Computational Modeling of Hypersonic Nonequilibrium Gas and Surface Interactions

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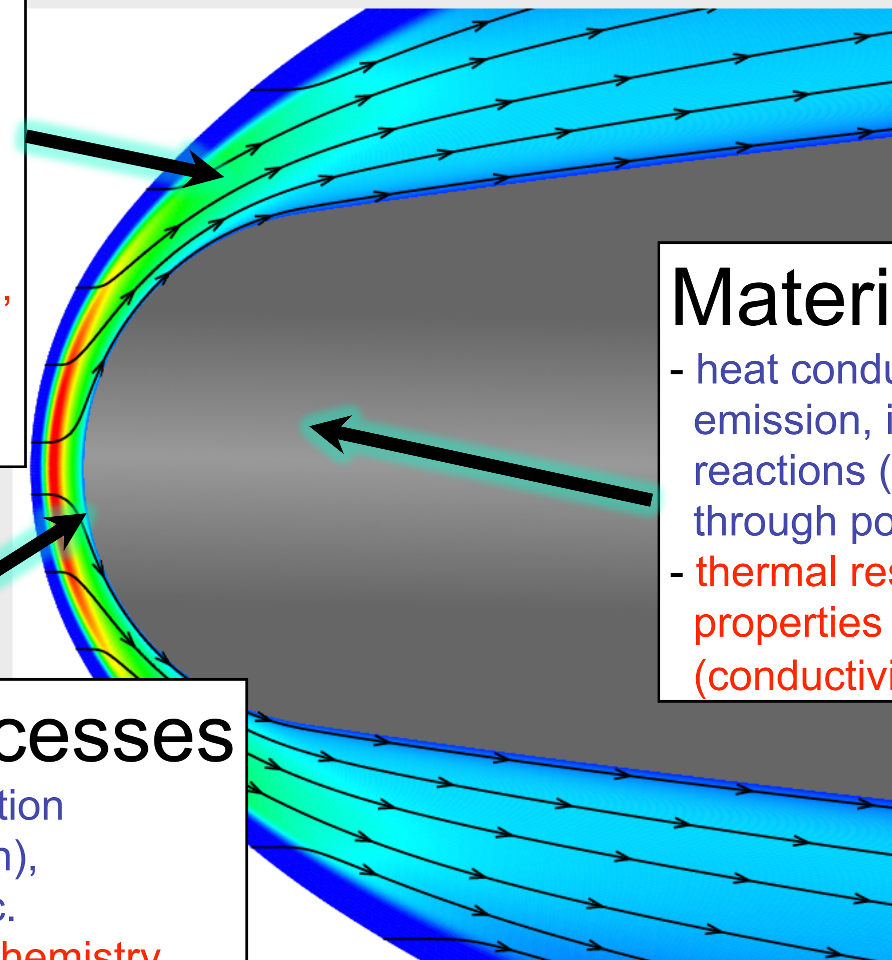
Hypersonic Vehicle Analysis



Gas Phase

- strong shocks, thermochemical nonequilibrium, boundary layer, etc.
- CFD, relaxation times, Arrhenius rate coefficients with two-temperature model

Material Response

- heat conduction, radiative emission, internal chemical reactions (pyrolysis), gas flow through porous media, etc.
- thermal response model, physical properties of complex materials (conductivity, emissivity…)

Surface Processes

- accommodation, ablation (oxidation, sublimation), catalysis, melting, etc.
- coefficients, surface chemistry mechanism and rates

Project Goals

- Nonequilibrium gas-phase processes:
  - use computational chemistry and Master Equation analysis to perform detailed studies of:
    - thermal relaxation processes (T-R-V)
    - chemical processes (dissociation, exchange)
  - develop reduced order models for use in CFD
- Nonequilibrium gas-surface processes:
  - use coupled CFD-surface chemistry-material response tools to study gas-surface interactions (e.g., catalysis, ablation)
  - assess models using experimental data (flow and surface) generated in high-enthalpy facility (Fletcher, Univ. Vermont)

