on accuracy of Gladstone Dale constants for the high temperature air species

Next Steps

- Continue development of AFRL ANDEE code (aerothermal nonequilibrium detailed energy exchange code)
  - State-specific transport coefficients
  - Parallelization to allow complex flows: double cone, realistic geometries
  - Reacting turbulence to assess signal distortion of turbulent flows in thermochemical nonequilibrium
- Collaborate with experimentalists to validate STS rates
- Develop automatic threshold criteria to distinguish regions with varying degree of nonequilibrium for use in reduced order models

Publications (June 2016-June 2017)

[1] Burt, J.M. and Josyula, E. , "Vibrational Nonequilibrium Quantification for State-Resolved Simulation of a Hypersonic Flow", Journal of Thermophysics and Heat Transfer, DOI: 10.25141/1.T5044, 2017

[2] Burt, J.M. and Josyula, E. , "Direct Simulation Monte Carlo Modeling of Gas Electronic Excitation for Hypersonic Sensing", Journal of Thermophysics and Heat Transfer, DOI: 10.25141/1.T5058, 2017

[3] Josyula, E., Suchyta, C.J., Vogiatzis, K., and Vedula, P., "State-to-State Kinetic Modeling of Select Air Species in Hypersonic Nonequilibrium Flows," American Institute of Aeronautics and Astronautics, AIAA 2017-3489

[4] Vogiatzis, K., Josyula, E., and Vedula, P. "Double-Cone Flows in Nonequilibrium: Comparison of CFD

with Experimental Data," American Institute of Aeronautics and Astronautics, AIAA 2017-0664

[5] Mackey, L., Boyd, I., Leger, T., Gosse, R., and Vogiatzis, K. "Effect of Hypersonic Flow Physics Modeling on Electro-Optical Sensor Assessment," American Institute of Aeronautics and Astronautics, AIAA 2017-3836

[6] Burt, J.M., and Josyula, E., "Nonequilibrium Radiation Modeling for a Low Enthalpy Hypersonic Shock Layer," American Institute of Aeronautics and Astronautics, 2015, AIAA 2015-0478

Publications (June 2016-June 2017)

[7] Josyula, E. Burt, J.M., Laporta, V., and Vedula, P., “State-to-State Kinetic Modeling of Oxygen in Hypersonic

Nonequilibrium Flows”, AIAA 2016-4316

[8] Burt, J.M., and Josyula, E., “Adaptive State Resolved Vibrational Energy Modeling for Hypersonic Flow Simulation”, AIAA 2016-4024

[9] Vogiatzis, K., Josyula, E., and Vedula, P., “Role of High Fidelity Nonequilibrium Modeling in Laminar and Turbulent Flows for High Speed ISR Missions”, AIAA 2016-4317

[10] Wang, X. and Josyula, X., “Effects of Vibrational Relaxation and Dissociation on Hypersonic Boundary-Layer Stability” AIAA 2016-3955

Technical Challenges Remaining

- PES-Based Rates: Known: N_3, O_3, In the works: N_4, O_4. Still to know: Other atom-molecule and molecule-molecule combinations in air
- Understanding validity of QCT rates
- Include electronic excited states for air species in PES and in QCT calculations
- Evaluate vibrational and chemical nonequilibrium effects on aero-optic phenomena for both laminar and turbulent cases
- Determine influence of molecular-scale gas surface interaction phenomena on window heating and surface contamination

Questions?

Budget update

Budget

6.1(LRIR 15RQCOR192)

AFOSR PO: I. Leyva

FY15	FY16	FY17	Total
275K	280K	285K	840K

- In-house Research Contractors
  - Lauren Mackey
  - Casimir Suchyta
  - K. Vogiatzis
- Summer Researchers
  - Iain Boyd (Michigan)
  - Prakash Vedula (Oklahoma)
- Expected to obligate funds by end of FY