Supplement of

Assessing acetone for the GISS ModelE2.1 Earth system model

Alexandra Rivera et al.

Correspondence to: Kostas Tsigaridis (kostas.tsigaridis@columbia.edu)

The copyright of individual parts of the supplement might differ from the article licence.
Chemical sources

The acetone molar yields of propane, butane, pentane, and higher alkanes were derived with suggestions from the literature (Fischbeck et al., 2017; Jacob et al., 2002; Weimer et al., 2017). We used a molar yield of 0.73 for propane, derived by averaging 0.72 from Jacob et al. (2002) and 0.736 from Weimer et al. (2017). Our molar yield of 0.95 for butane was derived by averaging 0.96 from Fischbeck et al. (2017) and 0.93 from Jacob et al. (2002). Our molar yield of 0.63 for pentane was derived by averaging 0.72 from Fischbeck et al. (2017) and 0.53 from Jacob et al. (2002). Finally, we used a molar yield of 0.79 for higher alkanes, derived from averaging the following four values: 0.96 for isobutane and 0.72 for isopentane in Fischbeck et al. (2017), and 0.93 for isobutane and 0.53 for isopentane in Jacob et al. (2002).

Global acetone budget and burden

Figure S1. The data recorded in the literature was used to determine a mean for each budget flux value, and the distance from that mean for each paper was expressed as a z-score (Arnold et al., 2005; Beale et al., 2013; Brewer et al., 2017; Dufour et al., 2016; Elias et al., 2011; Fischer et al., 2012; Folberth et al., 2006; Guenther et al., 2012; Jacob et al., 2002; Khan et al., 2015; Marandino et al., 2006; Singh et al., 2000, 2004; Wang et al., 2020). The z-scores for the literature are in shown as light-blue bars, and the Baseline model’s z-score is highlighted in yellow.
Figure S2. Net oceanic acetone fluxes in the Baseline simulation for December-February (top left), March-May (top right), June-August (bottom left), and September-November (bottom right), with red indicating a net source and blue indicating a net sink. Nonlinear colorbars are used to better differentiate the details in the map. The weighted global means of the net ocean fluxes are shown in boxes on the lower right of each subplot.
Figure S3. Comparison between the GISS ModelE2.1 simulations (Baseline in purple and Nudged_ATom in blue) and the ATom-1 field measurements (July-August 2016). Individual data points are shown with dark grey symbols, and their average values are shown in black, with error bars representing the one-sigma range of the averages. The root mean square error (RMSE) of each simulation is noted at the top right of each subplot.
Figure S4. Similar to Figure S3, except for the ATom-3 field measurements (September-October 2017).
Figure S5. Similar to Figure S3, except for the ATom-4 field measurements (April-May 2018).
Figure S6. GISS ModelE2.1 spatial distribution of annual mean acetone at surface for the Baseline simulation in Europe over twelve months. Filled circles represent data from field measurements from Solberg et al. (1996). A nonlinear colorbar is used to better differentiate the details in the map.
Figure S7. Contribution of acetone sources and sinks in the Baseline simulation over twelve months on the regional level (10˚ x 12.5˚ grid boxes) at nine European sites. The sources and sinks are shown as various colored dashed lines, and their sums are shown as solid navy-blue lines.
Figure S8. Acetone over twelve months for various sites that do not have enough measurements to resolve seasonality (Australia, Antarctica, Africa, Asia, Europe, North America). The modeled estimates of acetone at the surface from the Baseline simulation are shown as dashed blue lines and the grey error bars represent the one-sigma range of the modeled concentrations in the climatological mean of 5 years. The modeled estimates are overlaid with monthly (solid circles) or seasonal (solid lines) field measurements, as found in the literature (de Gouw et al., 2004; Dolgorouky et al., 2012; Galbally et al., 2007; Guérette et al., 2019; Hu et al., 2013; Huang et al., 2020; Langford et al., 2010; Legrand et al., 2012; Li et al., 2019; Read et al., 2012; Schade and Goldstein, 2006).
Figure S9. Total atmospheric burden, fluxes, and lifetimes of acetone from the literature (shown in boxes and whiskers with outliers as open circles) (Arnold et al., 2005; Beale et al., 2013; Brewer et al., 2017; Dufour et al., 2016; Elias et al., 2011; Fischer et al., 2012; Folberth et al., 2006; Guenther et al., 2012; Jacob et al., 2002; Khan et al., 2015; Marandino et al., 2006; Singh et al., 2000, 2004; Wang et al., 2020), values from GISS ModelE2.1 Baseline simulation (solid blue circles), and values from the Chem_Terp0 sensitivity study (green circles).

