#### A SEASONAL AND YEARLY POLLUTION STUDY BY USING WRF/CHEM AND WRF-CMAQ NESTED WITH CCSM3 GLOBAL MODEL

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**Abstract**: The importance of relating the climate variables with the air pollution concentrations in different areas in Europe is an area which is receiving a high level of attention by researchers during the last years. The climate global models are successfully reproducing the yearly and seasonal changes in meteorological variables successfully during the last 20-30 years. The air pollution concentration changes within the same period are also simulated by using last generation of air pollution models. Statistical analysis of both variables has been carried out in the present contribution. We have simulated with the CCSM3 (NCAR, USA) global model the period between 1995-2005 and compared with observational data produced by NNRP2 and other observational data sets. The CCSM3 is applied in coupled form so that the CAM3 atmospheric model is coupled with the CSIM3 model (Sea Ice Model), the Land Model CLM3 and the ocean model CCSM POP model. The POP model has been simulated during the period 1985-2005. We have simulated the 10 year period with WRF-CHEM (NCAR, USA) and WRF-CMAQ (EPA, USA) over the European domain nested within CCSM3 global model. The model simulation domain includes the whole Europe with 54 km spatial horizontal resolution and 23 vertical layers. The results show that pollution concentrations and meteorological variables are correlated for seasonal and yearly periods. The PM10 and PM2.5 aerosol concentration feedbacks as a response to temperature changes are also shown.

Key words: Global models, climate models, air pollution models, mesoscale air quality models.

### **1. INTRODUCTION**

General circulation models use quantitative methods to simulate the interactions of the atmosphere, oceans, land surface and ice. All climate models balance, or very nearly balance, incoming energy as short wave electromagnetic radiation (which in this context means visible and ultraviolet, not to be confused with shortwave) to the earth with outgoing energy as long wave (infrared) electromagnetic radiation from the earth. Any imbalance results in a change in the average temperature of the earth. Four dimensional global climate models or general circulation models (GCM's) discretise the equations for fluid motion and energy transfer and integrate these forward in time. They also contain parameterization for processes – such as convection – that occur on scales too small to be resolved directly. Atmospheric GCMs (AGCMs) model the atmosphere and impose sea surface temperatures. Coupled atmosphereocean GCMs (AOGCMs, e.g. HadCM3, Collins et al. (2001); EdGCM, Educational Global Climate Modelling); GFDL CM2.X, Russell et al. (2006); ARPEGE-Climat, Déqué et al. (1994), Tyteca (2005)) combine the two models. In this contribution we use the CCSM3 3.0 global climate model (Blackmon et al., 2001; Sarmiento et al., 2004) to simulate with the base control run the global climate for 1995-2005. The information is used to run two mesoscale air quality models over the European domain with higher spatial resolution. The CCSM3 3.0 global model is composed by four modules: 1) The CAM (Community Atmospheric Model) module which mimics the atmospheric dynamics to obtain all the needed meteorological variables; 2) The POP module (Parallel Ocean Program) which mimics the ocean dynamics during the simulated period. Current generation of ocean models, at resolutions that are practical in coupled climate integrations, can provide good simulations of variations in mass transport on time scales from days to seasons.

This success is relatively insensitive to details of the model formulation, e.g., vertical coordinate, parameterizations of dissipation, etc. However, at interannual-to-millennial time scales and for the equilibrium state of the ocean, current models show tremendous sensitivity to details of the representation of processes, such as deep convection, boundary-layer dynamics (lateral, surface, and bottom), interior redistribution of properties by mesoscale eddies, and mixing. These processes can be identified with the branches of the global thermohaline circulation, such as sinking at high latitudes (often within semi-enclosed seas), flow through narrow straits and over sills, rapid transport through deep and surface western boundary currents, weak and nearly adiabatic flow through the interior of ocean basins, and the return of deep water to the surface through spatially inhomogeneous mixing processes. Progress in ocean modeling for climate studies must address these sensitivities. Models certainly must be able to provide quantitative predictions of the ocean's response to changes in surface buoyancy fluxes, and hence of the role of the ocean in global climate change; 3) The exchange of energy, water, and momentum between the land surface and atmosphere must be provided to the atmosphere on short time scales (compared to a day) to adequately represent the couplings to boundary-layer processes and moist convection. These fluxes have substantial feedbacks on modelled precipitation, surface temperatures, and other aspects of climate simulations. Inputs from the atmosphere of precipitation and net radiation, as controlled by moist atmospheric processes, are also major determinants of surface climates. Soil and vegetation establish energy balances and temperatures and require geographically detailed data sets to provide their distributions and properties. Also important for fluxes is the loss of water by runoff and its storage in lakes and wetlands. Carbon fluxes to leaves must be calculated to determine water fluxes from leaves. Because of this dependence and a strong dependence of soil biogeochemistry on soil moisture and temperature, the land surface model provides a driver of biogeochemical and ecological processes and, finally

4) The Sea-Ice model mimics the fact that in virtually every scenario of warming due to greenhouse gases run in climate models, the largest increases in temperature occur in the high latitudes, especially near the edge of the sea ice. Meanwhile, observations show changes in the water mass structure of the Arctic Ocean, thinning of Arctic sea ice, and major icebergs breaking off the Antarctic ice shelves. Changes in the polar climate are becoming apparent, and understanding these changes is of great importance.