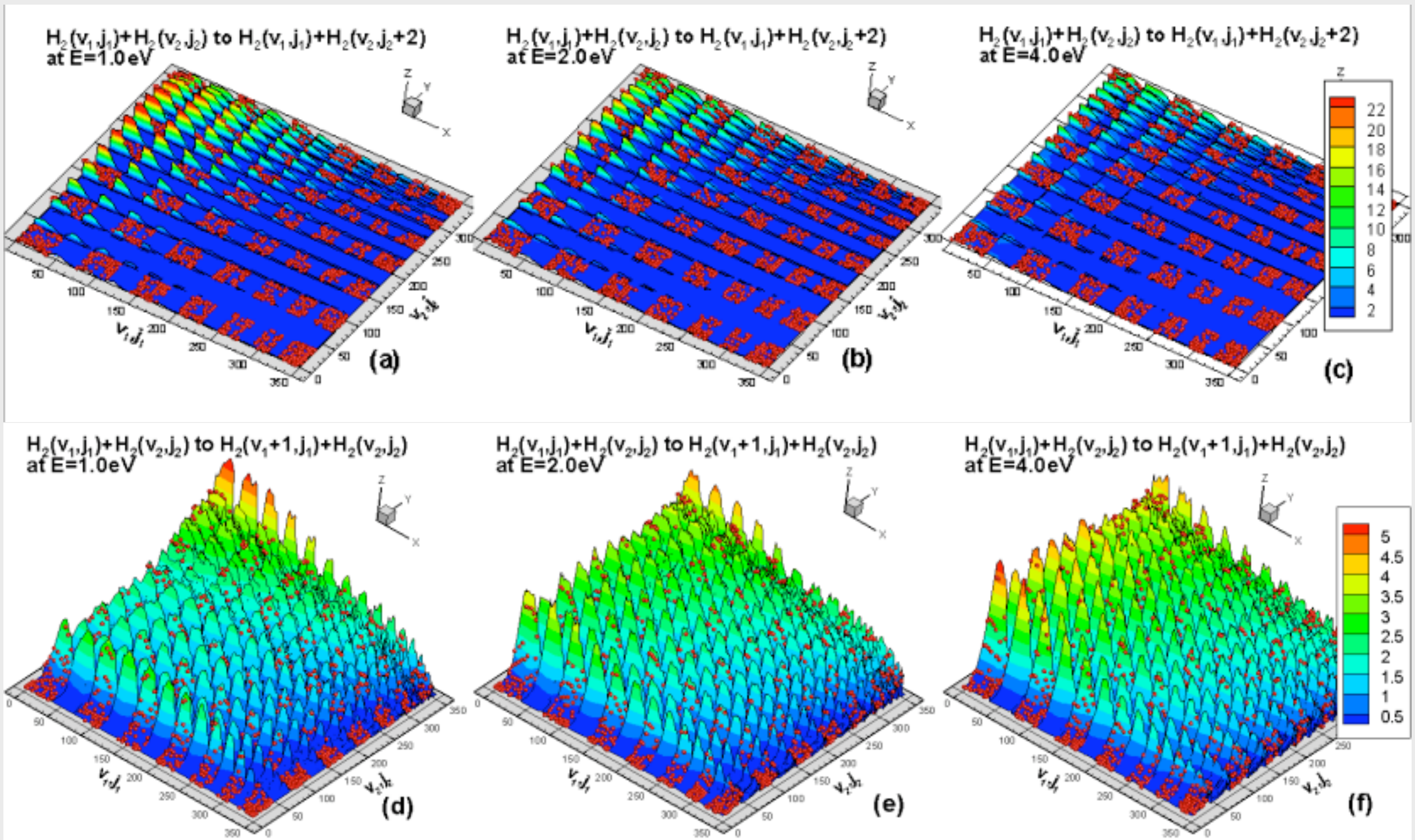
Gas Phase Studies: Technical Approach

- State-to-state transition cross sections and rate coefficients:
  - compute data for all ro–vibrational states, e.g. using QCT
  - reduce the number of state-to-state transition rates evaluated using a response surface design technique (Kriging)

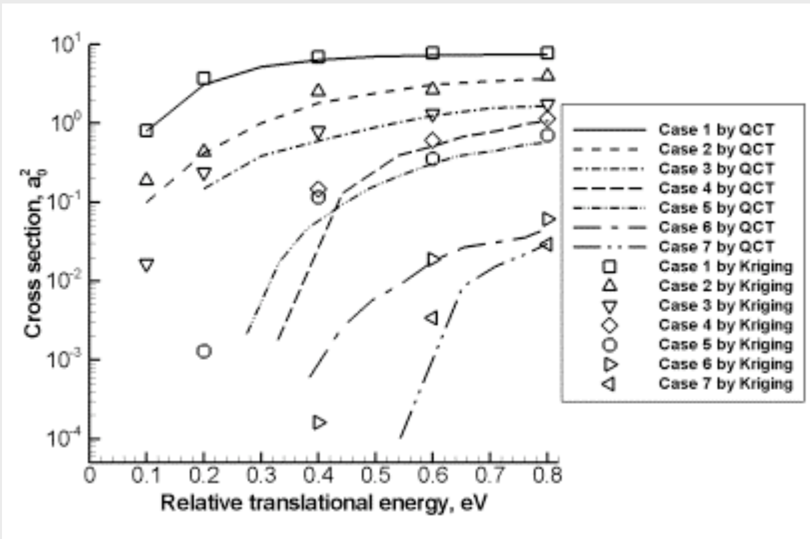
- Master Equation (ME) analysis of thermochemical relaxation:
  - constructed using complete sets of state-resolved transition rates for bound-bound and bound-free processes
  - compare results with existing measurements
  - use results to develop reduced-order thermochemistry models that can be implemented in CFD

