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CONCENTRATION EFFECT SIMULATION ON OZONE GAS ABSORPTION CROSS SECTION

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Abstract. The effect of concentration on ozone gas absorption cross section is reported. HITRAN 2012 - the latest available line list on spectralcalc.com simulator was used in this study to simulate ozone gas absorption cross section in relation to effect of varying ozone gas concentration in the visible spectrum. Results obtained for a 50 cm gas cell shows that transmittance vary continuously with concentration. However, ozone gas absorption cross section value of $5.1055 \times 10^{-25} \mathrm{m}^2/\mathrm{molecule}$ at wavelength 603 nm for concentration of 170 parts per million by volume (ppm) and above remains constant. Comparison of the simulated ozone gas absorption cross section with previous work show variation between 1.41 % and 2.44 %. The results obtained show that ozone concentrations between 170 ppm and 1200 ppm has no effect on ozone gas absorption cross section.

Keywords Absorption cross section; concentration; ozone gas; transmittance; visible spectrum

1.0 INTRODUCTION

The relevance of ozone gas as well as the advantages of using optical absorption spectroscopy to measure ozone gas have been previously emphasized by the authors [1, 2]. The importance of studying ozone gas absorption cross section has become important because of inconsistencies and discrepancies in ozone absorption data as seen in literature [3]. The work reported in this manuscript is an extension of previous work published by the authors on window size filter effect on ozone gas absorption cross section [4].

In previous study by the authors to investigate the effect of window size filter on ozone gas absorption cross section; at given flow rates of oxygen and ozone gas, there were fluctuations in the flow process which also resulted in varying of ozone gas concentration at a given flow rate [4]. In addition, at certain concentration especially at saturation points, it has been reported that Beer-Lambert law that governs the principle of gas measurement with optical absorption spectroscopy suffers from nonlinearity [5-7]. Thus, this emphasizes the possible effect of ozone concentration on ozone absorption

cross section. Hence, it has become obvious to examine the effect of concentration variation on ozone gas absorption cross section.

2.0 SIMULATION SOFTWARE AND METHODOLOGY

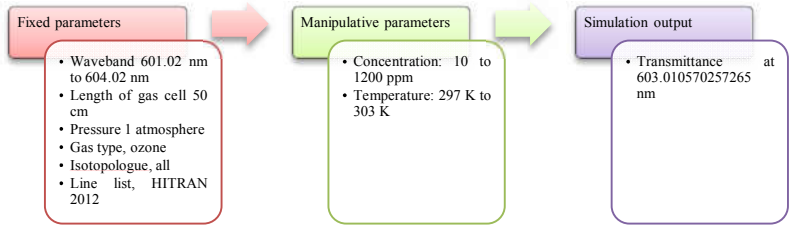

Figure 1 Spectralcalc.com simulation methodology and parameters

Spectralcalc.com is an online simulator for high resolution spectral modelling. HITRAN 2012 - the latest available line list on spectralcalc.com simulator was used in this study to simulate ozone gas absorption cross section in relation to effect of varying ozone gas concentration in the visible spectrum. Range of ozone gas concentration between 10 parts per million by volume (ppm) to 1200 ppm were investigated at different temperatures between 297 K and 303 K. The fixed parameters as shown in Figure 1 include: length of gas cell, 50 cm. Wavelength range of 601.02 nm to 604.02 nm and pressure of one (1) atmosphere. Ozone gas was selected as the gas of choice and all isotopologue of ozone gas were considered. The output from the simulator is transmittance at wavelength 603 nm (actual value is 603.0105702572658nm). In the visible spectrum, ozone gas has highest peak absorption at wavelength 603 nm [8, 9].

3.0 RESULTS AND DISCUSSION

Figure 2a and Figure 2b shows the effect of increase in temperature and increase in ozone concentration on transmittance. Increase in temperature resulted in increase in transmittance. The effect of temperature on transmittance increases along with increase in ozone gas concentration. From 297 K to 303 K, the rise is 0.00012 % (for 10 ppm concentration) and 0.01499% (for 1200 ppm concentration). On the other hand, light transmittance generally decreases along with increase in ozone gas concentration which is in good agreement with Beer-Lambert law [10]. There was an average decrease of 0.75% in transmittance from 10 ppm to 1200 ppm for each temperature considered. This is shown in Table 1.

