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Flow-radiation coupling for atmospheric entries using a Hybrid Statistical Narrow Band model



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ABSTRACT

In this study, a Hybrid Statistical Narrow Band (HSNB) model is implemented to make fast and accurate predictions of radiative transfer effects on hypersonic entry flows. The HSNB model combines a Statistical Narrow Band (SNB) model for optically thick molecular systems, a box model for optically thin molecular systems and continua, and a Line-By-Line (LBL) description of atomic radiation. Radiative transfer calculations are coupled to a 1D stagnation-line flow model under thermal and chemical nonequilibrium. Earth entry conditions corresponding to the FIRE 2 experiment, as well as Titan entry conditions corresponding to the Huygens probe, are considered in this work. Thermal nonequilibrium is described by a two temperature model, although non-Boltzmann distributions of electronic levels provided by a Quasi-Steady State model are also considered for radiative transfer. For all the studied configurations, radiative transfer effects on the flow, the plasma chemistry and the total heat flux at the wall are analyzed in detail. The HSNB model is shown to reproduce LBL results with an accuracy better than 5% and a speed up of the computational time around two orders of magnitude. Concerning molecular radiation, the HSNB model provides a significant improvement in accuracy compared to the Smeared-Rotational-Band model, especially for Titan entries dominated by optically thick CN radiation.

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1. Introduction

Spacecraft may undergo severe convective and radiative heating during atmospheric entry at high velocities from the surrounding aerothermodynamic environment. Its accurate prediction during the design of such vehicles is therefore paramount for the success and safety of future planetary missions. In particular, the radiative heat transfer in the shock layer ahead of the vehicle is known to significantly alter the aerothermodynamic environment, especially early in the entry when the velocity is high and

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http://dx.doi.org/10.1016/j.jqsrt.2016.04.008 0022-4073/© 2016 Elsevier Ltd. All rights reserved. the density of the atmosphere is low. The numerical simulation of hypersonic reactive plasma flows coupled with radiative heat transfer is an active research topic for the design of thermal protection systems of future space missions. Past numerical investigations have shown several major coupling effects including (i) radiative cooling of the shock layer due to the strong emission of the plasma [1–3], (ii) the production of precursor chemical compounds ahead of the shock [4], and (iii) the promotion of ablation products released by the heat shield which may in turn contribute to increased radiation blockage in the boundary layer [5]. At high altitudes corresponding to low densities, the need to consider detailed nonequilibrium radiation appeared since the middle of the 1980s [6] and thermodynamic and chemical nonequilibrium flowfield

solvers, coupled to radiative transfer, became common in the 1990s [7,8].

The numerical simulation of radiative transfer is a challenging problem because of the spatial, angular, and spectral dependence of the radiation field. The reference approach for treating the spectral dependence is the Line-By-Line (LBL) method which consists in finely discretizing the radiative properties over the relevant spectral range. These radiative properties depend on level populations and on fundamental spectroscopic data gathered in spectral databases such as NEQAIR [9,10], SPRADIAN [11], MONSTER [12], SPECAIR [13]. In the present study, we use the HTGR database (High Temperature Gas Radiation), which has been previously developed [14-18] for O_2-N_2 and CO₂–N₂ plasma applications. This database gathers up-to-date atomic spectroscopic data from various sources (such as NIST [19] and TOPbase [20]) together with ab initio calculations of diatomic molecular spectra and atomic line shapes. It includes bound-bound atomic and molecular transitions, bound-free transitions resulting from various mechanisms, and free-free transitions. The covered spectral range is [1000-200,000 cm⁻¹] and the targeted maximum temperature is 30,000 K. The HTGR database has been used in several studies for LBL radiative transfer calculations in hypersonic entries. In particular, Lamet et al. [21] performed uncoupled radiation simulations of the FIRE II flight experiment using a twotemperature approach to model the thermal nonequilibrium. More recently, Lopez et al. [22] carried out coupled flow-radiation simulations of the relaxation behind a shock wave in Air with a consistent state-to-state modeling of the atomic electronic levels.

A full LBL closely coupled flowfield-radiation model has been developed by Feldick et al. [23] for Earth hypersonic reentries. They used the tangent slab approximation and introduced optimized variable wavelength steps to decrease the computational costs. The full LBL simulations were successfully compared to a hybrid line-by-line-gray model where molecular radiation in optically thin systems was assumed to be gray inside narrow bands. However, although the LBL method is very accurate, the large number of radiative transitions that have to be taken into account makes it very computationally expensive and impractical for coupled simulations in complex geometries. The Smeared-Rotational-Band (SRB) model is a common way to simplify the calculation of molecular radiation but its accuracy is restricted to small optical thicknesses. It has been used for instance in Ref. [24], together with a LBL treatment of atomic radiation.

More sophisticated approaches for radiative property modeling include the k-distribution methods which are based on the distribution functions of the absorption coefficient over the whole spectrum (see e.g. [25]) or over spectral narrow bands [26]. They have been widely used for modeling IR radiation in the field of atmospheric physics or for combustion applications, but also for modeling visible, UV and VUV radiation of astrophysical (Opacity Distribution Function model of Ref. [27]) or thermal [28] plasmas. Recently such models have been developed in the framework of hypersonic nonequilibrium flows for air mixtures [29,30] and also in carbonaceous atmospheres [31]. They are based on the Full-Spectrum Correlated-k approach (FSCK) previously developed for IR applications [32] and use efficient tabulations and rescaling of the various required distribution functions against temperatures, molecular electronic state populations, and a typical Stark width of the atoms. The accuracy of these approaches was demonstrated by successful comparisons with LBL results. In the case of carbonaceous atmospheres [31], where only three non-overlapping molecular band systems are considered, such an approach is very efficient and easy to implement. Moreover, it retains a description of radiative properties in terms of absorption coefficients and is therefore applicable to any radiation solver. For more arbitrary gas mixtures, including for instance ablation products, a large number of overlapping, non-weak molecular electronic systems, absorbing in the Voigt regime, and whose induced emission contribution might not be negligible. have to be accounted for. In this case, the multi-scale MS-FSCK approach may become quite tedious to implement. Moreover, the spectral information is completely lost when using such full-spectrum approaches. This is not an intrinsic limitation if one is only interested in heat transfer with gray walls, but such models do not enable comparisons with experiments done in limited spectral ranges.

Recently, Lamet et al. [33] have developed a Hybrid Statistical Narrow Band (HSNB) model, which combines a Statistical Narrow Band (SNB) model for optically thick molecular systems with a box model for optically thin molecular systems and continua, and a LBL description of atomic line radiation. Band parameters have been computed using the HTGR database and tabulated against translational–rotational and vibrational temperatures. The HSNB model can easily include new radiating species and electronic systems, using the uncorrelation assumption inside narrow bands, and arbitrary electronic populations may be specified. Also, it can be applied to predict the radiative flux in the case of non-gray walls. Nevertheless, it might be less computationally efficient than k-distribution methods.

This study aims at showing the ability of the HSNB model to predict accurately and efficiently coupled radiation effects on hypersonic entry flows. For this purpose, a 1D stagnation-line flow model for blunt, hypersonic vehicles [34] has been coupled with a newly developed radiative transport code using the HSNB formulation. Earth entry conditions corresponding to the FIRE 2 experiment, as well as Titan entry conditions corresponding to the Huygens probe, are considered. Thermal nonequilibrium is described by a two temperature model, although non-Boltzmann distributions of electronic levels provided by a Quasi-Steady State model are also considered for radiative transfer. Section 2 details the 1D model for coupled flow and radiation along the stagnation-line of the vehicle. The HSNB model [33] is presented in Section 3 with new additional features. The results are finally discussed in Section 4.

2. Governing equations

We consider a plasma flow constituted of atoms, molecules and free electrons under chemical and thermal nonequilibrium conditions. The thermal state of the plasma is described according to a two-temperature model in which the translation of heavy species and rotation of molecules are assumed to follow a Boltzmann distribution at the temperature T, and the translation of electrons, vibration of molecules, and electronic excitation of heavy species are assumed to follow a Boltzmann distribution at the temperature T^{ve} . The energy of a species s per unit mass is then defined by

$$e_s(T, T^{ve}) = e_s^{tr}(T) + e_s^{ve}(T^{ve}) + e_s^f,$$
(1)

where e_s^{tr} , e_s^{ve} , and e_s^{f} are the translation–rotational, vibration–electronic-electron, and formation energies respectively, for species *s*. The rigid-rotor and harmonicoscillator models are used to describe rotational and vibrational modes when computing species thermodynamic quantities, while species electronic energies are computed from the electronic energy levels taken from Ref. [35].

