Contribution to:

12th CONFERENCE ON HARMONIZATION WITHIN ATMOSPHERIC DISPERSION MODELLING FOR REGULATORY PURPOSES

Cavtat, Croatia, October, 6-9, 2008

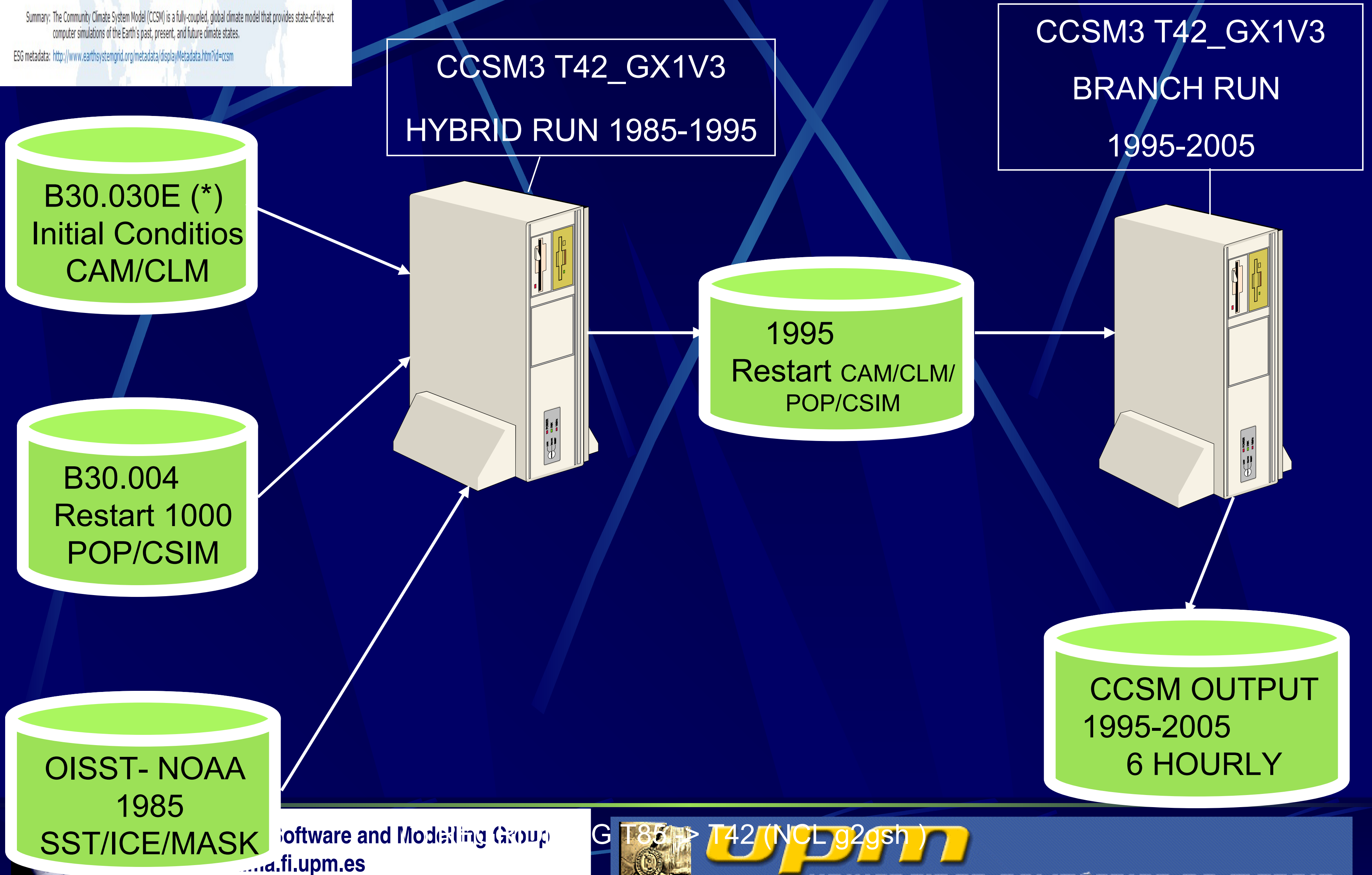
A SEASONAL AND YEARLY POLLUTION STUDYBY USING WRF/CHEM AND WRF-CMAQ NESTED WITH CCSM3 GLOBAL MODEL

R. San José, J. L. Pérez, J.L. Morant (a) and R.M. González (b)

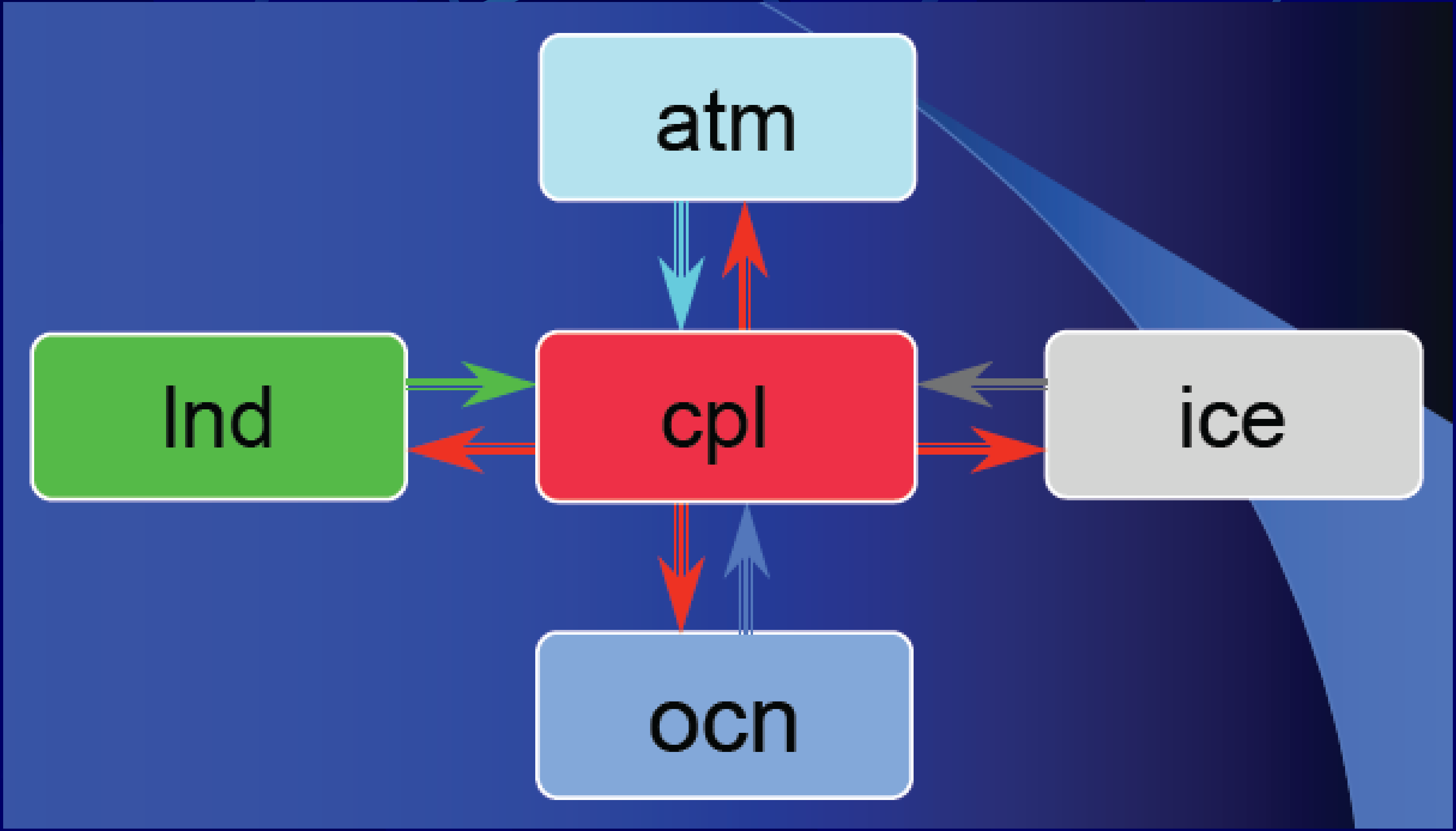
(a) *Environmental Software and Modelling Group*
Computer Science School – Technical University of Madrid (UPM)
Campus de Montegancedo – 28660 Madrid (Spain)
http://artico.lma.fi.upm.es

(b) *Spanish Observatory for Sustainability, Alcalá University,*
plaza de San Diego, s/n 28801 Alcalá de Henares, Madrid (Spain)
(c)*Department of Meteorology and Geophysics, Complutense University of Madrid (UCM),*
Ciudad Universitaria 28040 Madrid (Spain)

