Self-consistent vibrational and Electronic Kinetics a H_2/He Plasma

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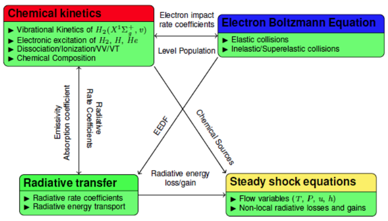
Introduction

The reliable prediction of radiative and convective thermal loads on a spacecraft's thermal protection system during an high speed entry in a planetary atmosphere requires proper consideration of the non-equilibrium character of the flow, taking into account the elementary processes of internal atomic an molecular excitation and ionization by heavy particle and electron collisions. In particular, electronic excitation is strongly connected to the instantaneous electron energy distribution function at a given point, since the latter dictates the actual rates of electron impact processes, while at the same time the instantaneous population distributions on the internal electronic and vibrational quantum states of the plasma components reflect on the shape of the EEDF through a complex interplay between inelastic and superelastic collisions, often leading to non-maxwellian EEDFs and corresponding non-Arrhenius impact rate coefficients.

Another important effect to be considered in the case of the high speed and low pressure conditions met during a planetary entry is the radiation-matter interaction. Radiation generated in one point of the flow can affect nearby locations through reabsorption, that tends to increase the local population of atomic excited states, while radiation escaping the heated gas lowers the overall excitation degree of the plasma and its temperature depending on the amount of reabsorption. A reliable quantitative analysis of the latter effect can be only performed introducing an explicit description of the radiation field solving a radiative transfer equation (RTE).

These aspects have been investigated in the case of a pure hydrogen plasma in previous works [1-4] . In this work that model has been improved extending the chemical kinetic scheme with a complete set of collisional and radiative processes for the He atom and a corresponding method for the calculation of the absorption coefficient and emissivity needed in the solution of the RTE. The resulting model has been applied to study a steady shock wave under conditions typical of an hypersonic entry in Jupiter's atmosphere.

COUPLING AMONG DIFFERENT SUB-MODELS



Shock Wave Solver

For the purposes of the present work, a suitable description of the fluid flow is obtained solving the following set of flow continuity equations for the mass density, momentum and energy fluxes [5]

FLOW CONTINUITY EQUATIONS

$$\rho_1 u_1 = \rho_2 u_2 = c_1$$
$$\rho_1 u_1^2 + P_1 = \rho_2 u_2^2 + P_2 = c_2$$
$$\tfrac{1}{2}u_1^2 + h_1 = \tfrac{1}{2}u_2^2 + h_2 = c_3 - \Delta Q_{\rm rad}$$

RADIATIVE LOSSES

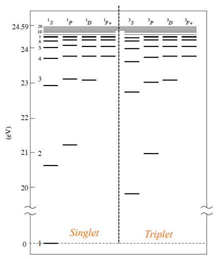
TRANSLATIONAL & INTERNAL ENTHALPY

$$h_T = c_P T$$
$$h_{\rm int} = \sum_s \left(h_{f\,s} + \sum_i \epsilon_{si}\chi_{si} \right) x_s$$

Collisional-Radiative Model

Jupiter's atmosphere is mainly composed by molecular hydrogen and atomic helium and for this work we have assumed an initial molar fraction ratio He/H_2=11/89. The chemical kinetics scheme considers a plasma comprising the H_2, H_2^+, He, He^+, H, H^+ and e^- species. Compared to our previous work, a model of the helium atom has been introduced, that closely follows that described in [6], using level energies from NIST's atomic database [7].

He ATOMIC MODEL



➔ *a total of 59 electronic states in the model of He*

➔ *for He^+ only the ground electronic state is considered*

CHEMICAL AND ELECTRON KINETICS

Specie	Process	Reaction
H_2	vv	$H_2(v)+H_2(w) \rightleftharpoons H_2(v+1)+H_2(w-1)$
	vTm	$H_2(v)+H_2 \rightleftharpoons H_2(w)+H_2$
	vTa	$H_2(v)+H \rightleftharpoons H_2(w)+H$
	drm	$H_2(v)+H_2 \rightleftharpoons 2H+H_2$
	dra	$H_2(v)+H \rightleftharpoons 2H+H$
	$e-V$	$H_2(v)+e^- \rightleftharpoons H_2(w)+e^-$
	$e-D$	$H_2(v)+e^- \rightleftharpoons e^-+H(n=1)+H(n=2,3)$
	$e-DI$	$H_2(v)+e^- \rightleftharpoons H+H^++2e^-$
	$e-I^+$	$H_2^++e^- \rightleftharpoons 2H^++2e^-$
	$e-D^+$	$H_2^++e^- \rightleftharpoons H+H^++e^-$
	$e-DR$	$H_2^++e^- \rightleftharpoons 2H$
H	$h\nu$	$H(n) \rightleftharpoons H(m<n)+\rightsquigarrow$
	rr	$H^++e^- \rightleftharpoons H(n)+\rightsquigarrow$
	HH	$H(n)+H(1) \rightleftharpoons H(m)+H(1)$
	HI	$H(n)+H(1) \rightleftharpoons H^++H(1)+e^-$
	eH	$H(n)+e^- \rightleftharpoons H(m)+e^-$
	eI	$H(n)+e^- \rightleftharpoons H^++2e^-$
He	$h\nu$	$He(n) \rightleftharpoons He(m<n)+\rightsquigarrow$
	rr	$He^++e^- \rightleftharpoons He(n)+\rightsquigarrow$
	eE	$He(n)+e^- \rightleftharpoons He(m)+e^-$
	eI	$He(n)+e^- \rightleftharpoons He^++2e^-$
e^-	in/sup	$X(s)+e^-(\varepsilon) \rightleftharpoons X(s'<s)+e^-(\varepsilon-\varepsilon^*)$
	DR	$AB(s)+e^-(\varepsilon) \rightleftharpoons A+B+e^-(\varepsilon-\varepsilon^*)$
	IR	$X(s)+e^-(\varepsilon) \rightleftharpoons X^++e^-(\varepsilon-\varepsilon^*)+e^-(0)$
	el	$X+e^-(\varepsilon) \rightleftharpoons X^++e^-(\varepsilon')$
	ee	$e^-(\varepsilon_1)+e^-(\varepsilon_2) \rightleftharpoons e^-(\varepsilon_1')+e^-(\varepsilon_2')$

