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A note on radiation preheating of some hydrocarbons by combustion products

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ABSTRACT

The aim of this paper is to provide upper bounds of the radiation emitted by hot combustion products, mainly CO_2 and H_2O, and absorbed by some gaseous cold hydrocarbons, or by cold CO_2 and H_2O. Line by line calculations with accurate spectroscopic data bases are used to compute the absorbed power under two geometrical configurations: a cold optically thin medium surrounded by spherical hot combustion products, and a thin cold slab in front of a hot combustion parallel slab. The absorbed power and the corresponding characteristic time scale are adjusted by simple and physically based formulas to provide quick estimations for various values of combustion product temperature, pressure, and the radius of the hot sphere or the hot slab thickness. The obtained time scales can be compared in a given application to hydrodynamic or diffusive time scales to decide whether it is necessary to take this preheating phenomenon into account or not.

1. Introduction

While radiation emission by hot combustion products is known to affect flame structure, temperature distribution and pollutant production, especially for large scale flames, the effects of radiation absorption by fresh fuel vapors or particles is less understood and is generally neglected. Joulin and Deshaies soon demonstrated the importance of radiation preheating on flame propagation when the gaseous mixture is seeded with inert or reactive particles [1,2]. For combustion processes involving pure gases, the partial overlapping between the emission spectra of hot products and absorption spectra of fuels may lead to significant radiation preheating of fuel vapors. Few studies have included this phenomenon in the investigation of flame structures [3,4]. Cai et al. show significant absorption by CH_4 when simulating the Sandia D flame [4]. They also show that accurate spectral models are required to compute accurately this absorption. On the other hand, several studies focused on the feedback of fuel vapor absorption on radiative transfer in pool fires [5–8]. It was shown for instance in [7] that, even for small scale pool fires, accurate gas-phase absorption spectra are required for calculating radiation heat transfer to the pool surface.

Another application where absorption by fresh gases was shown to be important is the measurement of flame speeds using spherical combustion chambers with various diluents [9–12]. The induced radiation uncertainties were found to be the most important when the fuels are diluted with H_2O and CO_2.

Depending on the combustion problem under consideration, and on the desired accuracy, radiative transfer through fresh gases can be neglected or not. Therefore, the aim of this paper is to provide quick estimates of the radiation preheating time scales to enable a researcher or engineer to neglect, when applicable, the cumbersome calculations of radiative transfer through fresh hydrocarbons or fresh H_2O and CO_2, on the basis of sound physical arguments. Upper bounds of net radiative powers (source term in the energy balance equation) are calculated by assuming that the fresh gases are optically thin, which leads to lower bounds of the associated time scales. In the following, we present first the spectroscopic data bases used for spectrum calculations (Section 2), then the geometrical configurations considered in this study (Section 3). The obtained volumetric absorbed powers and their adjustments by simple formulas are presented in Section 4, and some practical applications of the obtained results are finally discussed in Section 5.

2. Spectroscopic databases and line by line calculations

For each considered molecule and thermodynamic condition, the absorption coefficient κ_ν at wavenumber ν is given by

$$\kappa_\nu = \sum_{\ell \to u, E_\ell < E_u} S_{\ell u}(T) n_{\rm abs} f_{\ell u}(\nu - \nu_{\ell u}), \tag{1}$$

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where the sum extends to all radiative transitions $\ell \rightarrow u$ between molecular levels ℓ and u of respective energies E_ℓ and E_u. n_{abs} designates the absorbing molecule volumetric population, $S_{\ell u}(T)$ the intensity of the transition at temperature T, $\nu_{\ell u}$ is the central wavenumber of the transition, and $f_{\ell u}$ is the absorption spectral line shape. Contributing radiative transitions have been taken from up-to-date spectroscopic databases which provide for each listed transition $\nu_{\ell u}$, E_ℓ, and the line intensity $S_{\ell u}(T_{\text{ref}})$ at a reference temperature T_{ref}. The intensity at any temperature T is therefore obtained according to

$$S_{\ell u}(T) = S_{\ell u}(T_{\text{ref}}) \exp\left(-\frac{E_\ell}{kT} + \frac{E_\ell}{kT_{\text{ref}}}\right) \frac{1 - e^{-\frac{hc\nu_{\ell u}}{kT}}}{1 - e^{-\frac{hc\nu_{\ell u}}{kT_{\text{ref}}}}} \frac{Q(T_{\text{ref}})}{Q(T)}, \quad (2)$$

where $Q(T)$ is the internal partition function of the molecule at temperature T, h and k designate respectively the Planck and Boltzmann constants, and c the speed of light in vacuum. At high temperature, it is important to extend the sum in Eq. (1) to all contributing levels. The atmospheric HITRAN spectroscopic database [13] is known to be insufficient for CO_2 and H_2O at combustion temperatures.

The CDSD-4000 database [14] was selected for CO_2 since it has been shown to be accurate up to 4000 K at moderate spectral resolution [15]. The collisional broadening parameters are those provided in this database (air and self broadening Half Width at Half Maximum, and the temperature dependence coefficients). We use for H_2O the HITEMP 2010 database [16] which was obtained by merging the well established HITRAN 2008 data and a selection of lines from the extensive theoretical BT2 database [17]. The BT2 database was shown to provide accurate results by comparison with the few available experimental spectra of hot water vapor [16]. However, about ten lines in HITEMP 2010 appeared to be not reliable and were removed from the database (see Ref. [18] for more details). The HITEMP 2010 database provides also collisional broadening parameters in the case of air- and self-broadening (HWHM) but no temperature dependence coefficient in the case of self-broadening. We have thus retained the collisional broadening parameters of Ref. [19].

