Author response

Daniel Garduno Ruiz, Colin Goldblatt, Anne-Sofie Ahm

April 27, 2025

Dear Dr. Sander:

Here we provide responses to all of the comments made by the reviewer and specify the changes made to the manuscript. We have addressed all the comments and revised the manuscript accordingly.

Responses to reviewer comments

- The authors introduce a way of tracking the consequences of imbalances in the input data. However, they do not provide a remedy for such imbalances.

  Response: We would like to implement the method of balancing the concentration changes described in Lehman (2022) in a future version of Chempath.

- As the authors only provide a tracking of imbalances, the headline of Section 3.2 “Balancing of concentration changes" is misleading and should therefore be changed.

  Response: We changed the headline to “Tracking imbalances due to numerical errors"

- ... we assume that the difference between concentration changes and the total production by all reactions is due to the solver's numerical error...": In most applications the concentration change is calculated by the solver (with high accuracy), whereas the reaction rates are calculated separately after the main model run (from data with less temporal resolution than the internal calculations by solver), which introduces larger errors (and justifes a subsequent modification of the rates).

  As stated correctly by the authors, they request that the user ensures the balance of the input data. As explained above, this may be problematic for some users. Therefore a corresponding information (“warning") should be included in the abstract and introduction together with a notice that a part of the original algorithm of Lehmann (2004) was not implemented.

- **Response**: We include the following text in the abstract:

  “*Chempath* does not include the balance of concentration changes and reaction rates that Lehmann's algorithm uses to eliminate imbalances due to numerical errors”. Instead, *Chempath* quantifies the contribution of these imbalances to the production and destruction of a species.

  And the following text in the introduction:

  “Our implementation is based on the description of the algorithm in Lehmann (2004). However, there is one difference between Chempath and Lehmann's (2004) algorithm. Our implementation does not include the balance of concentration changes and reaction rates that

Lehmann's algorithm uses to eliminate imbalances due to numerical errors. Instead, *Chempath* requires input information about these imbalances to quantify the contribution of numerical errors to the production and destruction of a species."

- Table 1: [dci] should be explained as vector of the concentration changes..." (or the square brackets would have to be removed).

  Response: We specified that this variable represents a vector in table 1. We did the same with other variables representing vectors.

- Table 1 (last line): If $[c_i]$ and $[d_i]$ denote vectors, then $[\tau_i]$ must be calculated by element-wise division.

  Response: We specified that $[\tau_i]$ is calculated by the element-wise division of two vectors

- Eq. (1): This looks like a product of a matrix and a vector, but then the summation would not be correct (and there is one closing bracket too much)

  Response: We updated this equation to represent the multiplication of a matrix and a vector, to avoid the use of the sum notation. We did the same in all other equations containing sum notations.

- 200: where i = 1...ns seems to denote ns individual equations, which contradicts the vector notation in Eq. (14).

  Response: We deleted i = 1... ns to be consistent with the vector notation.

- You mention one vector [we], but calculate the sum over ne such vectors in Eq. (16). (Is the transpose symbol in Eq. (16) correct?)

  Response: We updated this equation to represent the multiplication of a matrix and a vector, to avoid the use of the sum notation. We also include an example of how this equation is fulfilled in our simple example (equation 24 in the corrected manuscript). You can see in that example why we need the transpose symbol.

- "keeping only the positive values" ⇒ keeping only the positive values and zero"? (analogously for negative values).

  Response: We deleted the sentences "keeping only the positive/negative values"

- I suggest to keep the deleted "as branching points" for clarity.

  Response: We re-included this sentence.

- We run Chempath ... in all the model times...": This sounds like points in time. What is the length of the time intervals analysed, corresponding to dt in Table 1?

  Response: We replaced "model times" with "model time intervals". For all points in time where there is a solution we use Chempath to obtain pathways, using the current point in time and the next point in time at which the solver obtains a solution. We use an adaptive solver with a varying dt. In our simulation dt varies from 10^{-8} seconds to 10^{3} seconds.

- We run Chempath ... at 32 time points...": cf. previous question.

  Response: Photochem also uses an adaptive solver with a varying dt. In our simulation dt varies from 0.1 to 10^{10} seconds.

