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Pressure Dependence of Ozone Absorption Cross Section

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Abstract. Accurate value of absorption cross section is required for correct measurement of ozone concentration. Measurement of ozone has been done at different altitude and pressure. However, previous work has failed to establish significant relation between pressure and ozone absorption cross section. Therefore, this work aims to establish relation between pressure and maximum ozone absorption cross section via spectralcalc.com gas cell simulator. Simulation results show maximum absorption cross section 1.148×10^{-21} m^2 $molecule^{-1}$ and maximum absorption wavelength 255.442 nm are independent of pressure changes from 0.1 atm to 3.0 atm. Thus, measurement of ozone concentration at maximum absorption wavelength is strongly recommended due to negligible pressure dependence.

Introduction

Ozone is earth natural protective layer in atmosphere at high altitude for absorption of harmful ultraviolet sun rays from reaching the earth. At low altitude, ozone is generated on site for killing micro-organisms in processed rice [1]. Although ozone is colourless, it has distinct smell. Its presence near earth is tracked constantly for pollution monitoring [2]. Today, fixed and portable ozone sensor devices are commercially available for measurement of ozone. Hence, ozone plays an important role in our daily lives and should be measured accurately.

Ozone concentration has been measured in different pressure environment, but little work has been done to investigate effect of pressure toward absorption cross section. Previous observation has failed to establish significant relation between pressure and ozone absorption cross section [3]. Accurate value of absorption cross section is important for correct calculation of concentration based on Beer–Lambert law in Eq. 1. Measurement of ozone concentration using maximum absorption cross section is important for maximum measurement sensitivity. Therefore, objective of this work is to establish relation between maximum ozone absorption cross section and pressure through simulation approach.

This work is important for accurate measurement of ozone in pressure changing environment. For example, measurement of ozone concentration profile in atmosphere is done using balloon from altitude 5 km to 35 km in pressure as low as 6.1 hPa [4]. Atmospheric pressure is 1 atm or 1013.25 hPa. Therefore, understanding of relation between pressure and absorption cross section is necessary for correct ozone concentration measurement.

Theoretical Background

In ultraviolet absorption spectroscopy, absorption cross section of ozone may be found using Beer–Lambert law in Eq. 1. Similar equation may be found in literature [5]. Transmittance, T_r is defined in Eq. 2. Absorption cross section, σ is dependent on absorption wavelength, λ [6]. The wavelength that corresponds to maximum absorption cross section ($\sigma = \sigma_{\max}$) is maximum absorption wavelength ($\lambda = \lambda_{\max}$). Maximum absorption wavelength, $\lambda_{\max}$ corresponds to wavelength at minimum transmittance, $T_{r\min}$. Thus, Eq. 3 may be deduced from Eq. 1 for calculation of maximum absorption cross section, $\sigma_{\max}$ using minimum transmittance, $T_{r\min}$. This work investigates if maximum absorption cross section, $\sigma_{\max}$ is dependent on pressure, P.

$$\sigma = -1000000RT/(c_{(\mathrm{ppm})}N_A P l_s)\times\ln(I_t/I_0). \quad (1)$$
$$T_r = I_t/I_0. \quad (2)$$
$$\sigma_{\max} = -1000000RT/(c_{(\mathrm{ppm})}N_A P l_s)\times\ln T_{r\min}. \quad (3)$$

$c_{(\mathrm{ppm})}$ = ozone concentration in ppm by volume.
I_0 = input intensity to ozone sample in count.
I_t = output intensity from ozone sample in count.
l_s = optical path length in m.
N_A = Avogadro's constant, 6.02214199×10^{23} molecule mol^{-1}.
P = pressure in atm.
R = ideal gas constant, 8.205746×10^{-5} atm m^3 mol^{-1} K^{-1}.
T = absolute temperature in K.
T_r = transmittance (no unit).
$T_{r\min}$ = minimum transmittance (no unit).
λ = absorption wavelength in nm.
$\lambda_{\max}$ = maximum absorption wavelength in nm.
σ = absorption cross section in m^2 $\mathrm{molecule}^{-1}$.
$\sigma_{\max}$ = maximum absorption cross section in m^2 $\mathrm{molecule}^{-1}$.

Methodology

Practical Concentration Calculation. Firstly, ozone concentration that corresponds to transmittance, $T_r = 0.5$ is calculated via Eq. 1 using the following parameters. The concentration, $c_{(\mathrm{ppm})}$ is calculated to be 123.5 ppm.

