The online coupled mesoscale climate-chemistry model MCCM - a modelling tool for short episodes as well as for climate periods

P. Suppan, R. Forkel and E. Haas

{Institute for Meteorology and Climate Research (IMK-IFU), Forschungszentrum Karlsruhe}

Correspondence to: P. Suppan (peter.suppan@imk.fzk.de)

Abstract

The online coupled regional meteorology-chemistry model MCCM (Mesoscale climate chemistry model, Grell et al. 2000), which is based on the non hydrostatic NCAR/Penn State University mesoscale model MM5, is presented. Recent applications of MCCM include short term studies such as simulations of high pollutant episodes for Mexico City, receptor analysis, as well as long term studies such as climate-chemistry simulations, simulations of yearly pollution conditions in the Alpine region, and daily real time forecasts of ozone and particulate matter for Germany. Some of these applications will be shown in this paper.

1 Introduction

Although online coupled models where meteorological and atmospheric chemistry processes are computed within one single model exist already since the 1990s, offline air quality models where the chemical processes are treated independently of the meteorological model are still widely used because of their lower computational costs. However, due to this separation of meteorology and chemistry there can be a loss of possibly important information of atmospheric processes, as the meteorological information is transferred to the CTM only once or twice per hour. The simulation of atmospheric chemistry with an online coupled

model can be regarded as more consistent than an offline treatment, as the chemistry part of the model receives all necessary meteorological information directly from the meteorological part of the model at each time step without any temporal interpolation. Especially on the regional scale with grid sizes down to 1 km, the wind field and other meteorological parameters are highly variable and neglecting these variances may introduce certain errors. Although the advantages of online coupled meteorology-chemistry simulations against an off-line treatment are most effective for fine horizontal resolutions, effects already become significant at horizontal resolutions of around 30 km (Grell et al., 2004).

2 Description of MCCM

The online coupled regional meteorology-chemistry model MCCM (Mesoscale climate chemistry model, Grell et al. 2000) has been developed at the IMK-IFU on the basis of the non hydrostatic NCAR/Penn State University mesoscale model MM5 (Grell et al., 1994). The full coupling of meteorology and chemistry ensures that the air quality component of MCCM is fully consistent with the meteorological component; both components use the same transport scheme, the same grid, and the same physics schemes for subgrid-scale transport. Similar to MM5 MCCM can be applied over a range of spatial scale from the regional scale (several thousand kilometres, with a resolution of 30-100 km) to the urban scale (100-200 km, resolution 1-5 km).

MCCM includes several tropospheric gas phase chemistry modules (RADM, RACM, RACM-MIM (Stockwell et al., 1990, 1997, Geiger et al., 2003)) and a photolysis module. Optional aerosol processes are described with the modal MADE/SORGAM aerosol module (Schell et al., 2001) which considers as single compounds sulphate, nitrate, ammonium, water, and 4 organic compounds. For the Aitken and the accumulation mode the gas phase/particle phase partitioning of the secondary sulphate/nitrate/ammonium/water aerosol compounds is based on equilibrium thermodynamics. The organic chemistry assumes that secondary organic aerosol compounds (SOA) interact with the gas phase and form a quasi-ideal solution.

Biogenic VOC and NO emissions are calculated online based on land use data, simulated surface temperature and radiation. Anthropogenic emissions of primary pollutants, like NO_x, SO_2, and hydrocarbons, as well as emissions of primary particulate matter have to be supplied either at hourly intervals or as yearly data from gridded emission inventories. Validation studies with MCCM have shown its ability to reproduce observed meteorological quantities and pollutant concentrations for different conditions and regions of the earth (Forkel and Knoche, 2006; Forkel et al., 2004; Grell et al., 1998; Grell et al., 2000; Jazcilevich et al., 2003; Kim and Stockwell, 2007; Suppan and Skouloudis, 2003, Suppan and Schädler, 2004; Suppan, 2007).

Furthermore the model is linked to other models like hydrological or/and biosphere based models in order to describe the interactions and feedback mechanisms from each compartment to the air quality and vice versa. A schematic description of the model is given in Fig. 1.

