Project No. 037005

CECILIA

Central and Eastern Europe Climate Change Impact and Vulnerability Assessment

Specific targeted research project

1.1.6.3.I.3.2: Climate change impacts in central-eastern Europe

D7.1: Coupling of the AQM's to the RCM's. Development of the preprocessors to convert RCM-output to AQM-input.

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Start date of project: 1st June 2006 Duration: 36 months

Lead contractor for this deliverable: University of Natural Resources and Applied Life Sciences, Vienna (BOKU)

Revision [final]

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Dissemination Level		
PU	Public	X
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

CECILIA WP4 DELIVERABLE D13 (or D7.1)

Lead partner for deliverable: BOKU

Contributing partners: CUNI, AUTH, CHMI, WUT, NIMH, BOKU

June 21, 2007

1 Introduction

The purpose of this deliverable is coupling of the air quality models (AQMs) used within CECILIA to the output of the regional climate models (namely RegCM and ALADIN). With this coupling the AQMs should be prepared for the following tasks, in particular the preparation of European background concentration runs with 50 km resolution, due in Delivrable D7.2 by month 18 of the project.
In particular, the following work was done:

- An interface between RegCM and CAMx was written by CUNI.
- AUTH prepared RegCM fields on the ENSEMBLES grid for the year 2000 with a 50 km resolution.
- BOKU prepared anthropogenic emissions for the year 2000 on the 50 km grid that can be combined with biogenic VOC emissions from the RegCM/CAMx interface.
- AUTH, BOKU and CUNI performed test model runs with CAMx.
- CHMI prepared the coupling between ALADIN and CAMx.
- WUT implemented regcm2camx.
- NIMH decided to use ALADIN with CMAQ and installed an interface.

2 Detailed description of the work done

2.1 *The interfaces between RegCM (ALADIN) and CAMx and the other models*

At CUNI the interface regcm2camx was written, that translates the output of the meteorological model RegCM to the input of the photochemical model CAMx. The transformation is performed without interpolation. Therefore both models should calculate on the same grid. Among the data fields required by CAMx are some, which can be used directly, others need to be diagnosed from the RegCM output.
In addition, biogenic VOC emissions are calculated by an algorithm by Guenther et al. (1993). They depend on the temperature and the global radiation. The same landuse data as needed by the CAMx model with 11 categories is used. NO_x emissions from soils are not considered.
A detailed manual for the use of RegCM2CAMx may be found in the appendix.

At CHMI the coupling between ALADIN and CAMx is in preparation, based on a similar coupling that is in use by BOKU and the Austrian Central Institute for Meteorology and Geodynamics (ZAMG) in a short term ozone forecast (Baumann-Stanzer et al., 2005) and similar to regcm2camx.
NIMH coupled the meteorological model ALADIN to the chemical model CMAQ.

2.2 *Preparation of emission input files*

The anthropogenic emissions are calculated with the emission model of BOKU-Met based on data from the UNECE/EMEP data base (http://webdab.emep.int/) for European emissions (Vestreng et al., 2005) for the year 2000. “Expert emissions“ are taken that are based on the national totals reported by the individual countries and have been completed and corrected/substituted for the use of dispersion modelling. These data comprise the annual sums of the emissions of NO_x, CO, non-methane hydrocarbons, SO_2, NH_3, fine particles (<2.5 µm) and coarse particles (2.5 µm to 10 µm) on a 50 km x 50 km grid. 11 sectors of anthropogenic activity are distinguished in accordance to SNAP97.
For the countries Austria, Czech Republic, Hungary, and Slovakia the EMEP data are downscaled to a spatial resolution of 5 km x 5 km. An emissions inventory for theses countries from the year 1995 (Winiwarter and Zueger, 1996) is used as data base for the spatial distribution of the emitters within the 50 km x 50 km EMEP grid cells for every sector.
For every sector the emission model applies different distributions for the month, the day of the week and the hour of the day for the temporal disaggregation. The disaggregation factors are taken from the

inventory by Winiwarter and Zueger (1996). They are available for the Pannonian countries. For all other countries the data for Austria have been used.
The emissions from the inventories must be splitted sector specific into the chemical compounds applied by the chemical mechanisms of the photochemical model. In the case of NOx it is assumed in all cases of anthropogenic emissions that 10 % are **NO_2** and 90 % are **NO** (molar percentages). The emissions of non-methane hydrocarbons are disaggregated in accordance with the needs of the chemical mechanism CBM-IV (Gery et al., 1989). This results in specific emissions of the following species, given in CBM-IV notation: **PAR** (alcane groups), **ETH** (ethene), **OLE** (alcene groups), **TOL** and **XYL** (aromatics of different reactivity), **FORM** (formaldehyde) and **ALD2** (aldehydes, ketones). In addition, the following species are emitted without chemical disaggregation: **CO**, **SO_2**, **NH_3**, **$PM_{2.5}$**, **$PM_{2.5\text{-}10}$**.
With the emission model 36 different sets of daily emissions were calculated, namely for every month these were three files containing weekday-, Saturday- and Sunday-emissions. Each set contains hourly emissions for every grid cell of the photochemical model in the units required by the CAMx model (Environ, 2006). These are mole per hour and grid cell for gaseous emissions and gram per hour and grid cell for particulates. By a small intermediate programme it is possible to add to these files the day specific biogenic emissions of isoprene and terpenes that depend on the meteorological data and were calculated with the regc2camx-programme, in order to prepare a complete emission input file for CAMx.

