Nonequilibrium Processes and Plasma Radiation in Hyperbolic Atmospheric Entry Flows

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Plan

1. Physical-Chemical-Radiative Problems of Hyperbolic Atmospheric Entries

2. Example for Radiative Calculations: Mars Atmospheric Entries


4. Concluding Remarks and Perspectives
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Space-Shuttle entries from orbit (parabolic trajectory) at $v < 7$ km/s.

Plasma radiation important for overall heat fluxes calculation at $v > 5$ km/s.

Extreme nonequilibrium conditions behind the strong shock-wave, $T_{tr} \gg T_{vib}$, $T_{tr} > 10,000$ K
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Hyperbolic Atmospheric Entries

Mars Atmospheric Entries Radiation

Nonequilibrium Processes in Shock-Heated Flows

Conclusions & Perspectives

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Estimation of the Spacecraft Aerodynamic and Thermal (Convective + Radiative) Loads

- Gas radiative properties determined by the wavelength-dependent emission and absorption coefficients:
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  \[ \alpha_{lu} = N_l B_{lu} \Delta E_{ul} \]

Besides the transition radiative properties \((A_{ul}, B_{lu})\), the state populations need to be known \((N_u, N_l)\), usually in a state-to-state approach.

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Calculation of transition probabilities can now be routinely carried for most chemical species

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Atmospheric Entry Radiation Research Activities at IST

- Line-by-Line numerical code SPARTAN: Simulation of PlasmA Radiation in Thermodynamic Nonequilibrium
- 63 atomic and molecular bound-bond, bound-free (Photodissociation, Photoionization, Photodetachment), and free-free (Bremsstrahlung) transitions from C, N, and O containing species (Earth & Mars)
- Online Gas & Plasma Radiation Database (GPRD) at http://cfp.ist.utl.pt/radiation for providing the scientific community with a database for molecular radiation
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Radiative Transition Probabilities Calculation

- Systematic calculation of the transition probabilities $A_{ul}$ by an "ab-initio" method
- Reconstruction of the molecular potentials using the RKR method and resolution of the Schrödinger equation

Example for the CN Violet System
Spectral Simulation of the Equilibrium Radiative Properties of a Martian-Type Plasma

- High resolution calculation of emission and absorption coefficients for a 100Å–100μm spectral range at 1000, 5000, and 10000 K using the full spectroscopic database (49 transitions)
- 30 min calculation time on a laptop for a spectrum of $\sim 10^5 – 10^6$ points
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Radiative properties at 1000 K

Emission coefficient

Absorption coefficient
Radiative properties at 5000 K

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Absorption coefficient
Radiative properties at 10000 K

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Equilibrium Radiation of a Martian-type Gas at 4300 Pa for the Temperature Range 200-10000 K

- Selected pressure of 4300 Pa which corresponds to the post-shock pressure in a aerocapture manoeuver in Mars atmosphere
- Calculation of the gas optically thin radiative power
- Calculation of the individual contribution of each system to the overall radiative power
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Quantitative Radiative Properties of a Martian-type Gas at 4300 Pa for the Temperature Range 200-10000 K

Optically thin radiative power of a Martian-type gas at 4300 Pa, in the temperature range 200-10000 K

Contribution from each atomic and molecular system.
Selection of an Appropriate Spectral Database

- For equilibrium conditions, few atomic and molecular systems contribute for overall radiative flux
- Not to be extrapolated to nonequilibrium conditions! (even for Boltzmann equilibrium of the flow, e.g. $C_2$ Swan Bands). Also for non-optically thin gas must account for absorbing transitions, e.g. $O_2$ Schumann–Runge
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Challenges Associated to the Development of a Nonequilibrium Entry Flow Model

- Definition of a self-consistent rate equations set valid in atmospheric entry conditions
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Different processes behind the shock-wave lead to the formation of an entry plasma.

- Dissociation, ionization processes with $E_{tr-rot} \gg E_{vib}, E_{el}$
- V–E Excitation of molecular electronic levels will contribute for gas radiation and Penning ionization ($N_2(A) + N_2(a') \leftrightarrow N_2(X) + N_2^+(X)$)
- Maxwellian EEDF may be assumed as the electrons are thermalized
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<th>Shock</th>
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<th>3</th>
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<td>Dissociation</td>
<td>Ionization (Penning?)</td>
<td>Plasma State</td>
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<td>V-T</td>
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<td>Electron-Impact Reactions</td>
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Reproduction of Inflight Flow Conditions in Ground-Test Facilities

- Shock-tube facilities typical of forebody flows, closer to entry flow conditions \( (E_{tr} > E_{el}) \) but short test times \( (<1 \text{ ms}) \) and typically with \( v < 10 \text{ km/s} \)

- Plasma facilities typical of afterbody flows and farther from entry flow conditions \( (E_{tr} < E_{el}) \) but virtually unlimited test times

Simulation of entry-like flows in different ground-test facilities
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Simulation of entry-like flows in different ground-test facilities

Expansion Flow
- Arc-Jet Facilities
- ICP Facilities
- Microwave Facilities

\(T<Te\)

Compression Flow
- Shock-Tubes

\(T>Te\)
Simulation of Dissociation Processes Behind Hyperbolic Shock-Waves

- Translational Temperatures up to 100,000 K
- V–T & V–V–T dissociation processes simulated by the FHO model
- Model more accurate than FOPT models, and compares well with more complex methods (QCT – Billing, Lagana)
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The Forced Harmonic Oscillator Model