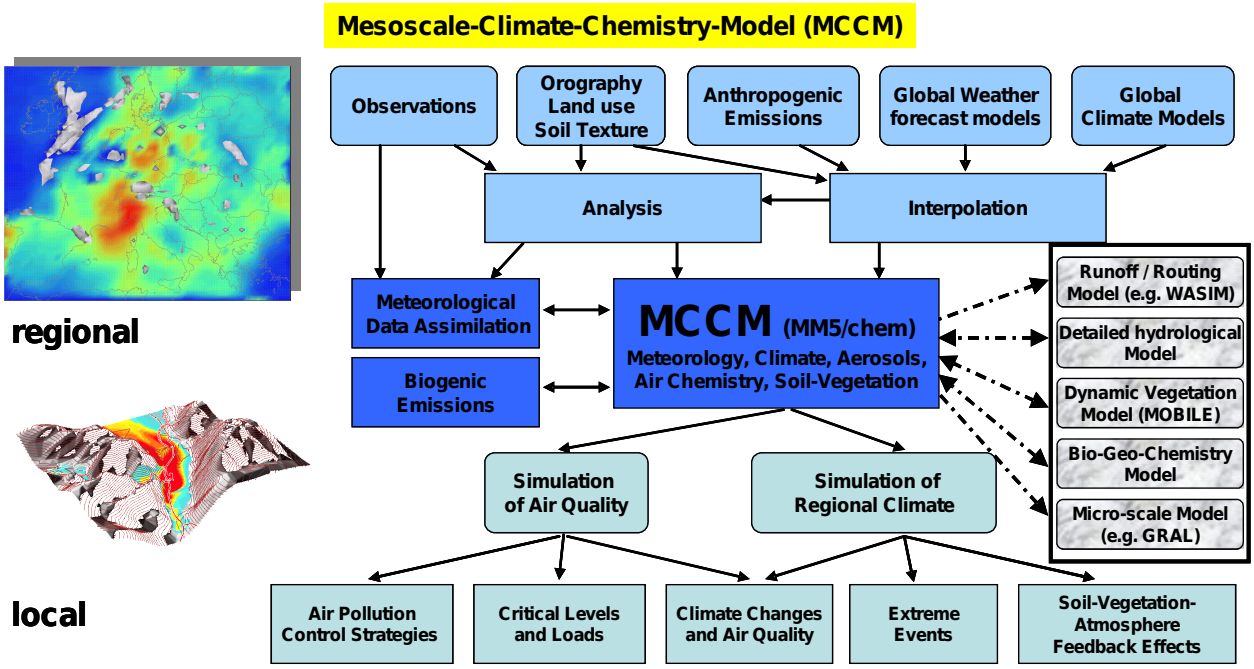

Fig. 1: Schematic description of MCCM as it is used on the local and regional scale for air quality simulations and the simulation of the regional climate including the introduced coupled models to hydrology and biosphere compartments.

3 Applications

The following examples show different applications of MCCM for short period simulations on air quality and emission reductions scenarios as well as simulations performed for the assessment of the impact on climate change to the regional air quality.

3.1 Evaluation studies

In order to evaluate the performance of the three chemistry mechanisms included in MCCM simulations over two months in summer 2003 were compared with observations.

The mechanisms were constructed using a software engineering tool for chemistry kinetics (Damian et al., 2002). By using a pre-processor for the construction of the numerical integration code, the solver (numerical integration scheme) and the underlying mechanisms were decoupled and by using identical integrations schemes, the influence of the numeric to the species evolution is comparable.

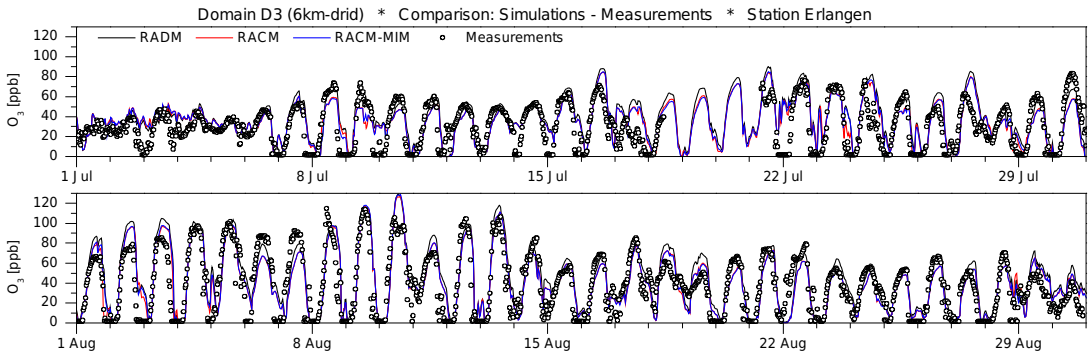

Fig. 2: Calculated and measured time series of ozone at the grid cell of the station Erlangen for 3 different chemical schemes.