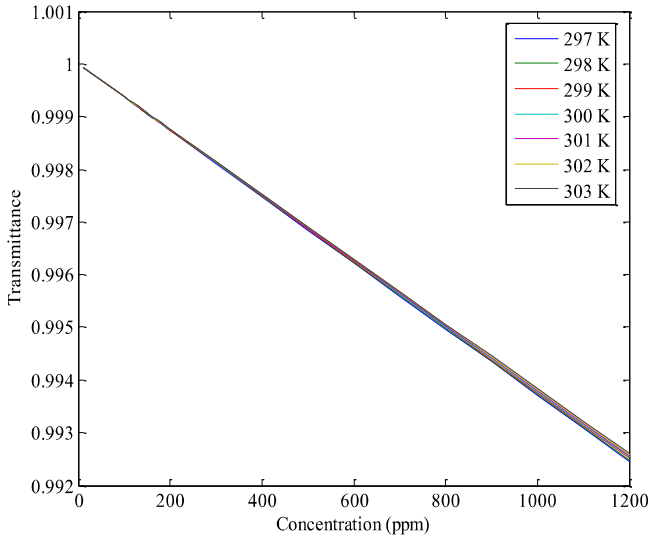

Figure 2a Graph of transmittance versus concentration for temperature 297 K to 303 K

Ozone gas absorption cross section and deviation were computed using equation 1 and equation 2 earlier described by the authors in their previous publications [4, 11].

$$\sigma = -\frac{10^6 \times R \times T_p}{c_{(ppm)} \times N_A \times P \times L} \times \ln T \quad (1)$$

where:
$c_{(ppm)}$ = Ozone concentration in ppm
R = Ideal gas constant (atm m^3 mol^{-1} K^{-1})
T_p = temperature (K)
σ = Absorption cross section (m^2/molecules)
N_A = Avogadro's constant ((molecule /mol))
P = pressure in atmosphere (atm)
L = Optical path length (m)
T = Transmittance

$$\frac{\sigma - \sigma_w}{\sigma_w} \times 100\% \quad (2)$$

where:
σ = ozone absorption cross section of previous work at wavelength 603 nm
σ_w = ozone absorption cross sectionof this simulation at wavelength 603 nm

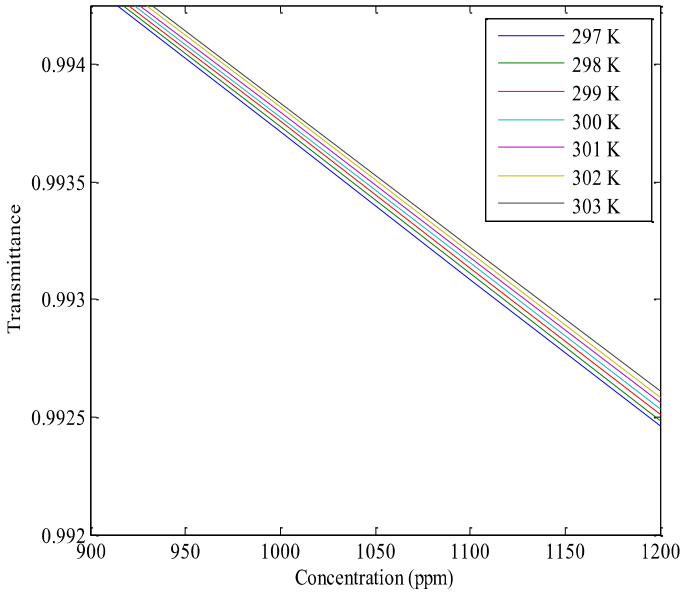

Figure 2b Zoom-in effect of transmittance versus concentration for temperature 297 K to 303 K

Table 1. Transmittance variation with temperature and ozone concentration

Temperature (K)	**297**	**298**	**299**	**300**
Concentration				
10 (ppm)	0.9999369	0.9999371	0.9999373	0.9999376
1200 (ppm)	0.9924591	0.9924843	0.9925094	0.9925342
Temperature (K)	**301**	**302**	**303**	
Concentration				
10 (ppm)	0.9999378	0.9999380	0.9999382	
1200 (ppm)	0.9925589	0.9925835	0.9926079	

Figure 3 and Figure 4 show the effect of varying ozone gas concentration on ozone absorption cross section. Both figures show the effects at different temperatures are overlapping. There was a rise in ozone gas absorption cross section from concentration 10 ppm to a maximum and a sudden fall to a constant level. The sudden rise and fall is below concentration 160 ppm for temperature range between 297 K and 299 K; and below concentration 170 ppm for temperature range between 300 K and 303 K. Sensitivity of sensors for ozone measurement in visible spectrum is lower as compared to the ultraviolet spectrum [9, 12, 13]. This has been attributed to lower absorption cross section in the visible spectrum[12]. Ozone measurement in the visible spectrum has thus been recommended for high concentration industrial applications [9]. From the results obtained in this study, effect of concentration variation on absorption cross section is negligible for 170 ppm concentration and above.

