Computational Modeling of Hypersonic Nonequilibrium Gas and Surface Interactions

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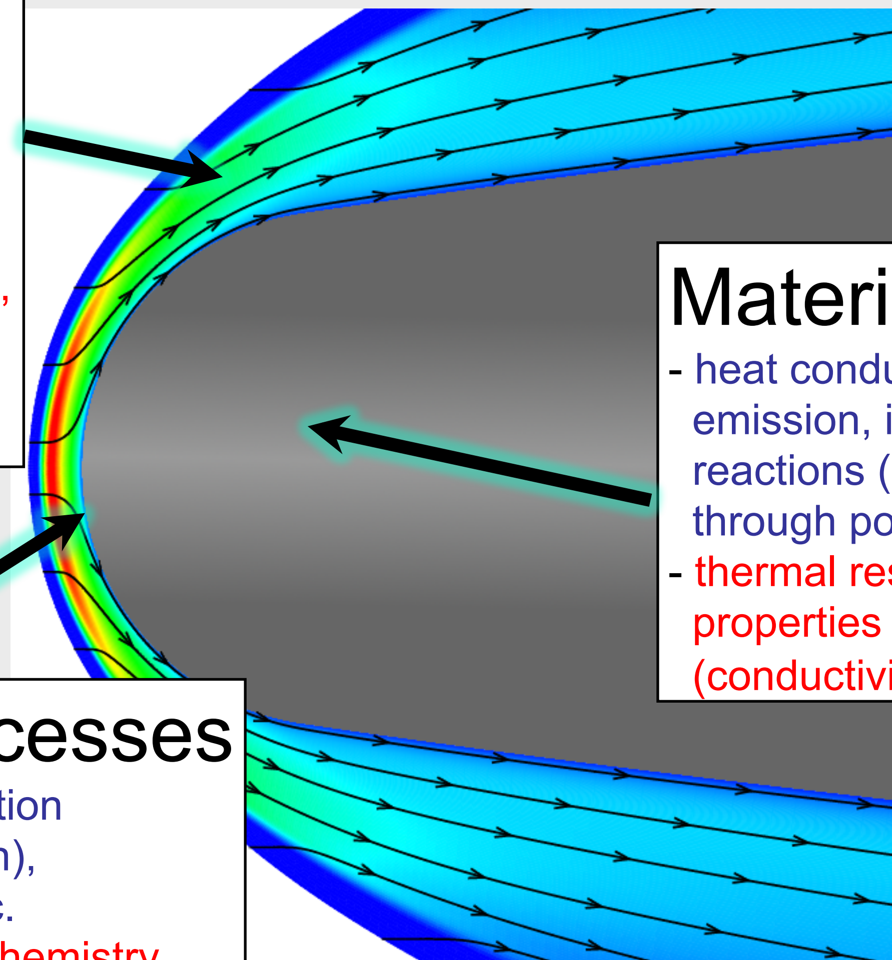
Hypersonic Vehicle Analysis

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 high-fidelity modeling (computational chemistry, Master Equation analysis) to perform detailed studies of:
    - thermal relaxation processes (T-R-V-E)
    - chemical processes (dissociation, exchange)
  - Assess models using experimental data
- 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-resolved analysis:
  - Go well beyond state-of-the-art 2-temperature modeling
  - FY12: ro–vibrational states of H_2 and N_2
  - FY13: extend to electronic states of N_2 and N
- Master Equation 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 codes

Thermochemistry: Two-Temperature Model (2-T)

- Energy pools of high temperature nitrogen (N_2, N, N_2^+, N^+, E^-):

Trans-rotational energy

$E_{trot}(T)$

E_{tr_N} $E_{tr_{N^+}}$ $E_{r_{N_2}}$

$E_{tr_{N_2}}$ $E_{tr_{N_2^+}}$ $E_{r_{N_2^+}}$

Electron-electronic-vibrational energy

E_e E_{ex_N} $E_{v_{N_2}}$

$E_{ex_{N_2}}$ $E_{v_{N_2^+}}$

$E_{eev}(T_{eev})$

- Nonequilibrium thermochemistry:
  a. Translational-rotational equilibrium
  b. Landau-Teller equation for vibrational relaxation
  c. Arrhenius rates evaluated using geometrically averaged temperature
  d. Chemical reactions:
     - Electron and heavy-particle impact dissociation
     - Electron impact ionization
     - Associative ionization
     - Charge exchange

Thermochemistry: Four-Temperature Model (4-T)

- Energy pools:

Translational energy: $E_{tr}(T)$ — E_{tr_N}, $E_{tr_{N^+}}$, $E_{tr_{N_2}}$, $E_{tr_{N_2^+}}$