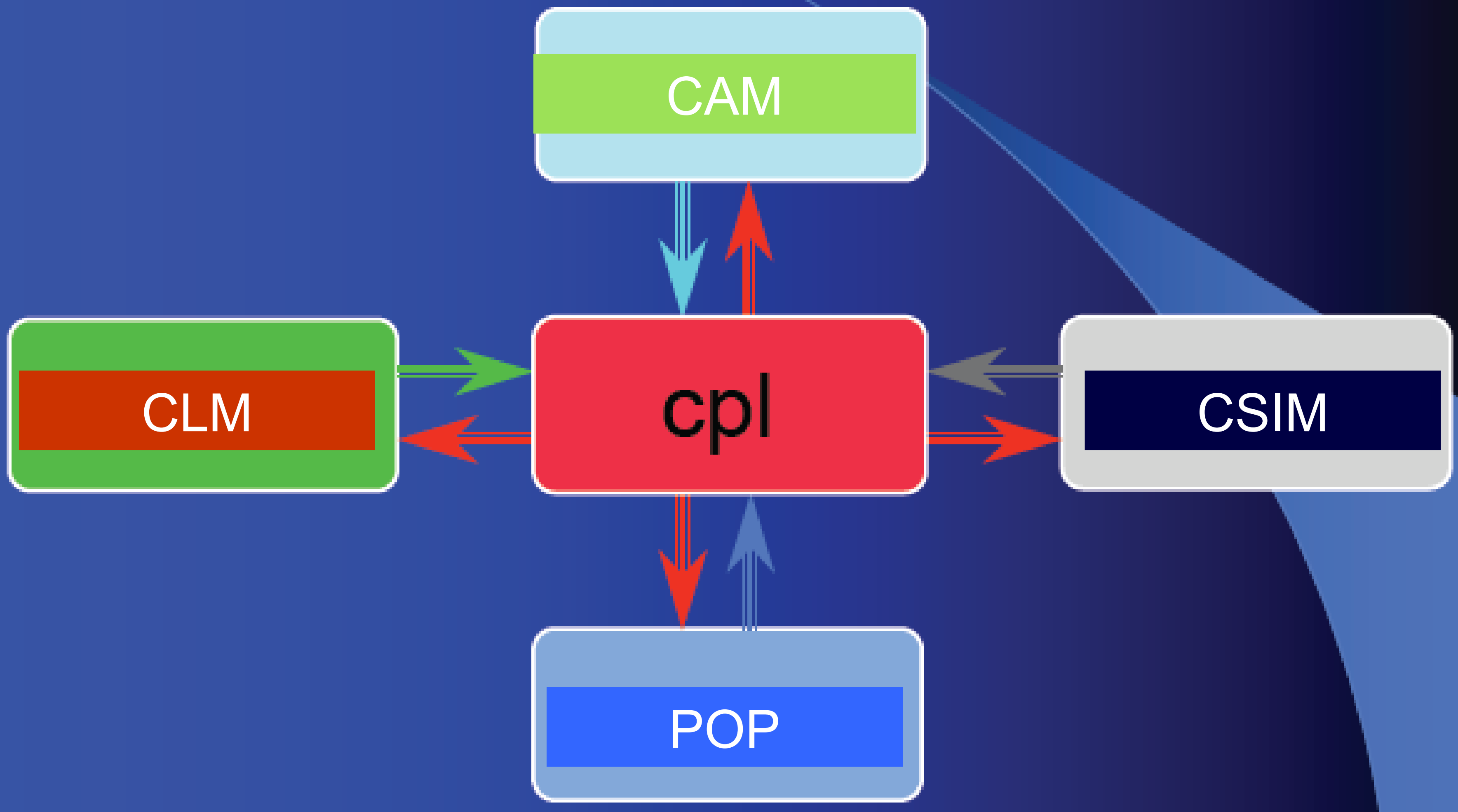
CCSM3 EXPERIMENT



CCSM 3.0



CCSM 3.0. COMPONENT SETS B



CCSM3 EXPERIMENT

B30.030E : T85 CCSM3 climate of the 20th Century run, 130 years (1870-01 -> 1999-12), fully coupled

B30.004: T42 CCSM3 Control run, 1000 years (0000-01 -> 1001-06), fully coupled.

OISST-NOAA: NOAA Optimum Interpolation (OI) Sea Surface Temperature (SST) V2. 1º Resolution. Sea Surface Temperature. Ice Concentration Land Sea Mask . Monthly Mean. (http://www.cdc.noaa.gov/cdc/data.noaa.oisst.v2.html)

T42 (CAM/CLM): 64(lat)*128(long)*26(vertical) . Approx. 2.8 degree resolution
T85 (CAM/CLM): 128(lat)*256(long)*26(vertical) . Approx. 1.4 degree resolution

GX1V3 (POP/CSIM) → 320*384*40 CELLS. Longitudinal resolution approximately one degree .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

CCSM3 EXPERIMENT

CSIM

Ice Thickness Distribution = Linear Remapping (Lipscomb(2001)).

Ice Dynamics = Elastic-Viscous-Plastic (Hunke and Dukowicz(1997)).

Strength Pack Ice = Based on Energetics (Rothrock(1975))

Damping Elastic Waves = False

Snow on Ice = True (snow on ridged ice falls into ocean)

Horizontal Transport Scheme = Incremental Remapping (Lipscomb and Hunke(2004)).

POP

Barotropic-mode solver = Chron-Gear preconditioned conjugate gradient

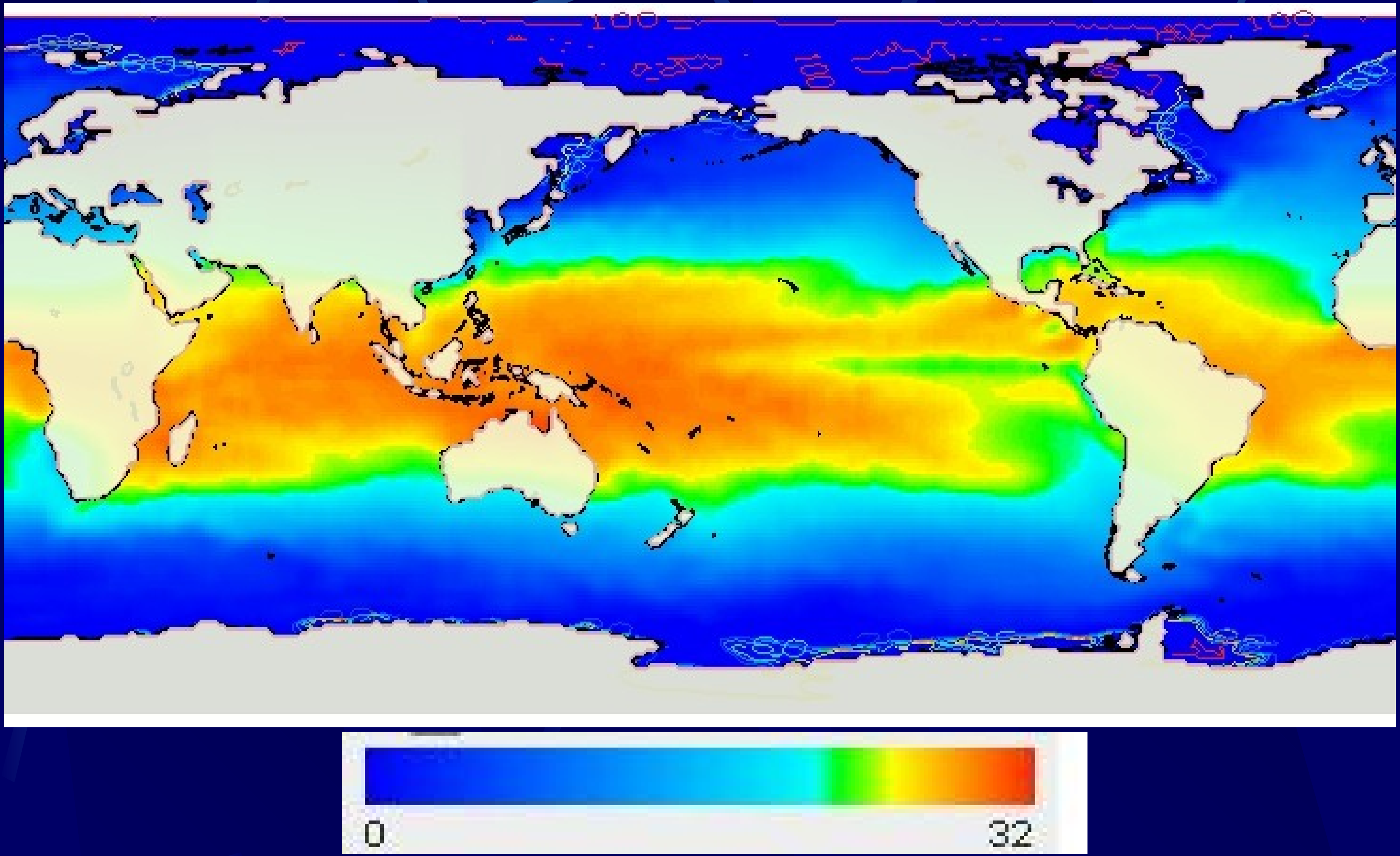
Advection methods = 3rd-order upwinding

Vertical mixing = KPP mixing (Large *et al.* 1994)