2.3 Test model runs for the year 2000

2.3.1 Meteorological runs with RegCM

A full year simulation of the regional climate model RegCM3 (http://www.ictp.trieste.it/~pubregcm/RegCM3/) was carried out for 2000, forced by the ERA-40 reanalysis fields (2.5°x2.5°, L23 pressure level) of ECMWF for a large European domain (similar to the common domain of the EU Project ENSEMBLES) with a grid resolution of 50 km x 50 km. The Global Ocean Surface Temperature (GISST), a set of SST (Sea Surface Temperature) data in monthly 1° area grids, was used to constrain the SST of the RegCM3 simulation. GTOPO30 Terrain and GLCC Landuse datasets, with 3 minutes resolution were used for the model topography and landuse, respectively. The Grell scheme with Fritsch-Chappell closure was used for the convective parametrization of the model simulation. The map projection choice was Lambert conformal. The meteorological output fields of RegCM3 were used to drive offline the air quality model CAMx. Indicatively, Figure 2-1 and Figure 2-2 show the comparison of RegCM3 simulated fields of surface temperature and total precipitation with the respective observed gridded dataset from Climatic Research Unit (CRU) for January 2000 and July 2000. Apart from some regional differences the overall comparison is satisfactory.

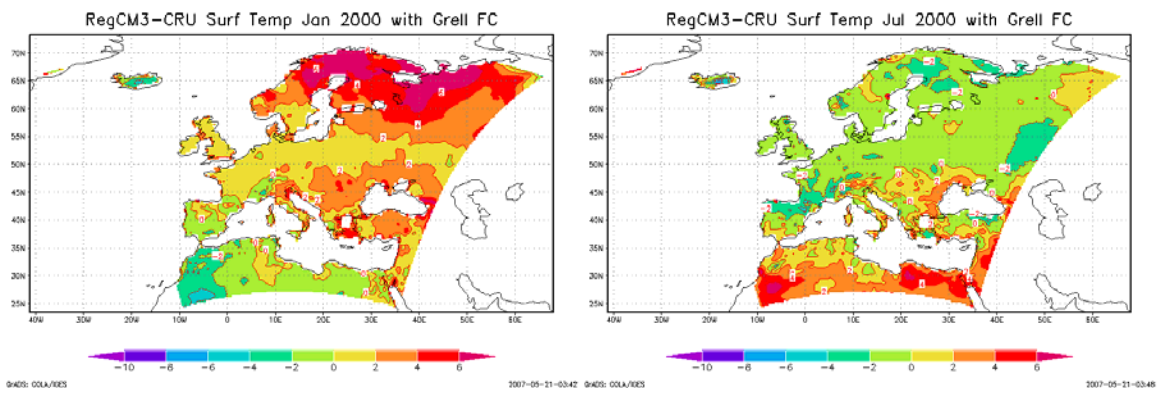

Figure 2-1: Comparison of RegCM3 with CRU surface temperature for January and July 2000**.**

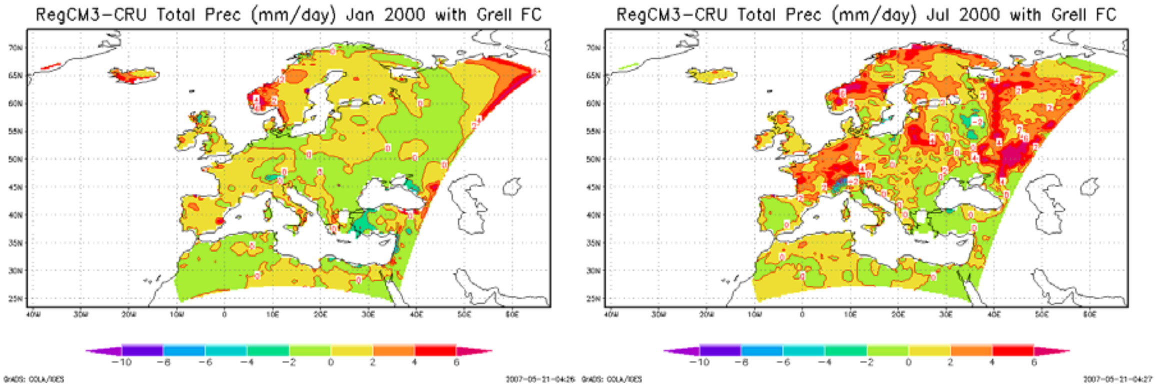

Figure 2-2: Comparison of RegCM3 with CRU total precipitation for January and July 2000.

2.3.2 Photochemical runs with CAMx

2.3.2.1 Runs at AUTH

The air quality model simulations were performed with the Comprehensive Air Quality Model with extensions (CAMx) version 4.40 (release date 25/10/2006). CAMx run with a coarse grid spacing over Europe in a spatial resolution of 50x50 km, identical to the grid defined for the meteorological runs. The domain's vertical profile contained 12 layers of varying thickness, extending up to 450 hPa. The meteorological fields were derived from RegCM runs performed by AUTH (see above). Hourly anthropogenic emissions of gaseous and particulate pollutants were compiled and provided by BOKU. Biogenic emissions were calculated using the RegCM-CAMx interface in a 6-hour basis. Biogenic and anthropogenic emissions were combined with AddEmiss software developed by BOKU. All emissions were treated as surface area emissions. Initial and boundary (top and lateral) conditions corresponded to concentrations of clean air. The chemistry mechanism invoked was Carbon Bond version 4 (CB4). This mechanism includes 117 reactions – 11 of which are photolytic - and up to 67 species (37 state gasses, up to 18 state particulates and 12 radicals). Photolysis rates were derived for each grid cell assuming clear sky conditions as a function of five parameters: solar zenith angle, altitude, total ozone column, surface albedo, and atmospheric turbidity. The rates were taken from a large lookup table that spans the range of conditions for each of the five dimensions. This table was developed using the TUV photolysis pre-processor following the discrete ordinates method (Madronich and Flocke, 1998). A file containing information on albedo, ozone column density and turbidity for the CAMx domain was also provided as input file (AHOMAP file) containing spatial and temporal distribution of the above mentioned parameters. These parameters are essential for photochemical simulations as they determine variation of photolysis rates. In order to prepare this file, seasonal average TOMS files were used (http://jwocky.nasa.gov). In Fig. XX3 are shown monthly mean ozone values over the European domain produced for the test run of year 2000 (January and July). Ozone mixing ratios follow well understood temporal and spatial patterns with the highest values during summer in Mediterranean and an increasing latitudinal gradient towards the southern latitudes due to more intense photochemical ozone production. Mind also the lowest ozone values during winter over highly polluted/industrialized regions due to O3 titration by NO.