The pressure p of the plasma is modeled using the perfect gas law

$$p = \sum_{s \in \mathcal{H}} \rho_s r_s T + \rho_e r_e T^{ve}, \tag{2}$$

where ρ_s is the species mass density, r_s the perfect gas constant per unit mass of species *s*, \mathcal{H} is the set of heavy species and the subscript *e* refers to free electrons.

2.1. Stagnation-line flow modeling

We follow the methodology of Ref. [36] for deriving a 1D plasma flow model along the stagnation-line of a spherical body (see Fig. 1). The problem is considered symmetric according to the azimuth angle ϕ and the velocity component u_{ϕ} is set to zero. Mass fractions and temperatures are assumed to be only a function of the radius r

$$y_s = \overline{y_s}(r), \quad T = \overline{T}(r), \quad T^{ve} = T^{ve}(r),$$
 (3)

while velocity and pressure are split into radial and tangential components following

$$u_r = \overline{u_r}(r)\cos\theta, \quad u_\theta = \overline{u_\theta}(r)\sin\theta, \quad p - p_\infty = \overline{p}(r)\cos^2\theta,$$
(4)

where the pressure is assumed to follow a Newtonian approximation [37]. Introducing this decomposition into the 3D Navier–Stokes equations in spherical coordinates and then taking the limit when θ tends to zero leads to a set of 1D equations for the stagnation–streamline quantities of



Fig. 1. Spherical body of radius R_0 subjected to a hypersonic flow at u_{∞} . Azimuth and zenith angles are ϕ and θ , respectively.

the form

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}^c}{\partial r} + \frac{\partial \mathbf{F}^d}{\partial r} = \mathbf{S}^c + \mathbf{S}^d + \mathbf{S}^{k} + \mathbf{S}^{rad}.$$
(5)

U is the conservative variable vector. \mathbf{F}^{c} and \mathbf{F}^{d} are the convective and diffusive fluxes. \mathbf{S}^{c} and \mathbf{S}^{d} are convective and diffusive source terms resulting from the expansion along the stagnation-line. \mathbf{S}^{k} is the kinetic and energy transfer source term vector and \mathbf{S}^{rad} is the radiative source term vector. Specifically, these vectors are written as

$$\mathbf{U} = \left[\rho_s, \ \rho u_r, \ \rho u_\theta, \ \rho E, \ \rho e^{ve}\right]^T, \tag{6}$$

$$\mathbf{F}^{c} = \left[\rho_{s} u_{r}, \ \rho u_{r}^{2} + p, \ \rho u_{r} u_{\theta}, \ \rho u_{r} H, \ \rho u_{r} e^{ve}\right]^{T}, \tag{7}$$

$$\mathbf{S}^{c} = -\frac{(u_{r}+u_{\theta})}{r} \bigg[2\rho_{s}, \ 2\rho u_{r}, \ 3\rho u_{\theta} - 2\frac{p-p_{\infty}}{u_{r}+u_{\theta}}, \ 2\rho H, \ 2\rho e^{ve} \bigg]^{T},$$
(8)

$$\mathbf{F}^{d} = \begin{bmatrix} j_{rs}, & -\tau_{rr}, & -\tau_{r\theta}, & q_{r} - \tau_{rr}u_{r}, & q_{r}^{ve} \end{bmatrix}^{T},$$
(9)

$$\mathbf{S}^{d} = -\frac{1}{r} [2j_{rs}, \ 2(\tau_{\theta\theta} - \tau_{rr} + \tau_{r\theta}), \ \tau_{\theta\theta} - 3\tau_{r\theta}, 2(q_{r} - \tau_{rr}u_{r} - \tau_{r\theta}u_{r} - \tau_{\theta\theta}u_{\theta}), \ 2q_{r}^{ve}]^{T},$$
(10)

$$\mathbf{S}^{k} = \begin{bmatrix} \dot{\boldsymbol{\omega}}_{s}^{k}, \ 0, \ 0, \ 0, \ \boldsymbol{\Omega}^{ve} \end{bmatrix}^{T}, \tag{11}$$

$$\mathbf{S}^{rad} = \begin{bmatrix} \dot{\omega}_{s}^{rad}, \ 0, \ 0, \ \mathcal{P}^{rad}, \ \mathcal{P}^{rad, ve} \end{bmatrix}^{T},$$
(12)

where the overline symbol introduced in Eqs. (3) and (4) to designate stagnation-line quantities has been omitted for the sake of clarity. The total energy and the vibrational-electronic-electron energy per unit volume are defined by $\rho E = \sum_{s} \rho_{s} e_{s} + \rho u_{r}^{2}/2$ (only the radial velocity component contributes to the kinetic energy due to the ansatz Eq. (4)) and $\rho e^{ve} = \sum_{s} \rho_{s} e_{s}^{ve}$. Note that the formation energy is not included in e^{ve} according to the definition given in Eq. (1). This choice is important for the source terms described below. The total enthalpy is defined by $H = E + p/\rho$.

The radial species diffusion fluxes j_{rs} are obtained by solving a simplified Stefan–Maxwell equation for heavy species [38]. The electron diffusion flux is computed from the ambipolar assumption that makes the electric current equal to zero. The radial heat fluxes are defined by

$$q_r = \sum_{s} j_{rs} h_s - \lambda^{tr} \frac{\partial T}{\partial r} - \lambda^{ve} \frac{\partial T^{ve}}{\partial r},$$
(13)

$$q_r^{\nu e} = \sum_s j_{rs} h_s^{\nu e} - \lambda^{\nu e} \frac{\partial T^{\nu e}}{\partial r},\tag{14}$$

where λ^{tr} and λ^{ve} are the thermal conductivities of the energy modes in equilibrium with the temperatures *T* and T^{ve} respectively, $h_s = e_s + p_s/\rho_s$, $h_s^{ve} = e_s^{ve}$ for $s \neq e$ and $h_e^{ve} = e_e^{ve} + p_e/\rho_e$. The components of the viscous stress tensor τ_{rr} , $\tau_{r\theta}$ and $\tau_{\theta\theta}$ are given by

$$\tau_{rr} = \frac{4}{3}\mu \left(\frac{\partial u_r}{\partial r} - \frac{u_r + u_\theta}{r}\right), \quad \tau_{r\theta} = \mu \left(\frac{\partial u_\theta}{\partial r} - \frac{u_r + u_\theta}{r}\right), \quad \tau_{\theta\theta} = -\frac{1}{2}\tau_{rr}, \tag{15}$$

where μ is the viscosity.

In Eq. (11) $\dot{\omega}_s^k$ are the collisional species mass production rates. Reaction rate constants are assumed to follow an Arrhenius law. Forward reaction constants are taken from the literature depending on the mixture considered. Backward reaction constants are computed such that equilibrium relations are satisfied [39]. The source term Ω^{ve} is written as

$$\Omega^{ve} = -p_e \left(\frac{\partial u_r}{\partial r} + 2 \frac{u_r + u_\theta}{\partial r} \right) + \sum_{s \in \mathcal{M}} \rho_s \frac{e_s^{v0} - e_s^v}{\tau_s^{VT}} + \rho_e \frac{e_e^{t0} - e_e^t}{\tau^{ET}} \\
+ \sum_s e_s^{ve} \dot{\omega}_s^k - \sum_{p \in \mathcal{R}} \Delta \mathcal{H}_p \dot{\chi}_p^k.$$
(16)

The first term on the right-hand-side of Eq. (16) represents the internal work done by the electron pressure. The second term represents vibration-translation energy exchange where e_s^{v0} and e_s^{v} are vibrational energies of species *s* at the temperature *T* and T^{ve} , respectively. The associated relaxation time τ_s^{VT} is computed from the experimental data of Ref. [40] taking into account the high temperature correction from Ref. [41]. The third term corresponds to electron-heavy translation energy exchange where e_e^{t0} and e_e^t are translational energies of electrons at the temperature T and T^{ve} , respectively. The expression of the relaxation time τ^{ET} is given in Ref. [42]. The fourth term represents the coupling between chemistry and vibrational-electronic energy. Finally, the fifth term accounts for the energy removed from the electron bath due to the set \mathcal{R} of electron impact ionization and dissociation reactions, where $\dot{\chi}_p^k$ is the molar rate of progress and $\Delta \mathcal{H}_p = \sum_s \nu_{sp} e_s^f / M_s$ is the chemical heat released per unit mole $(\overline{\nu_{sp}})$ is the stoichiometric coefficient for reaction p and M_s is the molar mass of species s) of reaction p. The set of chemical reactions considered will be specified for each case in Section 4.