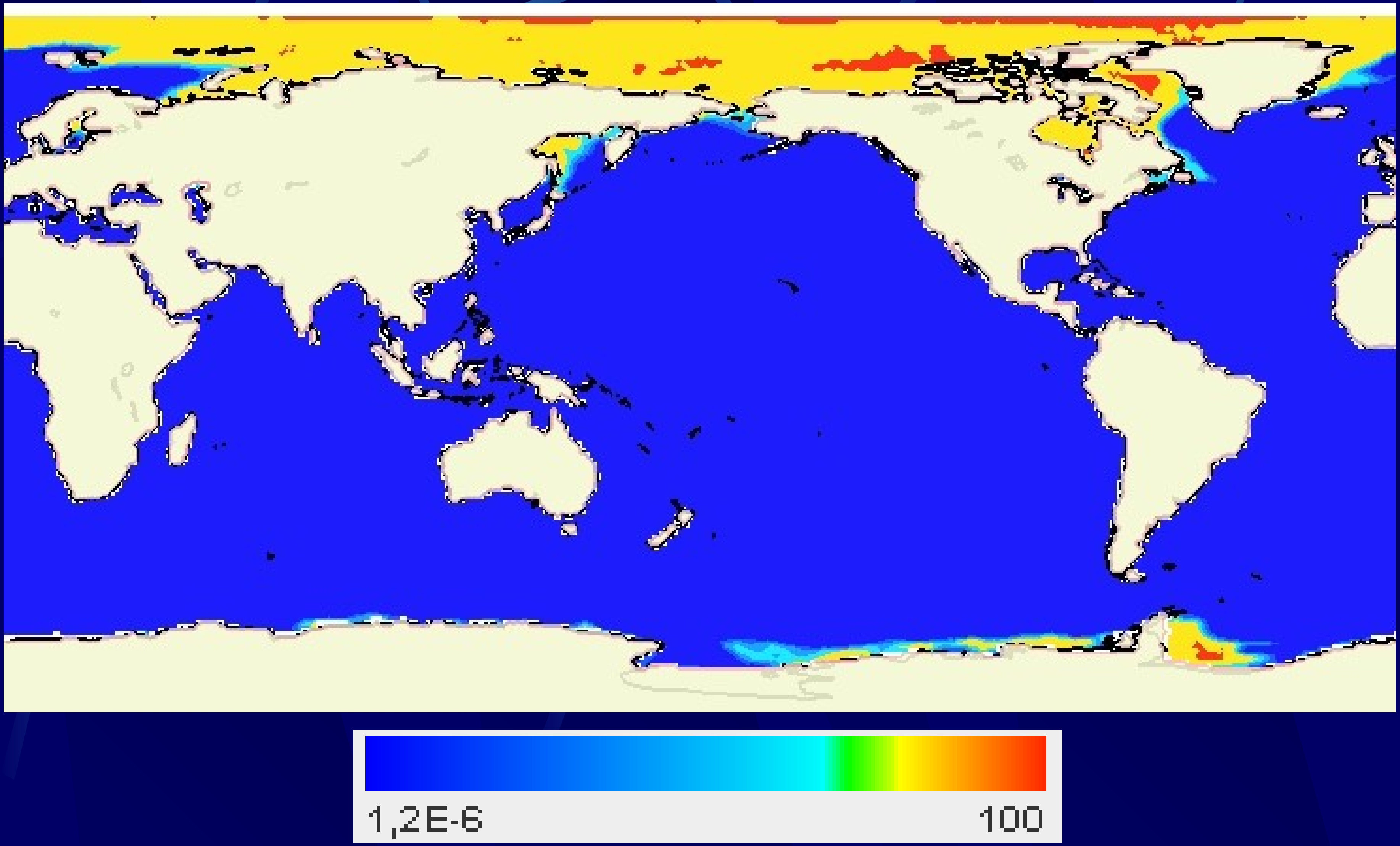
Horizontal mixing = Anisotropic Viscosity

Equation of state = (McDougall, Wright, Jackett and Feistel (2002))

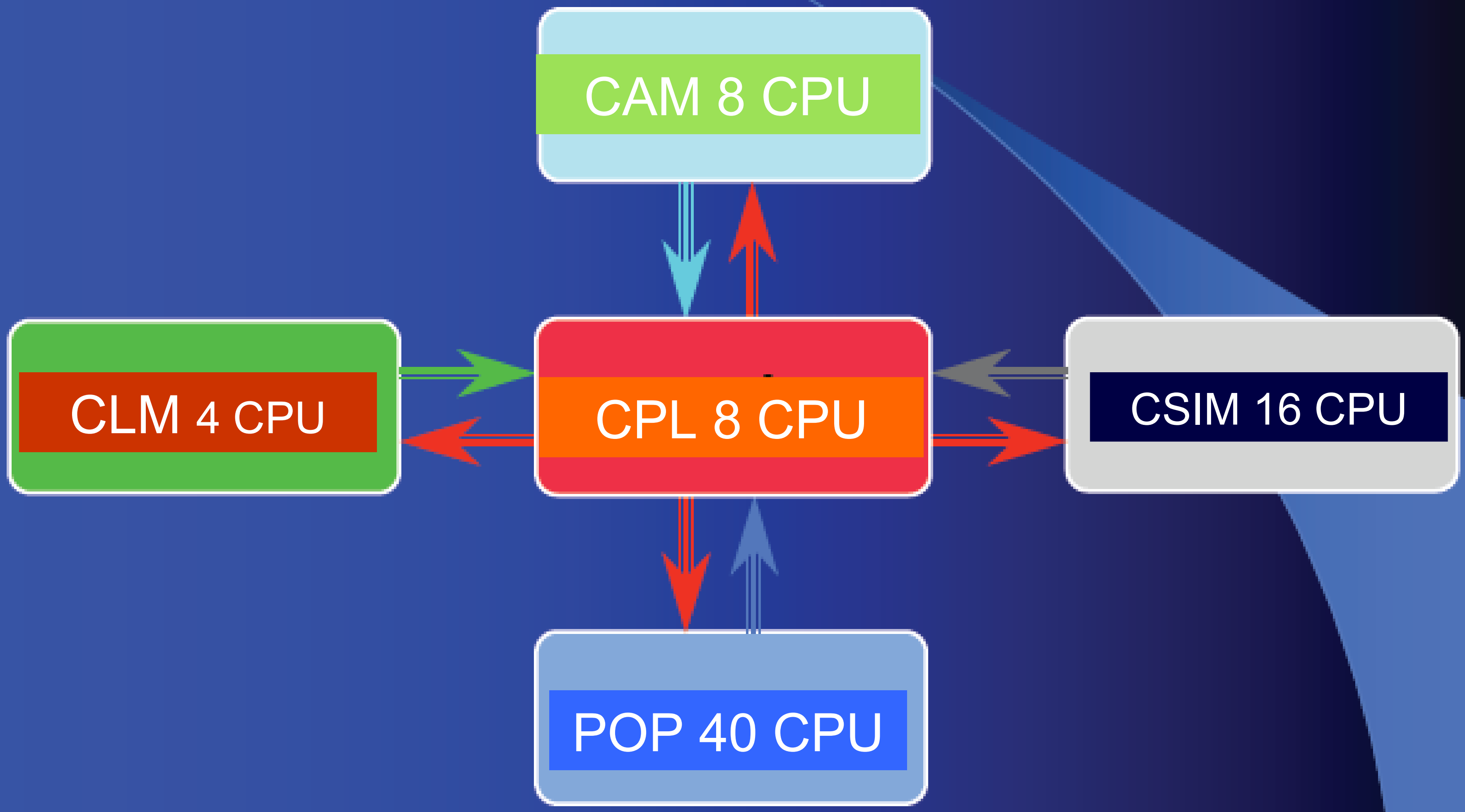
OISST-NOAA 1985-01 SST (ºC)



OISST-NOAA 1985-01 ICE FRACCTION (%)