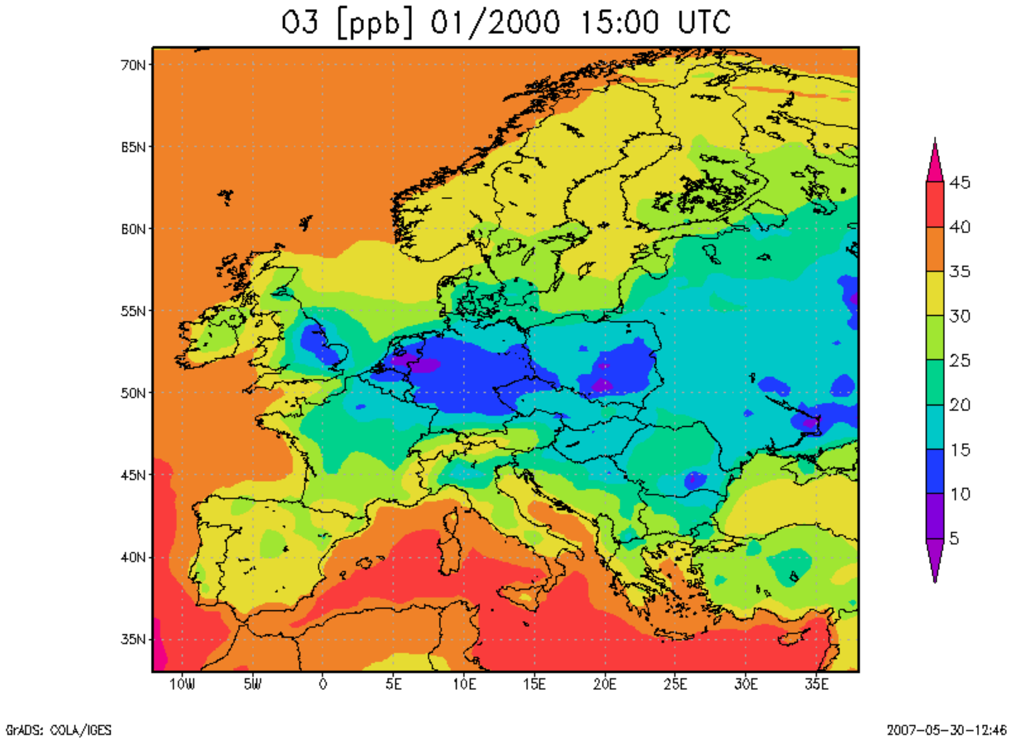

Figure 2-3: Ozone monthly mean values for January 2000 as calculated by CAMx at AUTH.

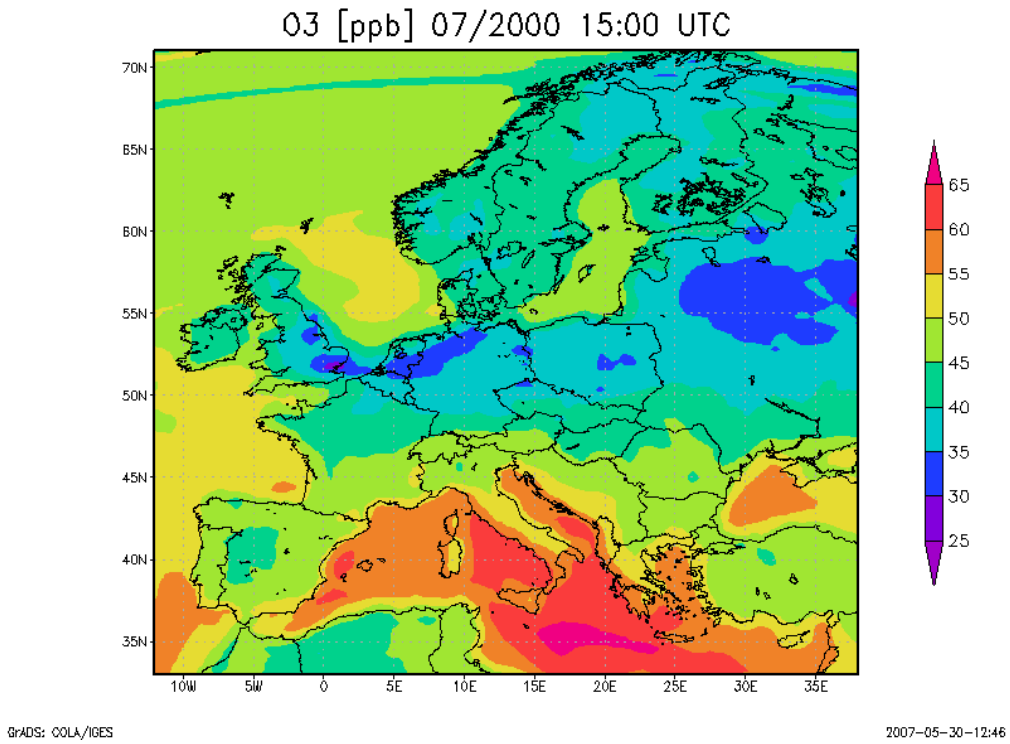

Figure 2-4: Ozone monthly mean values for July 2000 as calculated by CAMx at AUTH.

