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Simple parameterization of the absorption of the solar Lyman-alpha line

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Abstract. The absorption of the solar Lyman-alpha line by the terrestrial atmosphere is calculated, taking in account the wavelength variations of the emission line and of the O_2 cross-section, as well as the temperature dependence of the cross-section. A new parameterization is developed to reproduce in atmospheric models the results of this high-resolution calculation, up to an attenuation of 10^{10} for the incident solar radiation. The error made in most of existing models when computing the Lyman-alpha contribution to photodissociation rates in the middle atmosphere, using a constant O_2 cross-section of 10^{-20} cm^2, is shown to be important and this can affect the loss rate of mesospheric constituents such as H_2O or CH_4.

Introduction

Recently the interest of mesospheric water vapor has been emphasized in relation with anthropogenic increases in carbon dioxide and methane [*Thomas*, 1996; *Chandra et al.*, 1997]. Photodissociation of these constituents by the solar Lyman-α emission line H I at 121.56 nm is very important for the terrestrial middle atmosphere, since the low absorption cross-section of molecular oxygen in this wavelength region allows a penetration down to the lower mesosphere and even to the upper stratosphere. Furthermore, this line is the principal ionizing agent of nitric oxide in the ionospheric D region.

Most models use only one wavelength interval for this line, and assume that O_2 has a 10^{-20} cm^2 constant absorption cross-section in this interval. This approximation can lead to non-negligible errors in photodissociation rates [*Frederick and Hudson*, 1980]. Since detailed calculations using a coarse wavelength grid at Lyman-α are time consuming in multidimensional models, *Nicolet* [1985] developed a parameterization of the O_2 cross-section for the whole Lyman-α interval as a function of the O_2 slant column.

It is extremely useful for modellers to have access to simple and accurate parameterizations for the computation of photodissociation processes which require a high wavelength resolution. We develop here a new, robust parameterization of the solar Lyman-α line absorption which takes into account the wavelength and temperature dependence of the O_2 cross-section as well as the line profile. This technique is based on the reduction factors method [*Kockarts*, 1994] and it can be easily implemented in any atmospheric model for a low computing cost.

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Solar Lyman-α Line

Any parameterization taking in account the wavelength variation of this profile must depend of solar activity, at least through the Lyman-α total flux at the top of the atmosphere, Φ_∞. All the results shown here use the conventional value $\Phi_\infty = 3 \times 10^{11}$ photons cm^{-2} s^{-1} which is representative of a quiet Sun activity level, as shown recently by *Woods and Rottman* [1997] and *Tobiska et al.* [1997] , where time series of Φ_∞ have been extracted from satellite measurements, over a range as long as two 11-year solar cycles.

Although it has been shown that the Lyman-α profile changes with solar activity [*Vidal-Madjar*, 1975], it has not been measured over a time span long enough to reflect quantitatively its variation with solar activity. The present work uses a composite profile [*Lemaire et al.*, 1978] which represents the whole solar disk as seen from the top of the Earth's atmosphere under quiet sun conditions.

This solar Lyman-α intensity profile (see Figure 1) was digitized, normalized, and fit by a non-linear least-square method [*Marquardt*, 1963; *Press et al.*, 1989] to the sum of three gaussian functions, so that

$$\phi_\infty(\lambda) = \Phi_\infty \sum_{i=1}^{3} G_i(\lambda) \qquad (1)$$

where $\phi_\infty(\lambda)$ is the wavelength-dependent solar irradiance at the top of the atmosphere and $G_i(\lambda)$ are three gaussian functions

$$G_i(\lambda) = \frac{a_i}{s_i\sqrt{2\pi}} \exp\left(-\frac{(\lambda - \lambda_i)^2}{2\, s_i^2}\right) \qquad (2)$$

The parameters a_i, s_i and λ_i providing the best fit to the normalized intensity profile are given in Table 1.

The central core of the emission line is due to the absorption of the solar line by geocoronal hydrogen [*Meier and Prinz*, 1970]. This feature is reproduced by the second and third terms, G_2 and G_3, which have negative a_i values. This analytic representation of the solar Lyman-α intensity profile allows easy scaling to any wavelength grid, and may be adapted to other observed profiles simply by changing the fitting parameters.