The simulations were performed with four nested domains with 54, 18, 6 and 2 km grid resolution cover the time between 1st of July and 31st of August in 2003 and include episodes with high photosmog concentrations. The simulated species mixing ratios were compared to observations from the Bavarian measurement network (LFU). The evolution of the time series of the measured (LFU-Station Erlangen) and the simulated ozone (grid size 6 km resolution) is shown in Figure

2. On the one hand side the figure is demonstrating the good correlation between measurements and simulations, but on the other side it is also to see that the RADM mechanism is over predicting the ozone concentrations during the day, while the RACM and RACM-MIM simulation results fit much better to the observations (Haas et al., 2007).

3.2 Air quality studies

3.2.1 Effect of highway emissions

A typical application for assessing the influence of specific emission sources to the air quality is demonstrated within the next example. To assess the influence of highway emissions to the ozone and nitrogen dioxide concentration fields, the line source (highway) between Munich and Augsburg (ca. 35 km) was switched off and the emissions were set to the surrounding levels. This could be attributed to a reduction of 80 % of the traffic emissions.

As it can be seen in Figure 3, the increase on O_3 concentrations was up to 10 % whereas the NO_2 concentrations did show a decrease of close to 25 %. The red line marks the region of influence of this specific emission reduction.

Compared to the NO_2-influenced region, ozone has a smaller impact on the region (less than 800 km^2) but the impact is lasting longer (more than 12 h). The NO_2 influenced regions (close to 1000 km^2) are larger but are more short-lived (less than 6 h). The main time interval of influence for both, NO as well as for O_3 is during the night (Suppan and Schädler, 2004).

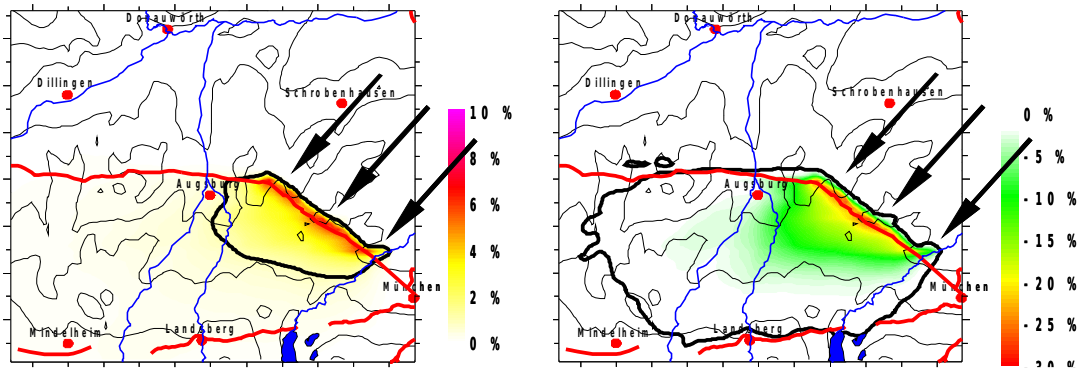

Fig 3: Traffic emission effect to O_3 (left) and NO_2 (right) concentrations at the nearby region of a highway during a 4 days period with strongly north easterly wind directions. The thick black line indicates the region of influence.