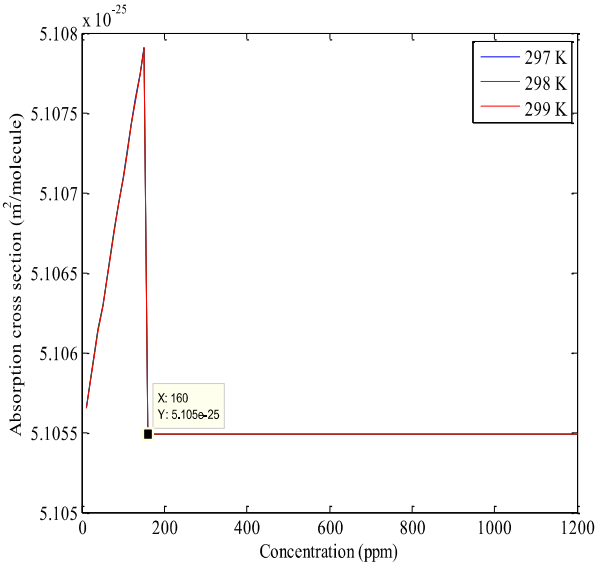

Figure 3 Simulated absorption cross section for temperature 297 K to 299 K

Absorption cross section for all temperature considered at concentration 10 ppm is averaged at $5.1057 \times 10^{-25}\mathrm{m}^2/\mathrm{molecule}$. Approximately $5.1080 \times 10^{-25}\mathrm{m}^2/\mathrm{molecule}$ absorption cross section is observed at the maximum point. At constant level, average of $5.1055 \times 10^{-25}\mathrm{m}^2/\mathrm{molecule}$ absorption cross section is observed. Percentage deviation of these values of absorption cross section from $5.18 \times 10^{-25}\mathrm{m}^2/\mathrm{molecule}$ at 603 nm [9, 14]; is in the range of 1.41% (at the maximum points) to 1.46% (at the points where the absorption cross section is constant). The difference is 0.05%. Similarly, comparison with $5.23 \times 10^{-25}\mathrm{m}^2/\mathrm{molecule}$ at 603nm [8], range of deviation in percentage is from 2.39% (at the maximum points) to 2.44% (at the points where the absorption cross section is constant). This also yields difference of 0.05%.