Some medium resolution spectroscopic data are available in the literature at relatively high temperature for several hydrocarbons (see e.g., Refs. [20,21] for several fuel vapors and Ref. [22] for CH_4). However, as we are mostly interested by radiation absorption by molecules at room temperature, we use the HITRAN-2012 database [13] for almost all considered hydrocarbons (CH_4, C_2H_2, C_2H_4, and C_3H_8). For C_2H_6, the linelist of HITRAN-2012 was combined with the pseudo-linelist developed by Harrison et al. in the 3 μm region, on the basis of absorption cross section measurements [23]. Indeed HITRAN-2012 only provides absorption cross sections in this important spectral region, and the use of a linelist enables to reproduce accurately temperature and pressure dependence of the absorption spectra. We have checked that the pseudo-linelist agrees very well with the HITRAN-2012 cross sections in this region (2550–3315 cm^{-1}). Note also that only cross sections are available for C_3H_8 in HITRAN-2012 database. These cross sections were used to produce high resolution absorption coefficients on the same spectral grid as for the other molecules.

For all line by line (LBL) calculations, the covered spectral range extended from 37.5 to 11262.5 cm^{-1} with a spectral resolution $\delta\nu = 0.01$ cm^{-1}. Line wing cutoff was taken at 500 cm^{-1} from line centers for hydrocarbons, while, for the heavy linelists of H_2O and CO_2 (111,346,008 and 573,881,316 lines, respectively), a variable cutoff between 50 and 500 cm^{-1} was used depending on temperature and pressure conditions. The Voigt line profile, combining Doppler and collisional broadening mechanisms, was considered in all LBL calculations.

Figure 1 shows examples of absorption spectra of H_2O and CO_2 at 2000 K, and of the considered hydrocarbons at 296 K, the total pressure being 1 atm The spectra have been downgraded to a resolution of 25 cm^{-1} for legibility reasons. It is clear that the most important overlapping spectral regions are in the red wings of 2.7 μm regions of CO_2 and H_2O bands and in the water vapor emission region between 6 and 10 μm. The important CO_2 ν_3 emission bands near 4.3 μm do not overlap significantly with hydrocarbon absorption spectra.

3. Radiative power and characteristic time scale

3.1. The two geometrical configurations

Two model geometries are considered in the following. In the first one, called *sphere*, the cold absorbing medium is a small sphere of negligible radius, to be considered as optically thin, surrounded by a concentric spherical hot mixture of combustion products of radius R. This configuration is representative of small fuel pockets surrounded by hot combustion products. In fact, the results from this simple geometry could be used for more general configurations as discussed below. The cold and hot gases are assumed to be isothermal at temperatures T_c and $T_{h,}$ respectively, and the whole system is at total pressure p. The molar fraction of the absorbing cold species is equal to 1 for all hydrocarbons and for CO_2 and H_2O. This has negligible incidence on the absorbed radiative power per unit partial pressure or on radiative time scales, except for H_2O whose absorption line widths at low temperature depend significantly on its concentration. Calculations of line broadening were therefore done with a more realistic value X_{H_2O}=0.16 at T_c. If we neglect emission by the cold gas, the absorbed power per unit volume is given by

$$Q^R = -\nabla \cdot \boldsymbol{q}^R = 4\pi \int_0^\infty \kappa_\nu^c(T_c)\left[1 - \exp(-\kappa_\nu^h(T_h)R)\right] I_\nu^0(T_h)\, \mathrm{d}\nu \quad (3)$$

where $\boldsymbol{q}^R$ is the radiative flux vector, κ_ν^c and κ_ν^h are respectively, the absorption coefficients of the cold and hot media given by Eq. (1), and I_ν^0 is the Planck's function.

It is worth noticing that Eq. (3) applies also in the case of spherical cold gases of finite radius R_1 surrounded by hot gases contained in a concentric spherical shell corresponding to $R_1 < r < R_2$. It is sufficient to replace the distance R by $(R_2 - R_1)$ in Eq. (3) to get the absorbed radiative power at the center of the two spheres assuming that the inner sphere remains optically thin. The configuration of concentric spheres is encountered for instance in spherical diffusion or premixed flames where the fuel is injected at the center of the system [24–28]. It is discussed in more details in Section 5.

Furthermore, the factor 4π (steradians) in Eq. (3) can be replaced by an actual angular integration to deal with more complex geometries. For fresh fuels surrounded by nonspherical burnt gases of thickness $R(\boldsymbol{u})$ and temperature $T_h(\boldsymbol{u})$ in incident direction $\boldsymbol{u}$, the absorbed power can be evaluated from

$$Q^R = \int_{4\pi} \frac{Q^R(\boldsymbol{u})}{4\pi} \mathrm{d}\Omega \quad (4)$$

where $Q^R(\boldsymbol{u})$ is the result of Eq. (3) with $R = R(\boldsymbol{u})$ and $T_h = T_h(\boldsymbol{u})$.

In the second model geometry, called *slab*, the absorbing cold medium at T_c is an infinite planar layer of negligible thickness, and is covered on one side by a parallel slab of width L containing the emitting hot mixture at T_h. This configuration is representative of counterflow diffusion or premixed flames and is discussed in more details in Section 5. Pure absorbing species are considered as in the *sphere* configuration. The volumetric radiative power is given in this case by

$$Q^R = -\nabla \cdot \boldsymbol{q}^R = 2\pi \int_0^\infty \kappa_\nu^c(T_c)\left[1 - E_2(\kappa_\nu^h(T_h)L)\right] I_\nu^0(T_h)\, \mathrm{d}\nu \quad (5)$$