2.3.2.2 Runs at BOKU

At BOKU similar CAMx model runs for the whole year 2000 were performed as at AUTH. In particular, the same CAMx model version (4.40) was used as well as the same meteorological input data, and the emissions were prepared in the same way. However, there were differences with respect to the lateral and top boundary concentrations, to the calculations of the photolysis rates and (probably) the landuse input.

The photolysis rates were calculated with the same photolysis pre-processor (TUV, Madronich and Flocke, 1998), however, a constant value for the total ozone column of 300 DU over the whole model

domain and for all seasons was used. This was done in order to avoid estimates of the total ozone column in model runs for future climate projections.
Two methods for the lateral boundary conditions were tried. Constant values taken from a global photochemical model (IMAU, Roelofs and Leliefeld, 2000) were used on one hand. On the other hand the boundary concentrations were calculated dynamically, by using those concentrations that had been calculated by the model for the same hour on the day before in the grid cells at a distance of 2 cells from the boundary. The two sets of top concentrations were either the same (“clean air”) values as used by AUTH or data from the IMAU model, which differed mainly by a higher ozone concentration, relative to the other set.
The monthly average of the ozone concentration in the lowest model level from the run with IMAU lateral concentrations and AUTH top values is displayed in Figure 2-5.

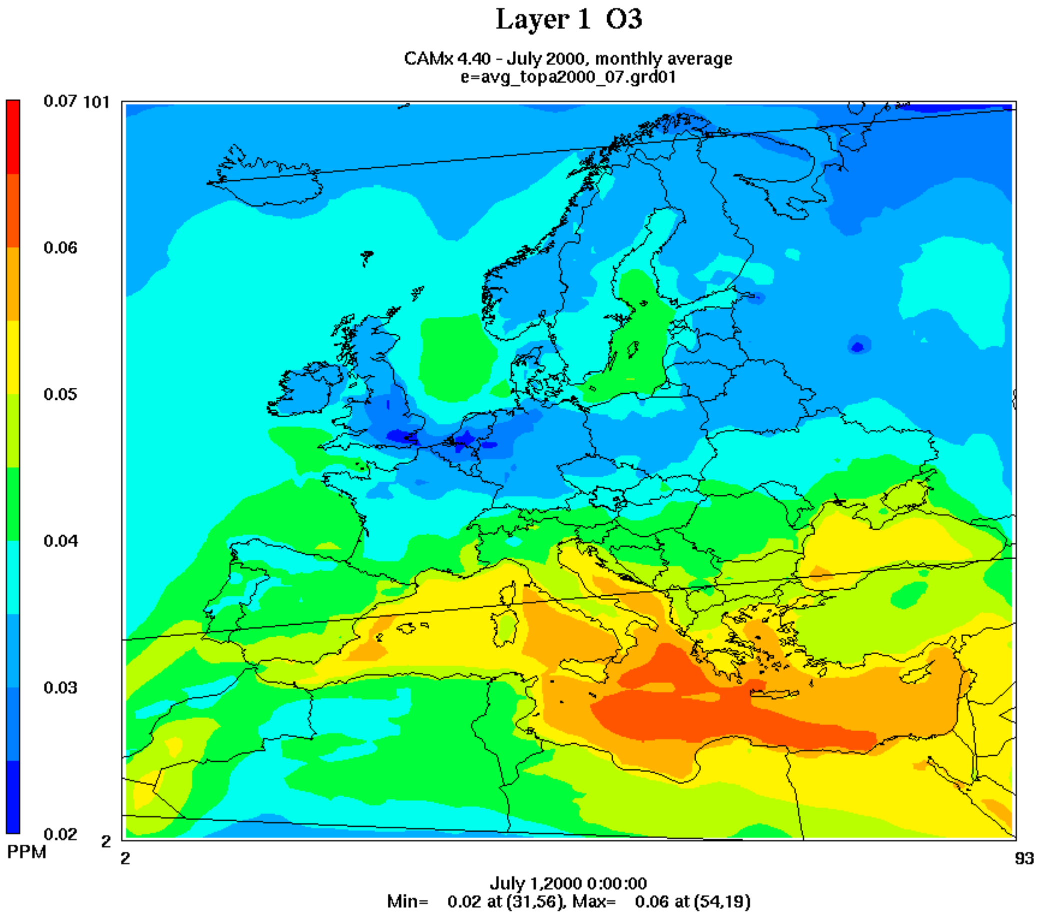

Figure 2-5: Ozone monthly mean values for July 2000 as calculated by CAMx at BOKU.

