A METHOD TO COMPUTE THE ATMOSPHERIC O_2 EXTINCTION SPECTRUM – ANALYSIS AND ESTIMATE OF SOME INPUT PARAMETERS

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Keywords: *O_2 atmospheric system, absorption, single scattering*

Abstract: *A method to compute the solar radiation extinction by the molecular oxygen in the atmosphere was developed. Absorption and single scattering towards the observer were included in the extinction model. Plane parallel atmosphere divided into layers with equal thickness was assumed. A computation following the "line-by-line" method was applied – the calculations were implemented consecutively for each rotational line from A (0,0) band of the oxygen atmospheric system. Study of some needed input parameters was carried out. The optimal number of included transitions and the optimal values of the atmospheric layers thickness and of the upper limit of the atmosphere were estimated. In the purpose of the study, the radiation extinction at different angles of observation and using different atmosphere model parameters was computed. The profiles of the separate rotational lines were obtained and the equivalent widths were calculated in the optimal way. The dependences assuming strong absorption were built for different models and different observation angles. The corresponding temperatures and atmospheric heights were obtained.*

МЕТОД ЗА ПРЕСМЯТАНЕ НА СПЕКТЪРА НА ЕКСТИНКЦИЯ НА АТМОСФЕРНИЯ КИСЛОРОД – АНАЛИЗ И ОЦЕНКА НА НЯКОИ ВХОДНИ ПАРАМЕТРИ

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Ключови думи: *атмосферна система на кислорода, абсорбция, еднократно разсейване*

Резюме: *Създаден е метод за пресмятане на екстинкцията на слънчевата радиация от молекулния кислород в атмосферата. В модела на екстинкцията абсорбция и еднократно разсейване в посока на наблюдателя. Разглежда се плоско паралелна атмосфера, разделена на слоеве с еднаква дебелина. Приложено е пресмятане по метода „линия по линия“ – изчисленията са извършени последователно за всяка ротационна линия от ивицата A(0,0) на атмосферната система на кислорода. Проведено е изследване на някои необходими входни параметри. Оценени са оптималният брой включени преходи, оптималните стойности на дебелината на атмосферните слоеве и на височината на горната граница на атмосферата. За целите на изследванията е пресметната екстинкцията на радиацията при различни ъгли на наблюдение и при различни параметри на модела на атмосферата. Получени са профилите на отделните ротационни линии и еквивалентните им ширини са пресметнати по оптимален начин. Построени са зависимостите при предположение за силна абсорбция за различни атмосферни модели и и различни ъгли на наблюдение. Получени са температурите и съответстващите височини при стандартна атмосфера.*

Introduction

Molecular oxygen is one of the main atmospheric constituents and that's why its extinction bands are between the strongest ones in the observed solar spectrum. A number of computations of the oxygen absorption (e.g. in [1, 2, 3, 4]) and studies of the O_2 scattering in the atmosphere [5, 6, 7] have been carried out.

In this work a method to compute the solar radiation extinction in the atmosphere is used when the solar radiation is registered at a given angle to the horizon. The method is described in detail in [8]. In the model absorption and single scattering by the oxygen molecules towards the observer are included. The absorption in the visible range is strongest in the atmospheric system of O_2. In this work we examine the A(0,0) band of this system.

The present work has 2 basic goals: to optimize the computations and to make a theoretical estimate of the expected differences between the results obtained for different conditions.

Atmospheric model and methods of computation

A plane parallel atmosphere was assumed. The absorption above the considered upper limit was neglected. The atmosphere was divided into parallel layers with equal thickness. Every layer was considered as homogenous and was characterized by a single value of the parameters $\boldsymbol{n}$, $\boldsymbol{T}$ and $\boldsymbol{p}$. The concentration $\boldsymbol{n}$, the temperature $\boldsymbol{T}$ and the pressure $\boldsymbol{p}$ were determined from the used atmospheric model.

Sunlight was considered as a parallel beam. During observations under different directions below the Sun current position (different angles towards horizon) and assuming single scattering in every observation direction rays scattered at different altitudes in the atmosphere are registered.

