EFFICIENT TECHNIQUE FOR DIRECT COMPUTING OF MOLECULAR ABSORPTION

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A quick procedure is proposed for computing of molecular absorption by line–by–line technique, which includes the known up–to–date algorithms reducing computation time by employing nonuniform grid over wavelengths together with a developed criterion for spectral line selection. The selection is made by the magnitude of the optical depth and is most efficient for inhomogeneous atmospheric path as the number of lines decreases with height.

The increasing interest in optimization of direct calculation of molecular absorption is caused by the increasing usage of this method in atmospheric optics applications. Analysis of available algorithms and computer codes[1–12] has revealed a number of factors important to computation efficiency. The present paper considers the selection of spectral lines, which makes it possible to drop out weak lines contributing little to the absorption in the course of numerical simulation.

Modern databases contain considerable number of spectral lines, not all of which contribute measurably to absorption. In this regard, of concern is the development of efficient algorithms for spectral line selection. Simplest of these algorithms drop lines weaker in intensity than some critical value adjusted empirically. More complex ones evaluate absorption coefficients or optical depth. Our analysis has shown all these criteria[4,7,12] to be insufficiently efficient. The error in transmittance due to the dropped lines can be estimated as

$$\Delta T(\nu)/T(\nu) = \Delta\tau_\nu , \qquad (1)$$

where $\Delta T(\nu)$ is the absolute error in the spectral transmittance $T(\nu)$, $\Delta\tau_m$ is the optical depth due to dropped lines, which determines the accuracy of $T(\nu)$ computation. By definition, $\Delta\tau_m$ is integral quantity being a function of not only spectral line strength, but also the altitude profile of gas concentration. Now existing criteria of selection by τ are based on dropping out lines, whose optical depth $\tau(z_1, z_2)$ is less than some threshold value ε (here z_1 and z_2 are the lower and upper altitude limits, respectively). Such a criterion excludes only the weakest lines. The remainder, however, may contain lines which are not necessarily important throughout the altitude range selected. In contrast, our algorithm evaluates the optical depth of the layer $z - z_2$, with z is a current altitude. Now, for each ith line we determine the altitude z_{0i} such that

$$\tau(z_{0\,i}, z_2) \le \varepsilon . \qquad (2)$$

The ith line is assumed to be contributing to absorption up to the altitude z_{0i}. As a result, the higher the altitude, the fewer lines are assumed as contributing ones. The algorithm is shown to be most efficient to treat gases like H_2O, whose concentration rapidly decreases with altitude. For CO_2, slowly decreasing with altitude, and for O_3, increasing with altitude, the algorithm is still applicable, although considering the absorption lines up to higher altitudes. Table I illustrates performance of our criterion of line selection, typical for the middle–IR range. Table I demonstrates that as the altitude increases, the number of nodes m_0 in the uniform frequency grid also increases, due to the decrease of the half–width with altitude. For a fixed altitude, the time of computing the spectral dependence of absorption coefficient is proportional to the product $m \cdot m_0$. Thus, even ozone absorption at the altitude of 40 km is computed 5 times faster with this algorithm. Also, water vapor transmittance within 0–50 km is sufficient to compute only up to z = 10 km.

This criterion not only allows selection of spectral lines, but also, in some cases of slant atmospheric paths, simultaneously fixes the upper altitude limit for transmission function computation.

TABLE I. The number of lines m included in computation of absorption coefficient at different altitudes, and the number of nodes m_0 at which the spectral transmittance is computed.

z, km	m_0	m		
		H_2O	CO_2	O_3
0	30	19	157	205
5	59	4	95	194
10	117	1	66	181
20	465	0	35	113
30	929	0	17	86
40	929	0	12	35

Molecular absorption can be computed with low spectral resolution using line spectrum within this wavelength interval. Generally, uniform frequency grids are employed. However, some algorithms[4,7,10,13,14] resort to adaptive procedures of numerical integration on nonuniform grids to reduce the number of integration nodes. The adaptive procedure of frequency integration used in Ref. 7, for example, allows accurate computation. However, grid steps are determined by the relative accuracy of spectral transmittance, yielding unjustified small integration step in the region of strong absorption, although these spectral ranges are not considerably contributing to transmission function. This shortcoming is avoided using adaptive procedure from Ref. 4. We have

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however shown that the use of this algorithm may require unjustified accurate computation in order to avoid line missing. An interesting procedure of dividing the frequency range is reported in Refs. 13 and 14; the frequency step is determined in terms of the equivalent line width so that it is possible to use coarser grid in the region of strong absorption. This algorithm is highly efficient for computing atmospheric transmittance through a fixed altitude range $z_1 - z_2$. The use of this for a different altitude range requires a change in the frequency grid thus resulting in complicated transmittance computations and repeated absorption coefficient computations.

As we think, the most efficient procedures of dividing the frequency interval are presented in Refs. 1 and 10; they propose the use of uniform grids instead of nonuniform ones, with small steps at line center and large ones at wings. It should be noted, that such an approach was realized in Ref. 1 through the use of an approximation for absorption line shape similar to that in Ref. 17, which may be very much in error in some instances; at the same time, the method of Ref. 10 is usable with any line shape.

We have implemented only the uniform frequency grid algorithm, with frequency step being proportional to the Voigt line half–width. In the infrared range there are more and shorter frequency steps with increasing altitude. That is, the absorption coefficient is calculated for a few frequency points at low altitudes and for more points for higher altitudes due to decreased Voigt line half–width. Our algorithm performs with frequency step that can be altered discretely, by halving an original step. This allows us to use a simple Lagrange interpolation with precomputed coefficients for changing the absorption coefficient or optical depth when transiting to a different grid. From above–mentioned we conclude that most problems with the approach arise at high altitudes, where the spectral lines are the narrowest and where, therefore, less expensive algorithms are required.

With time we plan to modify our algorithm to incorporate dividing the frequency range according to Ref. 10; this will give surprising, at first sight, result of increasing efficiency with increasing height.

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