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Line-sampling-based Monte Carlo method

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Null-collision Monte Carlo algorithms [1, 2, 3, 4] consist in adding a virtual null-collision coefficient to the real extinction one. These collisions, corresponding to pure forward scattering events, have no effect on the radiative transfer equation. A direct consequence of their introduction is that the resulting extinction coefficient $\hat{\beta}$ (defined as the sum of absorption, scattering and null-collision coefficients) can be defined arbitrarily. It can then be chosen as simple as desired to guarantee a rigorous free path sampling whatever the heterogeneity of the medium properties (pressure, temperature, mole fractions). The intermediate step of producing meshes, that can be the source of unquantifiable bias, is no longer required.

In more formal terms, the exponential extinction term does not depend on the real extinction coefficient anymore, but only on the arbitrary field $\hat{\beta}$. Thereby, the absorption coefficient appears only in a linear form in the recursive integral formulation of radiative transfer equation. Then it becomes possible when studying thermal radiation in a gaseous mixture to decompose the absorption coefficient as the sum of contributions of each molecular transition (or line) for each considered species.

This opens the door to the development of reference methods for which the costly step of producing numerous high-resolution absorption spectra vanishes. The absorption coefficient evaluation is no more required, only some molecular transitions are sampled during the Monte Carlo simulation and their exact contribution to absorption coefficient (for a given wavenumber and a given location) are computed from parameters gathered in molecular spectroscopic databases [5, 6, 7]. Nevertheless, it implies that probabilities must be associated to each molecular species and to each transition. The choice of these probabilities is fully arbitrary and has only an influence on the convergence rate of the algorithm.

Such a probabilistic model is proposed, and the considered Monte Carlo approach is tested and validated against six unidimensional and non-scattering configurations gathered by André and Vaillon in [8]. The description of these cases, that cover a wide variety of high-temperature applications, is depicted in Fig. 1.

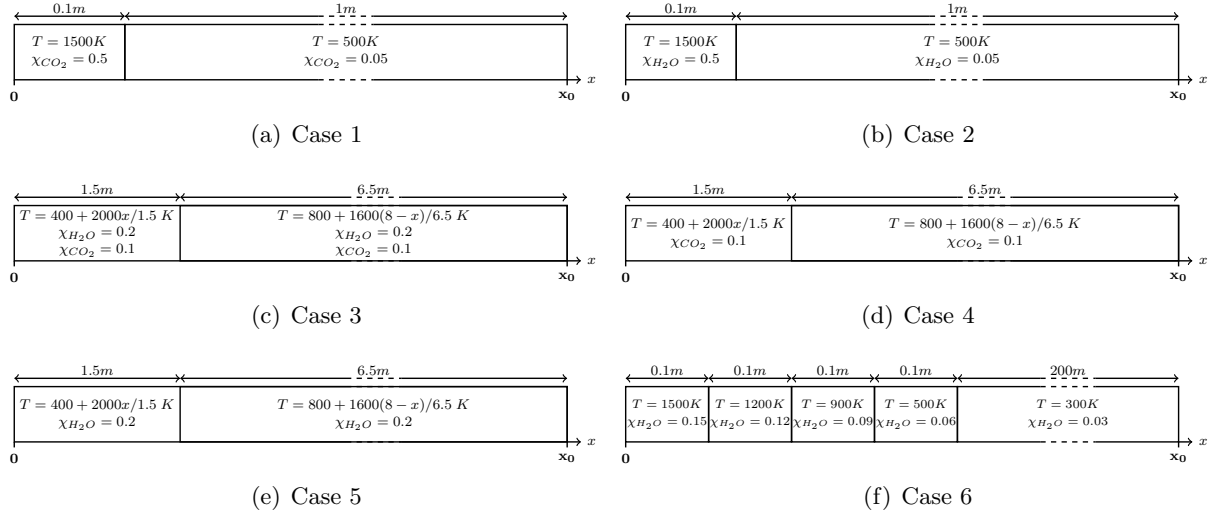


Figure 1. Description of the six test cases. Dimensions, temperature and mole-fractions fields are given. Fields are piecewise defined and atmospheric pressure is retained.

For each case, the considered quantity is the spectrally integrated intensity at location x_0 resulting from the emission/absorption of the gaseous column $[0, x_0]$. The considered range for spectral integration is $[10 - 15000\text{cm}^{-1}]$. Results obtained with the proposed approach (denoted I_{mcm}) and 10^6 independent realizations are given in Tab. 1 with their associated standard deviations. The computation times¹ required to reach a 1% standard deviation are

Table 1. Intensities integrated over the 10 to 15000cm^{-1} range for the six considered test-cases. Estimations obtained by the proposed approach I_{mcm} and 10^6 realizations are given with their associated standard deviation. Also displayed are the computation times required to reach a 1% uncertainty. Results can be compared with those of a line by line simulation I_{lbl} .