The principal scheme used for the computations for the assumed atmospheric model is shown in fig.1. The observation is carried out from point *A* under angle *α* towards horizon, in direction l_1. The

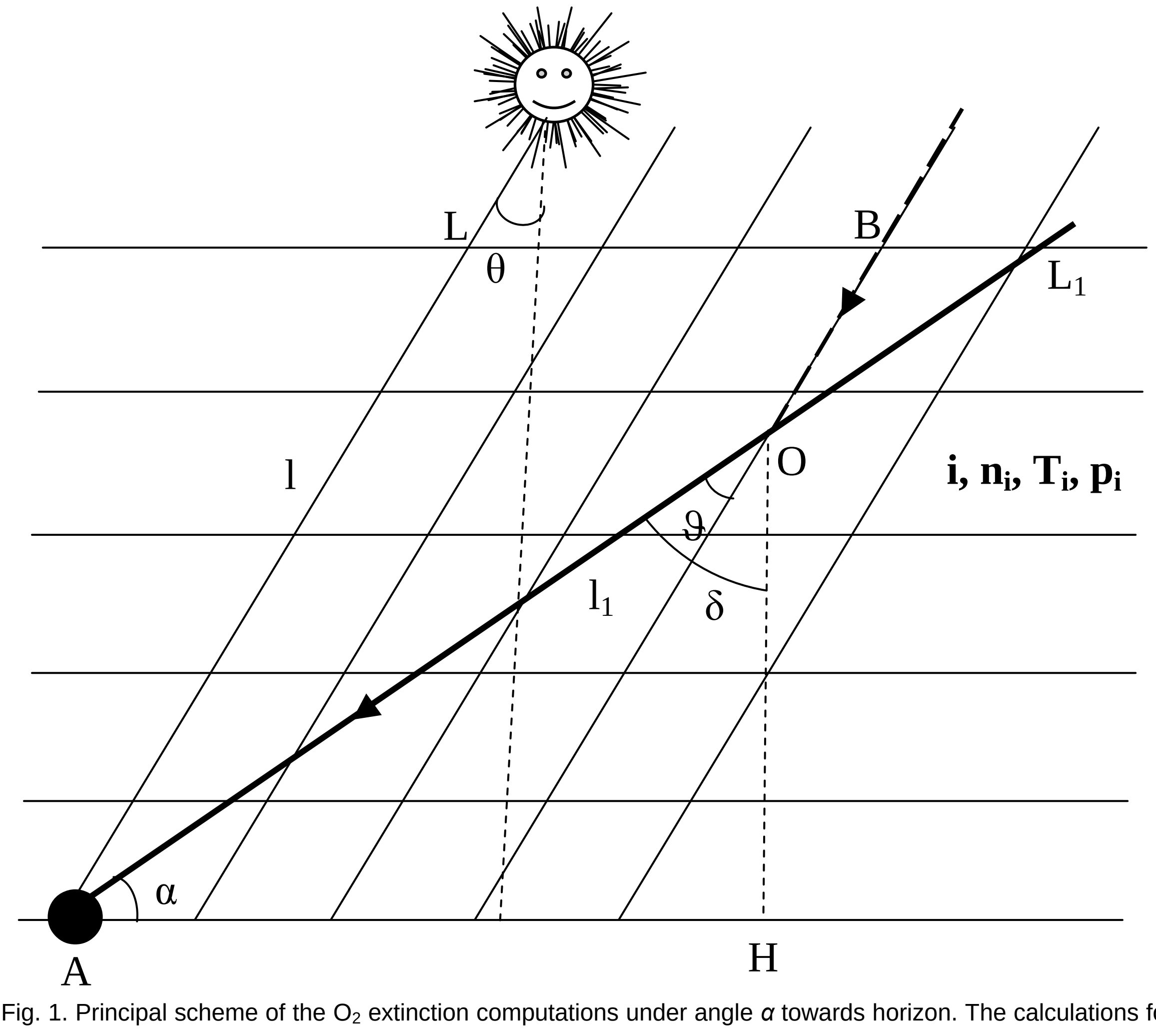

Fig. 1. Principal scheme of the O_2 extinction computations under angle *α* towards horizon. The calculations for every considered ray are divided into 3 parts: calculation of the absorption from the upper edge of the atmosphere to the layer where the ray crosses the direction of observation l_1 (point *O),* absorption and single scattering in direction l_1 in this layer and absorption of the obtained radiation from this layer to the Earth in the direction of observation.

line of observation intersects the upper limit of the atmosphere in point L_1. The zenith angle of the Sun is θ, the direction to the Sun from the point of observation A (l) crosses the upper limit of the atmosphere in point L. Rays, crossing the direction of observations in every atmospheric layer are included in the calculations, i.e. the number of rays is equal to the chosen number of atmospheric layers.