Load Balancing CCSM3 Components



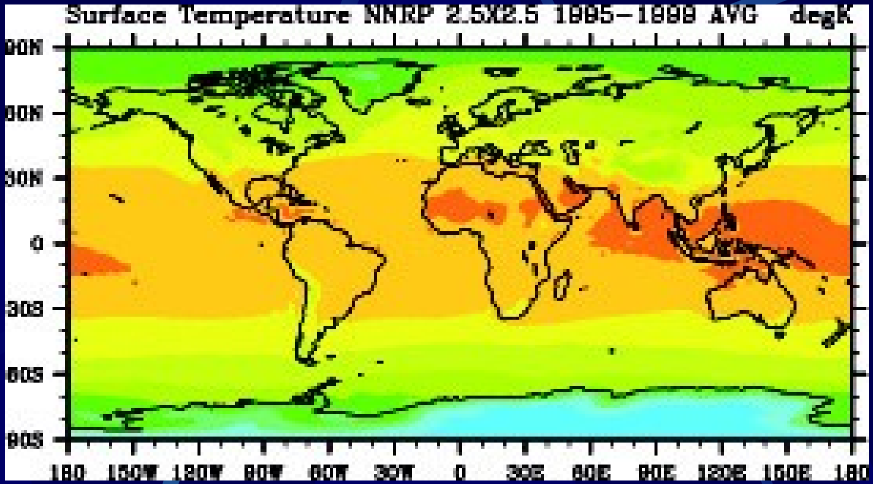
CCSM EXPERIMENT

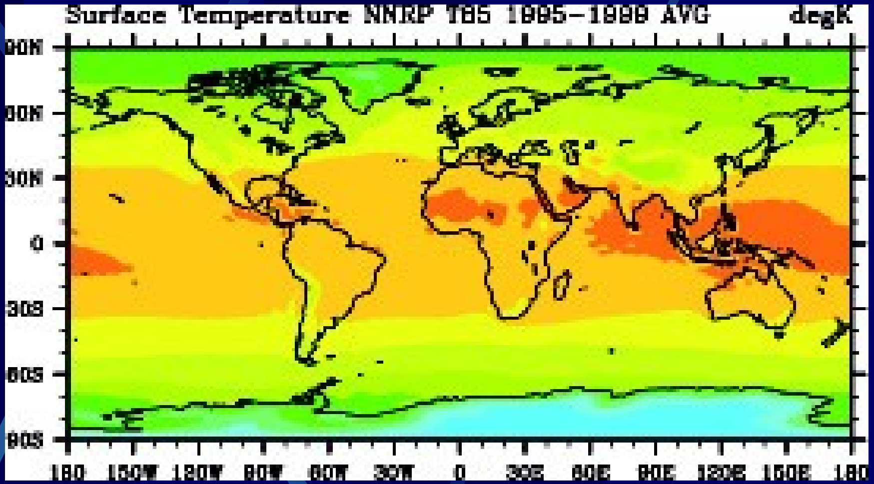
COMPUTER SYSTEM:

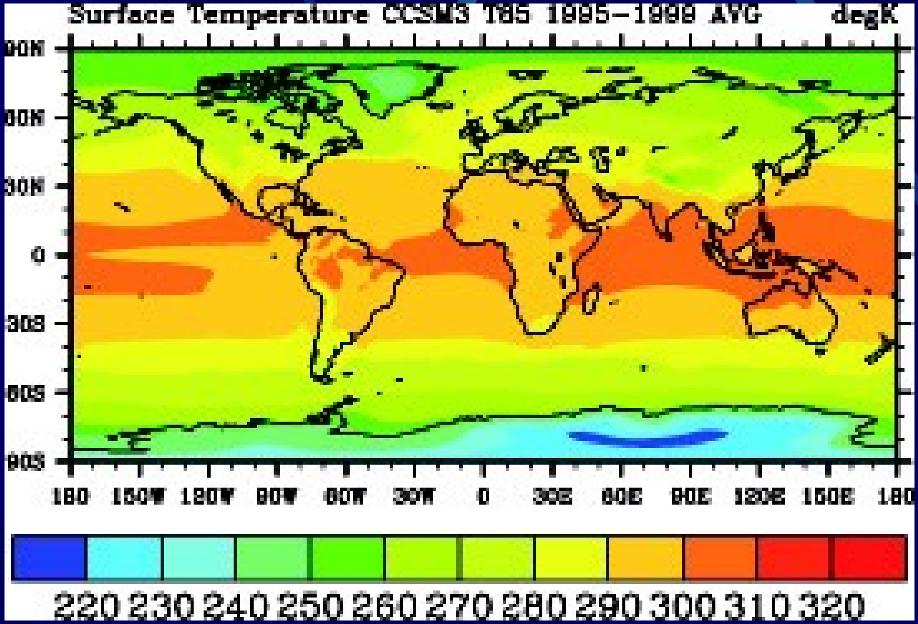
- Magerit clúster
- 1200 node eServer BladeCenter JS20
- PPC de 2'2 GHz and 4 Gb de RAM
- Myrinet network
- I**BM XL Fortran10.1**
- LoadLeveler queque software