Finally, $\dot{\omega}_s^{rad}$ is the radiative mass production rate of species *s*, \mathcal{P}^{rad} is the total radiative energy source term and $\mathcal{P}^{rad,ve}$ is the radiative energy source term for the energy modes in equilibrium with T^{ve} .

2.2. Radiative source terms

For computing the radiative source terms of Eq. (12), we make use of the 1D tangent slab approximation [43,44]. The radiative properties of the medium are assumed to vary only along the stagnation-line direction and are assumed to be constant in planes that extend to infinity, perpendicular to this direction. It is a reasonable approximation in this work as we will consider shock layer of which the size is small compared to the radius of the vehicle.

The radiative source terms are functions of the spectral radiative intensity I_{σ} which is governed by the radiative transfer equation

$$\cos \,\vartheta \frac{\partial I_{\sigma}(r,\vartheta)}{\partial r} = \eta_{\sigma}(r) - \kappa_{\sigma}(r)I_{\sigma}(r,\vartheta), \tag{17}$$

for a non-scattering medium of optical index equal to 1, where η_{σ} and κ_{σ} are the emission and absorption coefficients at wavenumber σ , *r* designates the position along

the stagnation-line and ϑ is the angle made between the optical path and the stagnation-line.

The radiative mass production rate in Eq. (12) corresponds to the production or destruction of a species *s* during a bound-free radiative process *p* (photoionization $A+hc\sigma \rightleftharpoons A^+ + e^-$ or photodissociation $AB+hc\sigma \rightleftharpoons A+B$)

$$\dot{\omega}_{s}^{rad}(r) = \sum_{p} \frac{\nu_{sp} M_{s}}{\mathcal{N}_{A}} \int_{0}^{\infty} \frac{2\pi \kappa_{\sigma}^{p}(r) \int_{0}^{\pi} I_{\sigma}(r,\vartheta) \sin \vartheta \, d\vartheta - 4\pi \eta_{\sigma}^{p}(r)}{hc\sigma} \, d\sigma,$$
(18)

where ν_{sp} is the stoichiometric coefficient for the bound free process *p* and species *s* (positive for product, negative for reactant), N_A is the Avogadro number, *h* is the Planck constant and *c* the speed of light.

The total radiative energy source term \mathcal{P}^{rad} is equal to the opposite of the divergence of the radiative flux q^{rad} , which gives

$$\mathcal{P}^{rad}(r) = -\frac{\partial q^{rad}(r)}{\partial r}, \ q^{rad}(r) = 2\pi \int_0^\infty \int_0^\pi I_\sigma(r,\vartheta) \cos \vartheta \sin \vartheta \, d\vartheta \, d\sigma.$$
(19)

For computing the source term $\mathcal{P}^{rad,ve}$, we first neglect the radiative energy exchanges with translational and rotational modes. Then, we take into account the fact that during a photoionization process, a part of the photon energy goes into the formation energy [22]. This leads to

$$\mathcal{P}^{rad,ve}(r) = \mathcal{P}^{rad}(r) - \sum_{p \in \mathcal{J}} \Delta h_p \dot{\omega}_{p,e}^{rad}(r),$$
(20)

where \mathcal{J} is the set of photoinization processes, $\dot{\omega}_{p,e}^{rad}$ is the electron mass production rate for the bound-free process p, and Δh_p is the ionization energy per unit mass of electron.

2.3. Numerical implementation

When radiation is ignored ($S^{rad} = 0$) we follow the implementation of Munafò and Magin [34] for the numerical solution of Eq. (5) of which we recall the main features. Equations are discretized in space by means of the finite volume method. The Roe scheme [45] is used to compute the convective flux at cell interfaces. Boundary conditions, which will be specified in Section 4, are implemented through ghost cells and are imposed in terms of primitive variables. The time integration is fully implicit and is performed until steady state is reached. In order to advance the solution from the time-level *n* to the time-level *n*+1, the fluxes and source terms are linearized around the solution at the time-level *n* by means of a Taylor-series expansion where the Jacobians are computed numerically.

When radiation coupling is considered the radiative source terms are added explicitly to the previous algorithm. They are not computed at each flow time step but are typically updated every 200 flow time steps. Starting from an uncoupled solution, time integration is performed until steady state is reached. In order to reduce the computational time, radiative calculations are carried out on a coarse mesh in which the convective cells are grouped by five based on an extensive grid convergence analysis. The angular integration of the intensity field is achieved by computing the intensity at each point for 20 regularly spaced cos ϑ values between -1 and 1. This relatively coarse angular discretization was found sufficiently accurate for the planar geometry associated with the tangent slab approximation. The spectral integration over the wavenumber σ in Eqs. (18) and (19) is achieved using the Hybrid Statistical Narrow Band model, which will be detailed in Section 3. Finally, radiative source terms are linearly interpolated from the cell centers of the radiation mesh to the cell centers of the flow mesh.

3. The Hybrid Statistical Narrow Band model for radiative transfer

The spectral radiative intensity at an arbitrary point *s* of an optical path starting at point s=0 is given by the solution of the radiative transfer equation, such that

$$I_{\sigma}(s) = I_{\sigma}(0)\tau_{\sigma}(0,s) + \int_0^s \eta_{\sigma}(s')\tau_{\sigma}(s',s) \, ds', \qquad (21)$$

where $\tau_{\sigma}(s', s) = \exp(-\int_{s'}^{s} \kappa_{\sigma}(s'') ds'')$ is the spectral transmissivity between points s' and s. We search for an expression of the averaged intensity $\overline{I_{\sigma}(s)}^{\Delta\sigma}$ over a spectral narrow band $\Delta\sigma$. First, the radiative mechanisms are grouped into different contributions: e.g. a molecular electronic system, a set of atomic lines, or a continuum process. These contributions are assumed to be statistically uncorrelated, which allows us to write

$$\overline{I_{\sigma}(s)}^{\Delta\sigma} = \overline{I_{\sigma}(0)}^{\Delta\sigma} \prod_{k} \overline{\tau_{\sigma}^{k}(0,s)}^{\Delta\sigma} + \sum_{k} \int_{0}^{s} \overline{\eta^{k}(s')\tau_{\sigma}^{k}(s',s)}^{\Delta\sigma} \prod_{k'\neq k} \overline{\tau_{\sigma}^{k'}(s',s)}^{\Delta\sigma} ds', \quad (22)$$

where the index k refers to a radiative contribution. Numerical tests have shown that the uncorrelation assumption between atomic lines and molecular lines was valid with an accuracy of about 1%. Note that we also assume in Eq. (22) the mean intensity at the starting point of the path (s=0) to be uncorrelated with the total transmissivity as we will only consider gray radiation leaving the boundaries of the domain.

For the evaluation of the term $\overline{\eta_{\sigma}^k(s')\tau_{\sigma}^k(s',s)}^{\Delta\sigma}$ in Eq. (22), we use different procedures which are presented in the following subsections: (i) a SNB model for optically thick molecular systems; (ii) a box model for optically thin molecular systems and continua; (iii) a LBL treatment for atomic lines. When all contribution types are included, the resulting method is named the Hybrid Statistical Narrow Band (HSNB) model.

The criterion retained to decide whether a molecular system is thick or thin is based on the maximum value of the optical depth $\kappa_{\sigma}l$ for a plasma at thermodynamic equilibrium with T=8000 K, p=2 atm and l=10 cm. If the maximum value of $\kappa_{\sigma}l$ is greater than 0.1, the molecular system is considered as thick.

3.1. Statistical narrow band model for optically thick molecular systems

For an optically thick molecular system, the emission coefficient and transmissivity are strongly correlated. However, the ratio $\eta_{\sigma}/\kappa_{\sigma}$ can be considered uncorrelated to the transmissivity τ_{σ} , allowing us to write

$$\overline{\eta_{\sigma}^{k}(s')\tau_{\sigma}^{k}(s',s)}^{\Delta\sigma} = \frac{\overline{\eta_{\sigma}^{k}(s')}}{\kappa_{\sigma}^{k}(s')} \frac{\partial \tau_{\sigma}^{k}(s',s)}{\partial s'}^{\Delta\sigma} \simeq \frac{\overline{\eta_{\sigma}^{k}(s')}}{\kappa_{\sigma}^{k}(s')} \frac{\partial \tau_{\sigma}^{k}(s',s)}{\partial s'}^{\Delta\sigma}.$$
(23)

.