Let's look at a ray starting from point B at the upper limit of the atmosphere (fig.1). It crosses the direction of observation in i-th layer with parameters n_i, T_i and p_i (point O). The computations can be divided into 3 principal parts: 1) calculation of the O_2 absorption from the upper limit of the atmosphere to layer *i-1*; 2) calculation of the absorption and the single scattering of the transmitted radiation in the direction of observation in layer *i*; 3) calculation of the absorption of the obtained up to here radiation from layer *i+1* to the observer in the direction of observation, using as zenith angle $\delta=90^o-\alpha$. The theory and the computations of the absorption and the single scattering are described in detail in [8] and the citations herein.

Optimization of the computations and estimate of the obtained results

In order to study the atmospheric processes and parameters, including temperature, based on spectroscopic methods, to spectroscopic measurements implementation, the processes in the atmosphere are to be modeled. The computed extinction spectra and the derived parameters are intended to be compared with the measured ones. For this reason, precise theoretical spectra are needed. Contrariwise, for more precise results, more sophisticated and time consuming calculations are to be carried out. That is why an optimization of the computing process is indispensible to obtain an adequate and satisfactory result and to facilitate the computations, as well.

Optimization of some input parameters

First, the number of lines to include in the computations was studied. All the lines, enumerated in HITRAN 96 data base of Rothman et al. [9] were used for the calculations. We examined the (0,0) band of the O_2 atmospheric system. The spectra of the P branch alone and of the P and R branches differ considerably because of the strong influence of the intense R branch lines, broaden and superimposed on the R branch spectrum. Thus it is necessary to make all computations for the whole (0,0) band.

The second input parameter that we have studied was the atmospheric layers thickness. It is important, because the number of considered rays and the computation cycles, respectively, depend on it. Thinner layers presume a more correct result, but the computation time may reach inadmissible length. Computations for layer thicknesses 5 km, 2 km, 1 km and 0.5 km were performed. The relative differences between the obtained spectra for consecutive layer thicknesses are presented in fig.2. The relative difference between the spectra with the use of 1 km and 0.5 km layer thickness doesn't exceed 0.1%. This difference was assumed low enough to be neglected. A layer thickness of 1 km was assumed sufficiently low to obtain good results.

Another input parameter that influences the computations and the result correctness is the upper limit of the atmosphere, assumed in the model. Usually, in O_2 spectra computations, a maximal height of 100 km is used, and the O_2 presence at higher altitudes is disregarded. But the O_2 concentration may be low enough at lower altitudes, too. Computations were made with the assumption of upper limit of the atmosphere 100 km, 80 km, 60 km, 50 km, 40 km and the relative differences towards the spectrum for upper limit 100 km were obtained. The result for 60 km and 80 km height is shown in fig.3. The relative difference for 40 km height reaches 0.5%, for 50 km height –

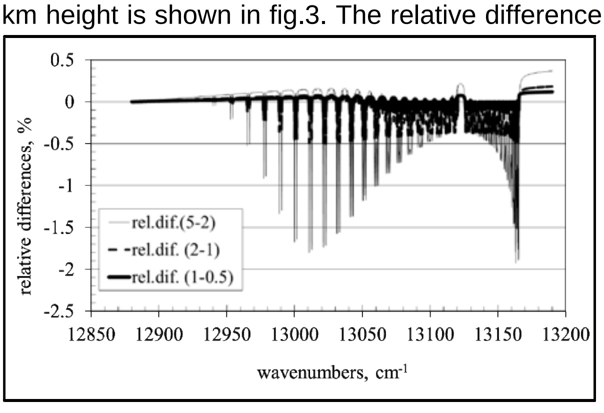

Fig. 2. Relative differences between the spectra computed for atmospheric layers thickness 5 km, 2 km, 1 km and 0.5 km. In the parenthesis the used layer thicknesses for the spectra of the respective relative differences chain are marked.