Figure S10. Similar to Figure S9, except values from the Chem_Par0.5 sensitivity study as green circles.
**Figure S11.** Similar to Figure S9, except values from the Chem_Par2.0 sensitivity study as green circles.

**Figure S12.** Similar to Figure S9, except values from the Veg_0.7 sensitivity study as green circles.

**Figure S13.** Similar to Figure S9, except values from the Ocn_2.0 sensitivity study as green circles.
Figure S14. Similar to Figure S9, except values from the Dep_f0.0 sensitivity study as green circles.
Figure S15. Similar to Figure S8, but with the chemistry sensitivity studies added. The modeled estimates of acetone at the surface from the Baseline simulation are shown as solid black lines, and the sensitivity studies are as follows: removing the acetone + chlorine reaction (dashed green lines), removing the production of acetone from terpenes (dashed blue lines), halving the yield of acetone from paraffin (dashed orange lines), and doubling the yield of acetone from paraffin (dashed pink lines). The modeled estimates are overlaid with monthly (solid circles) or seasonal (solid lines) field measurements, as found in the literature (de Gouw et al., 2004; Dolgorouky et al., 2012; Galbally et al., 2007; Guérette et al., 2019; Hu et al., 2013; Huang et al., 2020; Langford et al., 2010; Legrand et al., 2012; Li et al., 2019; Read et al., 2012; Schade and Goldstein, 2006).
Figure S16. Chemistry sensitivities anomalies from Baseline, with red indicating an increase and blue indicating a decrease of the column-integrated net acetone chemistry flux. Nonlinear colorbars are used to better differentiate the details in the map. The fourth chemistry sensitivity study, Chem_Cl0, is omitted as the anomalies from Baseline are negligible.
Figure S17. Acetone over twelve months at nine European sites with the terrestrial and oceanic sensitivity studies added. The modeled estimates of acetone at the surface from the Baseline simulation are shown as solid black lines, and the sensitivity studies are as follows: reducing vegetation emissions to 0.7 acetone from MEGAN (dashed light-green line), doubling ocean acetone concentration (dashed blue line), changing the reactivity factor for dry deposition (dashed brown line), and doubling biomass burning emissions (dashed orange line). Field measurements from Solberg et al., (1996) are shown as solid black dots.
Figure S18. Similar to Figure S8, but with the terrestrial and oceanic sensitivity studies added. The modeled estimates of acetone at the surface from the Baseline simulation are shown as solid black lines, and the sensitivity studies are as follows: reducing vegetation emissions to 0.7 acetone from MEGAN (dashed light-green line), doubling ocean acetone concentration (dashed blue line), changing the reactivity factor for dry deposition (dashed brown line), and doubling biomass burning emissions (dashed orange line). Field measurements from Solberg et al., (1996) are shown as solid black dots. The modeled estimates are overlaid with monthly (solid circles) or seasonal (solid lines) field measurements, as found in the literature (de Gouw et al., 2004; Dolgorouky et al., 2012; Galbally et al., 2007; Guérette et al., 2019; Hu et al., 2013; Huang et al., 2020; Langford et al., 2010; Legrand et al., 2012; Li et al., 2019; Read et al., 2012; Schade and Goldstein, 2006).
Figure S19. Similar to Figure S3, except a comparison between the GISS ModelE2.1 sensitivity simulations and the ATom-2 aircraft measurements (January-February 2017). Individual data points are shown with dark grey symbols, and their average values are shown in black, with error bars representing the one-sigma range of the averages. The root mean square error (RMSE) of each simulation is noted at the top right of each subplot. Note that all sensitivities are to be compared against the Baseline simulation.
Figure S20. Similar to Figure S19, except for the ATom-3 field measurements (September-October 2017).
Figure S21. Similar to Figure S19, except for the ATom-4 field measurements (April-May 2018).

References