This assumption is valid at thermal equilibrium where the ratio $\eta_{\sigma}/\kappa_{\sigma}$ is equal to the Planck function which is nearly constant within a narrow band. For thermal none-quilibrium conditions, Lamet et al. [33] checked that this assumption remains satisfactory for atmospheric entry flow applications. Discretizing the optical path into homogeneous cells of size $\Delta s_i = s_{i+1} - s_i$, the contribution of optically thick molecular systems to the mean intensity is thus written as

$$\frac{\overline{t}_{\sigma}^{\text{thick}}(s_{j})}{\sum_{k \in \mathcal{T}} \sum_{i=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{i+1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{i}, s_{j})}^{\Delta \sigma} \right) \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{i-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{i}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{i-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{i}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{i-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{i}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{i-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{i}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{i}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} - \overline{\tau_{\sigma}^{k}(s_{j-1}, s_{j})}^{\Delta \sigma} \right)} \frac{\overline{\eta_{\sigma}^{k}}}{K_{\sigma}^{k}} \Big|_{\substack{k \in \mathcal{S} \\ k \neq k}}}^{\sum_{j=0}^{j-1} \left(\overline{\tau_{\sigma}^{k}(s$$

where T is the set of optically thick molecular systems and S is the set of all the systems. A mean equivalent point s_i^* is introduced to simplify the spatial integration between s_i and s_{i+1} , such that

$$\overline{\tau_{\sigma}^{k}(s_{i}^{*},s_{j})}^{\Delta\sigma} = \sqrt{\overline{\tau_{\sigma}^{k}(s_{i+1},s_{j})}}^{\Delta\sigma} \overline{\tau_{\sigma}^{k}(s_{i},s_{j})}^{\Delta\sigma}.$$
(25)

This pragmatic choice does not cause any significant loss of accuracy.

From statistical assumptions concerning the intensity and the position of the lines within a narrow band $\Delta\sigma$, the SNB model [46] provides an expression for the mean transmissivity of a homogeneous column of the form

$$\overline{\tau_{\sigma}(l)}^{\Delta\sigma} = \frac{1}{\Delta\sigma} \int_{\Delta\sigma} \exp(-\kappa_{\sigma} l) \, d\sigma = \exp\left(-\frac{\overline{W}}{\delta}\right),\tag{26}$$

where δ is the mean spacing between the line positions within $\Delta \sigma$ and \overline{W} is the mean black equivalent width of these lines. The mean black equivalent width can be set as a function of three band parameters: the mean absorption coefficient $\overline{\kappa_\sigma}^{\Delta\sigma}$ of the absorbing species and two overlapping parameters $\overline{\beta_D}^{\Delta\sigma}$ and $\overline{\beta_L}^{\Delta\sigma}$ related to Doppler and Lorentz broadening. For addressing non-homogeneous optical paths, both the Curtis-Godson and the Lindquist-Simmons approximations have been considered. The Lindquist-Simmons approximation is known to be more accurate but also more computationally expensive compared to Curtis-Godson. Numerical tests have shown that the precision of the Lindquist-Simmons approximation was required during coupled calculations because it prevents numerical instability in the free-stream region. Details are given in Appendix A.

The required band parameters for radiative transfer calculations ($\overline{\eta_{\sigma}/\kappa_{\sigma}}^{\Delta\sigma}$, $\overline{\kappa_{\sigma}}^{\Delta\sigma}$, $\overline{\beta_L}^{\Delta\sigma}$, $\overline{\beta_D}^{\Delta\sigma}$) have been calculated in Ref. [33] for thick molecular systems of air and in Ref. [47] for thick molecular systems in Martian atmospheres. They have been tabulated according to two temperatures *T* and *T*^{ve} for 199 spectral bands of constant size $\Delta\sigma = 1000 \text{ cm}^{-1}$ in the range [1000–200,000 cm⁻¹]. As explained by in Ref. [33], the parameters can be converted for treating arbitrary electronic level populations as each electronic molecular system is treated independently.

3.2. Box model for optically thin molecular systems and continua

If a molecular system *k* is optically thin for all wavenumbers σ ($\kappa_{\sigma}^{k}l \ll 1$, *l* being a typical length of the problem), the mean transmissivity over a spectral narrow band can be simply expressed by $\overline{\tau_{\sigma}^{k}(s',s)}^{\Delta\sigma} = \exp\left(-\int_{s'}^{s} \overline{\kappa_{\sigma}^{k}(s')}^{\Delta\sigma} ds''\right)$. In addition, the correlation between the emission coefficient and the transmissivity is weak such that one can write $\overline{\eta_{\sigma}\tau_{\sigma}}^{\Delta\sigma} \simeq \overline{\eta_{\sigma}}^{\Delta\sigma}\overline{\tau_{\sigma}}^{\Delta\sigma}$. These two simplifications also hold for continua because of their weak spectral dynamics.

Therefore, the contribution to the mean intensity of the set of optically thin molecular systems and continua, B, is then written as

$$\overline{I_{\sigma}^{\text{box}}(s_{j})}^{\Delta\sigma} = \sum_{k \in \mathcal{B}} \sum_{i=0}^{j-1} \overline{\eta_{\sigma}^{k}} \Big|_{i}^{\Delta\sigma} \prod_{k \in \mathcal{S}} \overline{\tau_{\sigma}^{k}(s_{i}^{*}, s_{j})}^{\Delta\sigma} \Delta s_{i}.$$
(27)

Band parameters $(\overline{\eta_{\sigma}^{k}}^{\Delta\sigma}, \overline{\kappa_{\sigma}^{k}}^{\Delta\sigma})$ for optically thin molecular systems have been tabulated according to two temperatures *T* and *T*^{ve}. As for thick molecular systems, they can be converted for treating arbitrary electronic level populations.

Band parameters for continua have been tabulated according to one temperature (T^{ve} for free–free processes, photoionization and photodetachment, and T for O₂ photodissociation). For bound-free processes, three parameters have been tabulated in order to treat chemical non-equilibrium between the species involved in the process: the spontaneous emission coefficient $\overline{\eta}_{\sigma}^{eq} \Delta^{\alpha\sigma}$, the true absorption coefficient $\overline{\kappa}_{\sigma}^{abs} \Delta^{\alpha\sigma}$ and the induced emission coefficient $\overline{\kappa}_{\sigma}^{ie,eq} \Delta^{\alpha\sigma}$. For example, for a photoionization process ($A + hc\sigma \Rightarrow A^+ + e^-$), the spontaneous and induced emission coefficients have been tabulated according to the partial pressure of species *A*, assuming chemical equilibrium between *A* and A^+ concentrations. Under chemical nonequilibrium conditions, the actual radiative properties can be retrieved according to

$$\overline{\eta_{\sigma}^{k}}^{\Delta\sigma} = \overline{\eta_{\sigma}^{k, eq}}^{\Delta\sigma} \chi^{neq}, \qquad (28)$$

$$\overline{\kappa_{\sigma}^{k}}^{\Delta\sigma} = \overline{\kappa_{\sigma}^{k,\text{abs}}}^{\Delta\sigma} - \overline{\kappa_{\sigma}^{k,\text{ie,eq}}}^{\Delta\sigma} \chi^{\text{neq}}, \tag{29}$$

$$\chi^{\text{neq}} = \frac{n_{A^+} n_{e^-}}{n_A} \frac{Q_A}{2Q_{A^+} \xi} \exp\left(\frac{E_{\text{ion}}}{k_B T^{\text{ve}}}\right),\tag{30}$$

where n_s is the number density of species s, Q_s is the electronic partition function of species s, ξ is the volumetric translational partition function of free electrons, E_{ion} is the ionization energy of species A and k_B is the Boltzmann constant. Similar relations can be derived for photodissociation processes.

For both continua and thin molecular systems, the size of the spectral bands and the spectral range are the same as for thick molecular systems.

3.3. Line-by-line treatment of atomic lines

For atmospheric entry applications, many atomic radiative transitions are optically thick. Attempts have been made to derive a SNB model for atoms but the results were not sufficiently accurate due to the weak spectral density of atomic lines [33]. Therefore, the contribution of atomic lines to the mean intensity is treated in a LBL manner,

$$\begin{split} & \frac{\overline{\rho}_{\sigma}^{\text{It}}(s_{j})}{\sigma}^{\Delta\sigma} = \sum_{i=0}^{j-1} \frac{\eta_{\sigma}^{\text{It}}}{\kappa_{\sigma}^{\text{It}}} \Big| \left(\tau_{\sigma}^{\text{at}}(s_{i+1},s_{j}) - \tau_{\sigma}^{\text{at}}(s_{i},s_{j}) \right) \\ & \times \prod_{\substack{k' \in S \\ k' \neq a}} \overline{\tau_{\sigma}^{k'}(s_{i}^{*},s_{j})}^{\Delta\sigma}, \end{split}$$
(31)

where the first average is computed exactly over the narrow band.