Results:
Bound-Bound H_2 Transitions

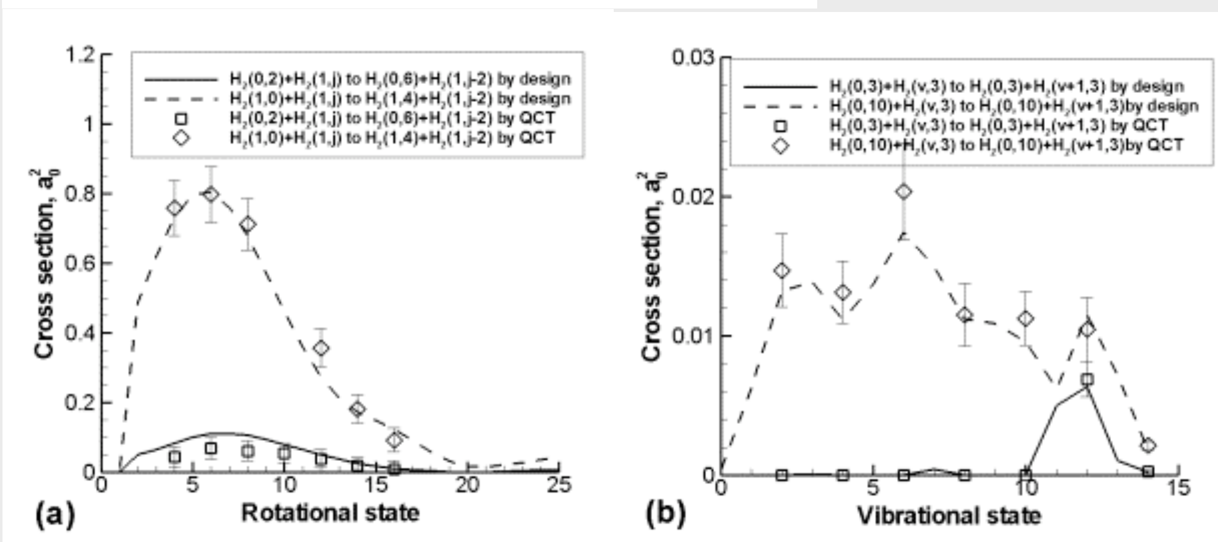
State-to-state cross sections obtained using response surface design method



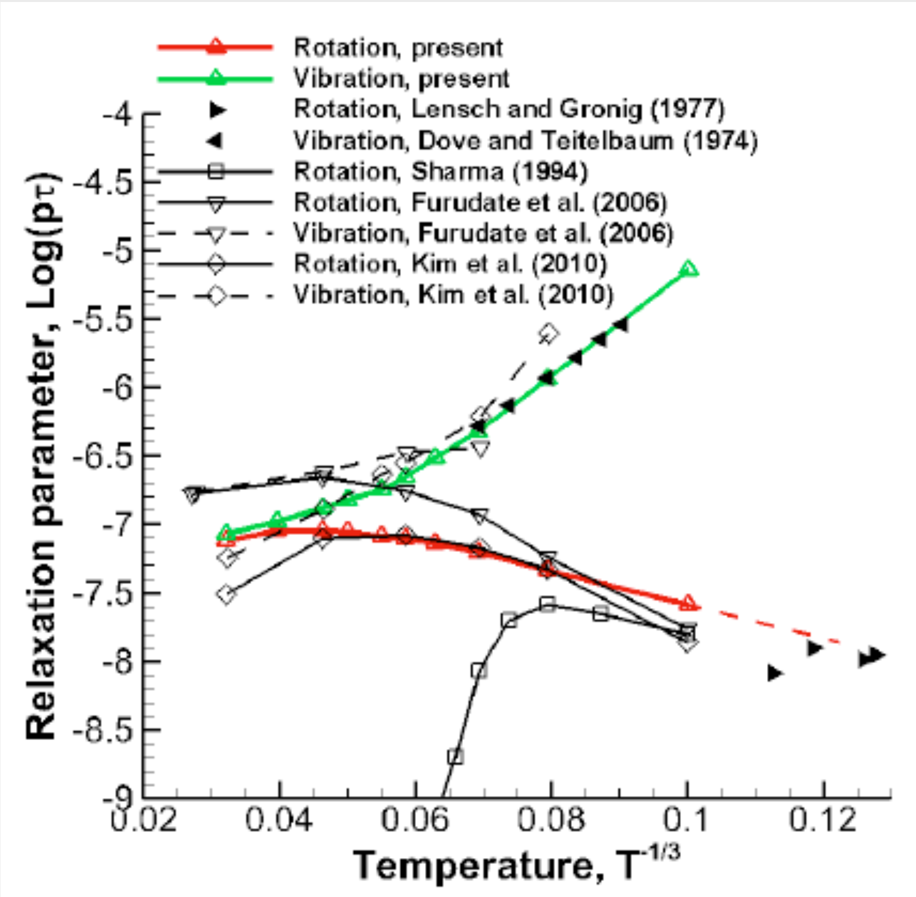
Results: Bound-Bound H_2 Transitions



State-to-state cross sections obtained using response surface design method calibrated using a small number of QCT evaluations (1,800 instead of 60,000!)