The WRF mesoscale non-hydrostatic meteorological model (Skamarock et al., 2005) simulates the atmospheric dynamics in a regional and/or continental environment. The MM5 model (PSU/NCAR) (Grell et al., 1994) was started to be developed in the 80's and has continued to be developed until the end of 90's. The WRF model has substituted to MM5 with much modern coding and new paradigms and capabilities. The modularity of WRF is superior to MM5. The WRF/CHEM is an on-line version of WRF model which means that the chemical reactions are incorporated into the WRF code, so that the transport and diffusion is integrated into WRF and the transportation numerical schemes are exactly done simultaneously with the meteorological solving processes. The advantage of the pollution *on-line* models is that the climate aspects can be investigated in a more realistic way than in *the off-line* models. WRF/CHEM continues to be under developing in many aspects. In this case we have used the WRF/CHEM May 2008 version (V 3.0). The WRF-CMAQ model is an off-line chemical transportation model developed by EPA (CMAQ module) in 2000. The CMAQ version used in this contribution is CMAQ 4.6 (October, 2006). CMAQ is run using the meteorological BC's and IC's provided by WRF in a separate run.

### 2. EXPERIMENT

In order to initialize CCSM3 in 1985, we have used B30.030 data sets with T85 Gaussian resolution (aprox. 2.8 degrees resolution). This dataset has been regridded to T42 (aprox. 1.4 degrees resolution) by using NCL g2gsh program. This data is used as initial conditions for CAM/CLM modules and B30.004 restart 1000 is used to run the POP/CSIM modules with GX1V3.

Additionally, SST values are taken from OISST NOAA 1985 SST/ICE/MASK (see Fig. 1). This configuration guarantees the maximum reliability to reproduce the condition during 1985-1995. In 1995 the system is configured to get outputs every 6 hours to serve as BC's and IC's for WRF/CHEM and WRF-CMAQ. CCSM3 is run in a fully coupled mode. The vertical resolution for the atmospheric and land processes modules is 26 vertical layers. In case of POP, we have 320\*384\*40 cells with a longitudinal resolution one degree (aprox.). The latitudinal resolution is variable, with finer resolution near the equator (approximately 0.3 degrees). 40 levels in the vertical associated with the gx1v3 resolution, with level thickness monotonically increasing from approximately 10 to 250 meters. This is based on previous experiments made by San José et al. (1994, 1996,1997,1998, 2002, 2004). Figure 2 shows the comparison between observations (NNRP) and modelling data (CCSM3) for 1995-1999 averaged surface temperatures with excellent results.



# OISST-NOAA 1985-01 SST (°C)

Figure 1. OISS-NOAA 1985-January SST average temperature. This temperature is taken as initial data for running CCSM3 in 1985.



# **CCSM – NNRP SURFACE TEMPERATURE**

Figure 2. Comparison between observations (NNRP) and modelling results (CCSM3) for surface temperature.

The VCCSM3 and mesoscale models have been run in the MAGERIT supercomputer (CESVIMA, Supercomputer Center of Madrid, Spain) which has 1200 node eserver BladeCenter JS20 with PowerPC 2,2 Ghz and 4 Gb RAM. Figure 3 shows a CPU balance configuration for running CCSM3. This is the configuration used in this work which took 200 CPU hours with 72 CPU's.



### Load Balancing CCSM3 Components



### 3. RESULTS

The results show a good agreement between meteorological variables – observed and modelled – with CCSM3 global climate model. The configuration made for 1985-1995 seems to play a good role and the BC's and IC's which are provided to WRF/CHEM and WRF-CMAQ are considered to be good. The 10 year monthly averaged values are compared for PM10 modelled concentrations from WRF/CGEM and WRF-CMAQ with Planetary Boundary layer Height (PBL) (right axis of the graphics) (see Figure 4) and 2 m temperature. PBL and PM10 values compare in anti-cyclic phase for monthly values, 2m temperature and PM10 values com pare also in anti-cyclic phase for yearly

values and finally O3 values obtained with WRF/CHEM compare poorly with those obtained with WRF-CMAQ. The WRF-CMAQ O3 values compare good with observations ( $R^2=0.57$ ) but the WRF/CHEM compare poorly with the observations ( $R^2=0.05$ ). Figure 6 show some correlations between 2m temperature values and SO2 (WRF-CMAQ), O3 (WRF-CMAQ) and PM10 (WRF/CHEM) concentrations.



Figure 4. Comparison between PM10 concentrations modelled with WRF/CHEM and WRF-CMAQ and PBL height and T. Also, O3 concentrations modelled with WRF/CHEM and WRF-CMAQ and PBL height.



Figure 5. Squared correlation coefficients between monthly surface temperature and O3, PM10 and SO2 concentrations during the 1995-2005 period.

As a conclusion, we should say that WRF/CHEM (in the actual version it seems to have problems with the photolysis rate code and it should be made more robust) for O3 concentrations needs more work since the comparison with the observations (and WRF-CMAQ) is very poor. WRF/CHEM is doing an excellent work for PM10 concentrations, even better than MM5-CMAQ. Probably because the MOSAIC aerosol model is used instead the MADE model but this should be confirmed with further experiments.

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