Electron energy distribution function

Electron impact rate coefficients are calculated by integrating the relevant cross section over the EEDF determined by solving the following Electron Boltzmann Equation. Inelastic collisions deplete the high energy tail of the EEDF and correspond to excitation and ionization by electron impact, while superelastic collisions correspond to de-excitation and recombination and tend to enhance the tail of the EEDF.

ELECTRON BOLTZMANN EQUATION

Elastic collisions with heavy particles — Elastic electron-electron collisions

$$\frac{df_e(\varepsilon,t)}{dt} = -\frac{dJ_{\rm el}}{d\varepsilon} - \frac{dJ_{\rm e-e}}{d\varepsilon} + S_{\rm in} + S_{\rm sup}$$

Inelastic collision — Superelastic collisions

$$K_e = \int_0^\infty f_e(\epsilon)\sigma(\epsilon)v_e(\epsilon)d\epsilon$$

ELECTRON IMPACT RATE COEFFICIENTS

Radiation modeling

The spectral intensity in the post-shock is described in the present work by solving the radiative transfer equation (RTE)

RADIATIVE TRANSFER EQUATION

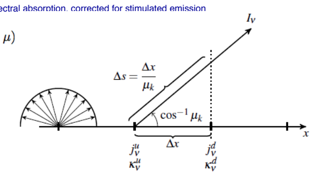
$$\mu\frac{dI_\nu(x,\mu)}{dx} = j_\nu^e(x) + \kappa_\nu'(x)I_\nu(x,\mu)$$

Spectral absorption, corrected for stimulated emission

Spectral Emissivity

INTEGRATION OF THE RTE ALONG THE LINE OF SIGHT

$$I_\nu(\Delta s) = I_\nu(0)e^{-\Delta\tau_{ud}} + j_\nu^u\frac{1-e^{-\Delta\tau_{ud}}}{\Delta\tau_{ud}}\Delta s + \left(\frac{j_\nu^d - j_\nu^u}{\Delta s}\right)\frac{\Delta\tau_{ud}-1+e^{-\Delta\tau_{ud}}}{\Delta\tau_{ud}^2}\Delta s^2$$



HELIUM LINE BROADENING

Electron Stark

$$w + id = \frac{2}{3c}N_e\left(\frac{\hbar}{m}\right)^2\int\frac{dv}{v}f(v)\left\{\frac{3}{4}\left(\frac{mv}{\hbar}\right)^2\rho_{\rm min}^2 + \sum_{i'}\mathbf{R}_{ii'}^2[a_{ii'}(z_{ii'}^{\rm min}) - i\varepsilon b_{ii'}(\tilde{z}_{ii'}^{\rm min})] + \sum_{f'}\mathbf{R}_{ff'}^2[a_{ff'}(z_{ff'}^{\rm min}) + i\varepsilon b_{ff'}(\tilde{z}_{ff'}^{\rm min})]\right\}$$

$$\rho_{\rm min}^2 = \frac{2}{3}\left(\frac{\hbar}{mv}\right)^2\left|\sum_{i'}\mathbf{R}_{ii'}^2[A_{ii'}(z_{ii'}^{\rm min}) - i\varepsilon B_{ii'}(\tilde{z}_{ii'}^{\rm min})] + \sum_{f'}\mathbf{R}_{ff'}^2[A_{ff'}(z_{ff'}^{\rm min}) + i\varepsilon B_{ff'}(\tilde{z}_{ff'}^{\rm min})]\right|$$

Ion Broadening Parameter

$$A = \frac{4\pi N_i}{3}\left[\frac{1}{3w}\left(\frac{\hbar}{m}\right)^2\left|\sum_{i'}\frac{\mathbf{R}_{ii'}^2}{2\pi c\bar{\nu}_{ii'}} - \sum_{f'}\frac{\mathbf{R}_{ff'}^2}{2\pi c\bar{\nu}_{ff'}}\right|\right]^{3/4}\left[\sum_{{\rm ions},z_i} z_i n_i^{2/3}\right]^{3/2}$$