3.2.2 Scenario simulations for Mexico City

Mexico City suffers from severe air quality problems with maximum ozone values up to 250 ppb. In order to investigate the effect of different precursor emissions and possible mitigation measures on the ozone levels in Mexico City MCCM was applied in the Greater Area of Mexico City (Jazcilevich et al., 2003; Forkel et al., 2004). Figure 4 reveals that, in agreement with observations, the simulated maximum ozone concentrations occur in the south west of the city (measurement station PED), which is down-wind of the city centre, as an uphill flow is prevailing during the afternoon. The minimum ozone concentrations are found in the centre of the city (measurement station MER), where the NO emitted by traffic titrates the ozone, and in the northern part of the city at places where the NO emissions from industry and power plants locally reduce the ozone concentrations (near measurement station XAL).

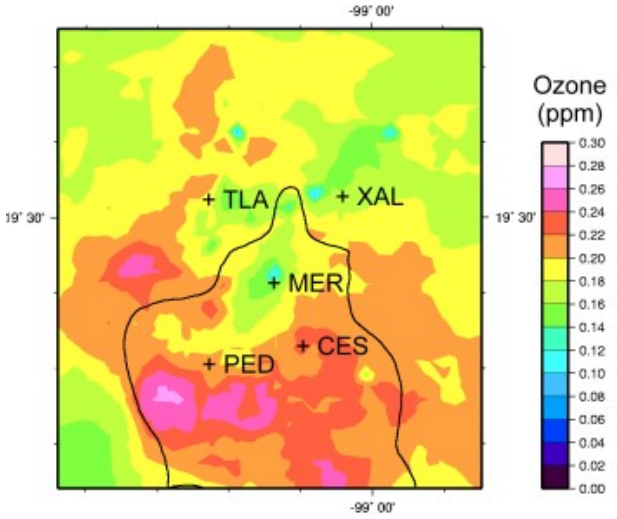

Fig 4: Average surface ozone concentration (in ppm) over 8 days at 4 p.m. Mexican summer time for the baseline 2010 emission scenario.

Compared to the ozone concentrations predicted for the 2010 baseline emissions, the emissions for a mitigation scenario including the replacement of old private cars, low sulphur diesel standards, the replacement of microbuses, and the

relocation of two power plants (corresponding to a reduction of anthropogenic emissions of NO_x by about 20 % and of VOC by 10 %) result in a decrease of the daytime ozone concentrations between 5 and 25 ppb at most locations. However, in the centre of the city and for the locations where power plants are switched off, the noontime ozone concentrations are higher for the mitigation scenario than for the baseline case since less ozone is titrated in case of the reduced NO emissions at these locations. The model results indicate that taken the projected emissions for the year 2010, extremely strong emission reduction measures for Mexico City would be necessary in order to significantly improve the air quality in Mexico City.

3.2.3 Source receptor analysis

Source-receptor analyses were made to allocate the air chemistry parameters to the individual emission sources. To estimate the impact of a source group on a certain pollutant, several simulations have to be accomplished. To minimize the associated uncertainties (non-linearity of chemical processes), the source group to be analyzed was suppressed. Due to the non-linear chemical processes, background concentrations and advection a “non-linear” fraction has to be introduced (DG-ENV, 2001). The source-receptor analysis is an important tool for abatement and emission reduction strategies.

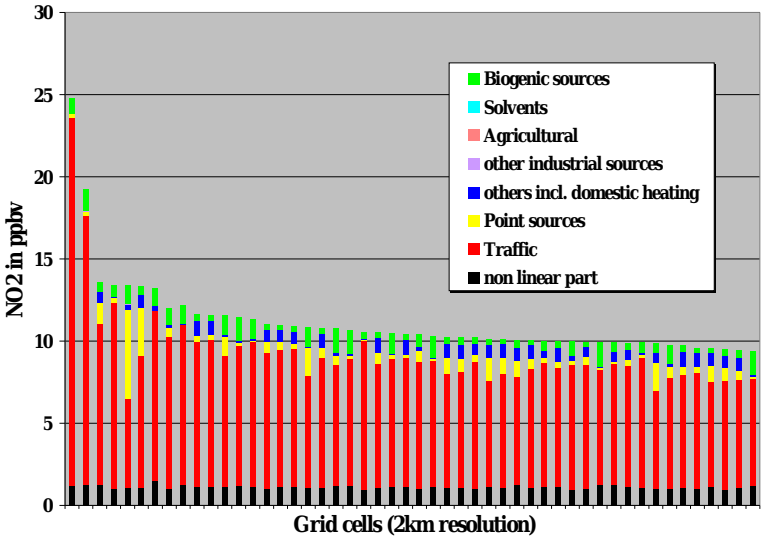

Fig 5: Source-receptor relationship for the 50 grid cells with highest NO_2-concentrations within the conurbation of Munich during a 4 days period.