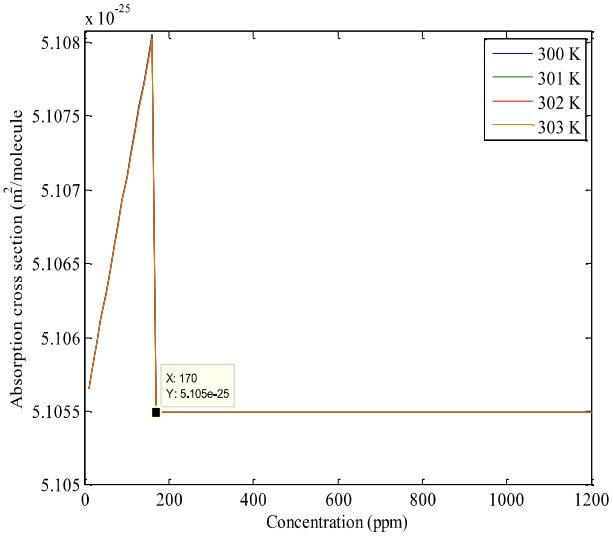

Figure 4 Simulated absorption cross section for 300 K to 303 K

4.0 CONCLUSION

In this manuscript, we have reported the investigation on effect of varying concentration on transmittance and absorption cross section of ozone at different temperatures. For temperature range from 297 K to 303 K, there was increase in transmittance of 0.00012 % (for 10 ppm concentration) to 0.01499% (for 1200 ppm concentration). There was an average decrease of 0.75% in transmittance from 10 ppm to 1200 ppm concentration at constant temperature. The percentage difference between ozone gas absorption cross section of $5.1080 \times 10^{-25}\mathrm{m}^2/\mathrm{molecule}$ (at maximum points) and $5.1055 \times 10^{-25}\mathrm{m}^2/\mathrm{molecule}$ (where absorption cross section becomes constant) is 0.05%. In comparison to previous work, the ozone gas absorption cross section deviation in percentage is between 1.41% and 2.44%. From the results obtained in this study, effect of concentration variation on absorption cross section is negligible for concentration 170 ppm and above. Outcome of the study show that there is no variation in absorption cross section for range of concentration between 170 ppm and 1200 ppm. For research activities in the visible spectrum on absorption cross section in the future; variation that could arise from concentration variation can be avoided by considering concentrations above 170 ppm. It is recommended that the results obtained be further verified with experiments.

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REFERENCES

[1] M. David, M. H. Ibrahim, S. M. Idrus, A. I. Azmi, N. H. Ngajikin, T. C. E. Marcus, M. Yaacob, M. R. Salim, and A. Abdul Aziz. Progress in Ozone Sensors Performance: A Review. *Jurnal Teknologi,* 73(6):23-29, 2015.

[2] M. David, M. H. Ibrahim, S. M. Idrus, and T. C. E. Marcus. Fundamental Review to Ozone Gas Sensing Using Optical Fibre Sensors. *TELKOMNIKA (Telecommunication Computing Electronics and Control),* 13(4): 1133-1144, 2015.

[3] A. Serdyuchenko, V. Gorshelev, M. Weber, W. Chehade, and J. Burrows. High spectral resolution ozone absorption cross-sections–Part 2: Temperature dependence. *Atmospheric Measurement Techniques,* 7: 625-636, 2014.

[4] M. David, M. H. Ibrahim, and S. M. Idrus. Sampling frequency effect on the absorption cross section of ozone in the Visible Spectrum. *Journal of optoelectronics and advanced materials,* 17(3-4):403 -408, 2015.

[5] T. C. Marcus, M. David, M. Yaacob, M. R. Salim, N. Hussin, M. H. Ibrahim, N. H. Ngajikin, A. I. Azmi, S. M. Idrus, and Z. Buntat. Alternative wavelength for linearity preservation of Beer–Lambert Law in ozone concentration measurement. *Microwave and Optical Technology Letters,* 57(4):1013-1016, 2015.

[6] K. Fuwa and B. Valle. The Physical Basis of Analytical Atomic Absorption Spectrometry. The Pertinence of the Beer-Lambert Law. *Analytical Chemistry,* 35(8): 942-946, 1963.

[7] M. Yasin, S. Harun, C. Tan, S. Phang, and H. Ahmad. Fiber optic chemical sensor using fiber coupler probe based on intensity modulation for alcohol detection. *Microwave and Optical Technology Letters,* 53(8):1935-1938, 2011.

[8] J. Brion, A. Chakir, J. Charbonnier, D. Daumont, C. Parisse, and J. Malicet. Absorption spectra measurements for the ozone molecule in the 350–830 nm region. *Journal of atmospheric chemistry,* vol. 30(2):291-299, 1998.

[9] S. O'Keeffe, C. Fitzpatrick, and E. Lewis. An optical fibre based ultra violet and visible absorption spectroscopy system for ozone concentration monitoring. *Sensors and Actuators B: Chemical,* vol. 125(2):372-378, 2007.

[10] R. C. Denney. Dictionary of spectroscopy. *Willey 2nd Edition* 119-120, 1982.

[11] T. C. E. Marcus, M. David, M. Yaacob, M. R. Salim, N. Hussin, M. H. Ibrahim, N. H. Ngajikin, A. I. Azmi, S. M. Idrus, and Z. Buntat. Pressure Dependence of Ozone Absorption Cross Section. *Applied Mechanics and Materials*, 735:260-264, 2015.

[12] K. Teranishi, Y. Shimada, N. Shimomura, and H. Itoh. Investigation of Ozone Concentration Measurement by Visible Photo Absorption Method. *Ozone: Science & Engineering,* 35(3):229-239, 2013.

[13] J. Orphal. A critical review of the absorption cross-sections of O_3 and NO_2 in the ultraviolet and visible. *Journal of Photochemistry and Photobiology A: Chemistry,* 157(2):185-209, 2003.

[14] E. Vigroux, *Contribution à l'étude expérimentale de l'absorption de l'ozone, par Ernest Vigroux*: Masson, 1953.