

Title: Benchmarking Photolysis Rates with Socrates (24.11): Species for Earth and Exoplanets

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Dear reviewer,

*Thank you very much for your comments. They have been very helpful and constructive and we believe have greatly improved and clarified the manuscript. Below we have listed all the comments, with our responses in **red** and italic. The corresponding updates in the manuscript are shown in **bold** text.*

Kind regards,

Sophia Adams and co-authors

This paper calculates photolysis rates using Socrates and evaluates the results through a comparison with two other reference models, UCI-ref and UCI-Jxr. The evaluation was conducted using both Earth's atmosphere, and an example exoplanet. The absorption cross-sections and quantum yields used were mostly based on expert panel reviews from IUPAC and JPL where available, with other sources used when necessary. The paper is a useful contribution to the field, especially as absorption cross-sections and quantum yields have been updated through this work, however more work needs to be done to extend the analysis of the discrepancies between the models, and improve consistency and readability before it can be published. Additionally, the quality of many of the figures (and their captions) does not seem to be up to GMD standards and should be improved.

Primarily, there are too many technical mistakes. Although many of them are minor, their quantity indicates a more thorough read through and edit is required by the authors (in addition to correcting those I have noticed in the 'Technical corrections' section).

A few sections mention the rates of reactions (lines 227,234), but there is no reference of how this was obtained, where are the quantum yields and absorption cross-sections from? Even if this is mentioned in Table A1, it should be referred to in the text.

Additionally, the analysis of the discrepancies between the models is missing depth. Is this work considered better than UCI (which may have quantum yields/absorption cross-sections that are not up-to-date)? Or is UCI already the standard, and this comparison is just to check the reliability of this work? Does UCI use pressure and temperature dependent quantum yield? It is

unclear from reading your paper. Differences between the two photolysis models should be explored further.

Thank you very much for these comments. The technical mistakes have now been fixed. We address each point below. Mentions of where our data was obtained is specified within the text as well as Table A1.

We have provided a more in depth analysis behind the discrepancies. We have also revised and recalculated new photolysis rates based on previously missed temperature dependent cross sections which explained some of the difference for species: HNO_3 , N_2O , N_2O_5 and H_2O_2 .

Finally, figures are not of a high quality and should be improved generally. Here are some specific examples, where detail, readability and consistency are lacking:

- Any mention of molecules should be correctly written i.e. ' O_2 ' not ' O2 ' in Figure 2.

Thank you, this has now been fixed.

- Ensure that the labelling is consistent: in most figures it should be ' μm ' instead of 'micron', and 'J rate (s^{-1})' instead of 'J rate s^{-1} '

All labels have been changed to " $\text{J} (\text{s}^{-1})$ " and all wavelengths are reported in nm.

- Many caption descriptions are not detailed enough to stand alone. Some examples: Figure 3 should have clearer references to the legend used in the figure, Figures 4 and 5 bottom row have no mention of where that data comes from (along with all other figures that include a J rate against wavelength), Figure 7 caption is missing detail (legend not explained)

Caption descriptions have been adjusted to provide more useful information.

- Some of the figures are misaligned (such as Figures 7 and 16, but there are many examples)

Figures have been adjusted so that they are all aligned.

- The text and numbers are very small, should be increased for visibility

The font size of the titles, axis ticks and legends have all been increased.

Specific Comments:

Line 176: Why was Part 1a used, and not another set-up? Can you provide a sentence or two to explain? Can you discuss how only looking at one very specific scenario 'clear sky, no aerosols, high sun (Solar Zenith Angle, SZA = 15°) over the ocean' will affect the results?

We only use Part 1a because other tests conducted by Photocomp were to test radiative transfer accuracy but this has been rigorously tested in Socrates's case so was not needed. The explanation in the paper is given as follows: "The PhotoComp study also included tests of the accuracy of the actinic flux calculations for different atmospheric compositions. However, the accuracy of the Socrates radiative transfer calculations has been extensively validated previously for both Earth (Pincus 2020) and exoplanets (Amundsen 2014), therefore we restrict our work here to benchmarking the photolysis rates only."

Lines 226,247: You mention that there are differences due to input data, do you know why absorption cross-sections and quantum yields are different? Is one more up-to-date, do they use a different source?

Yes, we are using more up-to-date cross sections. This has been clarified in the paper: "The UCI-ref model is based on JPL recommended cross-sections from 2010 while Socrates is using an updated temperature dependent cross-section from HITRAN 2020."