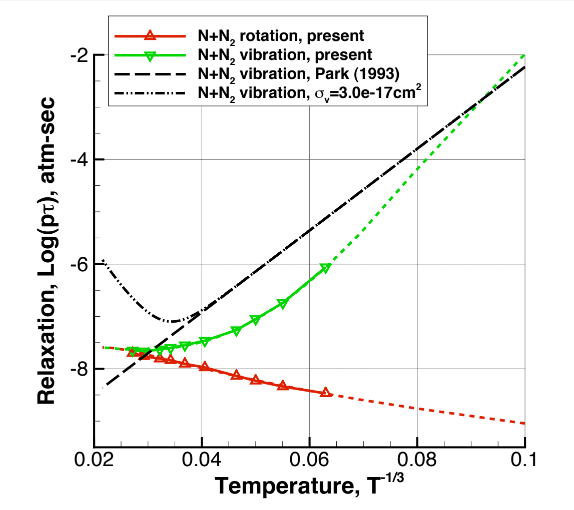
Results: H_2 Thermal Relaxation



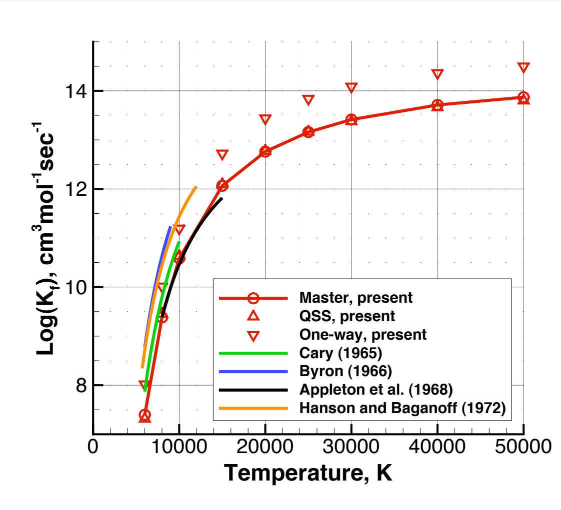
- Global relaxation parameters of the rotational and vibrational modes for H_2+H_2
- Rotational and vibrational relaxation times become similar at high temperature
- Technical details: Kim & Boyd, AIAA-2012-0362, Jan. 2012.

Analysis of N_2-N: Heat Bath Studies

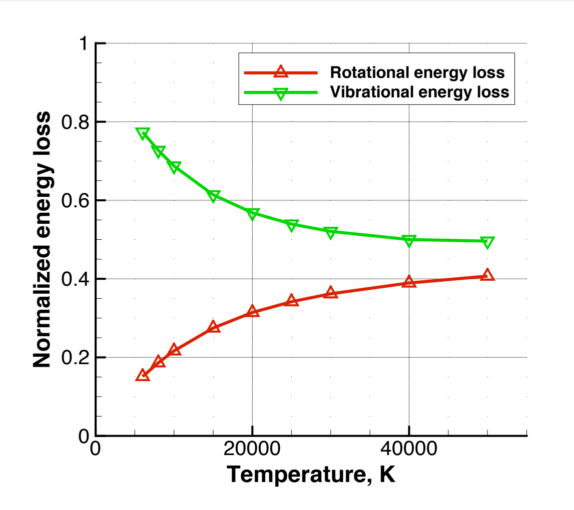
- State-to-state transition cross sections and rate coefficients:
  - use database of cross sections computed by Jaffe et al, NASA ARC
  - ME analysis involves solution of 9,390 equations
  - technical details: Kim & Boyd, AIAA-2012-2991, June 2012