Reduction Factors Parameterization

An exact calculation of the penetration of Lyman-α is based on Beer-Lambert's law using 500 wavelength intervals of 10^{-3} nm from 121.4 nm to 121.9 nm and an altitude grid of 1 km between ground level and 120 km. The vertical profiles of temperature and O_2 number density were provided by the semi-empirical MSIS model [*Hedin*, 1991] for day number 81 (March 22), latitude 0° and local solar time of 12h. The introduction of an exact calculation is extremely time consuming

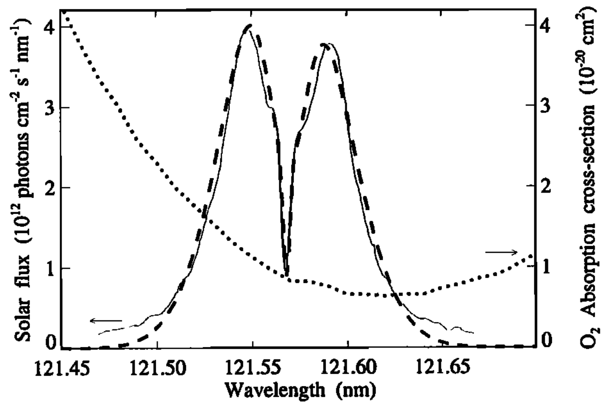

Figure 1. Lyman-α profile [*Lemaire et al.*, 1978] (solid line), fit to this profile (dashed line, Eqs. 1 and 2) and O_2 cross-section at the same wavelengths for a temperature of 203 K [*Lewis et al.*, 1983] (dotted line). The two Lyman-α profiles have been rescaled to a total flux of 3×10^{11} photons cm^{-2} s^{-1}.

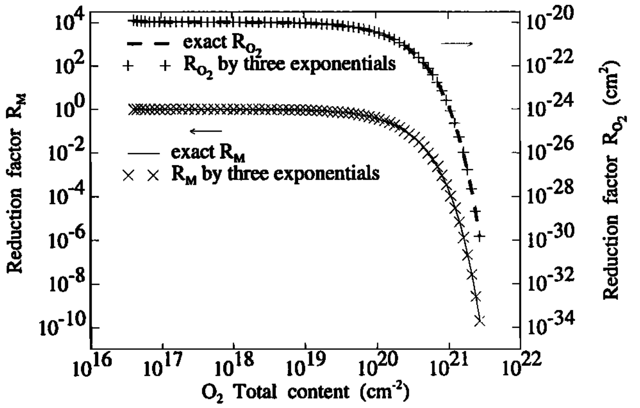

Figure 2. Comparison between exact computation of the reduction factor $R_M(z)$ (solid line) and the approximation given by Eq. 7 (×). Comparison between exact computation of the reduction factor $R_{O_2}(z)$ (dashed line) and the approximation given by Eq. 8 (+).

in multidimensional models. We develop, therefore, a parameterization based on the method introduced by *Kockarts* [1976, 1994] for the Schumann-Runge bands of molecular oxygen.

The detailed calculation is based on the O_2 absorption cross-section measured by *Lewis et al.* [1983] . This team measured σ_{O_2} at Lyman-α with a high spectral resolution and at four different temperatures ranging from 84 K to 366 K. Their results for 203 K, typical of mesospheric conditions, are shown by the dotted line on Figure 1.

For all minor constituents M, a single dimensionless reduction factor $R_M(z)$ can be defined as

$$R_M(z) = (1/\Phi_\infty) \int_{121.4\text{nm}}^{121.9\text{nm}} \phi(z,\lambda)d\lambda \qquad (3)$$

where $\phi(z, \lambda)$ is the wavelength-dependent solar irradiance at altitude z. The photodissociation rate of a minor constituent M is given by

$$J_M(z) = \Phi_\infty \times \sigma_M \times R_M(z) \qquad (4)$$

where σ_M is the constant cross-section of the minor constituent.

For molecular oxygen, the reduction factor in cm^2 is defined by

$$R_{O_2}(z) = (1/\Phi_\infty) \int_{121.4\text{nm}}^{121.9\text{nm}} \sigma_{O_2}(\lambda, T(z)) \times \phi(z,\lambda)d\lambda \quad (5)$$

where $\sigma_{O_2}(\lambda, T(z))$ is the wavelength and temperature-dependent O_2 absorption cross-section. The photodissociation rate of O_2 is now given by

$$J_{O_2}(z) = \Phi_\infty \times R_{O_2}(z) \qquad (6)$$

Table 1. Parameters used for the solar Lyman-α profile $\phi_\infty(\lambda)$ (Eq. 2)

	a_i	s_i	λ_i
$i=1$	1.33726	2.72491×10^{2}	121.568
$i=2$	-0.317024	1.05895×10^{2}	121.569
$i=3$	-0.0198859	1.68298×10^{3}	121.568

The reduction factors $R_M(z)$ and $R_{O_2}(z)$ can be computed with the detailed O_2 cross-sections and the detailed Lyman-α profile. The temperature dependence of the O_2 cross-section is introduced in the detailed computations by linear interpolation of the measurements of *Lewis et al.* [1983] at every 1 km altitude interval. The full and dashed lines in Figure 2 correspond to the exact calculation of, respectively, $R_M(z)$ and $R_{O_2}(z)$, for an overhead sun between 120 km and 40 km altitude where both reduction factors have decreased by a factor of 10^{10}. These results are parameterized by a sum of exponentials [*Kockarts*, 1994].

