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Geoscientific
Model Development
Discussions

Interactive comment on "A kinetic chemistry tagging technique and its application to modelling the stable isotopic composition of atmospheric trace gases" *by* S. Gromov et al.

Anonymous Referee #1

Received and published: 5 March 2010

General comment: The authors present a tagging methodology for isotopes, which is implemented in a box model. The paper is well written and I recommend publication after minor revisions. The topic is very complex and not straight forward. It is obvious that the authors are very familiar with the topic, but the reader might get lost without additional 'help'. Although most things are well described, it would be worth to have simple examples, before showing the chemical and mathematical details.

My main sugestions are:

1. Section 3 should start with the examples. When introducing the equations in the subsequent sections, the examples would be of great help, if the variables (incl. their

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values) are directly linked to the example.

2. A table of the used variables including the description and units would be helpful.

3. Some clarifying statement would be helpful: this tagging is a diagnostic in a sense that it helps to diagnose the regular chemistry. However, the method itself is based on prognostic equations.

4. Could you say someting about the solution of the tagging ODE: Stability, Attractivity? I.e. Do you always get the same equilibrium solution independent from the initial condition?

Specific comments:

page 214 line 16 The specific weight (or I assume molecular mass) q only takes into account the regarded element not the whole molecule?

page 217 l 18-20. I am puzzled by this sentence. Probably kr should read Ar in line 18? Otherwise eq (10) would lead to kr=Ar?

page 224 Why is qp/qe "the probability of the rare isotope to be transferred to the current product" (which is again a rare isotope?) I have difficulies to understand the idea behind the formula. (Well, after I saw the examples, I think I got it. If the whole text is better linked to the examples, this comment will be obsolete.)

page 225 line 1: It would be helpful to see the calculation, either in the appendix or in the supplement.

page 226 eq (15) 2nd line one 'maj' of Cb from the left side of the eq, should be moved to the right side of the eq.

page 229: The exmples are very important for the understanding of the methodology! I suggest to change the order in chapter 3 and to start with these examples. Further there should be a direct link between the numbers in the example and the variables in the previous sections. So, if the order in section 3 is changed, there could be a

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reference to the examples in the description of the methodology, e.g. qe=... qn=... in the 1st example of section 3.1.

page 231: eq 19:I was confused by the symbol e-, but it's probably a double "- -" ? page 231: eq (20), again an example would be nice. So if 16O2 is regarded than qn=2 and since you only consider 1 replaced O atom the rare chi is multiplied by 1/qn = 1/2.

page 232: For consistency reasons: the 1 in eq (21) should be bold.

page 233: Can you explain more detailed, why the equilibrium isotope effect introduce the deviations but not the 'normal isotope chemistry'? If I understand it right then MECCA produces a concentration cn of specie Cn at time t+tau. MECCA-TAG produces concentrations ˆmaj cn and ˆmin,i cn for time t+tau. I would have expected that the schemes give ˆmaj cn + sum_i ˆmin,i cn = cn This does not seem to be the case, which needs to be explained in more detail. It would be helpful, if (e.g. in the appendix / supplement) the authors could show mathematically that this holds or doesn't.

page 234: The re-scaling eq. (25) means that the left side is newly defined?

page 240 HL LL, it could be mentioned that this means high / low latitude ? (also in Fig. caption).

page 253 l 18 "JJ."

I am impressed by the second supplement.

Interactive comment on Geosci. Model Dev. Discuss., 3, 201, 2010.