Case	I_{mcm} (W/m ² /sr)	σ (W/m ² /sr)	$t_{1\%}$ (s)	I_{lbl} (W/m ² /sr)
1	3125.61	4.42	0.97	3126.06
2	3315.11	8.15	1.38	3311.88
3	39223.87	51.56	1.75	39202.5
4	12325.99	16.16	1.26	12320.1
5	38240.31	49.58	1.27	38215.0
6	885.93	3.93	9.86	886.55

also displayed. These results can be compared to those obtained with a line-by-line approach and denoted I_{lbl} ².

¹ The given computation times were obtained on a single core of an Intel Core i7 processor - 2.8GHz. They exclude the loading of spectroscopic data and of associated probabilities.

² Whereas the line-by-line computation requires, for test-cases 3 to 5, a discretization of the properties fields to be performed, the proposed approach does not need such an approximation. Indeed, the latter is an extension of null-collision algorithms that allow to compute at each collision a quantity depending strictly on the local properties (pressure, temperature, mole-fractions), see [3].

The computation is performed with the *CDS1000* spectroscopic database for CO₂ and with *HITEMP* for H₂O. A line-wing truncation at 25cm⁻¹ is also assumed.

The specific intensities obtained with the proposed Monte Carlo approach and the deterministic line-by-line one are fully consistent. The computation times required by the Monte Carlo approach to get a 1% confidence interval are comprised between 0.97 and 9.86 seconds according to the case study. Because of the stochastic nature of the proposed method, these computation times depend little on the spectral integration range or on the size of molecular spectroscopic database.

Beyond prospects of simulation, this approach offers an important versatility and possibility of analysis due to the fact that the computation does not rely on "rigid" precomputed spectra. For instance, it becomes possible to easily study the effect of a given spectroscopic database, parameter or hypothesis on a radiative observable with the very same algorithm, without having to recompute a large set of spectra to cover the heterogeneity of the medium. Two examples applied to test-case 2 are given in Fig. 2 where the effects of the choice of database and line-wing truncation distance are evaluated.

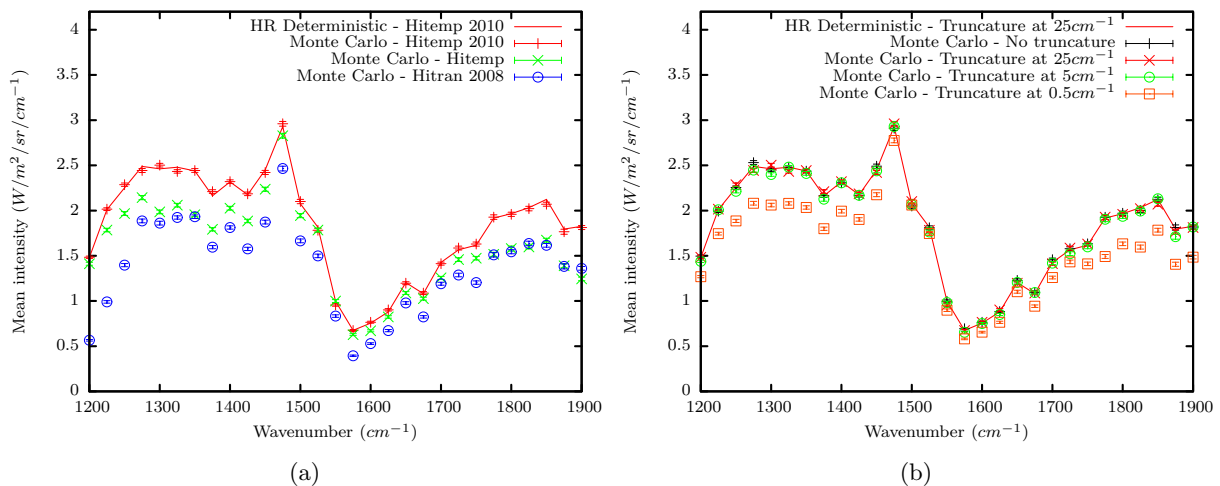


Figure 2. Intensities averaged over several narrowbands, computed for test-case 2, with different spectroscopic databases (a) and different line-wing truncation distances (b). Line-by-line computation are depicted in solid line.

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