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Ratios between formaldehyde, glyoxal and methylglyoxal as indicators on composition of None-Methane Hydrocarbons (NMHCs)

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Formaldehyde (HCHO), glyoxal (GLY) and methylglyoxal (MGLY) are typical oxidation intermediates in the atmosphere, the yield of which depend on the composition of precursor NMHCs and the concentration of HO_x and NO_x[1]. Previous work[2-3] uses the ratio of GLY to HCHO (RGF) as an indicator of the precursor VOCs, but few people combined the ratio of GLY to MGYL (RGM), and MGLY to HCHO (RMF) together to elucidate the premature VOCs. In this work, in order to fully explore the applicability of the ratio of the three species, we applied theoretical simulation of oxidation of different NMHCs and compared the results with field observations. A box model using MCM3.3.1 is deployed for simulating different NMHCs (including isoprene, monoterpenes, aromatics, alkanes, alkenes and alkynes) degradation processes. Under the given simulation conditions, various VOCs have different "ratio features". For RGF, nature VOCs range from 0.04 to 0.09 and low RGF is related to isoprene degradation, high RGF is related to monoterpene oxidation; aromatics (toluene and benzene) range from 0.4 to 3; the range of alkanes is 0 - 0.003; the ratio of ethylene and acetylene is around 0.011 and 13 respectively. For RGM, nature VOCs range from 0.5 to 5; the ratio of toluene and butane is around 2.2 and 20 respectively. For RMF, nature VOCs range from 0.007 to 0.2; the ratio of toluene and butane is around 0.18 and 0 respectively. In addition, through sensitivity analysis, it is found that RGF, RGM, and RMF obtained from the oxidative degradation of various VOCs are more sensitive to the change of NO_2 concentration and OH concentration. Taking isoprene as an example, the three ratios increase with the increase of OH concentration, and decrease with the decrease of NO_2 concentration. The above results were then compared with the data obtained during a field observation campaign in Yangtze River Delta region. Changes of RGF, RGM, and RMF with the observed NMHCs composition were investigated, and good agreement with model simulations was found.

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