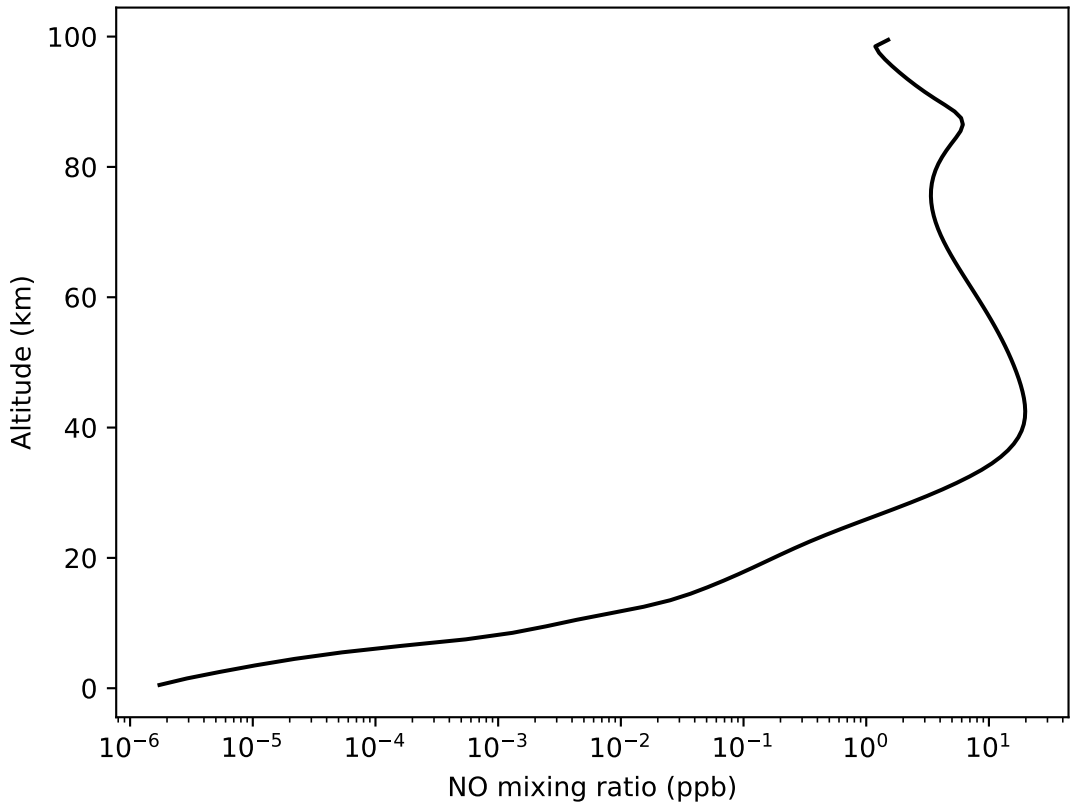

Figure 1: NO mixing ratio in our model run

- Does this sentence mean that the model run was 1 million years long (cf. also line 439)? If so, why do Table 4 and Figs. 3, 4, and 5 show results for .16 million years"?

  Response: We corrected these sentences to specify that the model was run for 1.2 million years.

- Probably the sequence of causes and effects is: decrease of the O2 input flux ⇒ decrease of the O3 production rate ⇒ decrease of the O3 concentration ⇒ decrease of the O3 loss rate.

  Response: We modified this sentence to include the sequence suggested here.

- Under conditions of present Earth (troposphere), the reaction CH3O2 + NO ..., which is included in your model, would ensure a short lifetime of CH3O2. However, the mixing ratio of NO in your model seems to be extremely small..

  Response: Figure 1 shows the NO mixing ratio corresponding to the red line in figure 3 on the manuscript. Its concentration is very small in the troposphere, as you notice. The concentration of NO in the model we are using is determined by chemistry, transport, and deposition. The model does not include lightning or anthropogenic emissions.

- “these species": which species (or why plural)? **Response**: We made the correction.
- The unit of the rates (molec/(cm2/s)) seems to imply vertically integrated rates. However, the figure caption says ... rates ... correspond to the height at which the pathways contribute the most..."

  Response: We made the correction.