2.3.3 Comparisons at the station Illmitz (A)

The comparison of the monthly ozone means from the calculations by AUTH and by BOKU for July 2000 in Figure 2-4 and Figure 2-5 show a general good agreement. This will serve as a base for the discussions at the next CECILIA workshop in June 2007. For the validation of the model systems, the results should also be compared with measurements. As a first approach, some model results have been compared with measurements at the Austrian station Illmitz, which is part of the EMEP network of background stations. Illmitz is located at the Neusiedler See close to the border to Hungary.
Figure 2-6 shows the comparison of the 6-hourly RegCM output for temperature as they were used for the CAMx model calculations with 0.5-hourly measurements at the station Illmitz for the year 2000. Both curves agree well, including the relatively low temperatures that occurred in July. However, the model with its lower temporal resolution does not reproduce the daily temperature maxima of the measurements.

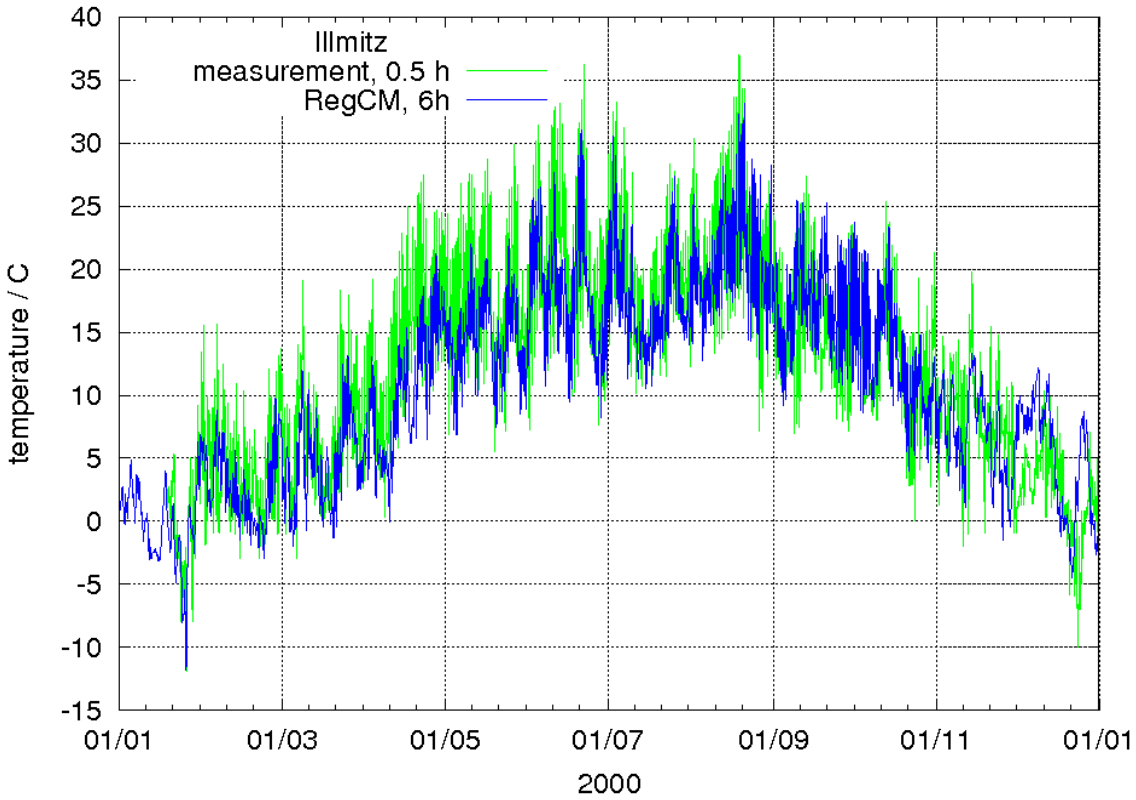

Figure 2-6: Comparison of 6-hourly RegCM output for temperature with 0.5-hourly measurements at the station Illmitz for the year 2000.