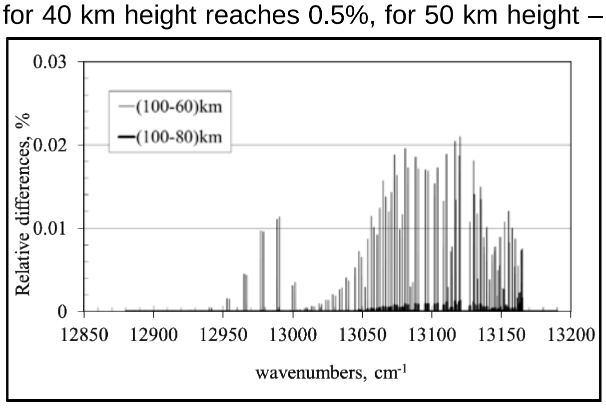

Fig. 3. Relative differences between the spectrum computed for atmospheric height 100 km and the spectra computed for 60 km and 80 km height.

0.09%, for 60 km height – 0.02%, and for 80 km height – 0.001%. Based on these results we admitted that for our computations an atmospheric height of 60 km is enough for our model.

Study of the change in the spectra, computed under different conditions

Using the assumed optimal input parameters, spectra at the same zenith angle (ZA), ZA=30º, under different angles of observation: 50º, 40º, 30º, 20º were computed. The stronger absorption for the smaller angles of observation is seen in the obtained spectra. To approach the real measured spectra, the computed spectra were convolved with a model triangle instrument function with half width 0.4 Å. The differences between the spectra under different angles of observation, and between the convolved spectra were obtained. These differences are of the order of several degrees.

Computations with all O_2 isotopes were implemented, and the differences between convolved spectra with and without O_2 isotopes are examined. The maximal contribution of the isotope lines is about 7-8%. This result necessitates the inclusion of the O_2 isotopes in the computations.

Further we performed computations using different atmospheric models: yearly mean temperatures, January and July temperatures from U.S. Standard atmosphere 1976. Convolved spectra were obtained as well. The relative differences between the spectra by the listed models for non-convolved and convolved spectra were studied. In fig.4 the differences between spectra (non-convolved and convolved ones) by the use of yearly mean temperatures and July temperatures are presented, for the case of ZA=30º and observation angle=50º. The maximal differences for the convolved spectra are about 4-5 times less, near 1.5%. The maximal differences between the spectra for different observation angles are in the frames of 1%.

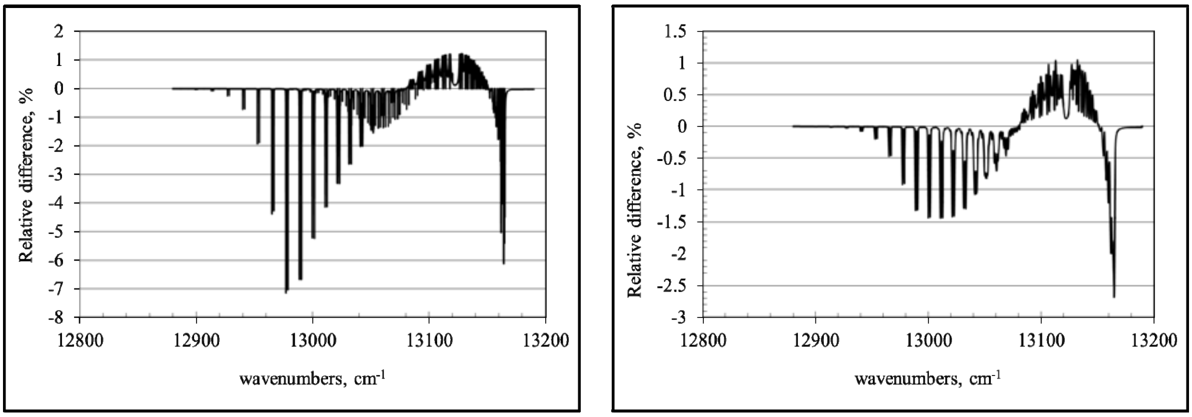

Fig. 4. Relative difference between the spectra obtained with mean annual temperatures and summer temperatures for ZA=30º and observation angle=50º: left – non-convolved spectra, right – convolved spectra.