CCSM 3.0 72 CPU (MPI ONLY) -> 10 YEARS (1985-1995) / 100 HOURS-CPU
-> 10 YEARS (1995-2005) / 100 HOURS-CPU

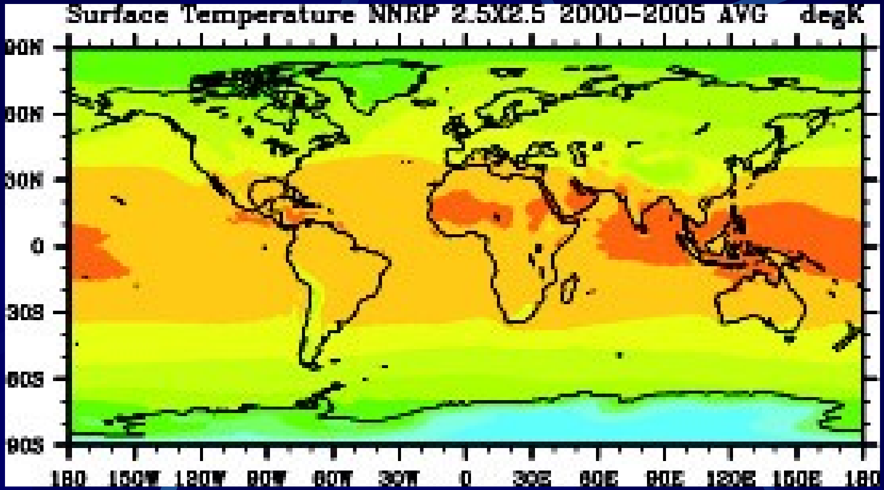
CCSM – NNRP SURFACE TEMPERATURE

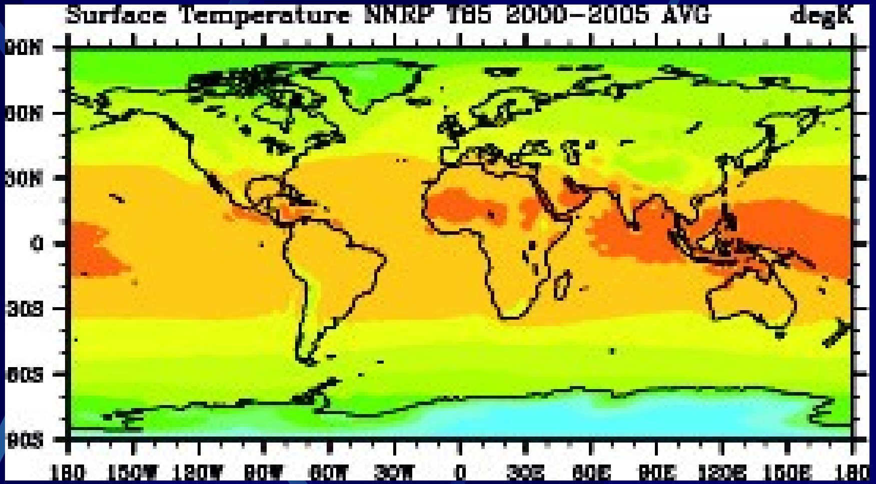


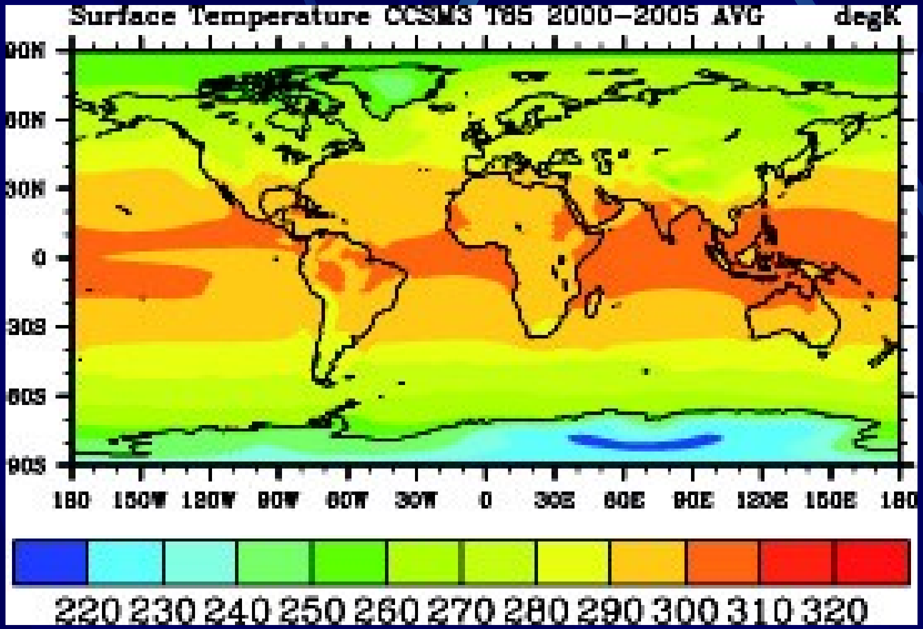




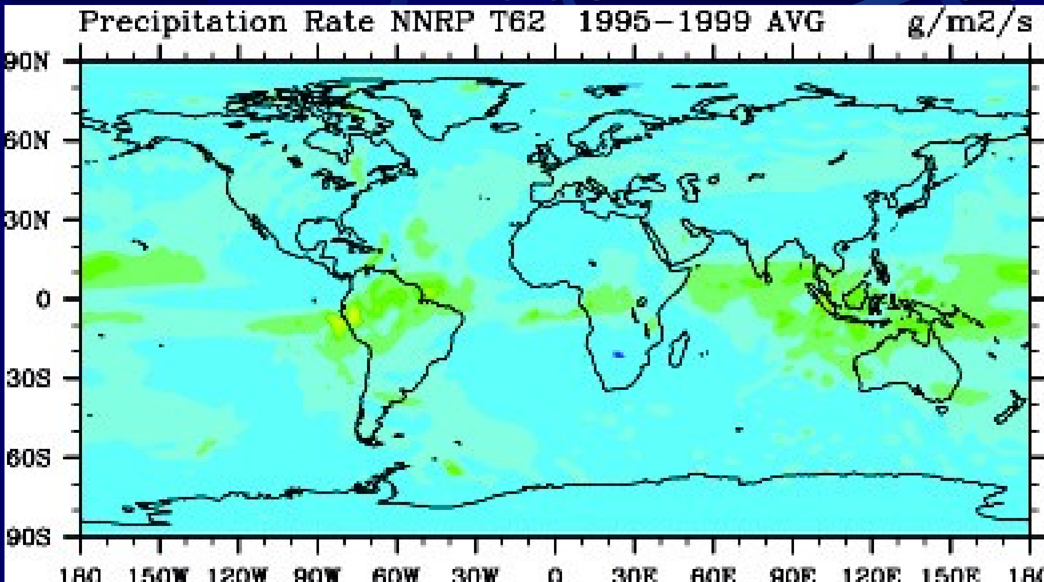
CCSM – NNRP COMPARATION

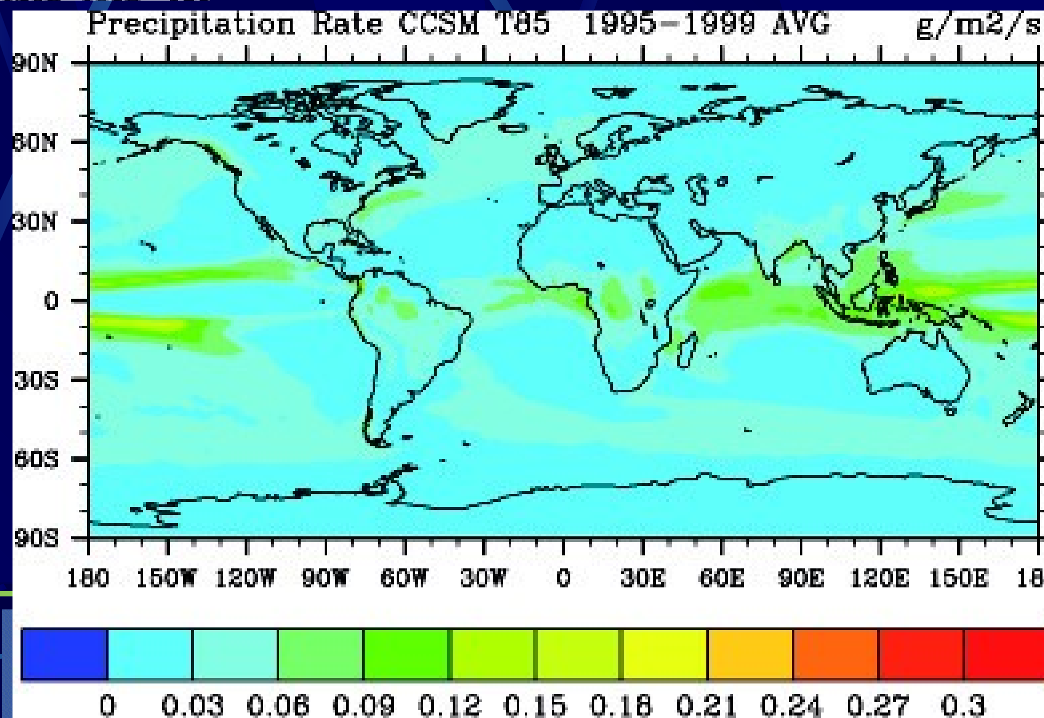