High resolution atomic radiative properties are computed according to

$$\eta_{\sigma} = \sum_{ul} n_u \frac{A_{ul}}{4\pi} \int_{ul}^{se} (\sigma - \sigma_{ul}) h c \sigma, \qquad (32)$$

$$\kappa_{\sigma} = \sum_{ul} \left[n_l B_{lu} f_{ul}^a (\sigma - \sigma_{ul}) - n_u B_{ul} f_{ul}^{ie} ((\sigma - \sigma_{ul})) \right] h\sigma, \tag{33}$$

where A_{ul} , B_{ul} and B_{lu} are the Einstein coefficients related to spontaneous emission, induced emission and absorption of the transition $u \rightarrow l$, n_u and n_l are the number densities of the upper and lower levels and σ_{ul} is the wavenumber of the transition, f_{ul}^{se} , f_{ul}^a and f_{ul}^{ie} are the line profiles associated to spontaneous emission, absorption and induced emission, respectively. The line shapes are related to one another to retrieve equilibrium at T^{ve} [46]

$$f_{ul}^{ie}(\sigma - \sigma_{ul}) = f_{ul}^{se}(\sigma - \sigma_{ul}) \left(\frac{\sigma_{ul}}{\sigma}\right)^3,$$
(34)

$$f_{ul}^{a}(\sigma - \sigma_{ul}) = f_{ul}^{se}(\sigma - \sigma_{ul}) \left(\frac{\sigma_{ul}}{\sigma}\right)^{3} \exp\left(\frac{hc(\sigma - \sigma_{ul})}{k_{B}T^{ve}}\right).$$
(35)

A Voigt profile is considered for the spontaneous emission line shape f_{ul}^{ee} . Einstein coefficients are taken from the NIST database and collisional broadening data are taken from Refs. [15,48].

The LBL treatment of atomic lines is not too penalizing because of the small number of atomic lines (of the order of few thousand) compared to the number of molecular lines (of the order of several million). Furthermore, the spectral grid dedicated to atomic radiation can be much smaller as compared to the LBL spectral grid including all radiative contributions. For this work, an adaptive spectral grid which combines the 11 point stencil per line proposed in Ref. [49] and a refinement procedure between two lines in order to accurately capture the far wing regions has been implemented. More details regarding this procedure are given in Appendix B.

4. Results

Three hypersonic entry conditions have been studied: two conditions of Earth entry corresponding to the trajectory points t=1634 s and t=1642.66 s of the FIRE 2 experiment and one condition of Titan entry corresponding to the trajectory point t=191 s of the Huygens probe entry. The FIRE 2 experiment has been the subject of many numerical studies because of the availability of flight data [50,51]. In addition, the study of the first trajectory point t = 1634 s allows to investigate strong thermal nonequilibrium effects. The Titan test case has been chosen to show strong molecular radiation effects coming from the CN-Violet system [39,52].

Boundary conditions for the numerical simulations are given in Table 1. The wall of the vehicle is assumed to be non-ablative, non-catalytic and isothermal at $T = T^{ve} = T_w$ and a no slip condition for the velocity is prescribed. In the free stream, temperature, velocity and mass densities are imposed. For radiation, we assume that the boundaries of the computational domain are black walls at T_w and T_∞ .

For Earth entries, a mixture of 11 species (e⁻, N, N⁺, O, O^+ , NO, N₂, N₂⁺, O₂, O₂⁺, NO⁺) is considered. Chemical reactions and rates are taken from Ref. [53]. The radiative systems taken into account are listed in Table 2. For photodetachment processes, the computation of N⁻ and O⁻ concentrations are based on a chemical equilibrium assumption with N and O. For Titan entries, a mixture of 13 species (N, C, H, N₂, C₂, H₂, CN, NH, CH, CH₂, CH₃, CH₄, HCN) at thermal equilibrium is envisaged. For the trajectory point considered, thermal nonequilibrium effects are weak and ionization is insignificant. Chemical reactions and rates are taken from Ref. [54]. Finally, all radiative systems taken into account are listed in Table 2.

4.1. Accuracy and efficiency of the HSNB model

In order to assess the accuracy and the efficiency of the HSNB model, a comparison with the rigorous Line-By-Line (LBL) method is carried out. In LBL calculations, radiative properties of the plasma are computed from the spectroscopic HTGR database [18] on a high resolution spectral grid of 4.4×10^6 points in order to capture correctly all the atomic and molecular lines.

It is also interesting to compare the HSNB model with the Smeared-Rotational-Band model, which is often used as a simple model to treat molecular radiation but may lead to a strong overestimation of radiative fluxes. For this purpose, we implemented a model similar to the Smeared-Rotational-Band that will be called hereafter HSNB-Weak. It consists in computing the mean transmissivity of thick molecular systems according to $\overline{\tau_{\sigma}^{k}(s',s)}^{\Delta\sigma}$ = $\exp\left(-\int_{s'}^{s} \overline{\kappa_{\sigma}^{k}(s')}^{\Delta\sigma} ds''\right)$ instead of Eq. (26). For the three entry conditions described previously

(FIRE 2 (1634 s, 1642.66 s) and Huygens (191 s)),

Table 1

Conditions for the trajectory points t = 1634 s and t = 1642.66 s of the FIRE 2 experiment and for the trajectory point t=191 s of the Huygens probe entry. Radius of the vehicle R_0 , wall temperature T_w and free stream conditions (temperature T_{∞} , velocity u_{∞} , total mass density ρ_{∞} and mass fractions y_{∞}).

Case	FIRE 2	FIRE 2	Huygens
	(1634 s)	(1642.66 s)	(191 s)
$R_0 (m) T_w (K) T_\infty (K) u_\infty (km/s) \rho_\infty (kg/m^3) y_\infty (%)$	$\begin{array}{c} 0.935\\ 615.0\\ 195.0\\ 11.36\\ 3.72\times10^{-5}\\ 77.0-23.0\\ (N_2-O_2) \end{array}$	$\begin{array}{c} 0.805 \\ 480.0 \\ 273.0 \\ 10.56 \\ 7.17 \times 10^{-4} \\ 77.0 - 23.0 \\ (N_2 - O_2) \end{array}$	$\begin{array}{c} 1.25 \\ 1000.0 \\ 183.0 \\ 4.788 \\ 3.18 \times 10^{-4} \\ 98.84 \\ -1.16 \\ (N_2 \\ -CH_4) \end{array}$

calculations have been performed with the LBL, HSNB-Weak and HSNB models from the same flowfield corresponding to the coupled result obtained with the HSNB model. Table 3 gives the incident radiative flux at the wall, together with the total computational time for one radiation calculation, for the different combinations of models and test cases. Compared to the reference LBL solutions, the HSNB model provides an accurate prediction of the incident radiative flux, with an error between 3% and 5% and a speed up factor around 80 for the computational time. Most of the computational gain comes from the calculation of LBL molecular spectra which is very expensive due to the large number of molecular lines.

From Table 3, the HSNB-Weak model provides reasonably accurate results for Earth entry with a difference of 3.5% and 4.5% for the two trajectory points. However, for the Titan entry case, the incident radiative flux is overpredicted by 26%. These are expected results based on a previous assessment of Smeared-Rotational-Band models in Ref. [24]. Concerning the computational times, the HSNB-Weak model is 5 times faster than the HSNB model for Earth entry cases. The Lindquist-Simmons approximation used for computing mean transmissivities over non-homogeneous paths for thick molecular systems (see Section 3.1 and Appendix A) is responsible for the lower computational efficiency of the HSNB model.

The spectral and cumulated incident radiative fluxes at the wall are displayed in Fig. 2 for the early trajectory point (1634 s) of the FIRE 2 experiment. It can be seen that the complex structure of the LBL spectral flux is correctly captured by both HSNB and HSNB-Weak models, with a good agreement on the total cumulated flux (see Table 3 for numerical values). The incoming radiation mostly arises from molecular and atomic transitions in the Vacuum Ultraviolet. The accuracy of the HSNB model should also be assessed regarding the total radiative energy source term along the stagnation line. Fig. 2 also shows this distribution together with the difference with LBL calculations normalized by the absolute maximum value of the total radiative source term. The differences do not exceed 5% for both HSNB and HSNB-Weak models. The highest discrepancies are located near the shock position, where the radiation emission is at a maximum.

Table 2

Radiative systems considered for Earth and Titan entries.