Thermal Relaxation Parameters



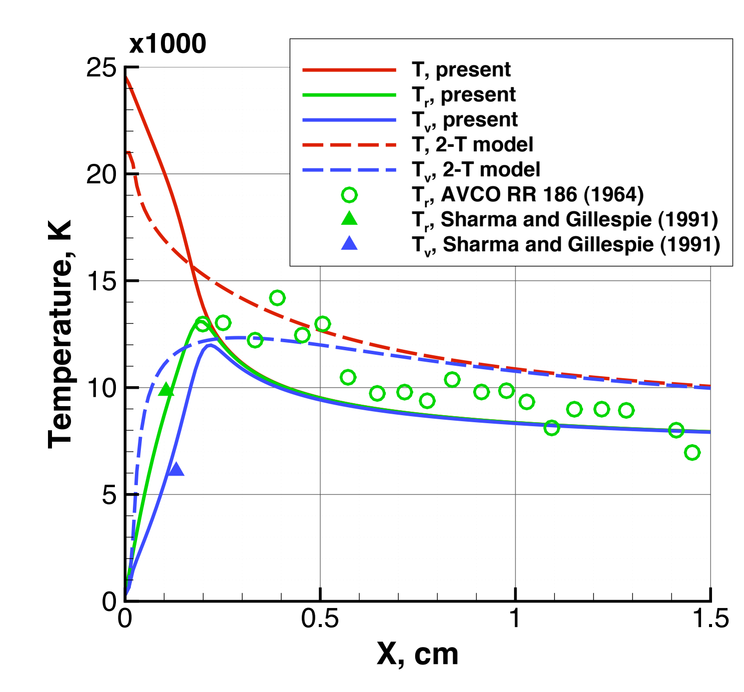
Chemical Reaction Rates



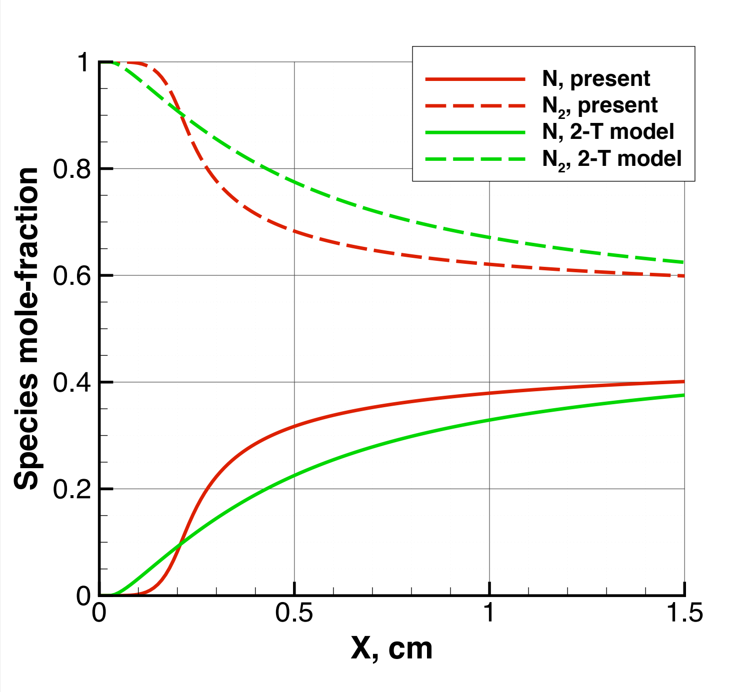
Energy Removal Due to Chemistry

Analysis of N_2-N: Shock Tube Studies

- One-dimensional flow equations combined with Master Equation:
  - N_2-N_2 included macroscopically using standard models
  - applied to experiment of AVCO / Sharma
  - technical details: Kim & Boyd, AIAA-2012-2991, June 2012



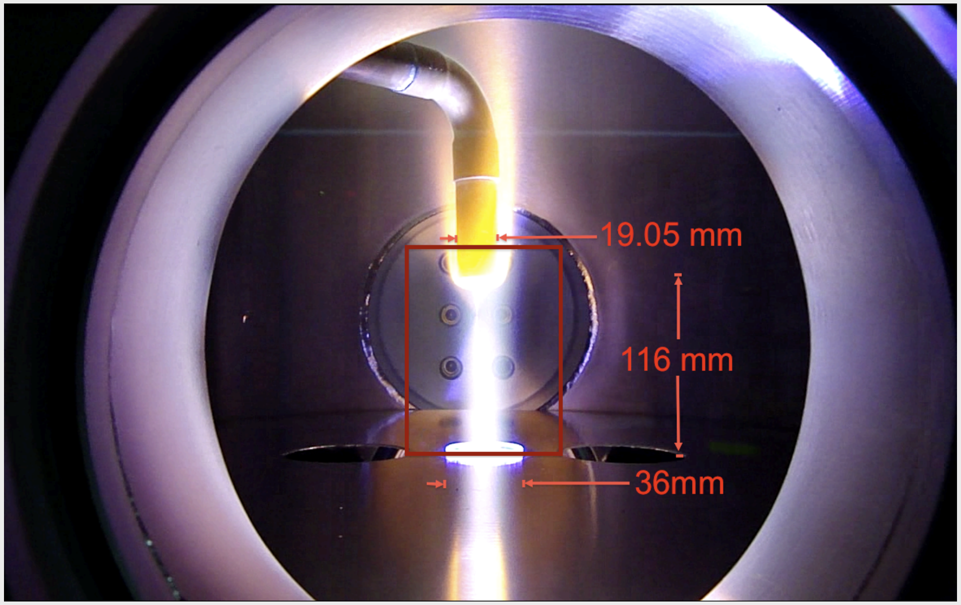
Temperature Profiles



Species Profiles

Gas-Surface Interactions: Assessment of Computations

- Collaboration with Prof. Doug Fletcher (UVM):
  - 30 kW Inductively Coupled Plasma (ICP) Torch Facility
- Samples exposed to high enthalpy gas flows
- Flow quantities measured using two-photon LIF:
  - N-atom number density
  - translational temperature
- Surface temperature and sample ablation also quantified



