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Global simulation of aromatic volatile organic compounds in the atmosphere

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Among the large number of chemical compounds in the atmosphere, the organic group plays a key role in the tropospheric chemistry. Specifically the subgroup called *aromatics* is of great interest. Aromatics are the predominant trace gases in urban areas due to high emissions, primarily by vehicle exhausts and fuel evaporation. They are also present in areas where biofuel is used (i.e residential wood burning). Emissions of aromatic compounds are a substantial fraction of the total emissions of the volatile organic compounds (VOC).

Impact of aromatics on human health is very important, as they do not only contribute to the ozone formation in the urban environment, but they are also highly toxic themselves, especially in the case of benzene which is able to trigger a range of illness under long exposure, and of nitro-phenols which cause detrimental for humans and vegetation even at very low concentrations.

The aim of this work is to assess the atmospheric impacts of aromatic compounds on the global scale. The main goals are: lifetime and budget estimation, mixing ratios distribution, net effect on ozone production and OH loss for the most emitted aromatic compounds (benzene, toluene, xylenes, ethylbenzene, styrene and trimethylbenzenes). For this purpose, we use the numerical chemistry and climate simulation ECHAM/MESSy Atmospheric Chemistry (EMAC) model to build the global atmospheric budget for the most emitted and predominant aromatic compounds in the atmosphere. A set of emissions was prepared in order to include biomass burning, vegetation and anthropogenic sources of aromatics into the model. A chemical mechanism based on the Master Chemical Mechanism (MCM) was developed to describe the chemical oxidation in the gas phase of these aromatic compounds. MCM have been reduced in terms of number of chemical equation and species in order to make it affordable in a 3D model. Additionally other features have been added, for instance the production of HONO via ortho-nitrophenols photolysis. The model results are compared with observations from different surface and aircraft campaigns in order to estimate the accuracy of the model.

keywords: aromatic, VOC, atmosphere, modeling.