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A study on interaction of a 4µm free electron laser beam with the rotational lines of sulphur dioxide

Surajit Bhuyan, Biswa Kr. Das

Department of Physics, Lakhimpur Girls' College, North Lakhimpur, India

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ABSTRACT

Sulphur dioxide is most noteworthy as an environmental pollutant. Interaction of a free electron laser beam of wavelength 4 µm with rotational lines of sulphur dioxide is studied. Values of transmittance, averaged over intervals of 0.1 cm^{-1}, are obtained for absorber thickness 0.01, 0.1 and 1 atm-cm, using the quasi-random model of molecular band absorption. From these values, intensities of the high resolution absorption lines of SO_2 are simulated in the frequency interval 2463.4983– 2464.919 cm^{-1}. The experimental data taken for this work agree well with the result. There is clearly a scope to apply this work in atmospheric optics.

Keywords: Sulphur dioxide lines, transmittance, free electron laser, quasi-random model.

INTRODUCTION

Sulfur dioxide (SO_2) is one of a group of highly reactive gasses known as "oxides of sulphur." Sulphur dioxide enters the atmosphere as a result of both natural phonomena and anthropogenic activities. The largest sources of SO_2 emissions are from fossil fuel combustion at power plants (73%) and other industrial facilities (20%). Smaller sources of SO_2 emissions include industrial processes such as extracting metal from ore, and the burning of high sulfur containing fuels by locomotives, large ships, and non-road equipment [1]. Atmospheric optics uses lasers for the remote probing of the atmosphere, including the measurement of traces of pollutant gases, temperature and water vapour concentration. The first precision measurement of ozone in the atmosphere was made using laser remote sensing. The attenuation and fluctuation of the optical parameters of the penetrating radiation are due to absorption by molecular bands or scattering by atmospheric species. Recently a linear relationship between concentration of sulfur dioxide and optical parameter (OP) is established using the Beer–Lambert law [2]. A precise knowledge of the spectra of sulphur dioxide is very important for accurate measurements involving the passage of a laser beam through this gaseous medium. In this work, a free electron laser is considered tuned to 4µm. The frequency interval in which the propagation of this free electron laser beam is considered, 2463.4983– 2464.919 cm^{-1}, lies in the combination vibration – rotation $\nu_1+\nu_3$ band of SO_2. The combination vibration – rotation $\nu_1+\nu_3$ band of SO_2 has been recorded under Doppler limited and atmospheric conditions with 3* 10^{-4} cm^{-1} instrumental resolution using a difference-frequency laser [3]. The $\nu_1+\nu_3$ band of SO_2 is strategically located in the 4 µm atmospheric window which is convenient for monitoring SO_2 in the air or observing extraterrestrial SO_2 through the atmosphere. The method used in this work, the quasi-random model [4] of molecular band absorption, is a variant of one of the methods described by Goody and Yung [5]. In their monograph, Goody and Yung have contrasted the use of random models with the line by-line method, and concluded that in some circumstances the random models might be sufficient, and require much less computer time. Infrared transmittances, based on the quasi-random model, have been calculated for H_2O and CO_2 and the results fitted with experimental measurements [6,7]. Using this model, simulations of intensities of absorption lines have been done for p-benzoquinone-H4 vapour [8] in the region 17800 - 24900 cm^{-1}, for water vapour [9] around 1.15 µm, and for nitrogen [10] around 575 nm. Potential use of this model in developing rapid models for accurately calculating atmospheric transmittances has been indicated [11]. Simulating the intensities of high-resolution lines of nitrogen around 570 nm, applicability of this model in optics of the atmosphere, especially of the upper atmosphere, has been shown [12]. Intensities of the high resolution absorption lines of sulphur dioxide are simulated in the frequency intervals 2499.0115-2499.9910 cm^{-1}[13] and 2523.336 - 2524.727 cm^{-1} [14, 15]. The frequency interval under consideration in the present study is another convenient sector in the sulphur dioxide spectrum for investigation of propagation of a laser beam through it.