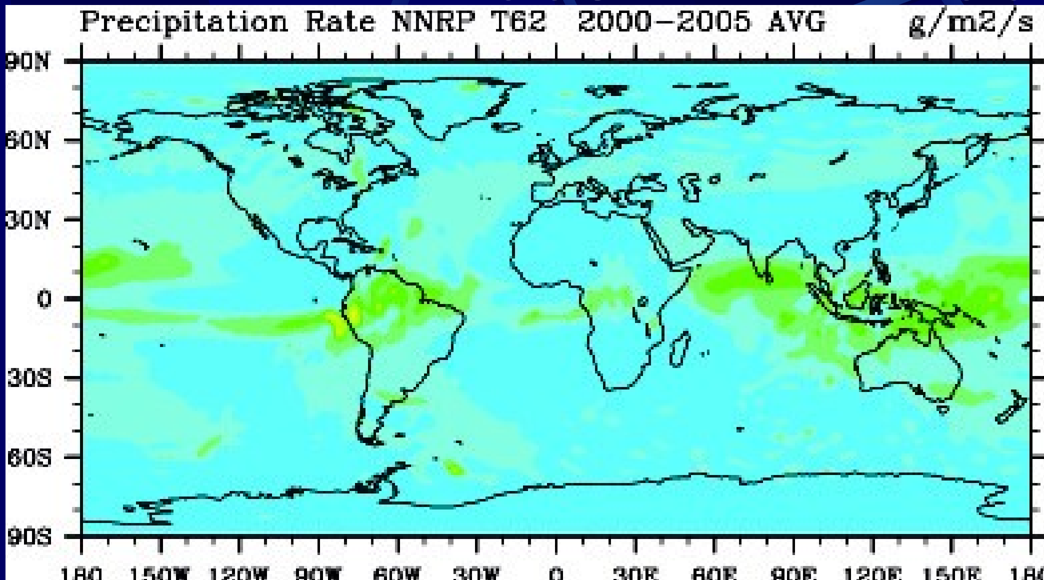


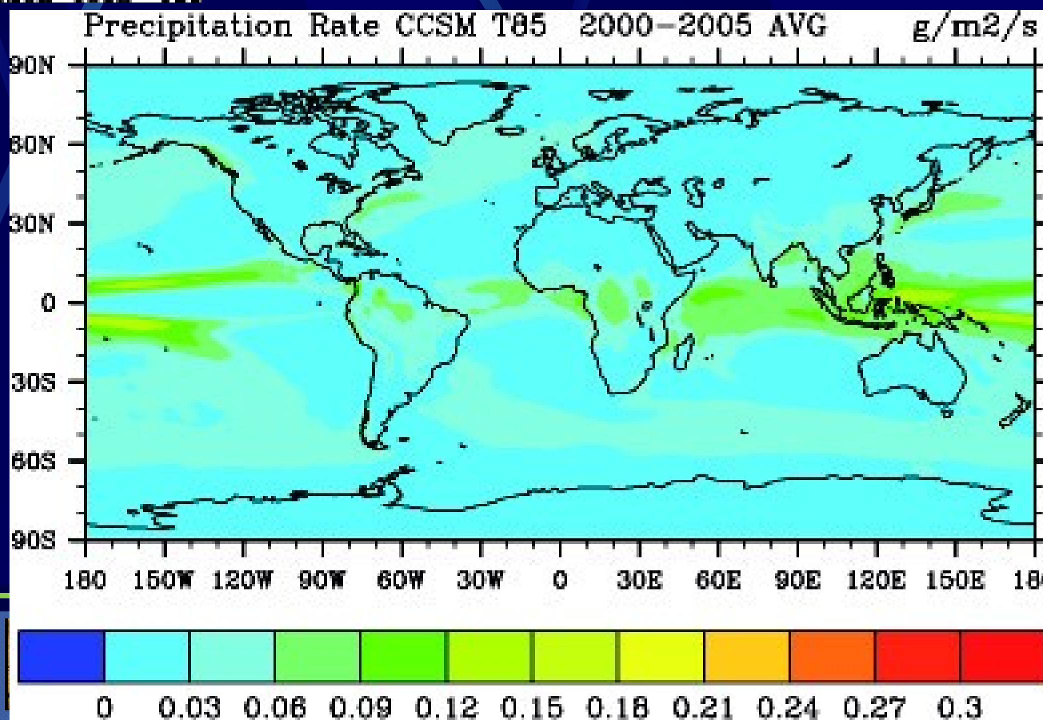
CCSM – NNRP COMPARATION



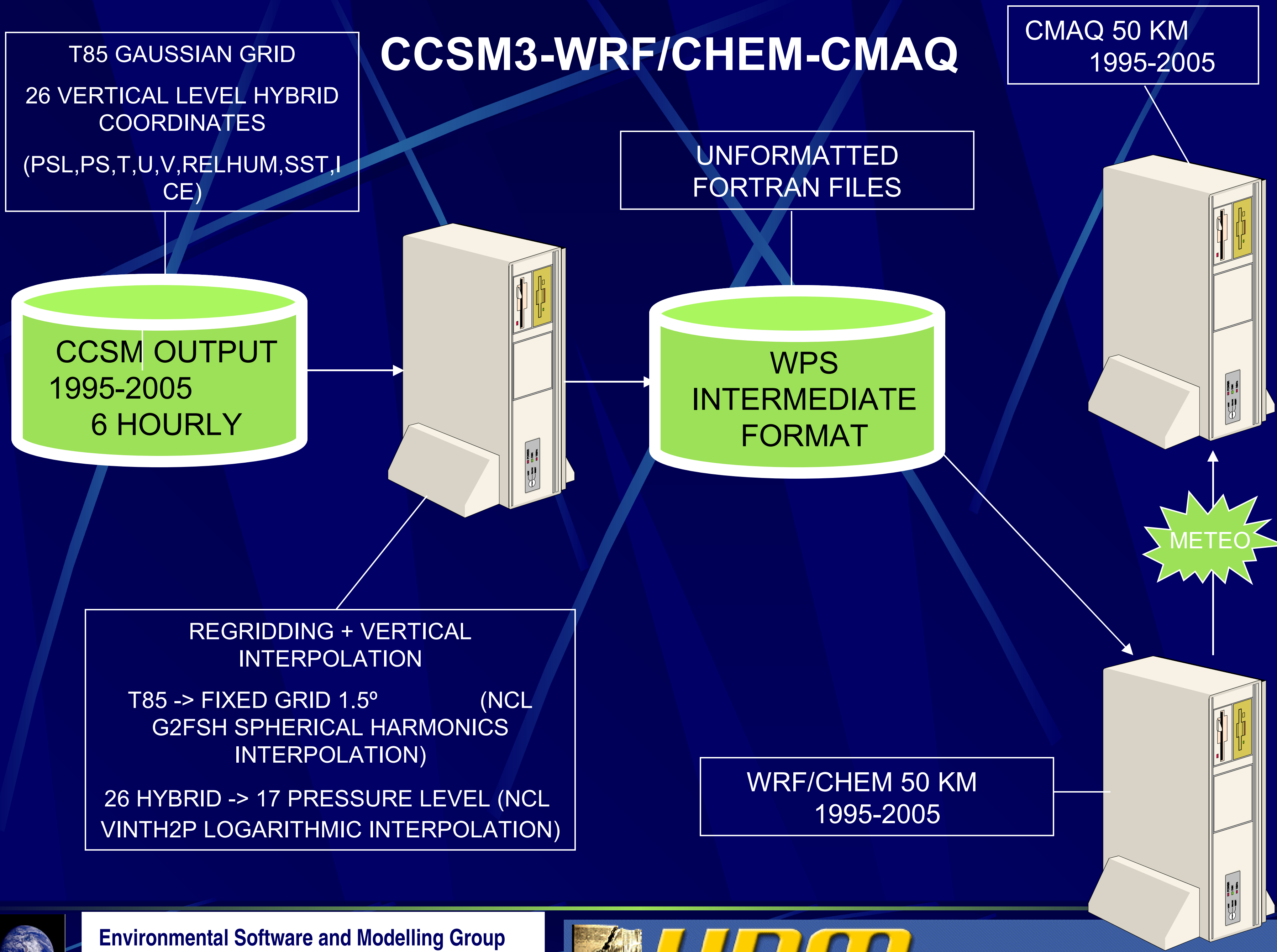


CCSM – NNRP COMPARATION

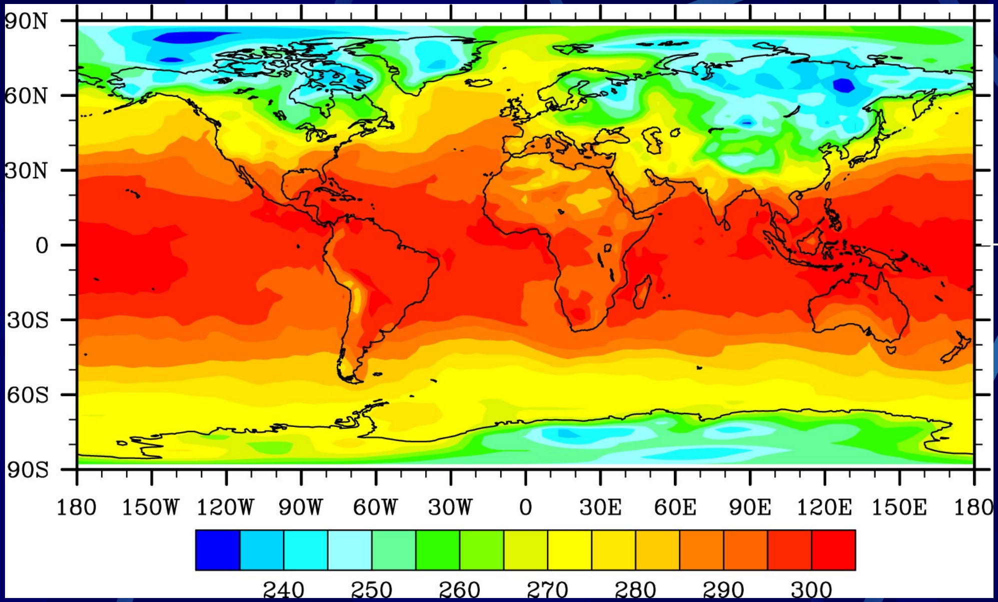




CCSM3-WRF/CHEM-CMAQ



REGRIDDING GAUSSIAN TO FIXED



TEMPERATURE (º k)

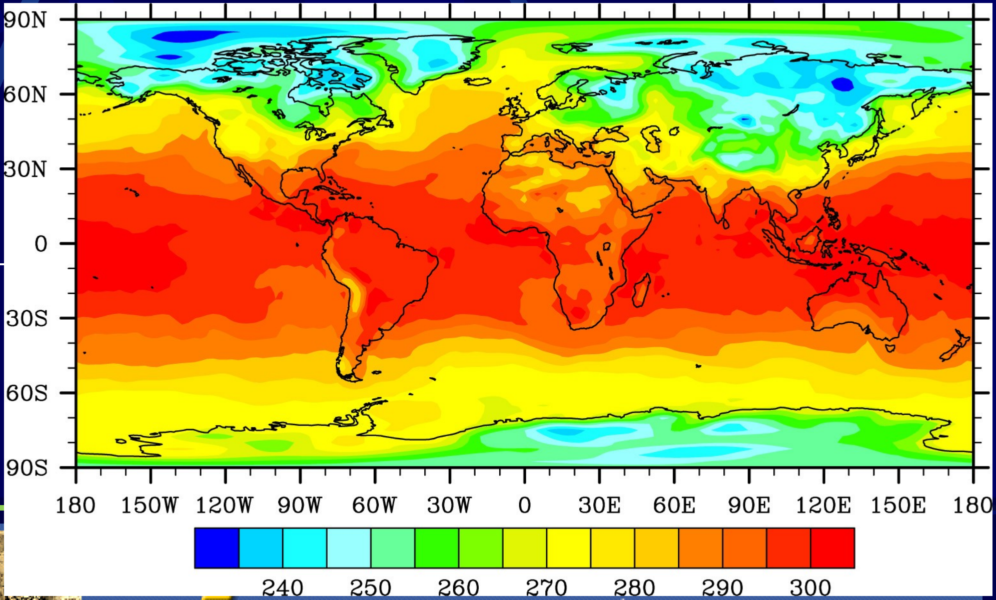
T85 GAUSSIAN GRID

CCSM OUTPUT 01-01-2003 12:00

TEMPERATURE (º k)