In order to cover a range of ten orders of magnitude in the decrease of both reduction factors, three exponentials are sufficient, i.e. $R_M(z)$ and $R_{O_2}(z)$ are respectively represented by

$$R_M(z) = \sum_{i=1}^{3} b_i \times \exp(-c_i \times N_{O_2}(z)) \qquad (7)$$

and

$$R_{O_2}(z) = \sum_{i=1}^{3} d_i \times \exp(-e_i \times N_{O_2}(z)) \qquad (8)$$

where $N_{O_2}(z)$ is the slant O_2 total content.

The coefficients are given in Table 2. The approximations obtained with Eqs. 7 and 8 are shown on Figure 2. For $R_M(z)$, the error is always smaller than 0.5% and for $R_{O_2}(z)$ it is always smaller than 2%.

O_2 Column-Dependent Cross-Sections

Instead of the direct calculation of photolysis rates using reduction factors (Eqs. 4 and 6), a more conventional formulation consists in using only one value of the O_2 cross-section for the whole Lyman-α spectral interval, but depending fictitiously on the slant column of oxygen molecules. The irradiance for the whole Lyman-α line is then

$$\phi(z) = \Phi_\infty \times \exp(-\overline{\sigma_{O_2}(z)}\, N_{O_2}(z)) \qquad (9)$$

where $\overline{\sigma_{O_2}(z)}$ is itself a function of $N_{O_2}(z)$. Such a formulation can be directly implemented in any atmospheric

Table 2. Parameters for the reduction factors $R_M(z)$ and $R_{O2}(z)$

	R_M		R_{O2}
b_1	0.68431	d_1	$6.0073 \times 10^{\ 21}$
c_1	$8.22114 \times 10^{\ 21}$	e_1	$8.21666 \times 10^{\ 21}$
b_2	0.229841	d_2	$4.28569 \times 10^{\ 21}$
c_2	$1.77556 \times 10^{\ 20}$	e_2	$1.63296 \times 10^{\ 20}$
b_3	0.0865412	d_3	$1.28059 \times 10^{\ 20}$
c_3	$8.22112 \times 10^{\ 21}$	e_3	$4.85121 \times 10^{\ 17}$

model, simply by replacing the constant value used for σ_{O_2} at Lyman-α (most often 10^{-20} cm^2) by an altitude dependent cross-section.

Since the irradiance $\phi(z)$, approximated by Eq. 9, must be equal to the integral of $\phi(z,\lambda)$ over the whole Lyman-α wavelength interval, an effective cross-section is given by

$$\overline{\sigma_{O_2}(z)} \;=\; -\;(1/N_{O_2}(z)) \times \ln(R_M(z)) \qquad (10)$$

where $R_M(z)$ is computed from Eq. 7.

Using Eqs. 10 and 9, it is possible to calculate easily the Lyman-α contribution to the photodissociation rate of a minor constituent M

$$J_M(z) \;=\; \sigma_M \times \phi(z) \qquad (11)$$

When calculating $J_{O_2}(z)$, σ_M must be replaced in Eq. 11 by $\overline{\sigma_{O_2}(z)}'$, a function satisfying

$$\overline{\sigma_{O_2}(z)}' \;=\; J_{O_2}(z)\;/\;\phi(z) \;=\; R_{O_2}(z)\;/\;R_M(z) \qquad (12)$$

Using the approximations for the reduction factors given in Section 3, we have checked that a formulation using effective cross-sections reproduces exactly the same photodissociation coefficients than the direct use of reduction factors. Although this technique requires à little more computations, it can be useful in photolysis models requiring the use of cross-sections, for example the models which calculate light scattering at all wavelengths.

However, this technique is less robust than the direct approach described in the previous section. At the bottom of the atmosphere, $R_M(z)$ can take an extremely small value, leading to numerical problems in Eqs. 10 and 12. This is not the case when using the direct approach (Eq. 4). Here, however, this case should be tested and if it arises, the efficient cross-sections should be set to non-zero values, *i.e* $\overline{\sigma_{O_2}(z)} = 8 \times 10^{-21}$ cm^2 and $\overline{\sigma_{O_2}(z)}' = 1.2 \times 10^{-20}$ cm^2 .

