Interactive comment on “Observed and simulated global distribution and budget of atmospheric C$_2$−C$_5$ alkanes” by A. Pozzer et al.

Anonymous Referee #1

Received and published: 12 February 2010

This manuscript reports on the inclusion of chemistry for C2-C5 alkanes in a global atmospheric model. Discussion focuses on the ability of the model to reproduce observations of these species and their calculated impact on the production of acetone and acetaldehyde. The analysis investigates two emission scenarios: one adhering to the EDGAR database and the other prompted by a recommendation by Jacob et al. (2002) that emissions should be distributed differently to better reflect observations. Although the analysis generally supports the recommendation of Jacob et al., the results are also presented in much greater detail (especially given the supplementary material) and are compared more extensively than previous work, taking advantage of multi-year observations from the NOAA/ESRL flask sampling network. This provides a clearer understanding of both the quality of the model improvement and the remaining discrepancies. The authors also identify a large underestimate in the total pentane
emissions used by Jacob et al. One concern is that some of the numbers used to describe the Jacob et al. emissions do not appear to match those found in that paper (see below for details). In the discussion of OVOC production, it would also be helpful if the authors would add some information on the relative importance of C2-C5 oxidation compared to other sources in the context of the total budgets for acetone and acetaldehyde. This paper should be published with minor modifications. Specific comments and questions are listed below.

1. On page 620 (line 21), the authors provide numbers for the Jacob et al. emissions that appear to disagree with those previously published. Jacob et al. report emissions of 3.6 and 5.0 Tg C/yr for i-butane and i-pentane, respectively, while the numbers reported here are 4.2 and 6.0 Tg/yr. It appears that the difference for i-pentane is a units difference (Tg C versus Tg C5H12), but that means that the 3.6 Tg C for butane should scale to 4.35 Tg. I am not concerned that there is a big problem here, but please be clear on both units and consistency with Jacob et al. so that readers going between the manuscripts do not get confused.

2. On page 629, the authors provide references regarding the importance of acetone in the upper troposphere, but all of these references are from 2001 or earlier. While I would not dispute that acetone has importance, more recent work on the temperature dependence of acetone cross sections and quantum yields have significantly downgraded the expected impact of acetone presented in those earlier references. More recent references should be added to this discussion and an acknowledgement that this more recent information is expected to alter the findings of these previous studies (including the Jacob et al. 2002 study on the acetone budget).

3. On page 630 (lines 20-22), the discussion of acetone yields is confusing in that Jacob et al. is quoted as using 0.52 for i-pentane (should actually be 0.53) and this study uses \( \sim 0.90 \). From the mechanism in Table 1, the yield is shown to be 0.616 and these reactions have been stated to represent “final degradation products” according to earlier discussion on Page 619 (line 5). Have I missed something here? If this is
not correct, some clarifying information would be useful. Another difference that is not mentioned is the acetone yield for i-butane (0.93 from Jacob and 0.794 from Table 1).

4. Why isn’t acetaldehyde from the oxidation of ethane mentioned in section 5.2?

5. In the abstract as well as section 5, it would be very helpful if the authors would comment not just on the absolute source strengths of acetone and acetaldehyde from alkane oxidation, but also provide some information on relative importance compared to other sources comprising the total budget for these species.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 615, 2010.