Problem of a more correct frequency integration in calculation of radiation characteristics

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Line-by-line calculations of IR radiative fluxes with the account of absorption by water vapor show that the fluxes and cooling rates are little sensitive to the step of frequency integration. This fact can be explained from the viewpoint of the probability theory. If the spectral absorption function of the water vapor molecule is considered as a random function, then the characteristics of its "spectrum" allow only a small number of points to be used to reconstruct it. The further decrease of the separation between the points gives the "excess" information in terms of the Shannon theorem.

1. Line-by-line calculation of the fluxes and cooling rates due to water vapor

Calculation of radiative characteristics in climate models is rather time consuming mostly because the application of line-by-line method to calculation of the transmittance imposes strict requirements on the frequency integration: the step of 0.01 cm^{-1} at a medium pressure is a usual practice, at large altitudes the integration step is, as a rule, even smaller (see, for example, Refs. 1 and 2).

At the same time, line-by-line calculations of IR radiative fluxes within the water vapor absorption spectrum indicate that the fluxes and cooling rates are not very sensitive to the step of frequency integration. Let us illustrate this statement by the examples of calculation of the net fluxes and cooling rates in two spectral regions involving water vapor absorption lines: $1.5-340$ and $980-1100$ cm^{-1} with the Voigt profile using different steps of the frequency integration. The former spectral region is characterized by a strong absorption, while the latter one is characterized by a weak absorption. The calculated results are shown in Figs. 1 and 2.

One can see that in the $1.5-340$ cm^{-1} spectral region the change of integration step over a wide range only slightly affects the fluxes and cooling rates in the region of medium pressure. Only the step $\delta\nu = 10.0$ cm^{-1} gives an obvious discrepancy. The calculation at large altitudes, above ~ 100 km (i.e., at low pressure less than $\sim 10^{-1-2}$ mbar) actually requires a small integration step; even the step of 0.01 cm^{-1} proves to be insufficient. The figure corresponding to the $980-1100$ cm^{-1} spectral region is somewhat less illustrative, but it is just this region where the step of 0.1 cm^{-1} is sufficient for close description of the fluxes and rates, while even the step of 1 cm^{-1} proves to be efficient for tentative estimates.
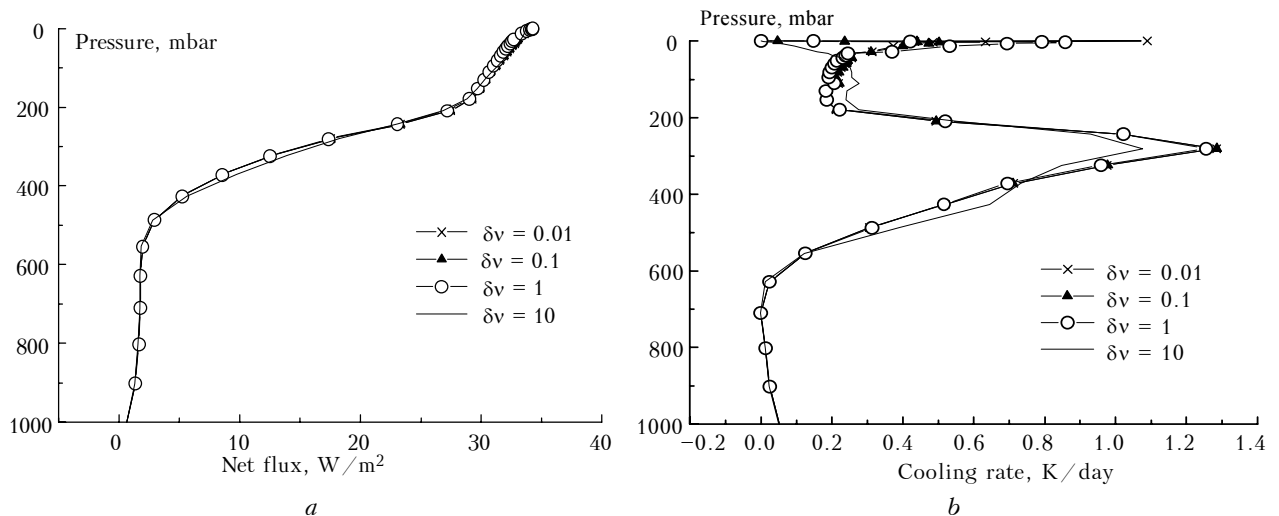