Earth entries	N N ⁺ O O ⁺
Thick molecular	N_2 (Birge-Hopfield 1 and 2. Worlev-lenkins.
systems	Worley, Caroll–Yoshino), O ₂ (Schumann– Runge), NO (β , β' , γ , γ' , δ , ε)
Thin molecular	N ₂ (first and second positive), NO (11,000 Å,
systems	infrared), N_2 (first and second negative,
Bound-free processes	$\frac{Meiner}{Meiner}$
bound-nee processes	dissociation (Ω_2) photodetachment
	$(N^-, 0^-)$
Free-free processes	N, O, N ⁺ , O ⁺ , N ₂ , O ₂
Titan entries	
Thick molecular	N ₂ (Birge–Hopfield 1 and 2, Worley–
systems	Jenkins, Worley, Caroll-Yoshino), CN violet, C ₂ Swan
Thin molecular	N ₂ (first and second positive), CN (red,
systems	LeBlanc), C ₂ (Philips, Mulliken, Deslandres-
	D'Azambuja, Ballik and Ramsay, Fox–
	Herzberg)

Table 3

Comparison between LBL, HSNB-Weak and HSNB models for FIRE 2 (1634 s), FIRE 2 (1642.66 s) and Huygens (191 s) cases. Incident radiative fluxes and computational times for one radiation calculation.

FIRE 2 (1634 s)	LBL	HSNB-Weak	HSNB
$q_w^{rad,i}$ (W/cm ²)	146.78	151.94	150.85
t_{CPU} (s)	20,480	41	242
FIRE 2 (1642.66 s)	LBL	HSNB-Weak	HSNB
q _w ^{rad,i} (W/cm ²)	553.78	578.81	581.97
t _{CPU} (s)	19,140	51	250
Huygens (191 s)	LBL	HSNB-Weak	HSNB
$q_w^{rad,i}$ (W/cm ²)	82.68	104.26	86.24
t_{CPU} (s)	13,158	5	105

The spectral and cumulated incident radiative fluxes at the wall and the total radiative source term along the stagnation line are shown for the Titan test case in Fig. 3. While the HSNB model reproduces with a good accuracy the LBL calculation, both the spectral flux and the total radiative source term are strongly over-predicted by the HSNB-Weak model. This failure comes from an incorrect treatment of the CN-Violet molecular system in the spectral range [25,000–29,000 cm⁻¹]. For this case, the value of the HSNB model is clearly realized.

An additional assessment of the accuracy of the HSNB model is proposed in Appendix C where we have reproduced the LBL results of Ref. [31] concerning the trajectory point t=189 s of the Huygens probe entry.

4.2. Analysis of radiation effects on flow and heat transfer

In this section, the results of coupled simulations obtained with the HSNB model are compared to the results of uncoupled simulations to show how radiative transfer affects the aerothermodynamic fields and the heat fluxes at the wall of the vehicle.

4.2.1. FIRE 2 (1634 s)

The FIRE 2 flight conditions of the early trajectory point t=1634 s correspond to a high velocity entry into a low density atmosphere (see Table 1). The plasma flow around the vehicle is then in strong thermal nonequilibrium that may not be correctly described by multi-temperature models [42].

In order to investigate non-Boltzmann effects, we implemented for this particular case the Quasi-Steady State (QSS) model proposed by Johnston [55]. For each radiation calculation, non-Boltzmann populations of electronic levels of N and O as well as the first electronic levels (X, A, B, C) of N_2 and N_2^+ are determined from simple correlations depending on the macroscopic state of the flow (electron temperature, total number densities). An additional assumption is made concerning N_2 VUV systems (Birge-



Fig. 2. FIRE 2 (1634 s). Comparison between LBL, HSNB-Weak and HSNB models. Left: spectral and cumulated incident fluxes at the wall. Right: total radiative source term along the stagnation line and differences with LBL calculations normalized by the maximum absolute value.



Fig. 3. Huygens (191 s). Comparison between LBL, HSNB-Weak and HSNB models. Left: spectral and cumulated incident fluxes at the wall. Right: total radiative source term along the stagnation line and differences with LBL calculations normalized by the maximum absolute value.

Table 4
FIRE 2. Standoff distance δ , conductive flux at the wall q_w , radiative flux at the
wall q_w^{Iau} and incoming radiative intensity at the wall I_w over spectral intervals
$\Delta \sigma_1 = [16, 667 - 33, 333 \text{ cm}^{-1}]$ and $\Delta \sigma_2 = [2500 - 50, 000 \text{ cm}^{-1}]$.

FIRE 2 (1634 s)	Uncoupled	Coupled	Coupled	QSS Flight data
δ (cm)	5.36	5.05	5.21	-
q_w (W/cm ²)	94.9	76.3	76.5	-
q_w^{rad} (W/cm ²)	203.6	150.0	74.7	-
$I_w(\Delta \sigma_1) (W/cm^2/sr)$	2.05	2.12	1.28	0.1
$I_w(\Delta \sigma_2) (W/cm^2/sr)$	8.57	7.16	4.71	1.3
FIRE 2 (1642.66 s)	Uncoupl	ed Co	oupled	Flight data
δ (cm)	4.06		4.01	-
$q_w (W/cm^2)$	635.6	6	17.0	-
q_w^{rad} (W/cm ²)	791.3	58	31.7	_
$I_w(\Delta \sigma_1) (W/cm^2/sr)$	11.65		9.28	10.5
$I_w(\Delta\sigma_2) (W/cm^2/sr)$	71.01	5	53.63	63

Hopfield 1 and 2, Worley–Jenkins, Worley, Caroll–Yoshino): the population of the upper energy levels of these transitions, which are above the dissociation limit, are computed according to a chemical equilibrium assumption with atomic Nitrogen. The non-Boltzmann populations are taken into account in the HSNB model using Eqs. (32) and (33) for atomic radiation and using expressions given in Ref. [33] for band parameters of molecular systems. It should be underlined that this QSS model used for radiation is not consistent with the flow modeling, though it provides a first approximation of thermal non-equilibrium effects. The full consistent state-to-state coupling between flow and radiation has been recently achieved for instance in Ref. [22] for atomic electronic states.

Table 4 compares the uncoupled, coupled, and coupled QSS results concerning the shock standoff distance, the conductive flux, and the radiative flux at the wall. The coupling effect is to decrease all of these quantities due to the radiative cooling associated with the strong radiative emission in the shock layer. The shock layer thickness decreases because the

plasma density increases and the heat fluxes decrease because the temperature levels are lower. In the coupled QSS case, the same trends are obtained but to a lesser extent. Table 4 also shows the incoming radiative intensity at the wall over two specific spectral ranges corresponding to the experimental flight data, given with an uncertainty of 20%. All uncoupled, coupled, and coupled QSS results are far from the flight data, although the QSS case is much closer than the two others.

Fig. 4 displays temperatures along the stagnation line for the uncoupled, coupled, and coupled OSS cases. The uncoupled temperature profile can be split into four regions from right to left: the free-stream, the shock, the equilibrium plateau and the boundary layer close to the wall. Because of the low density, the shock region is wide and in strong thermal nonequilibrium. In the boundary layer, T^{ve} is slightly greater than T, because of atomic recombination which creates vibrational energy. When radiation is considered (coupled case), the temperature distributions are significantly affected. The shock layer spreads out and the equilibrium zone is shortened. Radiative cooling lowers the peak and plateau temperatures. In particular, the maximum of T^{ve} decreases from 14,670 K (uncoupled) to 13,470 K (coupled). Another interesting feature is that the free-stream region is no longer at thermal equilibrium because the radiation absorption from the shock increases electronic and vibrational energy.

Fig. 4 also shows the species molar fractions along the stagnation line. For the uncoupled case, the main chemical mechanisms are the dissociation of molecular nitrogen and oxygen and the ionization of atomic nitrogen and oxygen through the shock. A significant amount of Nitrogen monoxide is also produced in the shock region. The ionization level is quite important in the plateau as the electron molar fraction reaches 0.15. In the boundary layer, the ionization level drops down and atomic nitrogen starts recombining. For the coupled case, the fall of the two temperatures slows down the ionization reactions and the electron molar fraction reaches a maximum of 0.08. The free-stream region ahead of the shock becomes chemically reacting under the effect of radiation: atomic oxygen is

produced by photodissociation and electrons are produced mainly by photoionization of molecular oxygen.

These coupling effects on temperature and composition are also noticeable in Fig. 4 for the coupled QSS case, however they are much weaker. In order to understand this behavior, the radiative source term along the stagnation line is plotted in Fig. 5 and split according to the atomic, molecular, and continua emission contributions. From uncoupled to coupled calculations, the peak of the radiative source term is decreased by a factor two due to radiative cooling. From coupled to coupled OSS calculations, the peak of the radiative source term is further reduced and atomic contribution almost vanishes at the shock location. The reason is that the T^{ve} Boltzmann distribution leads to an overestimation of the population of the highest electronic energy levels of atomic N and O, as well as N_2 and N_2^+ . In particular, for the N2 VUV systems, the dissociation equilibrium assumption makes the population of the upper electronic energy level associated with these systems close to zero and thus cancels their contribution to radiation. The remaining molecular emission peak in Fig. 5 comes mostly from NO radiation, of which electronic energy levels are assumed to be populated according to the temperature T^{ve}. An incorrect treatment of the thermal state of NO might be responsible of the remaining discrepancies between the coupled OSS results and the flight data.