Total Stark Broadening

$$w_{tot} \approx w + 1.75A(1-0.75R)w$$

HYDROGEN LINE BROADENING

Ion Stark

$$\Delta\bar{\nu}_{ion} = \frac{12.5}{2\pi c}(j^2 - i^2)\left[\sum_i z_i n_i\right]^{2/3}$$

Electron Stark

$$\Delta\bar{\nu}_e = \frac{32}{6\pi}n_e\sqrt{\frac{\pi m_e}{8kT_e}}\left(\frac{\hbar}{m_e}\right)^2\left(\ln\frac{R_D}{\rho_0} + 0.215\right)I(n,n')$$

Resonance

$$\Delta\bar{\nu}_{\rm res} = N_g\left(\frac{g_g}{g_i}\right)^{1/2}\frac{e^2 f_g i}{2\pi c^2 m_e\bar{\nu}_{ig}}$$

Doppler

$$\Delta\bar{\nu}_D = \frac{\bar{\nu}_0}{c}\sqrt{\frac{2\ln 2kT}{m_H}}$$

Line profiles modeled with a Voigt function

$$\phi(x,y) = \frac{1}{\Delta\bar{\nu}_D}\sqrt{\frac{\ln 2}{\pi}}\frac{y}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{y^2+(t-x)^2}dt$$

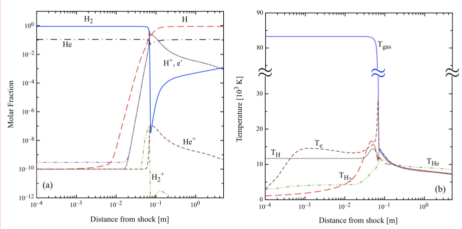
$$y = \sqrt{\ln 2}\Delta\bar{\nu}_L/\Delta\bar{\nu}_D$$
$$x = \sqrt{\ln 2}(\bar{\nu} - \bar{\nu}_0)/\Delta\bar{\nu}_D$$

convolution of Lorentzian and Gaussian lineshapes

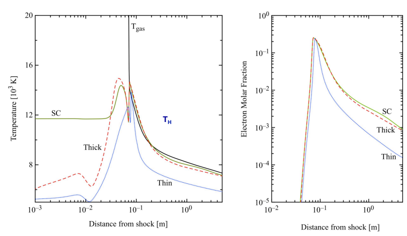
Study case: Hypersonic Entry in Jupiter's Atmosphere

- *7-species mixture: H_2, He, H, H^+, H_2^+, He^+, e^-*
- *Initial conditions: v=50 Km/s, P=27.5 Pa, T_g=160K, He/H_2=11/89*
- *Internal H, He and H_2 distribution are Boltzmann at 160 K*

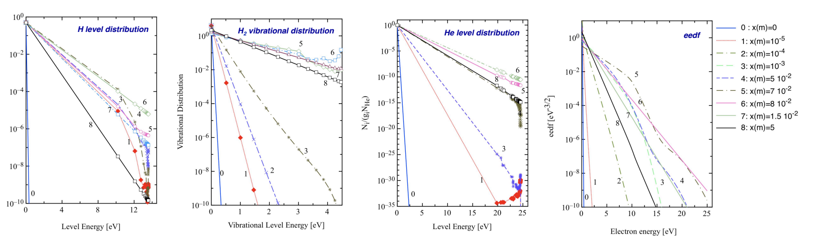
CHEMICAL COMPOSITION AND TEMPERATURE PROFILES



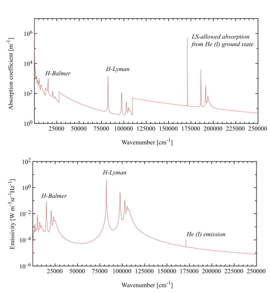
COMPARISON AMONG DIFFERENT RADIATION MODELS



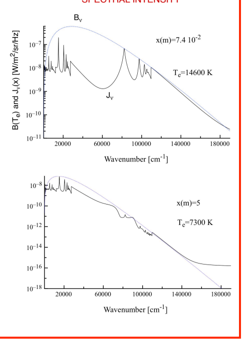
INTERNAL DISTRIBUTIONS AT DIFFERENT POINTS



ABSORPTION AND EMISSION COEFFICIENTS



SPECTRAL INTENSITY



Conclusions

A one-dimensional steady shock wave model coupling a comprehensive CRM of a H_2/He plasma, a Boltzmann solver for the EEDF and an RTE solver has been described. The model solves the steady state shock continuity equations, using the CRM to determine the non-equilibrium chemical composition and the distribution of atomic and molecular excited states. Electron-impact rate coefficients are directly calculated integrating the relevant cross-section over the actual EEDF determined by the Boltzmann solver, while radiative rate coefficients are self-consistently calculated using the local spectral intensity determined by the RTE solver. The RTE solver can also be used to determine non-equilibrium spectra, the radiative flux and its divergence in the post-shock region.

Acnowledgments

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