Geophysical Research Abstracts, Vol. 7, 00140, 2005
SRef-ID: 1607-7962/gra/EGU05-A-00140

The regional modeling of the stable carbon isotope ratio in the oxidation of hydrocarbons

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The NMHCs are oxidized by the OH radical in the atmosphere and lead to secondary pollutants such as ozone and aldehydes which play an important role in the creation of photochemical smog and secondary organic aerosols. Therefore, understanding the detailed sources and behavior of NMHCs is important. The study of the stable isotope ratio (δ^{13}C) can be useful to understand the history of an air parcel that include sources, mixing and photochemical processing.

A regional air quality model, MC2AQ, was modified to include isotope information for propene, toluene, propane, benzene, o-xylenes, and isoprene and it was run for the full month of July 1999. The possibility for nesting to a 5.3 km resolution from a 21.2 km resolution, has been added to the model in order to improve comparability with ambient observations.

These compounds (both ^{12}C and ^{13}C) were included as tracers in the model reacting only with OH, with no feedback on the main chemistry. This model structure can help to constrain the OH concentration and it could be a good parameter to evaluate the loss and production of OH radical in the model.

In this presentation we will show the results of the model which include:

1. The anti-correlation of the stable carbon isotope ratio with emissions and mixing ratio of NMHCs,
2. The diurnal pattern in the stable carbon isotope ratio which it is an indication of the effect of the processing by OH,

3. The back trajectories of the stable isotope ratio were determined to study the history of each hydrocarbon independently using the average photochemical age. The results can help in the determination of the possible sources of individual hydrocarbons and the effects of mixing and dilution during the parcel advection. The back trajectory analysis of the stable carbon isotope ratio provides information of the possible locations of the sources of the compounds being investigated,

4. The model was also set up to study the effect of the different emission types (area sources or point sources) of NMHCs on the stable carbon isotope ratio. Using this method can help us to identify the fractionation and location of these two different source types.