1.5º FIXED GRID

CCSM OUTPUT 01-01-2003 12:00



WRF/Chem & CMAQ DOMAINS

PROJECTION: Lambert Conformal Conic

Central Latitude: 50.86N Central Longitude: 7.14E

DOMAIN: 113*103 50 Km. RESOLUTION + 23 VERTICAL LEVELS
Lower-Left Corner LCC (-2825000, -2575000)

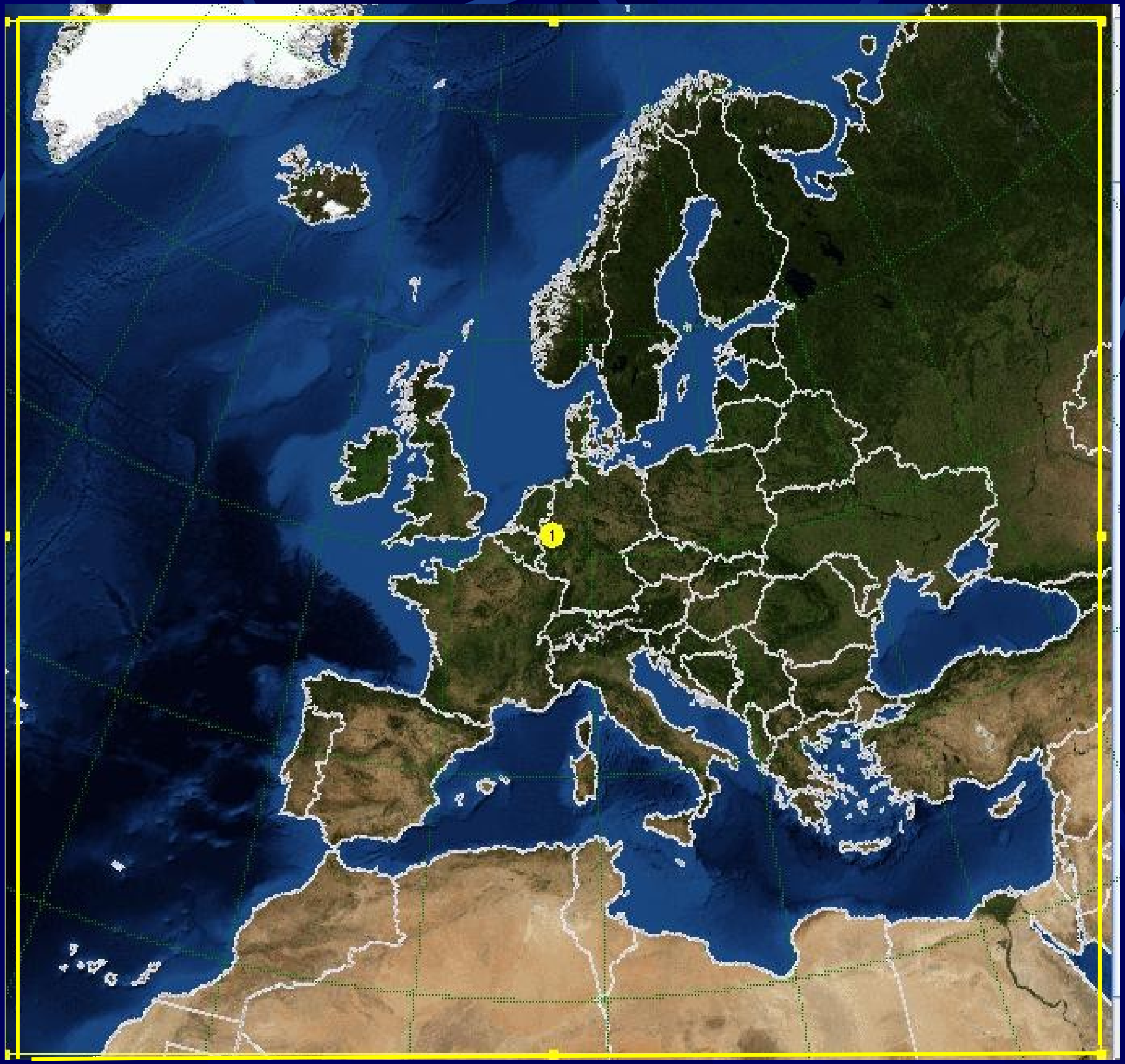
SIGMA VERTICAL LEVELS:
1.00,0.99,0.98,0.96,0.93,0.89,0.85,0.80,0.75,0.70,0.65,0.60,

0.55,0.50,0.45,0.40,0.35,0.30,0.25,0.20,0.15,0.10,0.05,0.00

LANDUSE DATA: USGS 24 CATEGORIES

GEOGRAPHICAL DATA: 10´ RESOLUTION

WRF/Chem & CMAQ DOMAINS



WRF/Chem CONFIGURATION

-**Physics Options in WRF**:

- **Cumulus Parameterization:**

  GRELL-DEVENYI ENSEMBLE SCHEME

- **PBL Scheme and Diffusion:**

  YONSEI UNIVERSITY (*YSU PBL)*

- **Explicit Moisture Scheme :**

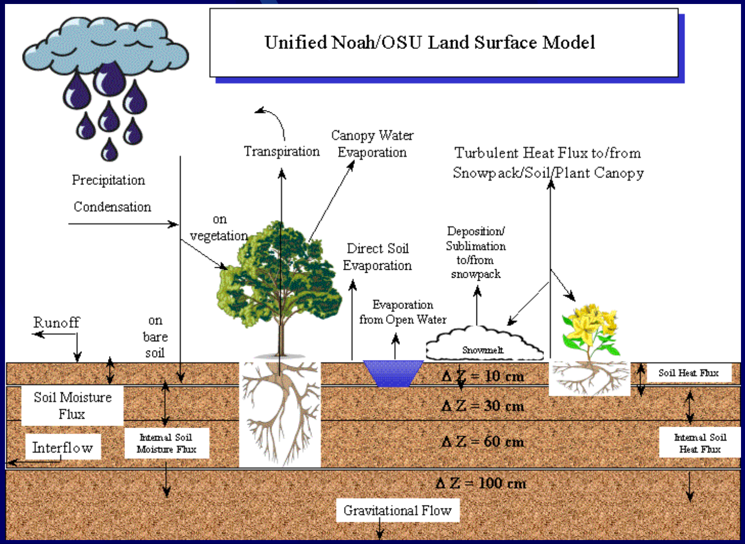
  WSM (WRF single-moment) 5-class microphysics