Fig. 1. Line-by-line calculation of the altitude behavior of the radiative flux (*a*) and the cooling rate (*b*) due to the absorption by water vapor in the $1.5-340$ cm^{-1} spectral region at different steps of frequency integration $\delta\nu$.
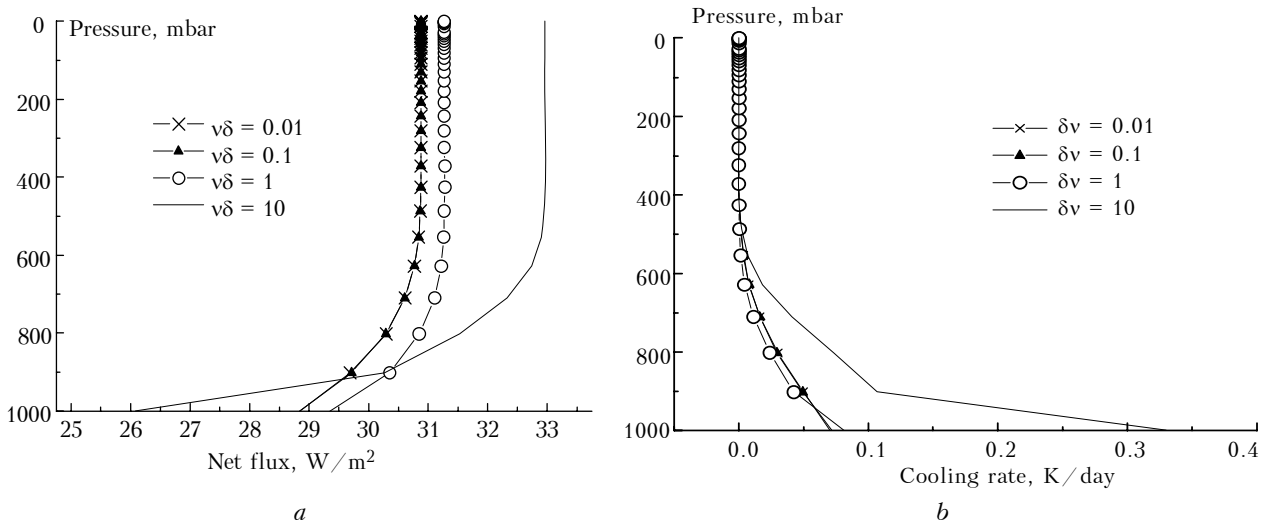
Fig. 2. Line-by-line calculation of the altitude behavior of the radiative flux (*a*) and the cooling rate (*b*) due to the absorption by water vapor in the 980–1100 cm^{-1} spectral region at different steps of frequency integration δν.

This fact is not surprising if we recall that statistical models for absorption bands of water vapor were used successfully in the pre-computer age.[3] The possibility of using not very small frequency step in the case of water vapor can be explained from the viewpoint of the probability theory. It turns out that if the spectral absorption function of the water vapor molecule is considered as a random function, then the characteristics of the "spectrum" of this function allow it to be reconstructed using only a small number of points. The further narrowing of the separation between points gives "excess" information in terms of the Shannon theorem.

2. Introduction into the problem from the viewpoint of the probability theory

Assume that we have a random function $f(x; a)$ for (now conditional) variable x; the set of random parameters (for example, coefficients of series expansion of a random function over the orthogonal determinate functions (referred to as the Karhunen–Loeve expansion). Let $\Phi(a)$ be the distribution function of the parameters a, so the statistical mean can be presented as

$$A_{\mathrm{st}} = \int f(x, a)\, \Phi(a)\, \mathrm{d}a. \qquad (1)$$

The situation is assumed stationary, that is, the mean determined by Eq. (1) is independent of x.