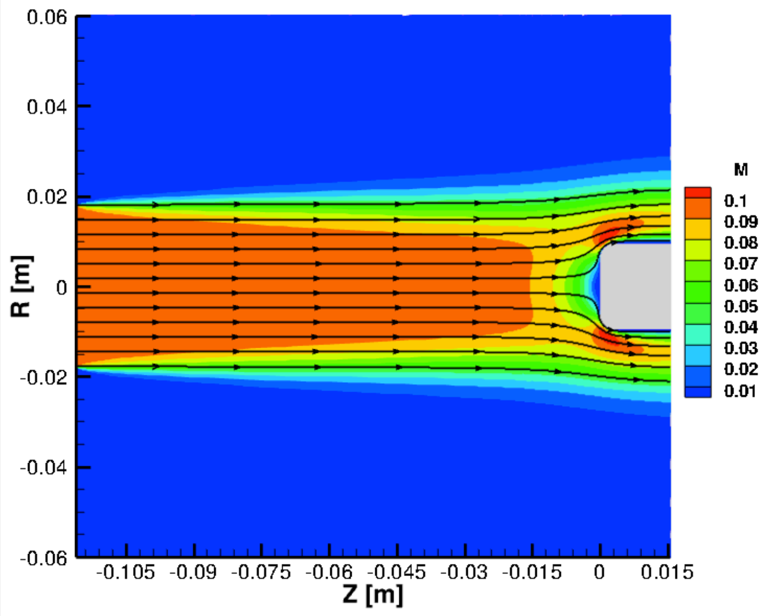
Graphite sample in nitrogen flow
(section in box is the portion simulated)
Source: Prof. D.G. Fletcher

Gas-Surface Interactions: Conditions Investigated

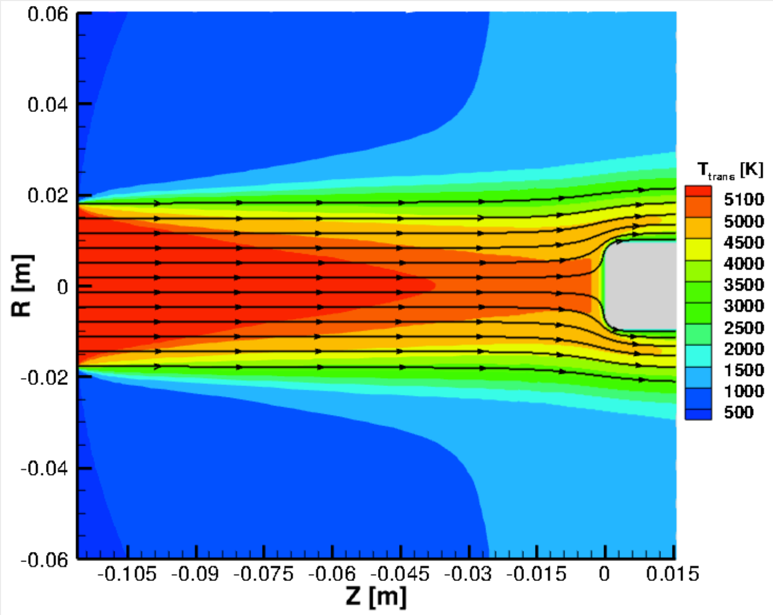
Free Stream:

Mass flow rate [kg/s]	*Temperature T_∞ [K]*	*Pressure [kPa]*	*Wall temperature T_w [K]*
0.001	5133	12	1590

Progress: subsonic inlet/outlet BCs added to LeMANS
sensitivity to various thermochemistry models