4.2.2. FIRE 2 (1642.66 s)

The FIRE 2 flight conditions of the trajectory point t=1642.66 s correspond to a quasi-thermal equilibrium situation. Due to the higher density, the kinetic energy transfer between the internal energy modes is much faster than for the trajectory point t=1634 s. Thus, the QSS model has not been considered in this case.

As it can be seen in Table 4, the standoff distance and the conductive flux slightly decrease and the radiative flux diminishes by around 25% when radiation is coupled to the flow. In addition, coupled results are in fair agreement with flight data which are given with an uncertainty of 20%. Temperatures and composition along the stagnation line are shown in Fig. 6. For the uncoupled case, the flow is in thermal equilibrium everywhere except in the shock region. A chemical equilibrium zone with flat molar fraction profiles is clearly distinguishable between the boundary layer and the shock. The electron molar fraction is around 0.07 in this zone. When radiation is considered, as for the previous trajectory point, the vibration-electronic-electron temperature T^{ve} increases and a slight fraction of O, e⁻ and O₂⁺ are produced in the free stream by photodissociation and photoionization of O₂. The temperature is slightly decreased in the shock layer, leading to a lower ionization level.

4.2.3. Huygens (191 s)

This Titan entry case has been selected to show the ability of the HSNB model to handle strong optically thick molecular radiation. For early trajectory points, a state-to-state electronic specific model of the CN molecule is required [39,55]. As thermal nonequilibrium modeling has been already discussed for the FIRE 2 t = 1634 s case, we will focus here on an quasi-equilibrium case at the trajectory point t = 191 s.

When coupled radiation effects are taken into account, the standoff distance decreases from 10.77 (uncoupled) to 10.33 cm (coupled), the conductive heat flux decreases from 24.2 to 22.0 W/cm² and the radiative flux decreases from 95.6 to 80.57 W/cm². The radiative flux obtained in the uncoupled case is in agreement with Ref. [52]. They found a radiative flux of 75 W/cm² but they applied to their results a correction coefficient of 0.75 to model the 3D effects.

The temperature and CN molar fraction along the stagnation line are plotted in Fig. 7. In the shock layer, we can notice a lower temperature due to radiative cooling and a higher CN molar fraction because of lower dissociation rates.

The role of CN radiation, especially the CN-Violet system, has been highlighted when discussing the accuracy of the HSNB model in Section 4.1. Indeed, it can be seen in Fig. 8 that the dominant contributors to radiation are the CN-Violet, followed by the CN-Red molecular systems. N_2 radiation also contributes



Fig. 4. FIRE 2 (1634 s). Temperatures and composition along the stagnation line.



 $x\ (m) \qquad \qquad x\ (m)$ Fig. 6. FIRE 2 (1642.66 s). Temperatures and composition along the stagnation line.

0.02

0.04

0

0.04

0.02



Fig. 7. Huygens (191 s). Temperature and CN molar fraction along the stagnation line.

significantly at the emission peak. However, C_2 radiation is weak. When radiation is coupled to the flow, the emission is reduced at the peak because of the lower temperature.

1e-05

0

5. Conclusion

We have shown in this paper the ability of the HSNB model to accurately and efficiently predict radiation effects on hypersonic entry flows. The HSNB model reproduces the LBL results with an accuracy better than 5% and a speed up of the computational time around two orders of magnitude. Concerning molecular radiation, the HSNB model provides a significant improvement compared to the Smeared-Rotational-Band model in the case of Titan entry dominated by optically thick CN radiation. Taking into account the coupling with radiation, both convective and radiative heat fluxes at the wall decrease. The standoff distance is reduced due to radiative cooling of the shock

NO₄

1e-05

0.06



Fig. 8. Huygens (191 s). Total radiative source term along the stagnation line.

layer. For Earth entry cases, we observed slower ionization levels as well as the appearance of O, e^- and O_2^+ in the free stream produced by the photodissociation and the photoionization of O_2 .

This study was focused on a 1D flow-radiation model in order to demonstrate the feasibility of coupled simulations with the HSNB model. However, 2D or 3D simulations may be required to determine the spatial distribution of the heat flux on the wall. For these geometries, coupled calculations are not practical with a LBL description of radiative properties. Though through the use of parallelization, the HSNB model may be used to compute radiative source terms accurately in a reasonable amount of time. The Monte Carlo method would be probably the best algorithm to solve the radiative transfer equation in this case.

The analysis of the first trajectory point of the FIRE 2 experiment has shown that the two temperature approach was not satisfactory to model the thermal nonequilibrium state of the plasma. The results obtained using non-Boltzmann electronic populations provided by the QSS model of Johnston [55] were closer to the flight data even if some discrepancies still remain. For such entry conditions (high velocity, low density), a self-consistent electronic specific collisional-radiative model should be developed. The HSNB model could be used since it is compatible with arbitrary populations of electronic states.

Finally, it is worth mentioning the usefulness of the presented HSNB model for studying coupled ablationradiation phenomena in the boundary layer of future entry vehicles. Light-weight carbon-phenolic ablators have already been extensively used for several recent missions and are likely to dominate future space missions as we look forward to evermore challenging entry environments. One notable effect that ablators may have on the radiation field is the ability of blown ablation products to absorb radiant energy from the shock layer and carry this energy down stream of the stagnation region. As several of the relevant carbonaceous species have already been included in the HTGR database and their HSNB band parameters have already been presented, the HSNB model could be used to significantly reduce the cost of ablation-radiation studies in the future.

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Appendix A. Curtis–Godson and Lindquist–Simmons approximations for SNB model

For a homogeneous optical path, analytical expressions can be derived for the mean black equivalent width \overline{W}/δ introduced in Eq. (26) for mean transmissivity calculations. These expressions depend on the broadening mechanism and a prescribed distribution law for line intensities within the narrow band and are functions of two parameters: a mean absorption coefficient \overline{k} per unit partial pressure of the absorbing species and an overlapping parameter $\overline{\beta}$.

For a non-homogeneous optical path, the Curtis–Godson approximation consists in using the expressions derived for homogeneous media with averaged parameters \overline{k}^* and $\overline{\beta}^*$ that we define according to

$$u = \int_{s'}^{s} p_a(s'') \, ds'', \tag{A.1}$$

$$\overline{k}^* = \frac{1}{u} \int_{s'}^{s} p_a(s'') \overline{k(s'')} \, ds'', \tag{A.2}$$

$$\overline{\beta}^* = \frac{1}{u\overline{k}^*} \int_{s'}^s \overline{\beta(s'')} p_a(s'') \overline{k(s'')} \, ds'', \tag{A.3}$$

where *u* is the mean pressure path length and p_a the partial pressure of the absorbing species. Expressions of the mean black equivalent width $\overline{W_L(s',s)}/\delta$ and $\overline{W_D(s',s)}/\delta$ for both Lorentz and Doppler broadening are given in Table 5. In order to obtain the mean black equivalent width in the Voigt broadening regime, we use the expression proposed of Ref. [56]

$$\frac{\overline{W_V}(s',s)}{\delta} = u\overline{k}^* \sqrt{1 - \Omega^{-1/2}},\tag{A.4}$$

Table 5

Expressions of mean black equivalent width for Curtis–Godson approximation and its derivative for Lindquist–Simmons approximation. The first column indicates the broadening type and the distribution function considered for line intensities. For Doppler broadening, the tailed-inverse exponential distribution is used for air systems (N_2 , O_2 , NO) and the exponential distribution is used for carbonaceous systems (CN, C_2).