Impact on Middle Atmosphere Modelling

In order to make a preliminary evaluation of the quantitative consequences of the approximations deduced in the two previous sections, we have computed exact total photodissociation coefficients for CH_4 and H_2O. Absorption cross-sections are taken from *DeMore et al.* [1994] , except for the Schumann-Runge bands of O_2 for which we used reduction factors of *Kockarts* [1994] . Although the H_2O cross-section varies smoothly over the Lyman-α line width [*Lewis et al.*, 1983], we used a constant value of value of 1.53×10^{-17} cm^2. The exact photodissociation coefficients take in account the wavelength variation of solar irradiance and O_2 cross-section at Lyman-α. Approximate photodissociation coefficients use only one spectral interval at Lyman-α, either with $\sigma_{O_2} = 10^{-20}$ cm^2, or with the parameterization described in Section 3.

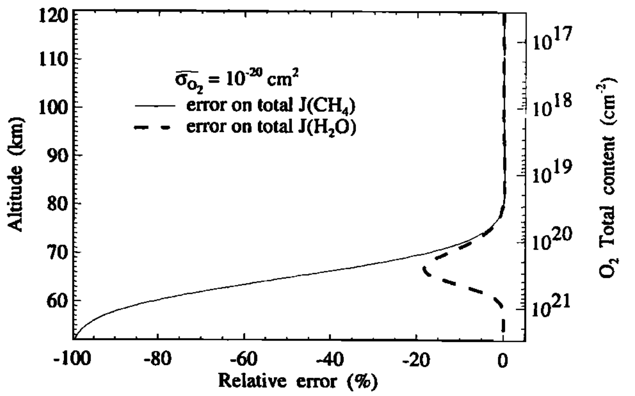

Figure 3. Vertical distribution of the relative error on CH_4 and H_2O photodissociation rates when a constant cross-section of 10^{-20}cm^2 is used for O_2. Negative values correspond to an underestimation with the constant cross-section. Overhead sun conditions.

For any photodissociation rate J a relative error is defined by

$$Error \;=\; 100 \times (J_{\text{approx}} - J_{\text{exact}})/J_{\text{exact}} \qquad (13)$$

Figure 3 shows the relative errors when a constant cross-section of 10^{-20} cm^2 is adopted for O_2. The maximum error for H_2O leads to an underestimation of 20% in the mesosphere. For CH_4, this underestimation can reach 100% in the lower mesosphere. The photodissociation rate of O_2 leading to $O(^1D)$ production is affected in a similar way, as well as the photoionization of nitric oxide in the D region.

When we use the approximation developed in the present paper the relative errors are drastically reduced as can be seen on Figure 4.

This has implications for mesospheric photochemistry. Using the $O(^1D)$ profile given by *Rodrigo et al.* [1991] , preliminary calculations of the total photochemical loss rates of H_2O and CH_4, including oxidation by $O(^1D)$, were made at all altitudes for overhead sun conditions. They indicate that at 70

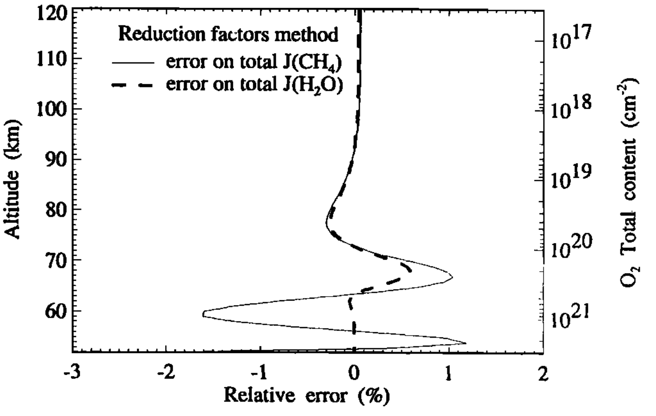

Figure 4. Same as Figure 3, but with the approximations developed in the present paper.

km, the loss rate of H_2O increases by 10% when the present parameterization is used instead of the old value $\sigma_{O_2} = 10^{-20}$ cm^2, and the loss rate of CH_4 increases by as much as 20%.

It appears, therefore, that the common approximation of a constant cross-section for O_2 at Lyman-α should be definitely abandoned in multidimensional middle atmosphere models.

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