MATERIALS AND METHODS

METHOD OF CALCULATION

High-resolution near-infrared absorption spectrum of sulphur dioxide is considered frequency interval 2463.4983–2464.919 cm^{-1}. The maximum relative intensity is normalized to unity and other values of intensity are taken relative to this one. The lines along with the assigned intensities are given in Table 1. The entire spectrum is divided into frequency intervals $\Omega = 0.1$ cm^{-1} wide. These Ωs are the intervals over which the average transmittances have been computed. Each interval is further divided into smaller intervals $\delta = 0.025$ cm^{-1}. The quasi-random model localizes each line within an error defined by the interval size δ. The transmittance at a frequency ν, as affected by n_p lines within the interval δ_p is computed from the expression [16]

$$\mathrm{T}(\nu) = \prod_{i=1}^{5} \left\{ \left(\frac{1}{\delta} \right) \int_{\delta_p} \exp\left[-S_i u b(\nu, \nu_i) \right] d\nu_i \right\}^{n_i} \tag{1}$$

where n_i represents the number of lines within the intensity range i, which itself is characterized by an average intensity S_i, u is the absorber thickness in atm-cm (atmosphere centimeter), and $b(\nu, \nu_i)$ is the Lorentz shape factor defined by (α is the half-width, i.e. half the frequency difference between the half-maximum points, ν_i refers to the center of the line).

The gases of the atmosphere are usually measured by the unit *atmosphere centimetre* (atm-cm). This measurement unit is used to define an atmospheric gas distributed along a path reduced to a layer at STP, provided the other gases

$$\mathrm{b}(\nu, \nu_\mathrm{i}) = \frac{\alpha / \pi}{(\nu - \nu_\mathrm{i})^2 + \alpha^2} \tag{2}$$

are excluded. The resulting thickness is then expressed in atm-cm, given by $u = cLP$, where c is the fractional concentration of the absorber, L is the path length in cm and P is the pressure in atmosphere.

For three different masses per unit area, u = 0.01, 0.1 and 1.0 atm-cm, and taking the half-width as α=0.015 cm^{-1}, equation (1) is evaluated with the help of a computer program based on Simpson's rule of numerical integration. First, the transmittance values are calculated at the centre of 0.1 cm^{-1} intervals. Transmittances by the wings of lines at the left and right adjacent intervals are also included. The transmittance at the centre of an interval is finally obtained as [17]

$$T = T_j \prod_{i \neq j} T_i \tag{3}$$

Next, transmittance values are obtained for another set of frequency intervals whose centres are shifted by half the interval size (0.05 cm^{-1}) from the original positions of the centres of the intervals. This is done in order to minimize the error associated with the occurrence lines at frequencies near the edges of a given interval. The results for the shifted and un-shifted intervals are averaged, and thus we obtain the average transmittance over a 0.1 cm^{-1} interval.

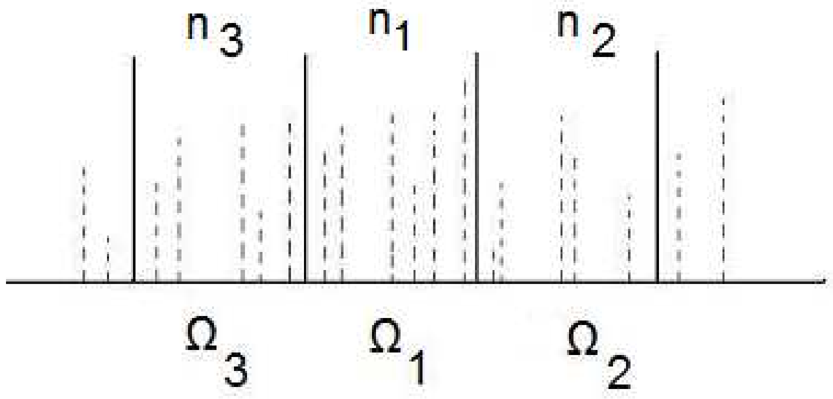

Figure 1: Three typical adjacent intervals showing the position and relative intensities of the lines contained in each.

Table 1: SO_2 lines affecting the propagation of the 4 μm laser beam

Frequency (cm^{-1})	Intensity (cm^{-1}/molecules-cm^{-2})	Frequency (cm^{-1})	Intensity (cm^{-1}/molecules-cm^{-2})
2463.4983	0.67	2464.200	0.28
2463.5305	0.70	2464.312	0.53
2463.551	0.33	2464.386	0.37
2463.6461	0.69	2464.546	0.61
2463.6527	0.74	2464.569	0.47
2463.693	0.37	2464.647	0.35
2463.704	0.18	2464.682	0.37
2463.7683	0.61	2464.688	0.42
2463.776	0.38	2464.7298	0.74
2463.832	0.27	2464.7773	0.90
2463.9421	1	2464.817	0.83
2463.9561	0.82	2464.843	0.24
2463.9822	0.78	2464.866	0.87
2464.025	0.52	2464.876	0.85
2464.0388	0.75	2464.905	0.77
2464.1415	0.74	2464.919	0.78
2464.1942	0.61		