Realizations of the random function $f^{(j)}(x)$ arise, if a acquires some values $a^{(j)}$ "allowed" by $\Phi(a)$. We can also introduce the mean over x (Δx is the averaging range):

$$A_{\mathrm{av}}^{(j)} = \frac{1}{\Delta x} \int \mathrm{d}x\, f^{(j)}(x), \qquad (2)$$

which must depend on j (the number of realization) if following the formal definition (2).

Usually the ergodic situation is considered irrespective of j (that is, for any realization)

$$A_{\mathrm{av}}^{(j)} = A_{\mathrm{st}}. \qquad (3)$$

Let us also note that if $K(x)$ is the correlation function of a random function $f(x; a)$ and $S(t)$ is its Fourier transform we have:

$$S(t) = \frac{2}{\pi} \int_0^\infty K(x)\, \cos xt\, \mathrm{d}x,$$

then the variances of these functions Δx and Δt relate to each other by the following "uncertainty relation"

$$\Delta x\, \Delta t \cong 2\pi. \qquad (4)$$

With these definitions a question arises: at what points should f be measured as a function of x in order is mean to be calculated accurately? The Shannon theorem gives the following answer to this question:

$$f(x) \sim \sum_{n=-\infty}^{+\infty} f\!\left(\frac{\pi n}{\Delta s}\right) \frac{\sin(\pi n - x\,\Delta s)}{\pi n - x\,\Delta s}, \qquad (5)$$

where Δs is the width of the spectrum of the random function. Different relations can be obtained, but it is for certain that $\Delta s > \Delta t$. For most common (canonical) distributions[4]:

$$\Delta s \cong 3\,\Delta t. \qquad (6)$$

Equation (5) states that "measurements" should be conducted at the points

$$x_n = \pi n / (\Delta s). \qquad (7)$$

Since

$$\int_{-\infty}^{+\infty} \frac{\sin by}{y}\, \mathrm{d}y = \pi, \qquad b > 0,$$

the integral (2) proves to be the sum $f(x_n)$.

The value of Δs is estimated from the relation following from Eqs. (4) and (6):

$$\Delta x\,\Delta s \cong 6\pi, \qquad (8)$$

in which

$$(\Delta x) = \frac{\int x^2\,f(x,\,a)\,\Phi(a)\,\mathrm{d}a\,\mathrm{d}x}{\int f(x,\,a)\,\Phi(a)\,\mathrm{d}a\,\mathrm{d}x} \ge (\Delta a)^2, \qquad (9)$$

where Δa is the width of the $\Phi(a)$ distribution. Inequality (9) arises because the integrals entering into Eq. (9) are treated as a convolution of two distributions what always increases the variance.

It follows from Eqs. (9) and (8) that the wider Δa, the smaller Δs. So, in view of Eq. (7), the points using which f is reconstructed prove to be separated more widely.

3. Application
to the absorption function

Assume that the statistical model of the spectrum is well justified. The frequency ω plays the role of x; the set of line centers and intensities forms a; $f(x,\,a)$ is the Bouguer exponent for random line centers and intensities. Within the framework of this model Eq. (1) corresponds to the absorption function. So we actually calculate Eq. (2). Besides, in calculations by the statistical model, ω disappears in Eq. (1), so the ergodicity of Eq. (3) can be considered valid.

However, for the statistical model Δs can be considered to be rather small. The point is that any position of a line is assumed equiprobable; the distribution Δa in this sense is wide. The situation with the intensities S is quite similar. Often the exponential distribution $\sim \exp(S/S_0)$ is written with parameter S_0, and it is also a wide distribution $(\Delta S = 0(S))$.

The "width of the distribution" Δx can be estimated directly using the database of spectroscopic information.

The calculation of the absorption coefficients and the estimation of the correlation function of distribution of the absorption coefficients and its variance made for some spectral ranges in the IR region give $\Delta x \sim 100$ cm^{-1}. It follows herefrom that $\Delta S \approx 5$ cm^{-1}, what gives a very rough upper limit for the integration step to be $1.0-0.1$ cm^{-1}.

Therefore, the points (7) can be separated rather wide, and a decrease in the separation between them simply gives the excess information in terms of the Shannon theorem.

Thus, the decrease of the integration step in radiative calculations is not always justified from the viewpoint of the calculation accuracy.

References

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