$\sigma = 1.147\times10^{-21}$ m^2 $\mathrm{molecule}^{-1}$ at maximum absorption wavelength, $\lambda_{\max} = 253.65$ nm [7].
$N_A = 6.02214199\times10^{23}$ molecule mol^{-1}.
$P = 1$ atm.
$R = 8.205746\times10^{-5}$ atm m^3 mol^{-1} K^{-1}.
$T = 300$ K.
$l_s = 0.20$ m.
$I_t/I_0 = 0.5$.

Spectralcalc.com Simulation. Secondly, spectralcalc.com [8] gas cell simulator is used to determine graphs of transmittance, T_r versus absorption wavelength, λ at different pressure, P. From the graphs, maximum absorption wavelength, $\lambda_{\max}$ and minimum transmittance, $T_{r\min}$ are extracted for further processing. The minimum value of transmittance, $T_{r\min}$ is used for calculation of maximum absorption cross section, $\sigma_{\max}$ via Eq. 3. Input to the simulator is as follow:

$N_A = 6.02214199 \times 10^{23}$ molecule mol^{-1}.

$c_{(ppm)} = 123.5$ ppm.

P = 0.1 atm, 0.2 atm, 0.3 atm... 3.0 atm or 101.325 mbar, 202.650 mbar, 303.975 mbar... 3039.750 mbar.

$R = 8.205746 \times 10^{-5}$ atm m^3 mol^{-1} K^{-1}.

T = 300 K.

l_s = 0.20 m.

Waveband = 0.24 µm to 0.27 µm.

Line list = HITRAN2008.

Gas = O_3.

Results and Discussions

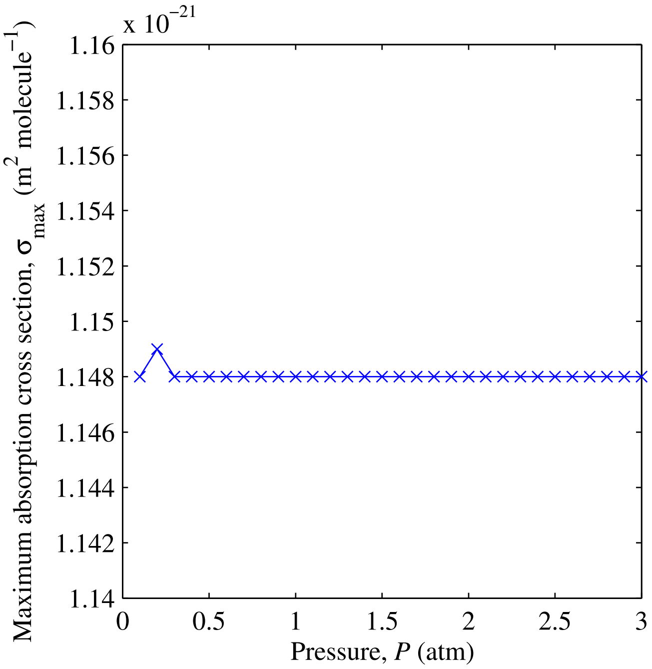

Fig. 1. Graph of maximum absorption cross section versus pressure based on spectralcalc.com simulation at concentration 123.5 ppm, temperature 300 K, optical path length 0.20 m and maximum absorption wavelength 255.442 nm.

Simulation result in Fig. 1 shows maximum absorption cross section, σ_{max} stays constant at 1.148×10^{-21} m^2 molecule^{-1} despite pressure, P changes from 0.1 atm to 3 atm. Sudden peak of 1.149×10^{-21} m^2 molecule^{-1} at 0.2 atm is due to rounding. Minimum value of transmittance, $T_{r\min}$ simulated from spectralcalc.com is rounded to 4 significant places for maximum absorption cross section, σ_{max} calculation via Eq. 3. Hence, maximum absorption cross section, σ_{max} is found to be not dependent on pressure, P. Simulation result is in good agreement with previous work. In previous work, absorption cross section is not significantly changed when pressure varies from 100 mbar to 1000 mbar due to short life of upper electronic state of ozone [3].