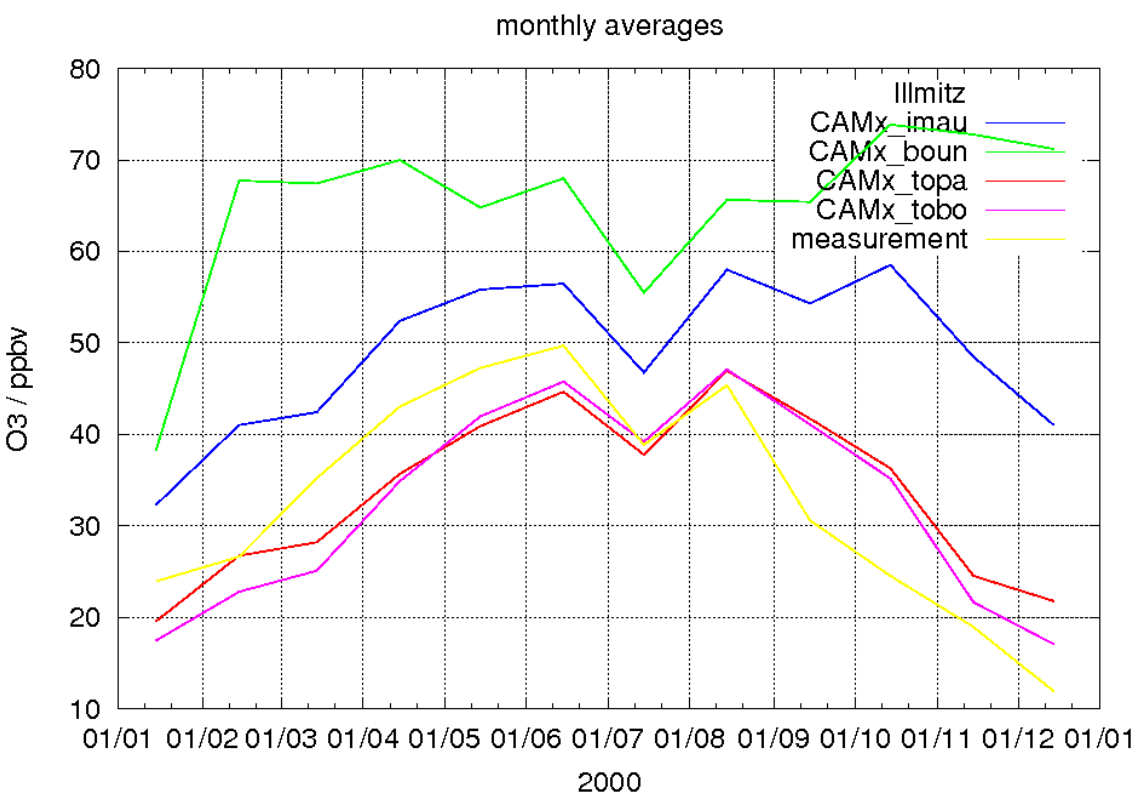

Figure 2-7: Comparison of monthly mean ozone values calculated with CAMx at BOKU for the station Illmitz (see text) with measurements.

Figure 2-7 displays a comparison of the monthly mean ozone values calculated with CAMx at BOKU for the station Illmitz with measured data. All curves show the relatively low ozone that occured in July due to the meteorological conditions (see temperature in Figure 2-6). Both runs with IMAU lateral concentrations follow the course of the measurements, however, the results of the run with high ozone at the top boundary (CAMx_imau) are generally too high while those calculated with the „clean air“ conditions by AUTH are too low (CAMx_topa). The run with dynamical boundary conditions and high ozone at the top (CAMx_boun) shows far too high ozone concentrations, in particular during the last months of the year. The run with dynamical boundary and low ozone top values (CAMx_tobo) gives results similar to CAMx_topa, but slightly closer to the measurements.

2.3.4 Runs at CUNI

As a first step, the distribution of pollutants were simulated for a long period of one year in the model couple RegCM and CAMx. CUNI used 23 vertical σ-levels reaching up to 70hPa, with a time step of 150 s at 45 km resolution in preliminary experiments for RegCM configuration and the same horizontal grid for CAMx. Initial and boundary conditions were set to CAMx's top concentrations (independent of time) (Simpson et al., 2003) for the 45 km resolution run, the results are used for driving the same couple of RegCM-CAMx in 10 km resolution on the smaller “CECILIA” region. In this setting, CB-IV chemistry mechanism is used (Gery et al.,1989). Some examples of the high resolution integration for the year 2000 are presented in Figure 2-8 for selected species. More interesting comparisons of the results with selected time series can be seen in Figure 2-9. Underestimation of the ozone concentration by the model especially during the warm season appears for some stations in Central Europe whereas significant overestimation is presented in the comparison for Ispra.

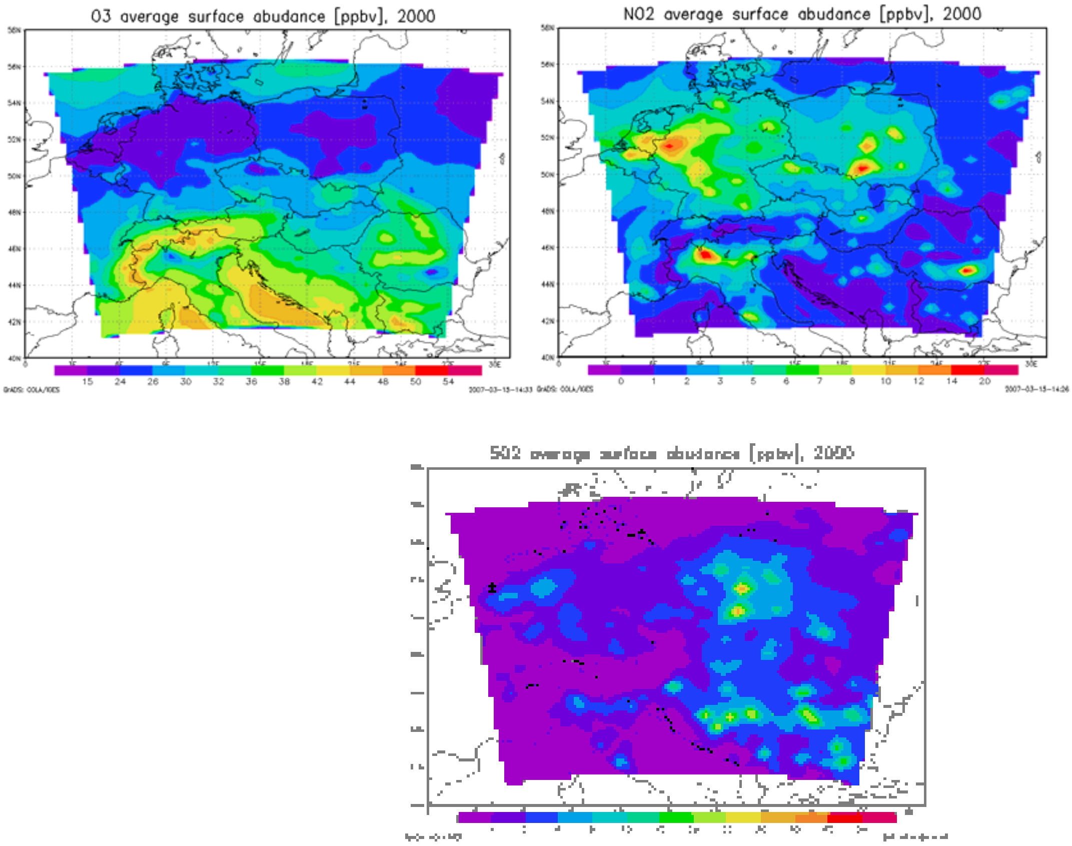

Figure 2-8: Average concentration of O_3 (upper left), NO_2 (upper right) and SO_2 (bottom panel) for the year 2000 in ppbv.