In Figure 5 the source-receptor distribution for NO_2 is shown for a short time period in the greater area of Munich/Germany. The concentration at each grid cell

includes several source categories. In accordance with the NO_x emission distribution the NO_2 concentrations caused by the traffic show also the highest values (Suppan, 2007).

3.3 Climate chemistry simulations

In order to investigate possible effects of global climate change on the near-surface concentrations of photochemical compounds in southern Germany, nested regional simulations with MCCM were carried out (Forkel and Knoche, 2006). The simulations with a horizontal resolution of 60 km for Europe and 20 km for central Europe were driven by meteorological boundary conditions provided by a long-term simulation of the global climate model ECHAM4. Two time slices of about 10 years were compared, one representing the 1990s and one representing the 2030s.

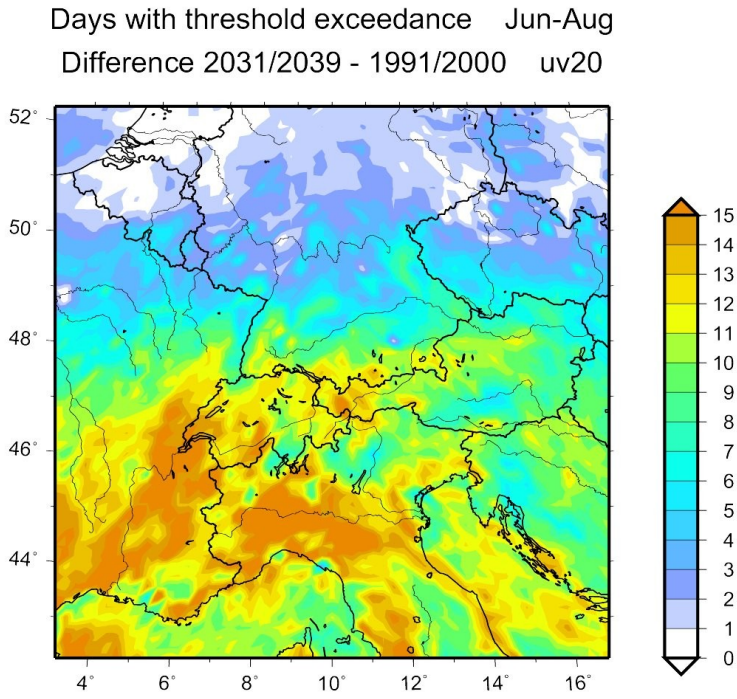

Fig. 6: Effect of climate change on the exceedance of the ozone threshold value

For the region of southern Germany the simulations show an increase of the mean summer temperature by almost 2° along with a decrease of cloud water and ice and a corresponding increase of the photolysis frequencies and the emissions of biogenic hydrocarbons. Under the model assumption of unchanged anthropogenic emissions this leads to an increase of the mean mixing ratios of most photooxidants. Because of the complex topography and the heterogeneous distribution of precursor emissions all parameters show pronounced regional patterns. The average daily maximum ozone concentrations in southern Germany increase for the considered scenario by nearly 10% in the summer months. Depending on the region the increase of the mean daily maximum ranges between

2 and 6 ppb. As a consequence, the number of days when the 8-hour mean of the ozone concentration exceeds the threshold value of 120 µg/m³ increases by 5 to 12 days per year (Fig. 6).

4 Conclusions

The online coupled model MCCM which is based on the well known and validated model MM5 has demonstrated its applicability to support and to address air quality issues, like emission reduction scenarios, abatement strategies or the impact of climate change to the air quality in sensitive and urbanized areas both on the regional and local scale. Furthermore the model is able to couple or to link also other models from different compartments like hydrology or biosphere.

References

Damian, V., Sandu, A., Damian, M., Potra, F., and Carmichael, G.R.: The Kinetic PreProcessor KPP - A Software Environment for Solving Chemical Kinetics, Computers and Chemical Engineering, Vol. 26, No. 11, p. 1567-1579, 2002.