Computing of the equivalent widths

The equivalent width W_e of a rotational absorption, resp. extinction line is a measure of the area of the line. It is connected to the absorption energy.

To obtain the right equivalent widths, we computed separately the shape of every rotational line. After that, it is necessary to extract correctly the baseline. First, we applied a linear fit below the rotational lines. But a more detailed examination has shown that this way was not entirely right. In fig.5 the lower part of the wavelength interval under considerable magnification is presented. For better clarity and to cover the whole range of lines, 3 lines were included: the first line (N=1), the last one (N=45) and a line of the middle of the P branch, with N=30. It is clearly seen that the baseline was not correctly extracted. Despite the maximal value that has to be extracted is 4 orders lower than the maximal lines intensities, taking into account the longitude of the wavelength range serious inaccuracies in the determined equivalent widths may occur. A polynomial fit of second order was drawn under each line in fig.5. These fits have depicted well the baselines. In fig.6, the lower part of the same lines is presented, after the baseline approach by a polynomial of second order. Such approach is suitable for the baseline extraction.

Dependence between the equivalent widths and the effective temperature

The effective temperature represents the temperature which the gas would take, if the temperature was uniform along the whole length of the atmospheric column, saving the internal gas energy. It was obtained that T_{eff} corresponds to the temperature at 6 km of altitude of the standard atmosphere.

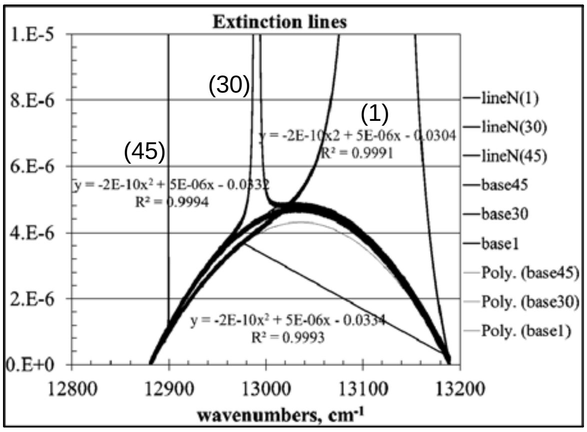

Fig. 5. Magnification of the lower part of 3 rotational extinction lines of the (0,0) P branch after the baseline extraction by a linear fit. The corresponding polynomial baselines and their equations are shown as well.

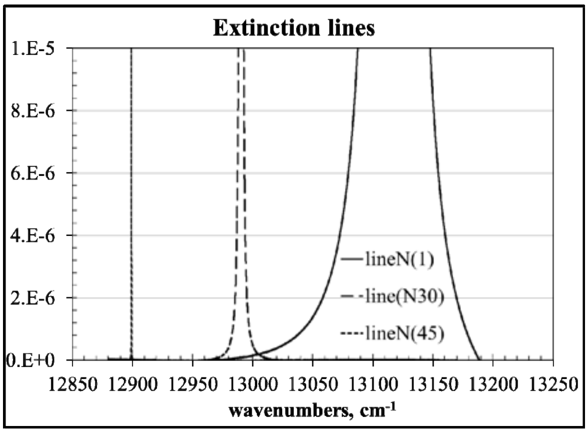

Fig. 6. Magnification of the lower part of the same lines as in fig.5 after the baselines extraction by a polynomial of 2 order.

T_{eff} is defined as:

$$T_{eff} = \frac{\int_0^\infty n(z)T(z)dz}{\int_0^\infty n(z)dz} = \frac{\int_0^\infty n(z)T(z)dz}{N} \tag{1}$$

The effective temperature is connected to the equivalent width. In the case of strong absorption, the following dependence is obtained:

$$\ln\left(\frac{W_e}{S_{JJ}^{1/2}}\right) = const - \frac{B_0 hc}{kT_{eff}} \frac{J(J+1)}{2} \tag{2}$$

where S_{jj} is the line strength, J is the rotational quantum number of the lower level and T_{eff} is the effective temperature.