Rotational energy: $E_r(T_r)$ — $E_{r_{N_2}}$, $E_{r_{N_2^+}}$

Vibrational energy: $E_v(T_v)$ — $E_{v_{N_2}}$, $E_{v_{N_2^+}}$

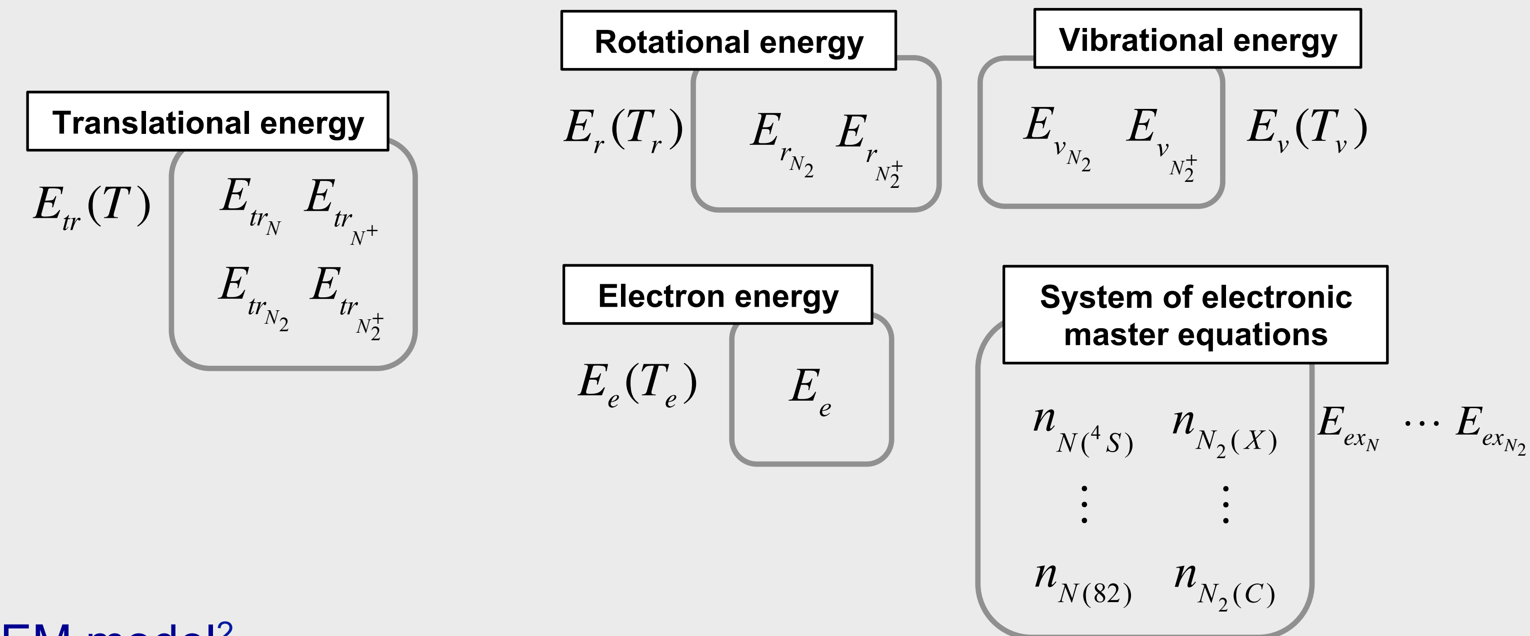
Electron-electronic energy: $E_{ee}(T_{ee})$ — E_e, E_{ex_N}, $E_{ex_{N_2}}$

- Rotational nonequilibrium[1]:
    a. Widely used Parker R-T model (1959)
    b. Modified Park model:
        - R-T relaxation time of Park (2004)
        - R-V energy transfer model of Kim & Boyd (2013)
        - Rotational-vibrational-translational (R-V-T) energy transfer of N_2+N by coupling the system of master equations with ro-vibrational state-to-state transition rates from NASA ARC (2008, 2009)

[1]Kim & Boyd, Chemical Physics, Vol. 415, 2013

Electronic Master Equation Model (EM)

- Energy pools:



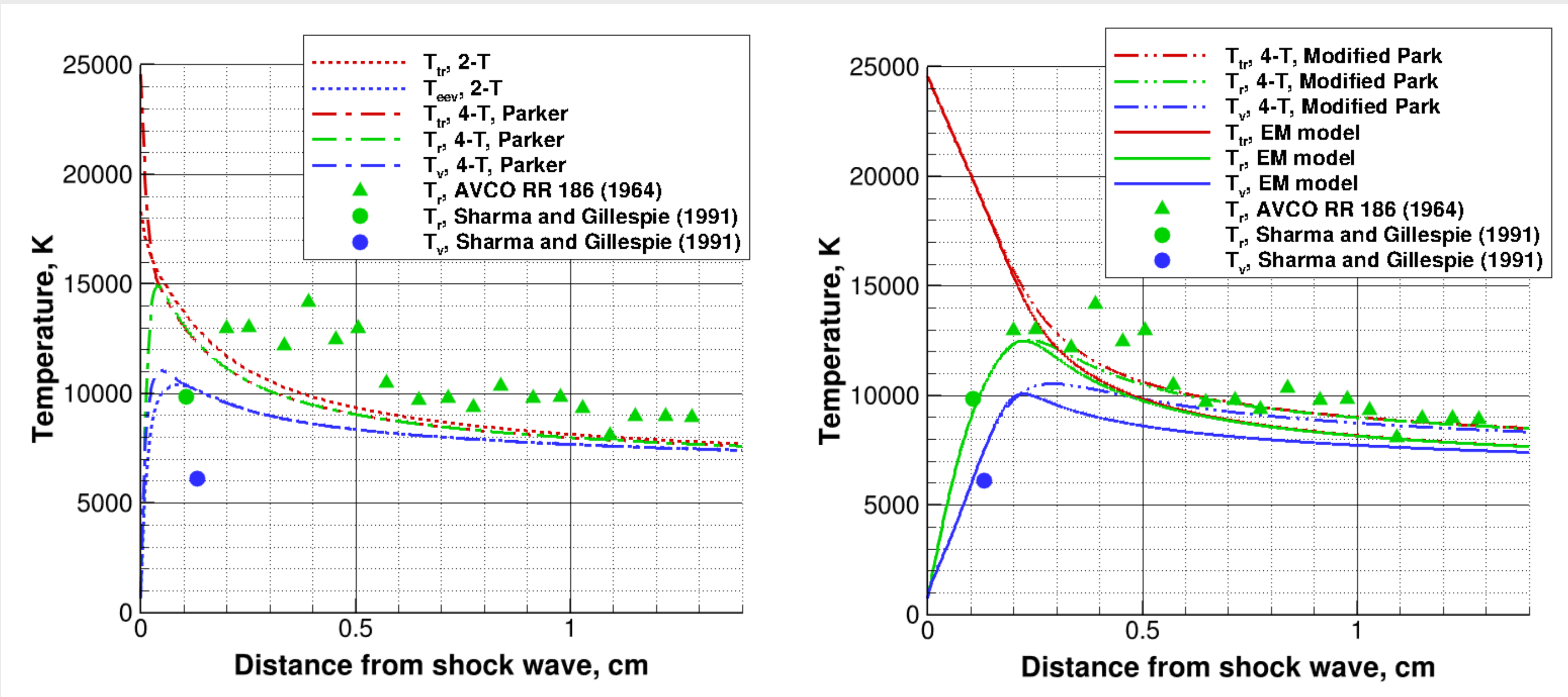
- EM model[2]
  a. Rotational nonequilibrium described by modified Park model
  b. Nonequilibrium populations of electronic states determined by solving system of electronic master equations
  c. Electronic master equations include radiative transitions from both electron and heavy-particle impacts

[2]Kim & Boyd, AIAA Paper 2013-3150, June 2013

Shock-Tube Analysis:
Nitrogen, 6.2 km/s

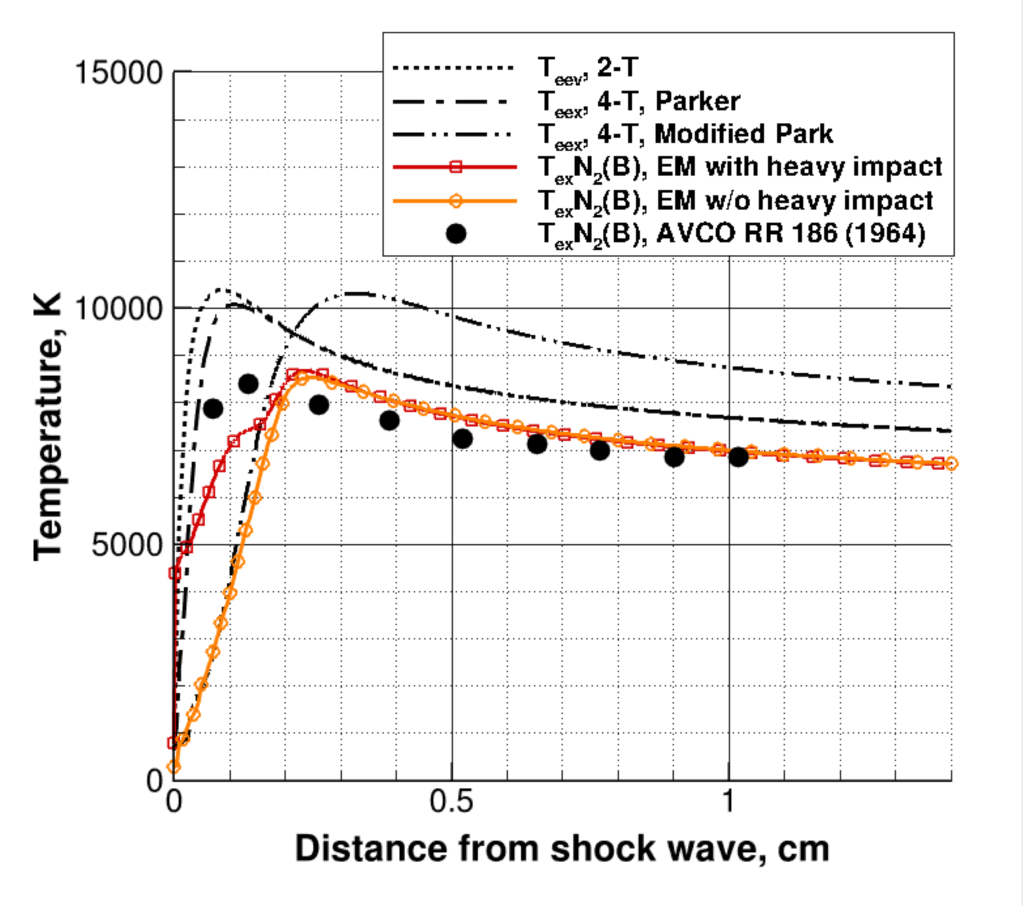
Electric-arc driven shock-tube experiments by AVCO (1964) and by Sharma and Gillespie at NASA ARC (1991):
- p=1.0 Torr, V=6.2 km/sec, $N_2(2+)$ band

