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Application and inter-comparison of the RADM2 and RACM chemistry mechanism including a new isoprene degradation scheme within the regional meteorology-chemistry-model MCCM

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Since the huge number of chemical species and reactions involved in the degradation of organic compounds does not permit an explicit treatment of these reactions, the use of condensed mechanisms in regional air quality models is necessary. Such mechanisms among some others are the RADM2 or the RACM mechanism, which are both widely applied in regional air quality models. With increased knowledge about biogenic VOC's chemistry, updates of the description of organic chemistry have become necessary. Geiger et al. (2003) introduced a new mechanism based on RACM with improved isoprene and biogenic VOC chemistry. To understand the behavior of the three mechanisms for the simulation of ozone episodes or daily ozone forecasts with regional air quality models, two case studies were performed for the three mechanisms: A box-model-inter-comparison of a standard test case and a cross-validation of a 60-day ozone episode simulation with the three-dimensional online-coupled regional air chemistry model MCCM. Focusing on ozone, the differences between the three mechanisms were rather small. In the regional air chemistry simulation with MCCM, the RADM2 mechanism did produce the highest daily ozone concentrations within the episode for three and one kilometer grid resolution simulations. An inter-comparison of the simulations with measurements results in good correlations of the simulated ozone concentrations for all three mechanisms. A statistic for selected continuous time periods of several days results in a correlation with the point measurements of r=0.93, while the correlation for the entire 60 day episode is around r=0.60.

Variations of correlation results for the three mechanisms are within 2 %. Applying a modern implicit integration method to the resulting differential equation systems for the chemistry mechanisms, the RACM mechanism costs about 30% more, for the modified RACM it is even up to 40% more consumed computational time compared to the integration of the RADM2 mechanism. Therefore the RADM2 gas phase chemistry mechanism is still a reasonable alternative for the use in regional ozone episodes, daily ozone forecasts or for long term air chemistry simulations.