Lines 294-295: Can you find the cause of the discrepancy, instead of listing potential causes

We hadn't included the effect of temperature dependent cross sections. This has now been rectified, and the results match more closely with the reference model.

Line 306: 'which the reference models may not' is there no way to know for sure?

Thank you for your comment. Our previous results did not take into account temperature dependence in the cross sections. We have recalculated based on this new input data and provided new results. The H₂O₂ section has been rewritten with this considered and we simply state exactly what input data we are using.

Lines 320-324: Can you add a figure (potentially in the appendix) demonstrating the effect of the pressure dependence on a J rate vs wavelength plot, at different pressures? This would be

similar to Figure 6 bottom panel, but showing the rate with and without pressure dependence of quantum yield? It would be good to do this for formaldehyde too

Thank you for your suggestion. However, Socrates does not currently have the functionality to consider pressure dependence in the quantum yield. Future work to include this functionality in Socrates will be undertaken and a subsequent analysis on the impact on the results will be undertaken.

Line 330: You mention there is a great deal of uncertainty with the input data, can you expand on this and provide examples? Especially as this is mentioned again in the last conclusion point

For example, we expand upon the uncertainty for CH_3ONO_2 and provide the following explanation: “The JPL 19-5 report does not provide recommended values of the quantum yield but reports conflicting values measured at particular wavelengths. We use a quantum yield of 1 for wavelengths ≥ 248 nm, 0.91 for wavelengths 241 - 248 nm and 0.7 for wavelengths < 241 nm. However the chosen limits are fairly arbitrary and likely to be the cause of the discrepancy between the Socrates and UCI-ref photolysis rates.”

Technical Corrections:

Generally:

- Fast-JX: capitalise the ‘X’ throughout the text

This has been amended throughout the paper.

- Molecule names should not be capitalised (formaldehyde lines 303 and 304, glyoxal line 326, carbonyl sulfide)

The molecule names are no longer capitalized.

Line 17: units should be separated with a space ‘25 km’

A space has been added.

Line 20: 'At the surface, UV irradiation has implications...' remove comma

The comma has been removed.

Line 24: This sentence is confusing, what do you mean by 'elements'?

*Thank you for your comment. This sentence has been reworded as follows: **"Work exploring the cycling of ozone has been performed which demonstrated features such as formation of secondary ozone layers, and shielding from flaring caused by ozone build-up from previous flares"***

Line 29-31: This sentence is very hard to read and understand, please rework

*This section had been reworded for clarity. The sentence now reads: **'In order to calculate photolysis rates, we need information on the absorption cross section of the species involved, the quantum yield of the reactions (i.e. the branching ratio indicating which particular photolysis pathway is most probable), the spectrum of the incoming irradiance from the star at the top of the atmosphere and a treatment of the radiative transfer to determine the resultant actinic flux at a given atmospheric layer.'***

Line 90: there is an extra space after 'remembered'

This section has been reworded therefore this is no longer an issue.

Line 154: EUV was mentioned for the first time without a definition. Wavelength range covered in extreme UV category would also be useful

*EUV has now been defined as **"extreme UV (EUV, <121 nm)"***

Line 202: What is 'N³', is that a mistake?

The "3" subscript was to indicate a footnote. This has been reformatted to avoid confusion.

Line 209: 'O(³P)' not just '(³P)'

This has been fixed.

Figure 8 caption: Needs space between 'pressure(Pa)' should be 'pressure (Pa)'

A space has been added.

Line 259: I think it should say '400-420 nm' not '300-420 nm'

This was a mistake and now reads as '400-420 nm'.

Line 319: the word 'significant' should only be used if it is statistically significant. Is that the case here?

Yes, it is the case where it is statistically significant here.

Line 344: FUV not defined

FUV had now been defined- ; The wavelength ranges have been defined as "far UV (FUV, 121 - 200 nm) "

Line 345: space needed '121.6nm'

A space has been added.

Line 359: NUV not defined, Figure 4 missing capital

This has now been defined as "near-UV (NUV, ~200-400 nm)" and the missing capital has been added.

Line 382: 'and so similar to'?

This section has been reworded and so this grammatical error is no longer an issue.

Line 412: 200nm, space needed

A space has been added.

Line 459: 50nm, space needed

A space has been added.

Table A1: Table caption should be above a table, not below. More description of the table is needed in the caption

The caption is now above the table, and more description of the table has been included.