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Benzene and toluene stable carbon isotope ratios: Global modelling and interpretation

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Global distributions and seasonal cycles of benzene and toluene concentrations have been calculated for the first time together with the respective stable carbon isotope ratios. The simulations were made using the global CTM MOZART3 (Kinnison et al. 2007), which has been extended to include the different rate constants for reactions of the isotopomeres with the OH radical. The model includes about 300 chemical reactions and a detailed description of meteorology, photochemistry, emission and deposition processes. The simulations cover the years 2003 and 2004 with a horizontal resolution of 1.875° and 60 vertical hybrid layers reaching from the surface to 0.1 hPa.

These numerical simulations extend our previous analysis of the concentrations and stable carbon isotope ratios for ethane as described in Stein & Rudolph (2007) by investigating volatile organic compounds with shorter atmospheric residence times. This provides the basis for studying the dependence of chemical processes occurring on different timescales on atmospheric mixing and dilution. We compare estimates of chemical ages derived from stable carbon isotope ratios with calculations based on the 'hydrocarbon clock' analysis using benzene and toluene concentration ratios. This will be used to evaluate the validity as well as the limitations of the various approaches to determine photochemical ages and to determine the contributions of dilution and chemical loss for spatial and temporal concentration gradients of species with different chemical lifetimes.

Kinnison, D. E. et al. (2007), J. Geophys. Res, 112, D20302, doi:10.1029/2006JD007879, 2007.
Stein O., J. Rudolph (2007), J. Geophys. Res., 112, D14308, doi:10.1029/2006JD008062.