- Translational, rotational, and vibrational temperatures



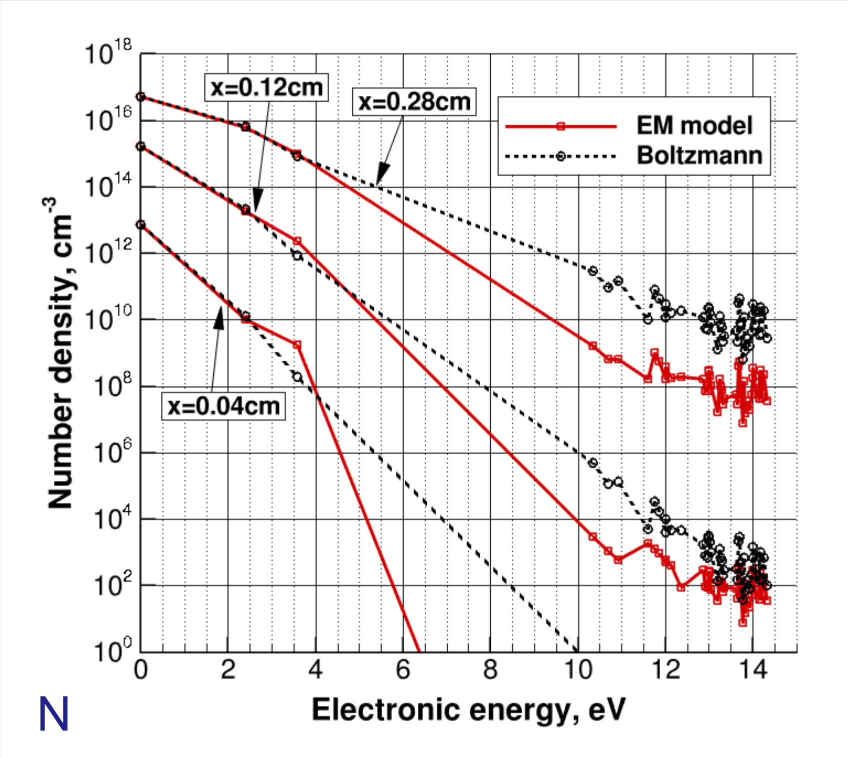
Shock-Tube Analysis:
Nitrogen, 6.2 km/s

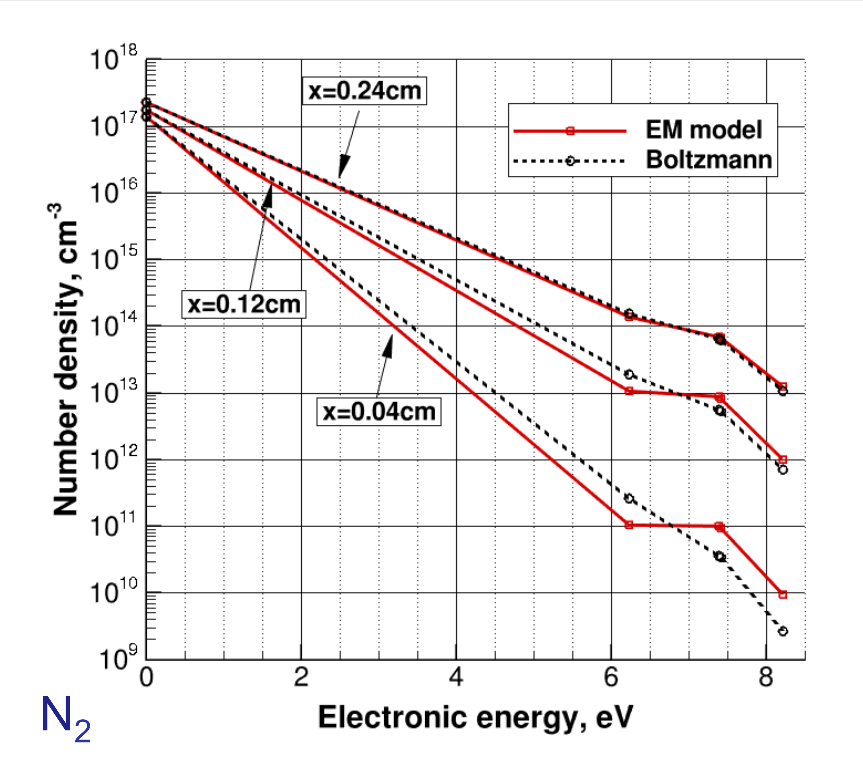
- Electronic temperature of $N_2(B^3\Pi_g)$



