

Interactive comment on “Recommendations for spectral fitting of SO₂ from MAX-DOAS measurements” by Zoë Y. W. Davis and Robert McLaren

Anonymous Referee #1

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Title: Recommendations for spectral fitting of SO₂ from MAX-DOAS measurements.

The aims of the article is to find the best fitting window for SO₂. Sulfur dioxide is a gas that is difficult to measure due to the proximity of its absorption band at low wavelengths, the main problems encountered: low ultraviolet radiation and stray light. The article is well structured and clear in its dissertation, considering the complexity of the research topic. The researchers working with SO₂ will find this article and its recommendations on the fitting window, errors and uncertainties, very useful.

â€” General consideration

1) How would you use the recommendations discussed in the article with satellite com-
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parisons? 2) Have you tried the 315-325 nm window fit?

3) Have you thought in a comparison, using the window fit recommend, with satellite? OMI? TROPOMI?

4) Is it necessary to correct the ring effect if active DOAS is used?

5) It would be very useful to include in the article measurement of calibration cells with high SO₂ concentrations ($\sim 1 \times 10^{19}$), applying the recommendations presented in the article and discussing the results.

â€” Specific consideration

Introduction Line 34: Rix et al., 2012, spectral range fit between 315 and 326 nm.

Line 43: verify reference “Wang and Christopher, 2003”, is it correct?

Methods Line 55: Instrument resolution (FWHM) are calculated or is the information provided by the company (in this case, Ocean Optics)? The company provides an average resolution of the entire spectral range of the instrument and not in the specific absorption range of a given compound (e.g. SO₂, NO₂, etc.).

Line 58: “using the DOASIS software package”. Why using DOASIS? In my opinion, QDOAS is currently the best and most widely used software for the fitting of contaminating compounds in the atmosphere with ground-based techniques.

Line 61-62: Be careful to use high and low concentration referring to the calibration cells. I disagree in considering a concentration of $\sim 1 \times 10^{17}$ as “high”. This is relative. What are you talking about? Contaminated areas? industrial areas? volcanic areas? Megacities? The SO₂ concentrations of $\sim 1 \times 10^{17}$ molec/cm² (occasionally $\sim 1 \times 10^{18}$) are “high” considering anthropogenic contaminated areas, such as megacities or/and industrial areas. Volcanic SO₂ concentrations can reach $\sim 1 \times 10^{19}$ molec/cm². Using instruments such as UV camera, very concentrated calibration cells are needed ($\sim 1 \times 10^{19}$ molec/cm²), to be able to calibrate the instrument for SO₂ concentrated plumes. I

suggest specifying the “high concentrations” in the atmosphere of polluted areas, like megacities.

Linea 63: “These SCDs would be equivalent to an air mass with SO₂ mixing ratios of 87 and 8.7 ppb. . .”. Is the calculation correct? How did you calculate these values?

â€” Final consideration

Personally, I tried to apply the recommendations, discussed in the article, on the best SO₂ fitting windows. I compared, using MAX-DOAS and Direct Sun techniques, the 307.5-319 nm window fit with other windows fit used in the literature. The 307.5-319 nm window fit work well in anthropogenic contaminated areas, I was able to recover more spectra and obtaining a lower RMS than other windows fit. On the other hand, the results obtained by testing the recommended window fit with very concentrated calibration cells ($\sim 1e19$), greatly underestimate the real concentration inside the cells. I consider the article important for the scientific community and I recommend publication in AMT. I therefore recommend minor revisions.

Please also note the supplement to this comment:

<https://www.atmos-meas-tech-discuss.net/amt-2019-420/amt-2019-420-RC1-supplement.pdf>

Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2019-420, 2020.