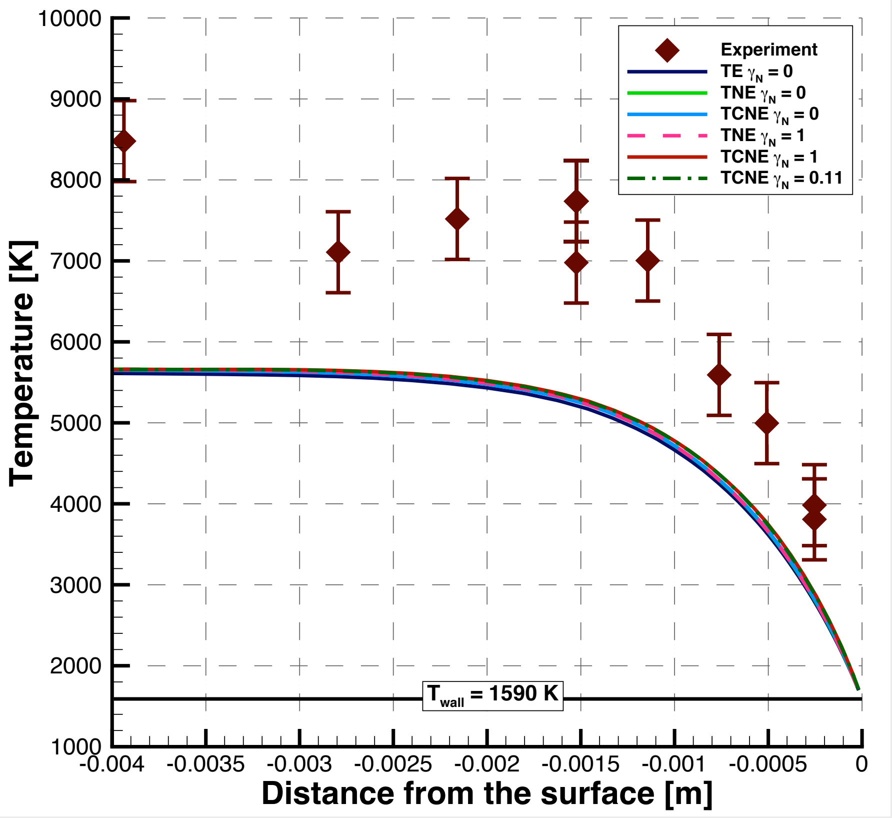
Mach number



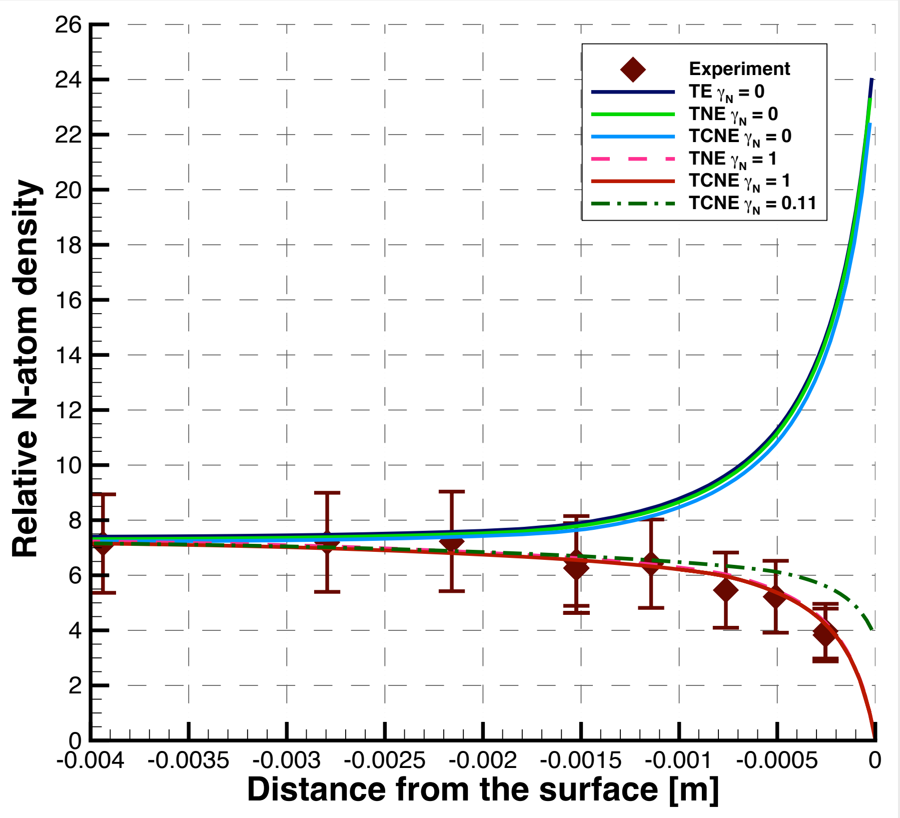
Translational temperature

Gas-Surface Interactions: Comparisons with Experiment

Comparisons along the stagnation streamline



Translational temperature



Relative N-atom density

Future Plans

- Nonequilibrium gas-phase processes:
  - develop T-R-V relaxation models for CFD from ME results
  - high fidelity CFD chemical reaction models including rotational mode will also be developed from ME analysis
  - continue analysis for other important air interactions
  - evaluation using existing experimental data sets

- Nonequilibrium gas-surface processes:
  - compare surface chemistry models (catalytic recombination, finite rate chemistry module of MacLean & Marschall)
  - model surface recession (material response code: MOPAR)
  - study sensitivity to gas-thermochemistry rates and models
  - assess modeling using Univ. Vermont experimental measurements of flow field properties and sample mass loss

Technical Challenges

- Nonequilibrium gas-phase processes:
  - large number of different air species interactions (N_2-M, O_2-M, NO-M, etc.)
  - fidelity required from computational chemistry?
  - Master Equation analysis becoming expensive
  - lack of modern, validation quality, experimental data
- Nonequilibrium gas-surface processes:
  - isolating contributions of competing mechanisms to effects observed (e.g. flow processes, catalysis, ablation)
  - uncertainties in facility operation (e.g. ICP exit conditions)