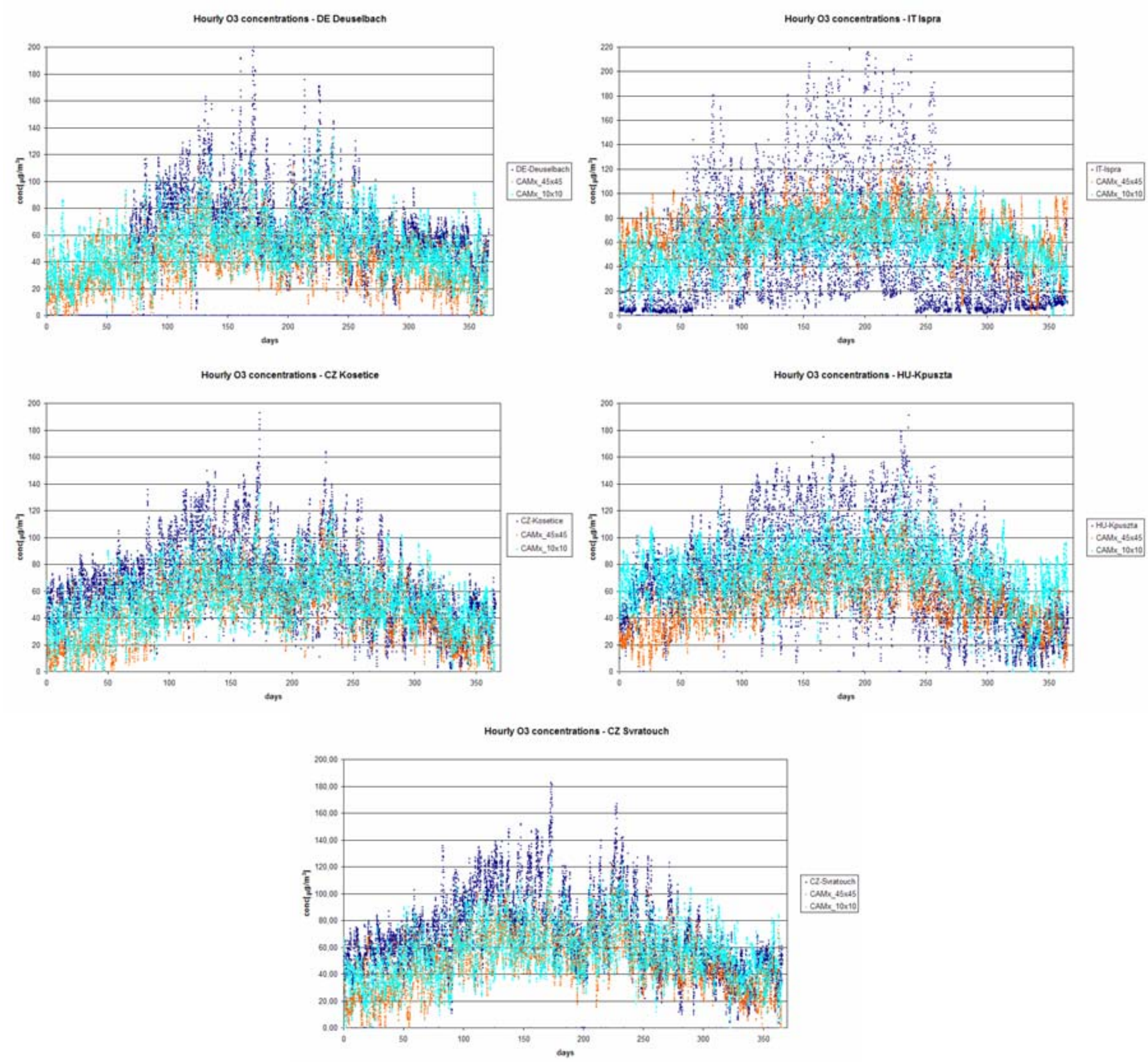

Figure 2-9: Comparison of simulated and measured hourly concentration of O3 for Deuselbach (upper left), Ispra (upper right), Kosetice (middle left), Kpuszta (middle right) and Svratouch station (bottom panel) in the year 2000 (µg/m3).

3 Summary

For the first deliverable of Workpackage 7 of the CECILIA project , the photochemical models were prepared for there further tasks. This included the installation of the interfaces between the meteorological models and the photochemical models as well as first test runs that will be used for the validation of the model systems.

4 References

Baumann-Stanzer, K., M. Hirtl and B. C. Krüger, 2005a: Pilotstudie zur Prognose von Sommersmog auf Basis operationeller regionaler Wettervorhersage in Österreich. Endbericht, Zentralanstalt für Meteorologie und Geodynamik und Institut für Meteorologie der Universität für Bodenkultur Wien, Mai 2005.

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5 Appendix

1. regcm2camx-manual by Peter Huszár.