Similarly, simulation result in Fig. 2 shows maximum absorption wavelength, λ_{max} stays constant at 255.442 nm despite pressure, P increases from 0.1 atm to 3.0 atm. Simulation result is comparable to previous work. In previous work, ozone has strong absorption at wavelength 253.65 nm [7], 254 nm [9], 255 nm [10] and 280 nm [11]. Measurement of maximum absorption cross section, σ_{max} at maximum absorption wavelength, λ_{max} is important for low uncertainty measurement between 1 % and 1.5 % [12].

Finally, simulation result in Fig. 3 shows transmittance, T_r decreases exponentially when pressure, P increases linearly. The finding agrees with Beer–Lambert law in Eq. 1. The higher the pressure, P, the lower the transmittance, T_r. Based on theoretical expectation, absorption cross section is a constant. Hence, absorption cross section is not significantly affected by pressure changes.

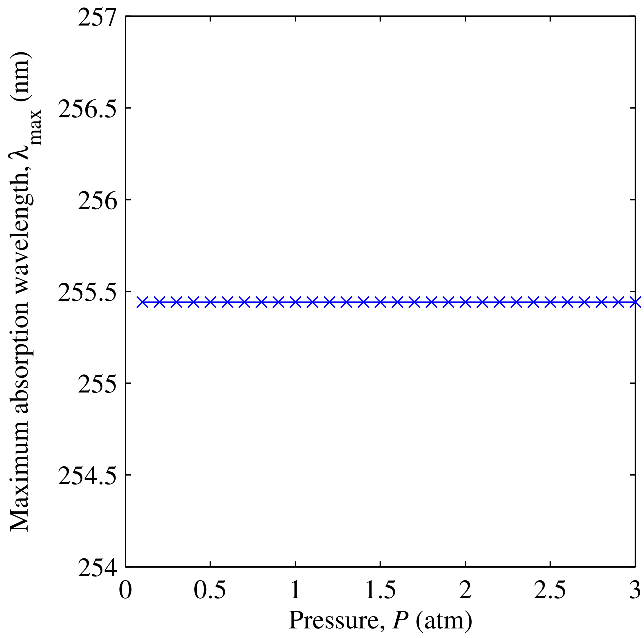

Fig. 2. Graph of maximum absorption wavelength versus pressure based on spectralcalc.com simulation at concentration 123.5 ppm, temperature 300 K and optical path length 0.20 m.

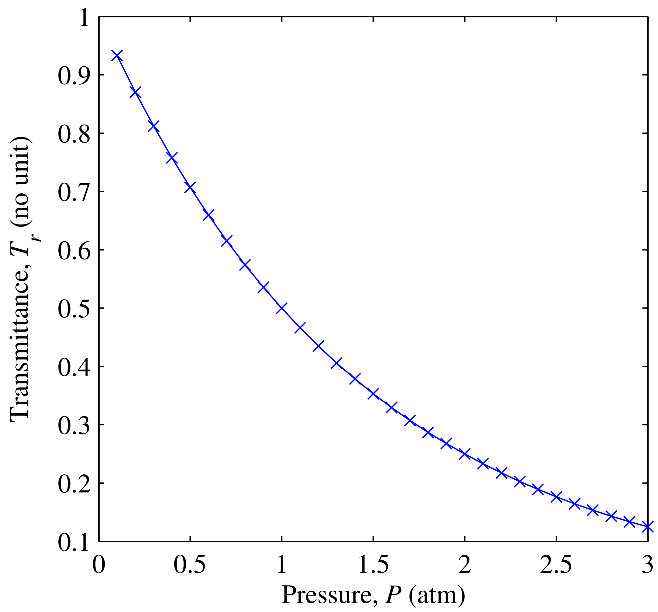

Fig. 3. Graph of transmittance versus pressure based on spectralcalc.com simulation at concentration 123.5 ppm, temperature 300 K, optical path length 0.20 m and maximum absorption wavelength 255.442 nm.

Conclusions and Recommendations

In conclusion, spectralcalc.com simulation result shows maximum absorption cross section of ozone at 1.148×10^{-21} m^2 $molecule^{-1}$ is not dependent on pressure changes from 0.1 atm to 3.0 atm. Similarly, simulation result shows maximum absorption wavelength at 255.442 nm is independent of pressure fluctuations. As a result, this work strongly recommends measurement of ozone concentration at maximum absorption wavelength, 255.442 nm because maximum absorption cross section, 1.148×10^{-21} m^2 $molecule^{-1}$ is stable at different pressure.

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