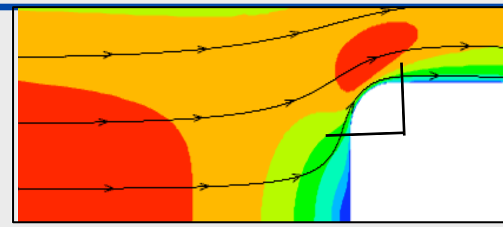
Technical Approach: Computational Tools

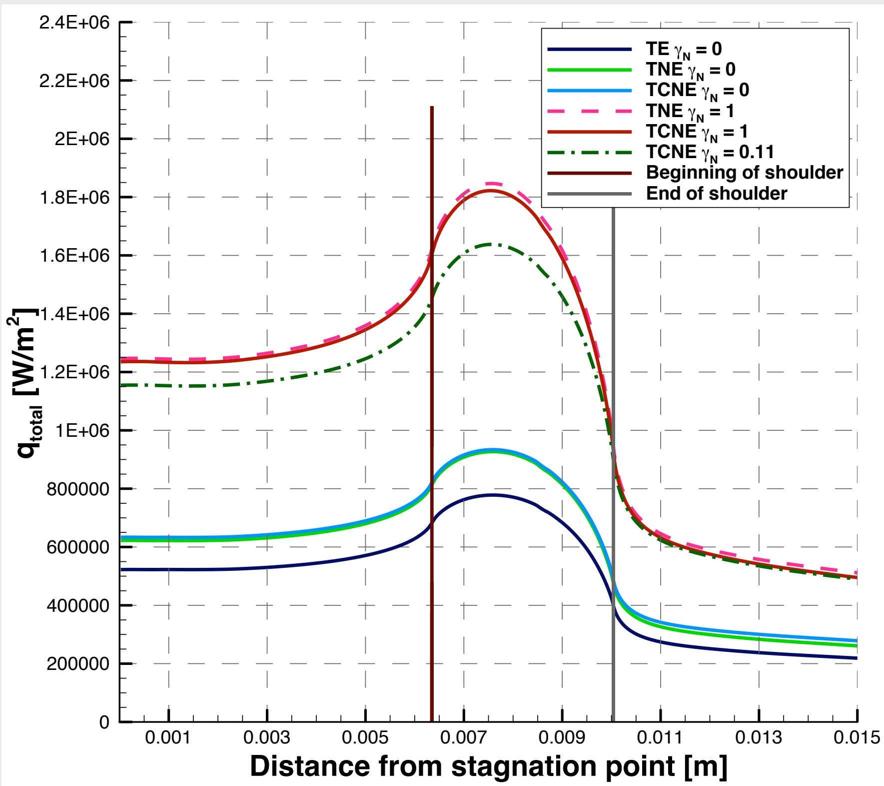
- LeMANS
  (Scalabrin and Boyd: AIAA-2006-3773)
  - Navier-Stokes CFD code
  - finite volume FVS
  - implicit time integration (point/line)
  - 2D/3D unstructured mesh
  - parallel, domain decomposition
  - finite rate thermo-chemical nonequilibrium effects
  - validated for hypersonic flow using experiments, codes

- MOPAR
  (Martin and Boyd: AIAA-2009-3597)
  - material response code
  - control volume finite element (CVFEM)
  - quasi-1D
  - pyrolyzing/non-pyrolyzing ablators
  - momentum conservation through Darcy's Law (or Forcheimer's Law)
  - moving boundaries
  - has been coupled to LeMANS

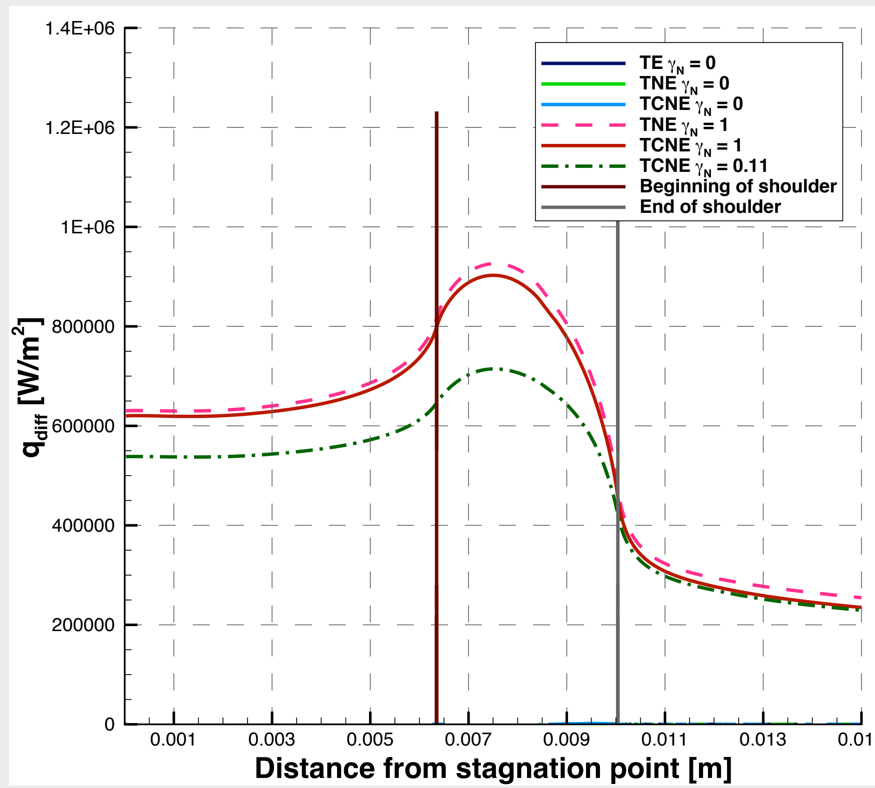
Results: Surface Properties

Total Heat flux = (Translational + Vibrational) convective heat flux + Diffusive heat flux





Total heat flux



Diffusive heat flux