Appendix 1:

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RegCM2CAMx

Version 4.40
User's Guide

Peter Huszár

Prague, Czech Republic

January 2007

1. Introduction

It is now well established that climatically important (so called radiatively active) gases and aerosols can have substantial climatic impact trough their direct and indirect effects on radiation, especially on regional scales. The study of these effects requires coupling of regional climate models (RCMs) with atmospheric chemistry/aerosols to assess the climate forcing to the chemical composition of the atmosphere and its feedback to the radiation, eventually other components of the climate system. There is a variety of chemical transport models (CTMs) available for treating the chemical composition of the atmosphere., thus it seems profitable to take the advantages if this against the possibility of development of chemistry module in an existing RCM.

This user guide introduces the reader the RegCM2CAMx interface for coupling RegCM regional climate model (Elguindi at al., 2006) and CAMx chemical transport model (Environ, 2006). CAMx is an Eulerian photochemical dispersion model that allows for integrated "one-atmosphere" assessments of gaseous and particulate air pollution (ozone, PM2.5, PM10, air toxics) over many scales ranging from sub-urban to continental. CAMx simulates the emission, dispersion, chemical reaction, and removal of pollutants in the troposphere by solving the pollutant (eulerian) continuity equation for each chemical species on a system of nested three-dimensional grids. These processes are strongly dependent on the meteorological conditions, so CAMx requires meteorological input from a NWP model or RCM for successful run. RegCM2CAMx is intended to act in this issue. Briefly, it takes RegCM's outputs and convert them to fields and formats accepted by CAMx. RegCM2CAMx v. 4.40 is adapted to work along with the same CAMx version (v. 4.40.) and RegCM Version 3.1 or later.

RegCM2CAMx has also included calculations of biogenic emissions of isoprene and mono-terpenes, but this is only an optional functionality which was developed for a particular use at the Charles University.

2. Meteorology in CAMx

As said in introduction, processes in CAMx responsible for chemical compound concentration evolution depend on meteorology. The following fields (with units and dimension) are required by CAMx:

- geopotential height at all model layer interface [m]
- average pressure of all model layer [mb] -3D
- average u-wind of all model layer [ms^{-1}] - 3D
- average v-wind of all model layer [ms^{-1}] - 3D
- surface temperature [K°] - 2D
- average temperature of all model layer [K°] - 3D
- average water vapour concentration of all model layer [ppm] – 3D
- average cloud water content of all model layer [gm^{-3}] – 3D
- average rain water content of all model layer [gm^{-3}] – 3D
- average snow water content of all model layer [gm^{-3}] – 3D
- average graupel water content of all model layer [gm^{-3}] – 3D

- integrated column cloud optical depth for all layers [dimensionless] – 3D
- vertical diffusivity at all model layer interface [m^3s^{-1}] – 3D

Some of these fields that RegCM does not provide need to be diagnosed. These are pressure, rain-, snow-, graupel water content, integrated column cloud optical depth and vertical diffusivity. RegCM2CAMx aims to calculate these fields and writes them to CAMx supported format.

3. How RegCM2CAMx works

RegCM2CAMx extracts meteorology from RegCM output for a particular day. It takes the ATM and SRF files, read them in and for the desired day it processes it for CAMx and writes CAMx meteorology input files. It does not provide horizontal and vertical interpolation, so the output is written to the same grid, except the possibility of choosing a subset of RegCM's vertical layers and write CAMx meteorological input for it. RegCM2CAMx assumes that ATM and SRF files start at the beginning of the month and the output frequency for ATM files is 6 hours, for SRF is 3 hours. If this assumption is not fulfilled, easy code editing in regcm2camx4.40.fmay adapt RegCM2CAMx for the new conditions. For detailed look into the code refer to the MM5CAMx interface (www.camx.com/down/support.php). RegCM2CAMx is a modification of it. It runs on GNU/Unix operating systems.
RegCM2CAMx package contains the source files (written in Fortran 77): regcm2camx4.40.f

clddiag.f

kvcalc_ob70.f

calcnatvoc.f

params.inc

fields.inc

Makefile

Makefile_IFC

Makefile_PGF

and a BASH job-file:

regcm2camx_6h_1day.sh.

During the run, temporary files are created: regcm2camx.param

timesdates.in

Steps needed for successful RegCM2CAMx run.

1.) Place ATM., SRF. and OUT_HEAD RegCM output in the directory where RegCM2CAMx files are copied.
2.) Edit RegCM's sigma-levels in regcm2camx4.40.fsource file. (18 or 23 vertical layers)
3.) Edit BASH regcm2camx_6h_1day.sh job-file
    1. Choose the day, you intend to process for CAMx by setting the *YYYY, MM, DD* and *JUL*
    2. Set the domain parameters:*NX, NY, NZ* and *DX*.
    3. If you do not want to do biogenic emission processing, set *ifbioemis* parameter to *.false.*
    4. Start RegCM2CAMx by command: ./regcm2camx_6h_1day.sh

(The Makefile expects ifort Intel Fortran Compiler. Alternatively, Makefile_PGF is provided for Portland Fortran Compiler.)

After these steps, the output files for CAMx meteorology should be created in the same directory named as follows:

camx.zp.${YYYY}${JUL}
camx.uv.${YYYY}${JUL}
camx.t.${YYYY}${JUL}
camx.kv.${YYYY}${JUL}
camx.q.${YYYY}${JUL}
camx.cr.${YYYY}${JUL},

where ${YYYY} and ${JUL} are variables that contain the year and the julian date of the processed day.

Literature

Elguindi, N., X. Bi, F. Giorgi, B. Nagarajan, J. Pal, F. Solmon, S. Rauscher, A. Zakey 2006: *RegCM Version 3.1 User's Guide*. PWCG Abdus Salam ICTP

ENVIRON Corp., 2006:CAMx Users' Guide, version 4.40