

Geochronology Discuss., author comment AC1
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Reply on RC1

Alexandria J. Koester and Nathaniel A. Lifton

Author comment on "Technical note: A software framework for calculating compositionally dependent in situ ^{14}C production rates" by Alexandria J. Koester and Nathaniel A. Lifton, Geochronology Discuss., <https://doi.org/10.5194/gchron-2022-16-AC1>, 2022

We thank Dr. Reto Trappitsch for their helpful feedback to our manuscript. We respond to each comment in detail below:

- *Major comments:*
- *You present production rates based on various minerals and give the composition of these minerals. Would it be easier / simpler to present elementary production rates and have the user ultimately calculate the overall production rate in a given mineral based on their specific composition? This could allow a user to easier work with the results from this manuscript. Please feel free to completely ignore this idea, I am not very familiar with the general approach in the field of terrestrial cosmogenic nuclides*

We appreciate the reviewer's comments, but the calculator already does what is suggested. It takes major elemental oxide data and calculates a theoretical production rate based on the sample composition. The production rate is then normalized to the calibrated production rate in quartz. Future work would include a geologic calibration for each mineral if possible. In response to the other reviewer, we have also derived an equivalent elemental production rate formula – this will be presented in the revised manuscript.

- *Section 3.1, second paragraph: In Reedy (2013), excitation functions for the production of ^{14}C from elementary O and Si are presented and not from ^{16}O and ^{28}Si . Generally, cross-sections are measured using materials with natural isotopic abundances. This makes more sense, since these elements also occur in geological samples of interest in their normal isotopic composition.*

We thank the reviewer for noting the inconsistency in our manuscript. We have changed the wording in our description of Reedy's measurements and updated the figures that show the measured excitation functions, noting that they are on natural isotopic abundances. We have also updated the text to reflect that most of the neutron excitation functions that Reedy presents are in fact not measured directly (with a few exceptions), but rather are derived from the measured proton excitation functions (line 130).

- *For excitation functions from JENDL/HE-2007: Did you take the values for pure isotopic compositions as stated in line 128? I don't expect that your samples contain, e.g., isotopically pure ^{48}Ti . Therefore, a $\text{Ti}(n,X)^{14}\text{C}$ excitation function where all isotopes are included in their terrestrial composition should be used for the calculations.*

The reviewer is correct - we are assuming essentially pure isotopic compositions for the modelled excitation functions. For each of the modelled excitation functions, we used the most abundant isotope for each element. Of the elements we are considering here for the modelled excitation functions, only three of the isotopes do not have natural abundances of essentially 100%. These are ^{39}K (93% elemental abundance), ^{40}Ca (97% elemental abundance), and ^{48}Ti (73% elemental abundance). While we agree that it would be more accurate to consider production from the natural abundances of each isotope for these elements, we note that the proportion of spallation production of in situ ^{14}C from each is only a small fraction of total production for the ranges of compositions we consider. For instance, the percentage of total production predicted from ^{39}K , as considered here, ranges from 0.1 to <0.01%, that from ^{40}Ca ranges from 0.2 to 0.01%, and the percentage of total production from ^{48}Ti is uniformly <0.001% in all cases considered (Table 3). Thus, we argue that any errors in our total predicted compositionally dependent production rates introduced by considering only the isotopes above, instead of the natural isotopic abundances for these elements, would likely be insignificant relative to other uncertainties in our calculations that we note. We have updated the text to clarify this argument in the manuscript. Also see our response below to the next comment.

- *Uncertainty determination for JENDL/HE-2007 excitation functions, last paragraph in Section 4.2. You estimate the overall uncertainties for the purely calculated excitation functions at 10-15%. The estimate is based on comparing the JENDL/HE-2007 (calculated, generally GNASH) with TENDL (calculated, TALYS). This comparison is not exactly fair. A better comparison would be to compare calculated excitation functions with measured ones, as, e.g., Broeders et al. (<https://doi.org/10.14494/JNRS2000.7.N1>), however, you obviously cannot do this for the reactions you are interested in. A better estimate to use for the uncertainty of calculated production rates is given in Reedy (2013), section 3.1, third-last paragraph: "[...] most formulae and codes give cross-sections for an individual nuclide that typically differ from measured ones by factors of ~ 2 (Ammon et al., 2009)". Your uncertainty estimate seems therefore far too optimistic.*

We agree that our uncertainty estimates for the modelled excitation functions could be more conservative. However, apart from ^{23}Na , all the modelled reaction excitation functions have only minor impact on the overall production rates we predict (see above response as well). The percentages of total production of in situ ^{14}C from ^{55}Mn , ^{40}Ca , ^{39}K and ^{31}P range from <0.001 to 0.2 for the compositions considered (Table 3). Even if reaction cross sections are off by a factor of 2, as suggested above from Reedy (2013), the impact to overall production is small. For instance, if we doubled the percentage of ^{14}C production from Ca for Wollastonite, it would only increase to 0.4 %. Thus, as noted above, we argue that the overall additional uncertainty in our results that might be introduced by using more conservative estimates of potential errors in the modelled cross-sections would be insignificant relative to other uncertainties in the calculations. Of course, as we note, particularly for ^{23}Na , this also points to the need for more measured excitation functions for in situ ^{14}C production – both from protons and the neutron excitation functions derived from those measurements. We note in our conclusion that measured excitation functions (or those derived from measurements at natural abundances, such as for neutrons in most cases, per Reedy) would greatly improve our predictions, and have modified the text to reflect the additional points above.

- *Minor comments:*
- *Section 3.1, first paragraph: This paragraph contains quite a lot of information that is not understandable without reading Lifton et al. (2014) first. You are already describing what goes into the model in a very good way in Section 2.1. For this paragraph, it would be good if you could explain all abbreviations (LSDn, PARMA, SHA.DIF.14k - if this is an abbreviation). Furthermore, could you provide some detail on what the gridded R_C and dipolar R_CD models of Lifton et al. (2016) are?*

We acknowledge that we skimmed over the details of Lifton et al. (2014) but argue that interested readers can go to the original publication for full details of the nuclide-specific LSDn scaling methodology. We expect that interested readers will be familiar with the term "LSDn" because it is a common scaling method (along with St and Lm, as seen in the online UW v3 online calculator that we reference in text). We have also included some minor edits in line 115 for clarification.

- *Figure 1: For the measured curves, it might be good to present the measurements as symbols, in order to easier distinguish between interpolated and measured values.*

We appreciate the comment to clarify the figure and have added symbols to make it easier to distinguish measured values (or those inferred from measurements, such as most of the neutron data) from interpolated values.