Shock-Tube Analysis:
Nitrogen, 6.2 km/s

- Electronic state populations of N and N_2 from EM Model



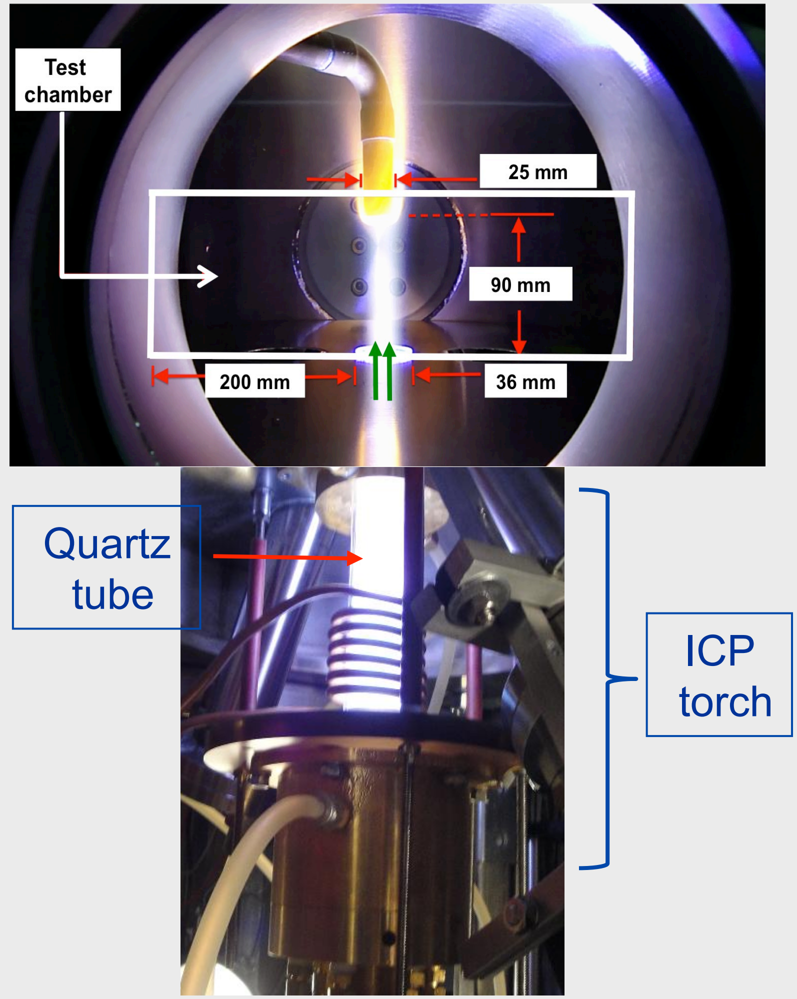


Gas-Surface Studies: Technical Approach

- External flow:
  - High-enthalpy flow CFD code with 2-T nitrogen thermochemistry (LeMANS)
- Surface chemistry:
  - Finite rate module (Marschall & McLean)
  - Implemented as a boundary condition in LeMANS
  - Catalysis and nitridation (ablation)
- Material response:
  - 2D code (MOPAR)
  - Communicates with LeMANS via surface chemistry module
  - POCO graphite grade DFP2

Gas-Surface Interactions: Assessment of Modeling

- 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:
  - Relative N-atom number density
  - Translational temperature
- Surface temperature, heat flux, and ablation rate also measured



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

Gas-Surface Interactions: Conditions Investigated

Flow exiting ICP:

Mass flow rate [kg/s]	*Temperature T_∞ [K]*	*Pressure [kPa]*	*Wall temperature T_w [K]*
0.82×10^{-3}	7000	21.3	1598

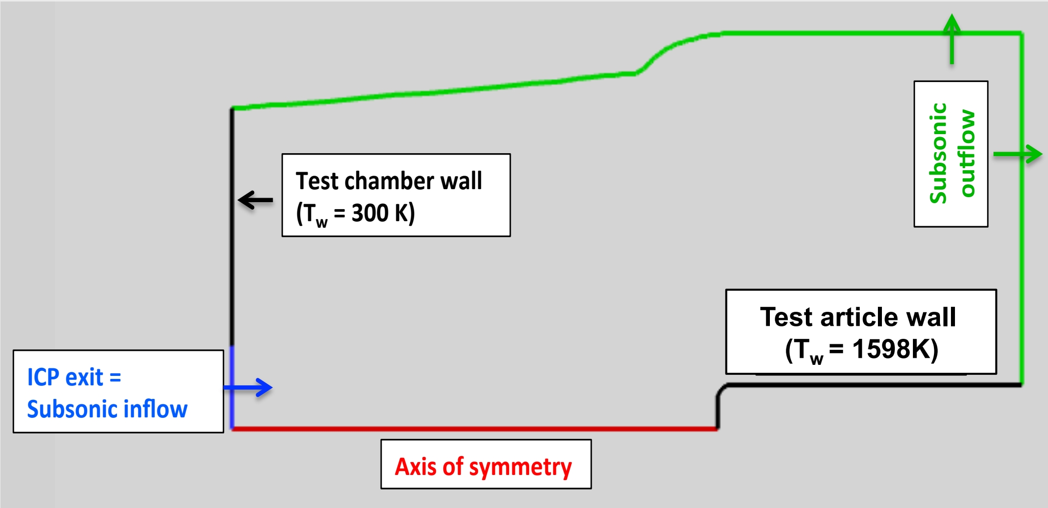
- Exit chemical composition calculated using:

(i) *Chemical Equilibrium with Applications (CEA)*

(ii) $Power = \dot{m}\Delta h$

$$\Delta h = \sum_{i=N,N_2} Y_i \int_{298}^{T} C_{pi}\, dT + \sum_{i=N,N_2} Y_i \Delta h^{\circ}_{fi}$$

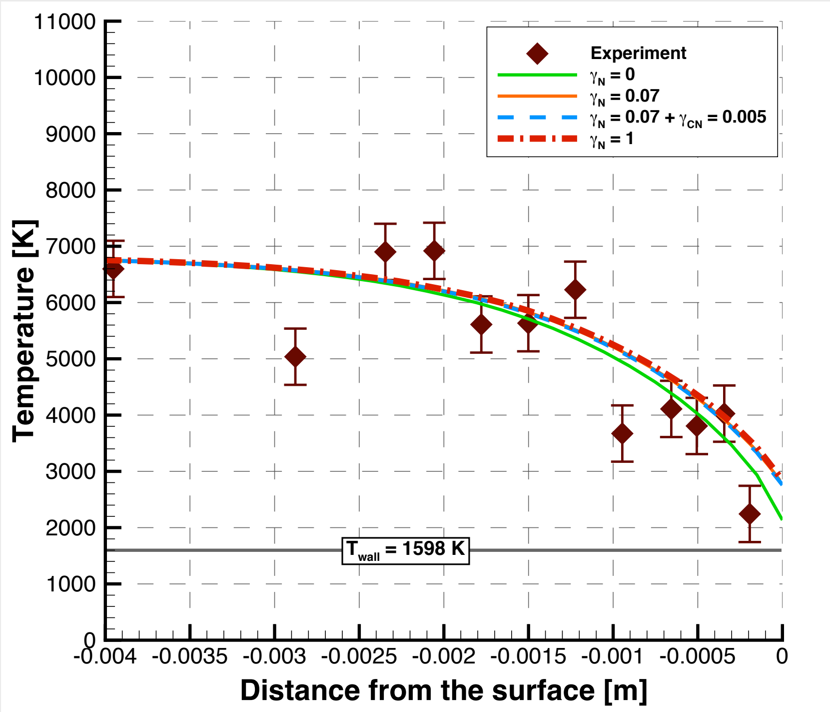
$$Inlet\ Power \approx 13.8kW$$



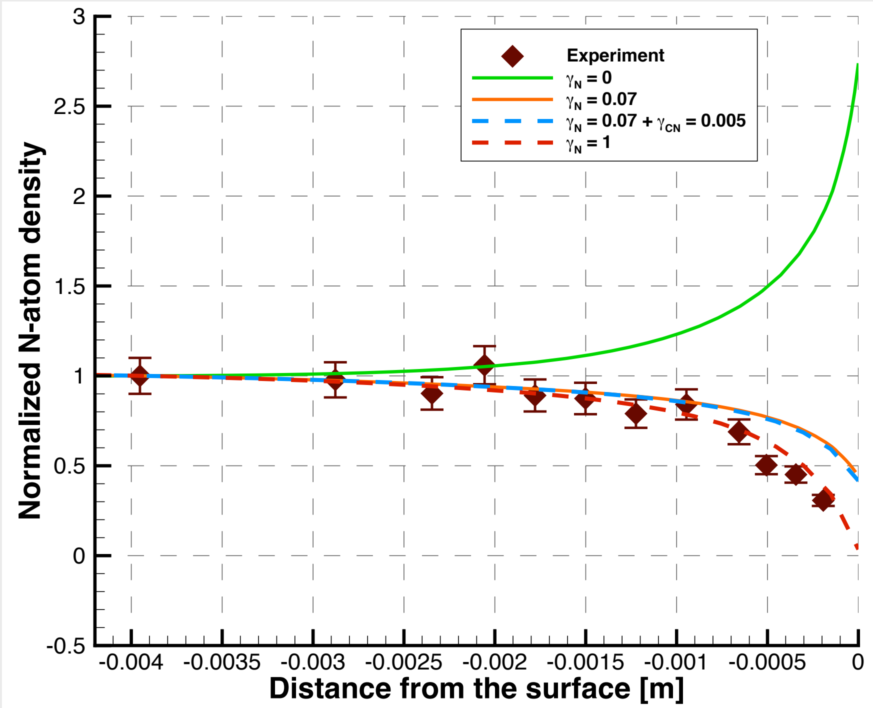
Boundary conditions

Gas-Surface Interactions: Flow Properties

Comparisons along the stagnation streamline for CEA composition

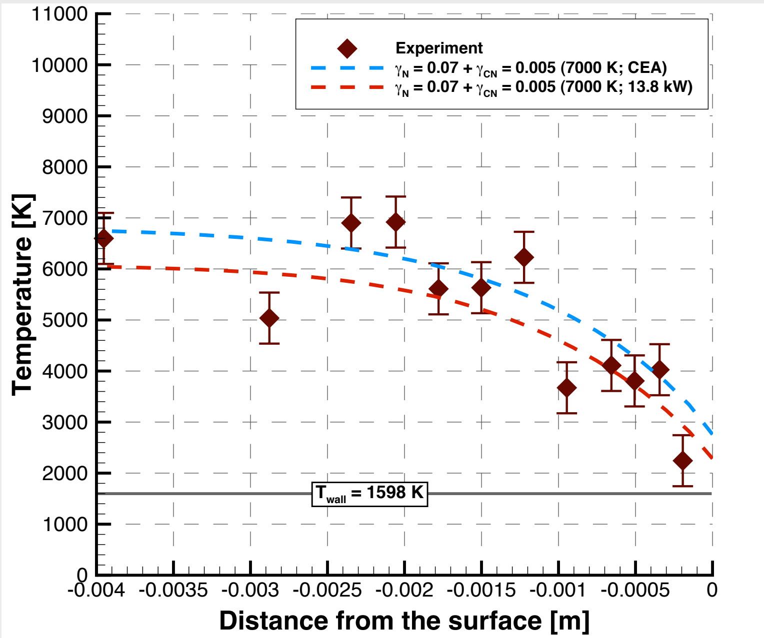


Translational temperature

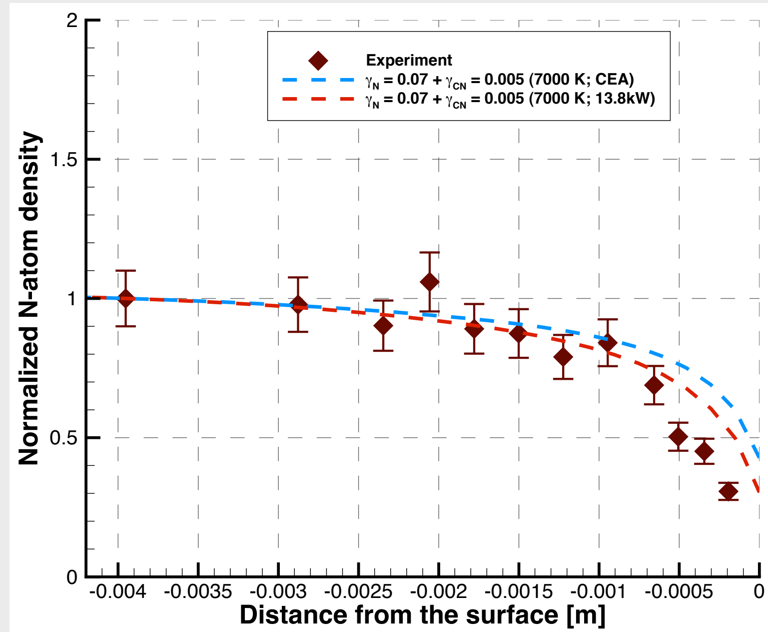


Normalized N-atom density

Gas-Surface Interactions: Sensitivity to Exit Composition



Translational temperature

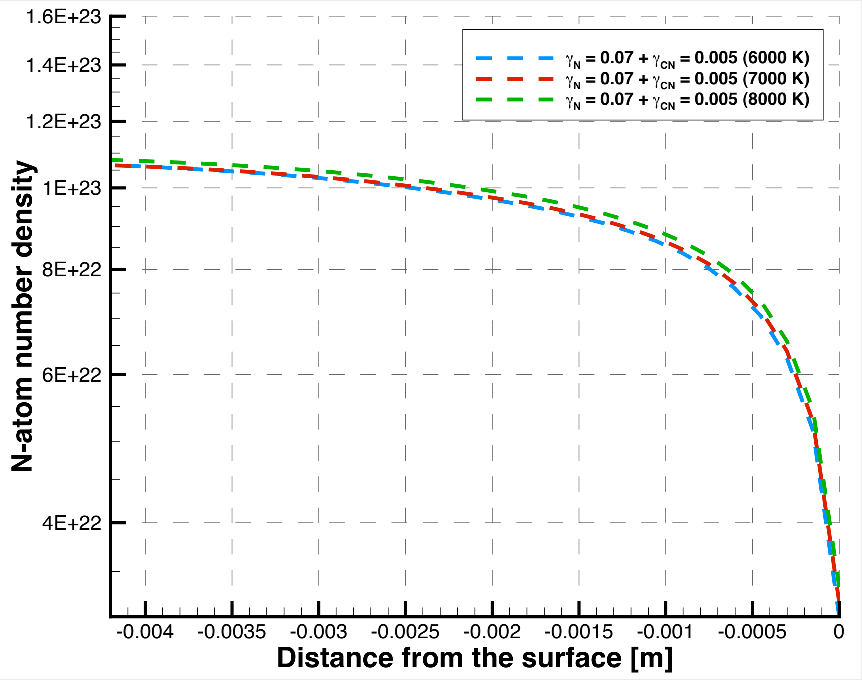


Normalized N-atom density

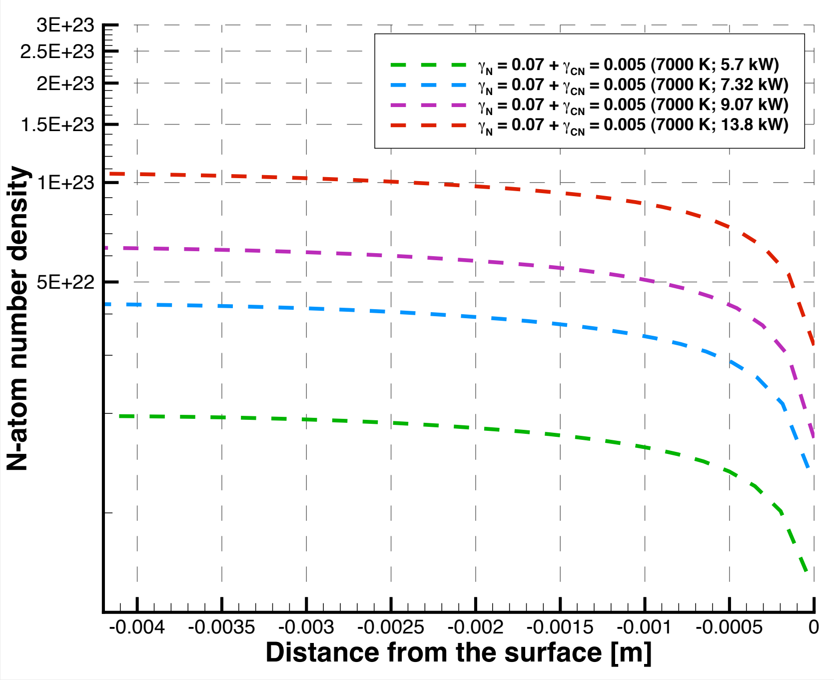
Exit Composition	T_∞ *[K]*	q_{stag} *[W/cm²]*	T_{stag} *[K]*	*Mass Loss Rate [kg/s]*
CEA	7000	270	2758	2.21
13.8 kW	7000	128	2284	0.86
Experiment	~7000	40 - 80	~1600	0.2 – 0.6