- **V–T probabilities for collinear atom-diatom non-reactive collisions** (Kerner:1958) & (Treanor:1965)

\[ P(i \rightarrow f, \varepsilon) = i!f!\varepsilon^{i+f} \exp(-\varepsilon) \left| \sum_{r=0}^{n} \frac{(-1)^r}{r!(i-r)!(f-r)!\varepsilon^r} \right|^2, \]

\[ n = \text{min}(i, f). \]

- **V–V–T probabilities for collinear diatom-diatom collisions** (Zelechow:1968)

\[ P(i_1, i_2 \rightarrow f_1, f_2, \varepsilon, \rho) = \left| \sum_{g=1}^{n} (-1)^{(i_12-g+1)} \times C_{g,i_2+1}^i C_{g,f_2+1}^f \varepsilon^{1/2(i_12+f_12-2g+2)} \exp(-\varepsilon/2) \right|^2 \]

\[ \times \sqrt{(i_12-g+1)!(f_12-g+1)!} \exp[-i(f_12-g+1)\rho] \times \sum_{l=0}^{n-g} \frac{(-1)^l}{(i_12-g+1-l)!(f_12-g+1-l)!!\varepsilon^l} \]

\[ i_{12} = i_1 + i_2, \quad f_{12} = f_1 + f_2, \]

\[ n = \text{min}(i_1 + i_2 + 1, f_1 + f_2 + 1). \]
Assumptions for Shock-Heated Flows

- V–V–T reaction rates for the 59 levels of: \( \text{N}_2: 59^4 \sim 10^7 \)
  
  \[ \Rightarrow P(i_1, \text{all} \rightarrow f_1, \text{all}, \varepsilon, \rho) = P(i_1 \rightarrow f_1, \varepsilon). \quad (\text{Adamovich:1995}) \]

- Dissociation occurs for a transition to a vibrational level \( \nu > 59 \) (quasibound level)
  
  \[ P(i \rightarrow, \varepsilon) = P(i \rightarrow \nu_{\text{qbound}}, \varepsilon) \cdot P_{\text{decay}}, \]
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Polynomial expansions prevent the calculation of quasibound vibrational levels $v_{qbound} > 81$. 

Vibrational levels energies for $N_2$.
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Possible Simplifications

- Asymptotical expressions by Adamovich simplify calculations and allow for rotation effects

\[ P(i \rightarrow f, \varepsilon) = J_s^2 \left( 2\sqrt{n_s \varepsilon} \right) \]

- No approximations used here. Variable precision arithmetics in MATLAB (64 digits numbers) used in calculations

\[ J_s^2 \left( 2\sqrt{n_s \varepsilon} \right) \approx \frac{(n_s)^s}{(s!)^2} \varepsilon^s \exp \left( \frac{-2n_s \varepsilon}{s+1} \right) \]
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Validation of the FHO model

- Comparison with experimental data and QCT calculations by Billing show very good agreement in general.
- Failure of the FHO model for near-resonant transitions at lower temperatures (not important for shock-heated flows).
- Near 100,000K reaction rates achieve a plateau.

Single-quantum V–V rates for $\text{N}_2$–$\text{N}_2$ (0, 1→1, 0) and (0, 1→20, 19) transitions and $\text{O}_2$–$\text{N}_2$ (0, 1→1, 0) transitions. — and ——, FHO model. ×, calculations of Billing:1979 for $\text{N}_2$–$\text{N}_2$. ⚫, interpolation of experimental data for $\text{N}_2$–$\text{O}_2$ (1, 0→0, 1), Taylor:1969.
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Simulation of Simplified Shock Geometries for Nitrogen flows

- V–T reaction rate database calculated up to $T_{tr} = 100,000\,\text{K}$ for 100 levels of $\text{N}_2$
- Simulation of a Shock at an altitude of 76 km and fixed translational temperatures of 1,000, 10,000 and 100,000 K.
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Shock Simulation at 1000 K

- Reaction Rates Database at 1000 K
- Time Evolution of the VDF
Shock Simulation at 10000 K

Reaction Rates Database at 10000 K

Time Evolution of the VDF
Shock Simulation at 100000 K

Reaction Rates Database at 100000 K

Time Evolution of the VDF
Evolution of the Molecular Dissociation at Different Shock Temperatures

- Dissociation times range from more than 1 s for \( T \leq 5,000\text{K} \) to 1 ns for \( T = 100,000\text{K} \)
- For lower temperatures, “ladder-climbing” phenomena enhance dissociation after a certain incubation time
- At higher temperatures, \( (T \geq 50,000\text{K}) \) dissociation proceeds equiprobably from all the vibrational levels
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Time evolution of N\(_2\) dissociation at different shock temperatures.
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- Development of radiation databases is a straightforward task, but needs extensive validations.
- Developed state-to-state models need to be valid for the most extreme hyperbolic shock-waves. Importance of multiquantum transitions.
- Computation time issues remain determinant as they prevent full-use of line-by-line calculations and state-to-state models. The errors induced by the used approximations (Boltzmann equilibrium, band models) remain unknown.
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Perspectives

- V–T dissociation models should include effects of molecular rotation.
- V–E processes need more theoretical developments. Only available experimental data obtained for gas-discharge applications with \( T_{tr} \sim 300 \text{K} \).
- Radiation re-absorption may be important for hyperbolic flows (see Park 2004 for Galileo probe entry simulations).
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V–E processes need more theoretical developments. Only available experimental data obtained for gas-discharge applications with $T_{tr} \sim 300\text{K}$

Radiation re-absorption may be important for hyperbolic flows (see Park 2004 for Galileo probe entry simulations)