DG-ENV: The AUTOOIL-II programme: Air-Quality report, EC DG-ENV, edited at JRC Ispra, Report EUR 19725 EN, version 7.2 and http://europa.eu.int/comm/environment/autooil/index.htm, 2001.

Forkel, R. and Knoche R.: Regional climate change and its impact on photooxidant concentrations in southern Germany: Simulations with a coupled regional climate-chemistry model, J. Geophys. Res., doi:10.1029/2005JD006748, 2006.

Forkel, R., Smiatek, G., Hernandez, F., Iniestra, R., Rappenglück, B., and Steinbrecher, R.: Numerical simulations of ozone level scenarios for Mexico City, 84th AMS Annual Meeting (6th Conference on Atmospheric Chemistry: Air Quality in Megacities), Seattle, Wa. 11-15 January 2004, Combined Preprint CD, contribution P1.2 (4pp.), http://ams.confex.com/ams/84Annual/techprogram/paper70640.htm, 2004.

Geiger H., Barnes, I., Benjan, I, Benter, T., and Splitter M.: The tropospheric degradation of isoprene: an updated module for the regional chemistry mechanism. Atmos. Environ. 37, 1503-1519, 2003.

Grell, G.A., Dudhia, J., and Stauffer, D.R.: A description of the Fifth-generation Penn State/NCAR Mesoscale Model (MM5). NCAR Tech Note TN-398 + STR, 122pp, 1994.

Grell, G.A., Schade, L., Knoche, R., and Pfeiffer, A.: Regionale Klimamodellierung, Final Report, Joint Proj. BayFORKLIM, Subproject K2, Fraunhofer-Institut für Atmos. Umweltforschung, Garmisch-Partenkirchen, Germany, 1998.

Grell, G.A., Emeis, S., Stockwell, W.R., Schoenemeyer, T., Forkel, R., Michalakes, J., Knoche, R., and Seidl, W.: Application of a multiscale, coupled MM5/Chemistry Model to the complex terrain of the VOTALP Valley Campaign, Atmos. Environ., 34, 1435-1453, 2000.

Grell, G.A., Knoche, R., Peckham, S.E., and McKeen, S.A.: Online versus offline air quality modeling on cloud-resolving scales, Geophys. Res. Lett., 31, 2004.

Haas, E., Forkel, R., and Suppan, P.: Application and Inter-comparison of the RADM2 and RACM Chemistry Mechanism including a new Isoprene Degradation Scheme within the Regional Meteorology-Chemistry-Model MCCM, Int. Journal of Environment and Pollution, in print, 2007,

Jazcilevich, A.D., Garcia, A.R., and Ruiz-Suarez, L.G.: A study of air flow patterns affecting pollutant concentrations in the Central Region of Mexico, Atmos. Environ., 37, 183-193, 2003.

Kim, D. and Stockwell, W.R.: An online coupled meteorological and air quality modeling study of the effect of complex terrain on the regional transport and transformation of air pollutants over the Western United States, Atmos. Environ., 2319-2334, 2007.

Schell B., Ackermann, I.J., Hass, H., Binkowski, F.S., and Ebel, A.: Modeling the formation of secondary organic aerosol within a comprehensive air quality model system, Journal of Geophysical research, 106, 28275-28293, 2001.

Stockwell, W., Middelton, P., and Chang, J.: The Second Generation Regional Acid Deposition Model – chemical Mechanism for Regional Air Quality Modeling. Journal of Geophysical Research, 95, 16343-18367, 1990.

Stockwell, W., Kirchner, F, Kuhn, M., and Seefeld, S.: A new mechanism for region atmospheric chemistry modeling. Journal of Geophysical Research, 102, 847-879, 1997.

Suppan, P., and Skouloudis, A.: Inter-comparison of two air quality modelling systems for a case study in Berlin. Int. J. Environment and Pollution, 20, pp 75-84, 2003.

Suppan, P., and Schädler, G.: The impact of highway emissions on ozone and nitrogen oxide levels during specific meteorological conditions, Science of the Total Environment, 334-335, 2004.

Suppan, P.: Assessment of Air Pollution in the Conurbation of Munich – Present and Future. Science of the Total Environment, 2007, in print.