Table 2: Absorption of a free electron laser beam for three different amounts of SO_2

Frequency	Absorptance (%) for path length		
(cm^{-1})	0.01 atm-cm	0.1 atm-cm	1 atm-cm
2463.5483	41.25	41.75	46.5
2463.6483	53.25	54.02	60.99
2463.7483	55.57	57.82	72.15
2463.8483	59.67	79.92	95.93
2463.9483	62.39	91.45	100
2464. 0483	62.3	91.23	100
2464.1483	58.28	73.1	89.09
2464.2483	55.43	56.52	65.95
2464.3483	55.35	55.71	59.1
2464.4483	55.33	55.51	57.3
2464.5483	55.32	55.46	56.75
2464.6483	55.33	55.49	57.05
2464.7483	55.33	55.51	57.25
2464.8483	50.74	50.92	52.69
2464.9483	41.56	41.73	43.32

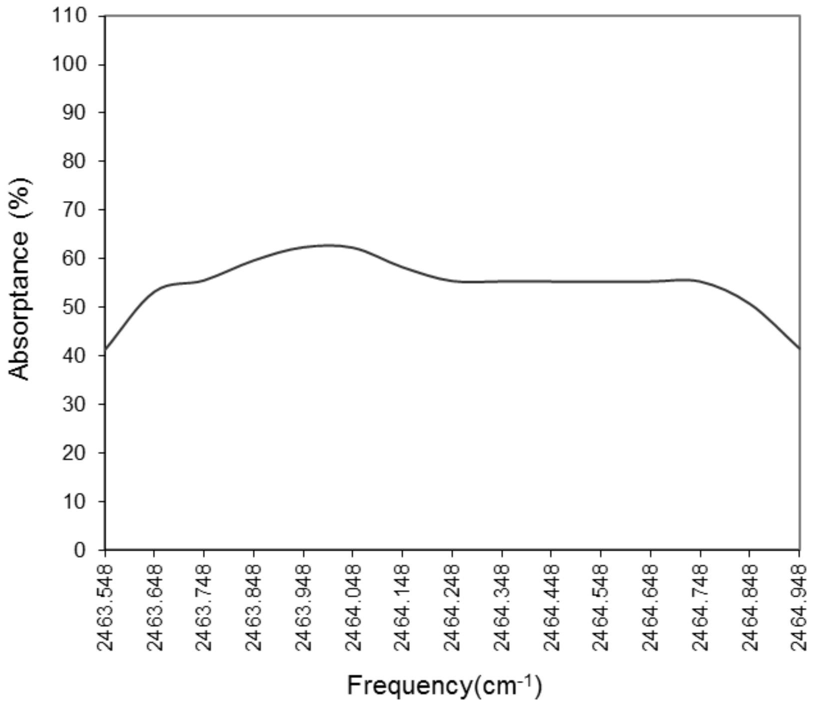

Figure 2: Absorptance of a 4 µm free electron laser beam for a 0.01 atm-cm path length of SO_2.