Approximation	Curtis–Godson $\frac{\overline{W}(s',s)}{\delta}$	Lindquist-Simmons $-\frac{1}{\delta} \frac{\partial \overline{W}(s^{'},s)}{\partial s^{'}}$
Lorentz, tailed-inverse exponential	$2\overline{\beta_L}^*\left(\sqrt{1+\frac{u\overline{k}^*}{\overline{\beta_L}^*}}-1\right)$	$p_a(s^{''})\overline{k(s^{''})}_{(1-r^2+2x)\sqrt{1+2x}}^{2xr+(1-r^2)\sqrt{1+2x}}$
		$X = \frac{u\overline{k}^*}{2\overline{\beta_L}^*}, \ r = \frac{\overline{\beta_L}(s')}{\overline{\beta_L}^*}$
Doppler, exponential	$rac{\overline{eta_D}^*}{\sqrt{\pi}} \int_{-\infty}^{+\infty} rac{\operatorname{xexp}(-\xi^2)}{1+\operatorname{xexp}(-\xi^2)} d\xi$	$\frac{p_a(s^{'})\overline{k(s^{'})}}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{\exp(-\xi^2)}{(1+x\exp(-r^2\xi^2))}d\xi$
	$X = \frac{u\bar{k}^*}{\bar{\rho}_D^*}$	$X = \frac{u\overline{k}^*}{\overline{\beta_D}^*}, r = \frac{\overline{\beta_D}(s^*)}{\overline{\beta_D}^*}$
Doppler, tailed-inverse exponential	$\frac{\overline{\rho_{D}}}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\ln\left(1+\operatorname{xexp}(-\xi^{2})\right)d\xi$	$\frac{p_a(s^{'})\overline{k(s^{'})}}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{\exp(-\xi^2)}{(1+x\exp(-r^2\xi^2))}d\xi$
	$X = \frac{u\overline{k}^*}{\beta_D^*}$	$X = \frac{u\overline{k}^{*}}{\overline{\beta_{D}}^{*}}, \ r = \frac{\overline{\beta_{D}(S^{*})}}{\overline{\beta_{D}}^{*}}$



Fig. 9. FIRE 2 (1634 s). Comparison between Curtis–Godson and Lindquist–Simmons approximations.

$$\Omega = \left[1 - \left(\frac{1}{u\overline{k}^*}\frac{\overline{W_L}(s',s)}{\delta}\right)^2\right]^{-2} + \left[1 - \left(\frac{1}{u\overline{k}^*}\frac{\overline{W_D}(s',s)}{\delta}\right)^2\right]^{-2} - 1.$$
(A.5)

An alternative approach for treating non-homogeneous optical path is the Lindquist–Simmons approximation [57]. It consists in finding expressions for the space derivative of the mean black equivalent widths in Lorentz $\partial W_L(s'', s)/\partial s''$ and Doppler $\partial W_D(s^*, s)/\partial s''$ broadening regimes. The expressions used is in this work are given in Table 5. They involve both local parameters $\overline{k}(s^*)$, $\overline{\beta}(s^*)$ and averaged parameters $\overline{k}^*, \overline{\beta}^*$. The non-uniform mean black equivalent widths in each broadening regime are then obtained by spatial integration, according to

$$\frac{\overline{W_{L/D}(s',s)}}{\delta} = \int_{s'}^{s} \frac{1}{\delta} \frac{\partial \overline{W_{L/D}(s'',s)}}{\partial s''} ds'', \tag{A.6}$$

and Eqs. (A.1) and (A.2) are used again to get the mean black equivalent width in the Voigt broadening regime.

A comparison between the HSNB Curtis–Godson and the HSNB Lindquist–Simmons is given in Fig. 9 for the FIRE 2 (1634 s) test case. The difference between the two approximations is very tiny and for most of the points is much lower than the difference between HSNB Lindquist– Simmons and LBL calculations. However, we can see a much larger discrepancy in the free stream: the radiative source term predicted by the HSNB Curtis–Godson model becomes negative while it remains positive for the HSNB Lindquist–Simmons and LBL models. A negative energy source term in this cold region is a major computational issue for coupling because negative temperatures can be predicted after few iterations. This is why the Lindquist– Simmons approximation has been chosen for the coupled simulations even though it requires around three times more computational time.

Appendix B. Adaptive spectral grid for atomic radiation

This appendix describes the method for generating an adaptive spectral grid for the LBL treatment of atomic radiation in the HSNB model (Section 3.3). We start from an 11 point stencil [49] defined by σ_{ul} , $\sigma_{ul} \pm \Delta$, σ_{ul} being the line center and Δ the 5 point half-stencil

$$\Delta = \left\{ \frac{1}{8} \gamma_V, \frac{1}{2} \gamma_V, \Delta \sigma_W, \Delta \sigma_{FW}, \frac{25}{2} \gamma_V \right\}.$$
(B.1)

The estimated distances from the line center to the line wing $\Delta \sigma_W$, and to the far wing $\Delta \sigma_{FW}$ are computed by $\{\Delta \sigma_W, \Delta \sigma_{FW}\} = \frac{2}{\pi}(1+\zeta)\gamma_L + \alpha\gamma_D$, where γ_L and γ_D are the half widths at half maximum of the line related to Lorentz and Doppler broadening respectively. The values of the ζ , α constants are taken to be {1, 1.8} for $\Delta \sigma_W$, while they are chosen as {2.6, 5.8} for $\Delta \sigma_{FW}$. $\gamma_V = \sqrt{\gamma_D^2 + \gamma_L^2}$ is the estimated Voigt half width at half maximum. It was shown that such stencil provides a reasonably accurate resolution of line intensities for low pressure atmospheric entry conditions due to the low degree of line broadening in that regime [49].

This fixed point method is likely to work well in spectral regions with a high number of electronic transitions and with a large degree of line overlap because the majority of the points are distributed around the line centers. For areas in which there are large distances between neighboring line centers, the method is likely to provide poor estimates of spectral quantities due to the large error in interpolating the spectral values in the far line wing regions.

For this reason, we implemented an adaptive refinement procedure in order to accurately compute the far line wing regions for atomic spectra which have a relatively weak spectral density. To begin, the complete line list for atoms considered is first ordered by ascending line center values. Then, each region between two consecutive lines is considered. For each consecutive line pair, an adaptive mesh is created based on the two corresponding line shapes. We will denote the left line shape properties with the superscript *L*, and the right properties with an *R*. First, the approximate center point between each line is defined simply as $\sigma_{LR} = (\sigma_{ul}^L + \sigma_{ul}^R)/2$. Next, the following set of points are added to the mesh based on the 11 point stencil, but ensuring that points added for each line do not overlap one another:

$$\sigma_{ul}^{L} + \Delta^{L}, \quad \forall \Delta^{L} < \sigma_{LR} - \sigma_{ul}^{L}$$
(B.2)

$$\sigma_{ul}^{L} - \Delta^{R}, \quad \forall \Delta^{R} < \sigma_{ul}^{R} - \sigma_{LR} \tag{B.3}$$

For lines which are sufficiently close, the above procedure will prevent unnecessary points from being added to the spectral grid. For lines which are very far apart in comparison to their line widths, the above set of points are augmented by adding points recursively to the center region by successively bisecting the two intervals closest to the last points added by the stencil above until the spacing between the outermost two stencil points for each line is at least half the size of the spacing between the outermost stencil point and the next point. In other words, two bisection fronts are propagated towards the line centers until the spacing between points matches that of the two outermost stencil points of each line.

The accuracy of this adaptive procedure has been successfully compared with the fine LBL spectral grid of 4.4×10^6 spectral points that we use for full LBL calculations [58]. The differences we obtained were negligible compared to the accuracy of the full HSNB model which is around a few percent (see Section 4.1). The spectral size of the adaptive mesh for atomic radiation was around 4×10^4 points for the applications considered in this paper, which allows the computational time to be two order of magnitude less. Thus this adaptive spectral mesh procedure constitutes a decisive development for the practical use of the HSNB model.

Appendix C. Accuracy of the HSNB model against literature results

The accuracy of the HSNB model has been assessed in Section 4.1 by comparison with LBL results, where both HSNB parameters and LBL radiative properties were obtained from the HTGR spectroscopic database. The purpose of this appendix is to compare the HSNB model with reference results obtained by other researchers.

We have considered the LBL radiation simulation of Bansal and Modest [31] of the trajectory point t = 189 s of



Fig. 10. Huygens (189 s). Comparison between LBL, HSNB and LBL results from Bansal and Modest [31]. Contribution of the CN red and violet systems to the radiative source term along the stagnation line.

the Huygens probe entry from uncoupled flowfield taken from Johnston [55]. The spectroscopic constants were taken from Laux [59] and nonequilibrium populations of the CN electronic states were considered.

In order to reproduce their results we have computed the radiative source term along the stagnation line with both the HSNB model and the LBL approach. For the CN electronic states, both Boltzmann populations and nonequilibrium populations based on the QSS model of Bose et al. [60] have been taken into account. The comparison is shown in Fig. 10 for the CN red and violet systems. First of all, we can see that for a given population assumption, our LBL and HSNB results give similar results. When the QSS model is used, we obtain a good agreement with the LBL results of Bansal and Modest [31] for both LBL and HSNB. Note that nonequilibrium effects are not negligible in the considered simulation and lead to about 16% difference at the peak value of the radiative source term.

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