The dependencies between ***$ln(W_e/S_{jj}^{1/2})$*** and ***$J(J+1)/2$*** at different observation angles for 3 cases: yearly mean, January and July data from U.S. Standard atmosphere 1976 were constructed, using the determined theoretically W_e. In fig.7 are shown these dependences for observation angles 50º and 15º. The corresponding temperatures are calculated. These temperatures correspond to atmosphere columns inclined towards horizon by 50º and 15º, respectively. At lower observation angles higher corresponding temperatures are obtained, which agrees with the used model of the temperature profiles.

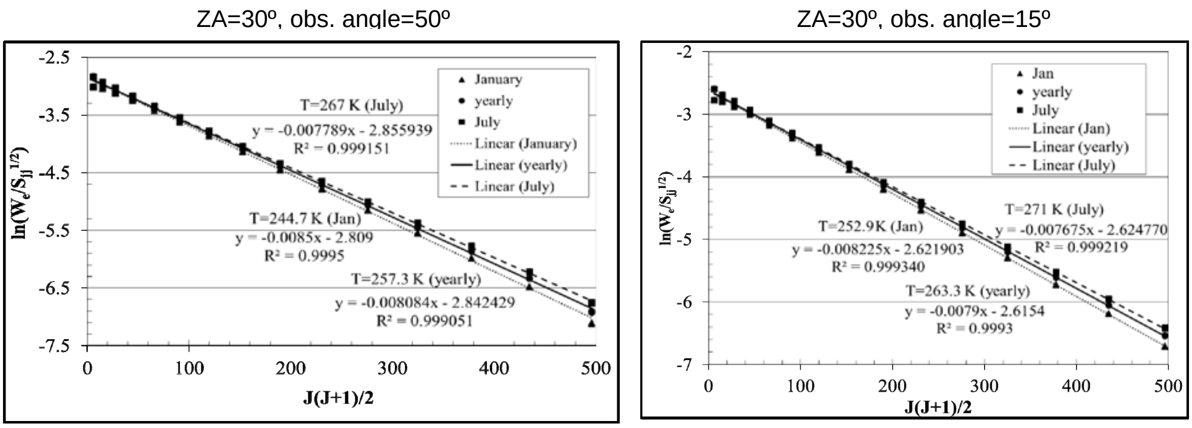

Fig. 7. Computed dependencies of ***$ln(W_e/S_{jj}^{1/2})$*** on ***$J(J+1)/2$*** at different observation angles for 3 cases: yearly mean, January and July data from U.S. Standard atmosphere 1976. The trend is linear, confirming the strong absorption. The corresponding temperatures are calculated.

The obtained temperatures by the January, July and yearly mean data are correct in regard to each other in reference to the used models.

These results confirm that the theoretically obtained extinction spectra and equivalent widths are of good accuracy and may be used to model real conditions and analyze atmosphere processes together with ground based extinction spectra measurements.

By the obtained temperatures, the corresponding standard atmosphere altitudes were determined. In Table 1 the results for the corresponding temperatures and standard atmosphere altitudes for the different models for some cases of absorption and extinction are presented. The effective temperatures and the corresponding heights are included as well.

Table 1. Temperatures and corresponding standard atmosphere altitudes, obtained by the We dependencies

	Absorption, ZA=0°	Extinction, ZA=30°, OA=50°	Extinction, ZA=30°, OA=15°	
US Standard 1976	T H	T H	T H	T_{eff} H
January		244.7 K 6 km	252.9 K 4 km	243.93 K 6 km
Yearly mean	263.22 K 4 km	257.3 K 5 km	263.3 K 4 km	250.27 K 6 km
July		267.0 K 5 km	271.0 K 4.5 km	258.33 K 6 km

Conclusions

The optimal number of included transitions and the optimal values of the atmospheric layers thickness and of the atmospheric height were estimated.

The radiation extinction at different angles of observation and using different atmosphere model parameters was computed. The obtained differences were examined.

The profiles of the separate rotational lines were obtained and a way to calculate correctly the equivalent widths was found out.

The dependences assuming strong absorption were built for different models and different observation angles. The corresponding temperatures and atmospheric heights were obtained.

Based on the obtained results it can be concluded that the computation of the extinction spectra and the equivalent widths is accurate. Therefore such computations can be used to model real measurement conditions. By the use of theoretical estimates and spectroscopic measurements the corresponding atmospheric temperature could be evaluated.

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