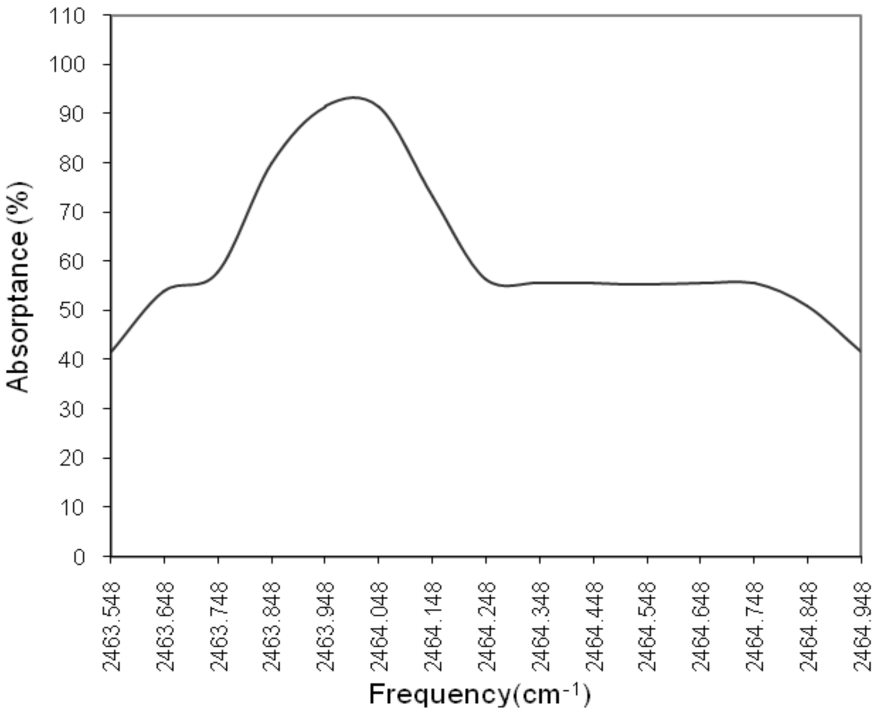

Figure 3: Absorptance of a 4 µm free electron laser beam for a 0.1 atm-cm path length of SO_2.

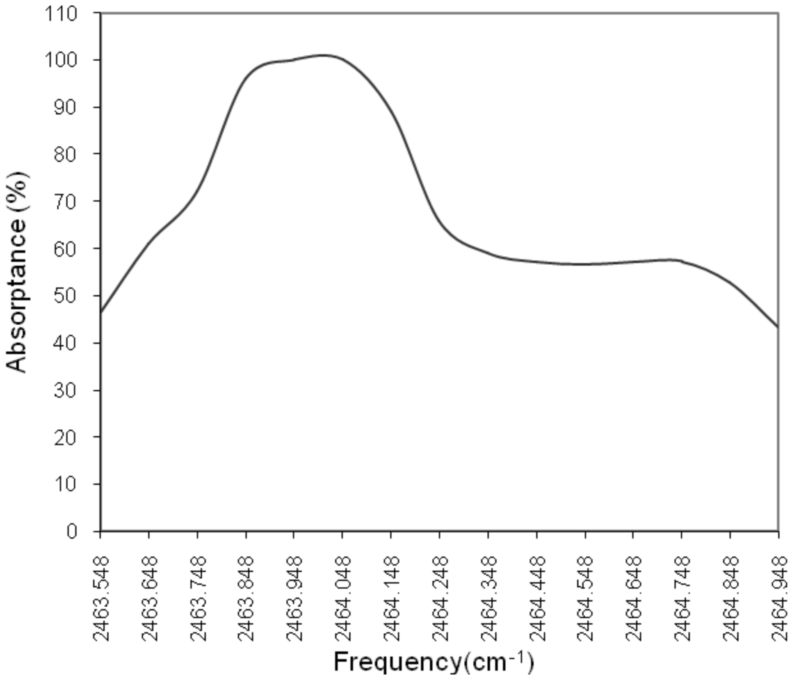

Figure 4: Absorptance of a 4 μm free electron laser beam for a 5 atm-cm path length of SO_2.

RESULTS AND DISCUSSION

Influences of 33 lines for the interval are worked out for 0.01, 0.1 and 1 atm-cm thickness of sulphur dioxide in the frequency intervals 2463.4983– 2464.919 cm^{-1}. The computational results for the propagation of a 4 μm laser beam through these three amounts of the absorber are presented in Tables 2 and shown in Figures 2 –4. It reveals from the figures that the smaller the amount of the absorber the more marked is the variation and with greater amounts of the absorber the absorptance values tend to saturate. From generated absorptance values intensities of the high resolution absorption lines in the above interval of SO_2 can be simulated. The absorption values agree well with the experimental data taken for this work. This concludes that the quasi-random model for simulating the intensity distribution by grouping the lines in a given frequency interval works reasonably well - a fact established in recent times for important atmospheric species like nitrogen sulphur dioxide and methane.

CONCLUSION

As the rotational lines are observed to be sufficiently fine, therefore in this work the broadening of the lines is assumed to be homogeneous. There is a scope to generalize the model for inhomogeneous broadening as well. Application prospect of this work in atmospheric optics is quite bright. Till now, a large number of high resolution absorption spectra of other diatomic and polyatomic molecules have been reported; the present work could easily be extended to these spectra. Temperature and pressure dependence of the linewidth, and consequently of the absorptance, is the aspect that calls for further research. The scopes of error in these computations are (a) the size of the small intervals, δ, as mentioned in the description of the model, and (b) the number of divisions taken in the Simpson-rule based program, which is known to any programmer.

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