Gas-Surface Interactions: Sensitivity to Exit Conditions

Comparison of N-atom number density along the stagnation line

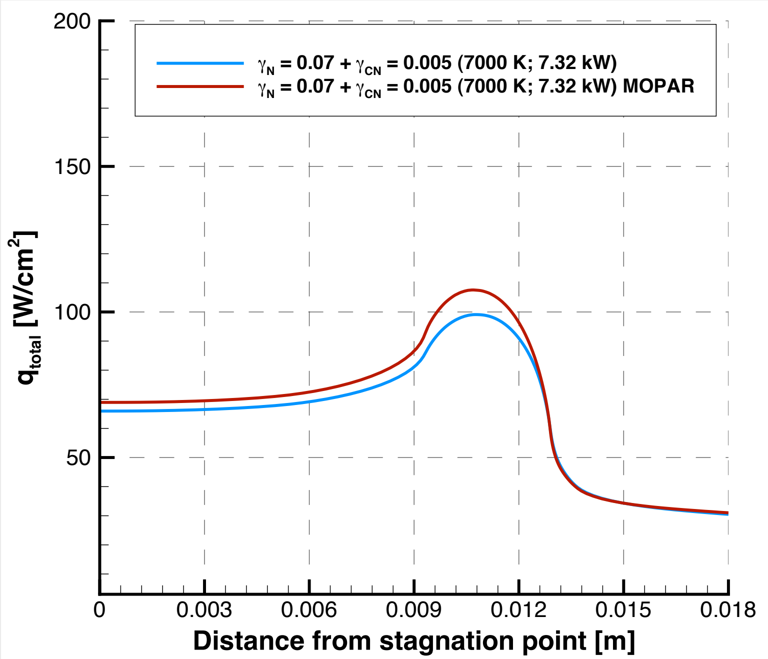


N-atom number density
(Varying Temperature)



N-atom number density
(Varying Power)

Gas-Surface Interactions: Effects of Conduction



Power [kW]	X_N	T_∞ *[K]*	q_{stag} *[W/cm²]*	T_{stag} *[K]*	*Mass Loss Rate [kg/s]*
7.3 (Rad. Eq.)	0.1	7000	66	1934	0.26
7.3 (MOPAR)	0.1	7000	69	1654	0.27
Experiment		~7000	40 - 80	~1600	0.2 – 0.6

Summary

- Nonequilibrium gas-phase processes of nitrogen:
  - 2T model: neglects strong rotational nonequilibrium in shock front
  - 4T model: better agreement obtained when modified Park model used for rotational relaxation (in place of Parker model)
  - EM model: allows direct comparisons with electronic temperature, good agreement with all measurements

- Nonequilibrium gas-surface processes for nitrogen on graphite:
  - Identified measurements needed from experiments to allow clearer conclusions about modeling:
    - Absolute atom number density
    - Will allow accurate estimate of ICP power absorbed by flow
  - Good agreement with all experimental measurements:
    - Flow: temperature and relative atom density
    - Surface: heat transfer rate, temperature, mass loss rate

Technical Challenges

- Nonequilibrium gas-phase processes:
  - Large volume of chemistry computations required, Master Equation analysis becoming expensive
  - What fidelity is required from computational chemistry?
  - Significant number of different air species interactions (N_2-M, O_2-M, NO-M, etc.)
  - Lack of modern, validation quality, experimental data
  - New AFOSR-BRI effort (Michigan/Stanford/G-Tech/Texas)

- Nonequilibrium gas-surface processes:
  - Isolating contributions of competing mechanisms to effects observed (e.g., flow processes, catalysis, ablation)
  - Identifying data required from experiments to enhance conclusions drawn from modeling work