- **Radiation Scheme:**

  RRTM - Dudhia radiation

- **Surface Scheme :**

  Noah Land-Surface Model

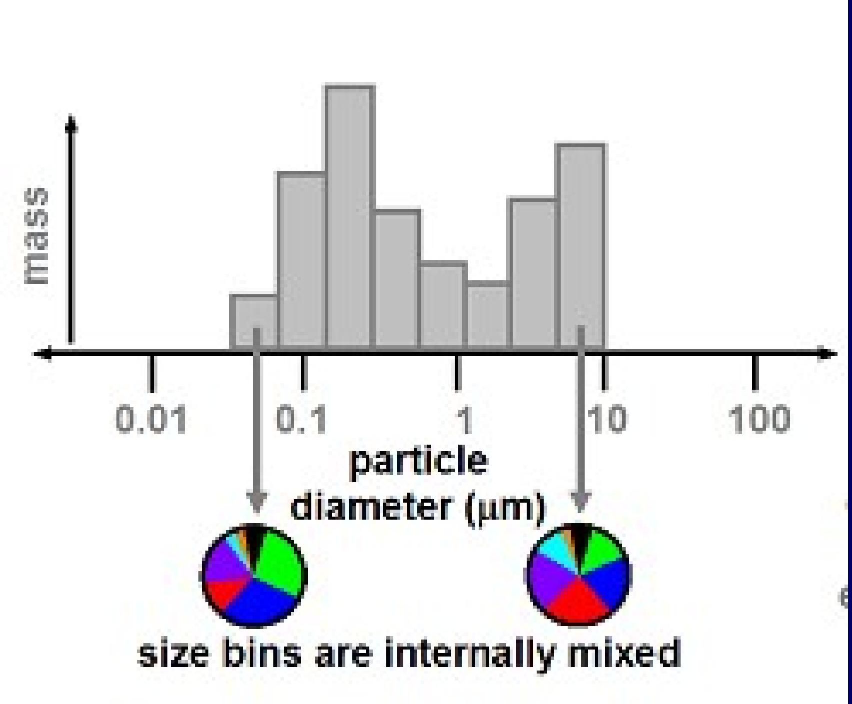


WRF/Chem CONFIGURATION

-**CHEMICAL Options:**

- CBMZ chemical mechanism (Carbon Bond).
- MOSAIC Aerosol 4 bins (Zaveri et al. 2004)
- Aqueous chemistry OFF
- Cloud chemistry OFF.
- Biogenic Emission (Gunther et al. 1994)
- FTUV Photolysys

Sectional Approach

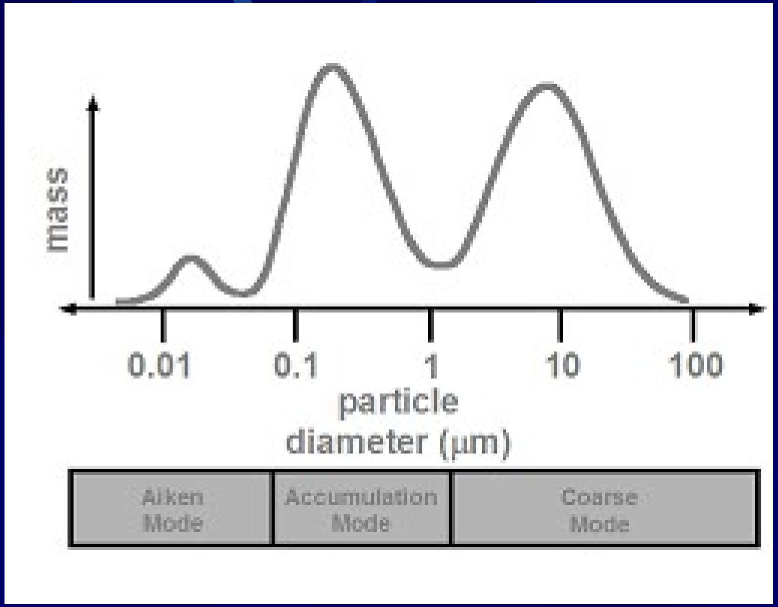


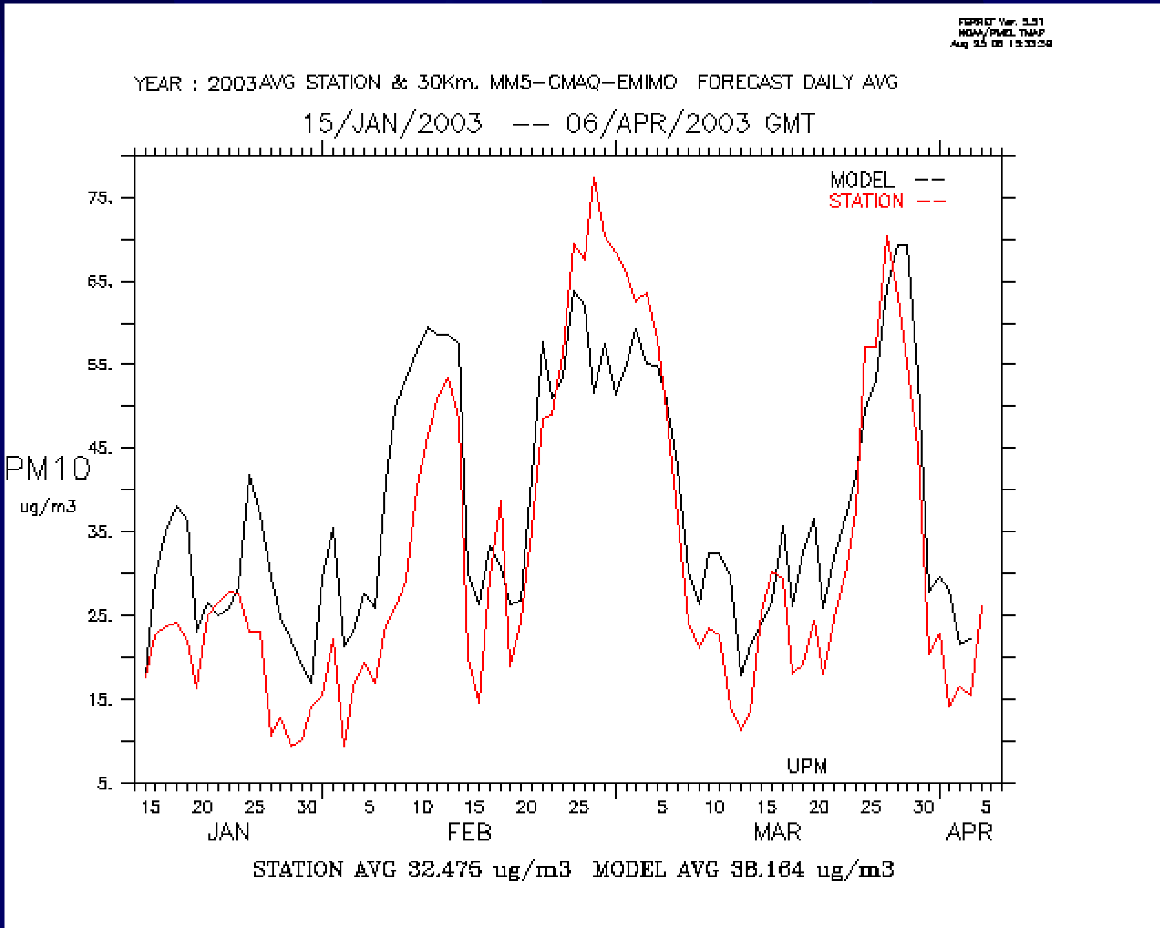
CMAQ CONFIGURATION

-**CCTM Options in CMAQ**

- Advection scheme: global mass-conserving scheme (Yamartino)
- Vertical Difussion: Asymmetric Convective Model (ACM2)
- CB05 chemical mechanism (Yarwood et al. 2005).
- Euler Backward Solver (EBI) solver
- CMAQ Aerosol : The 3rd generation modal CMAQ aerosol model
- Aqueous/cloud chemistry ON.

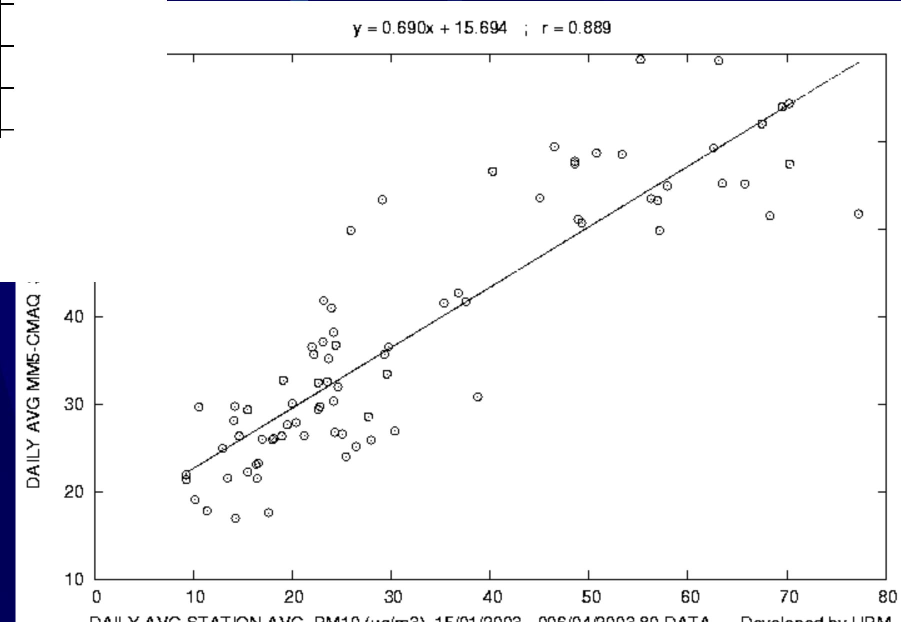
Modal Approach



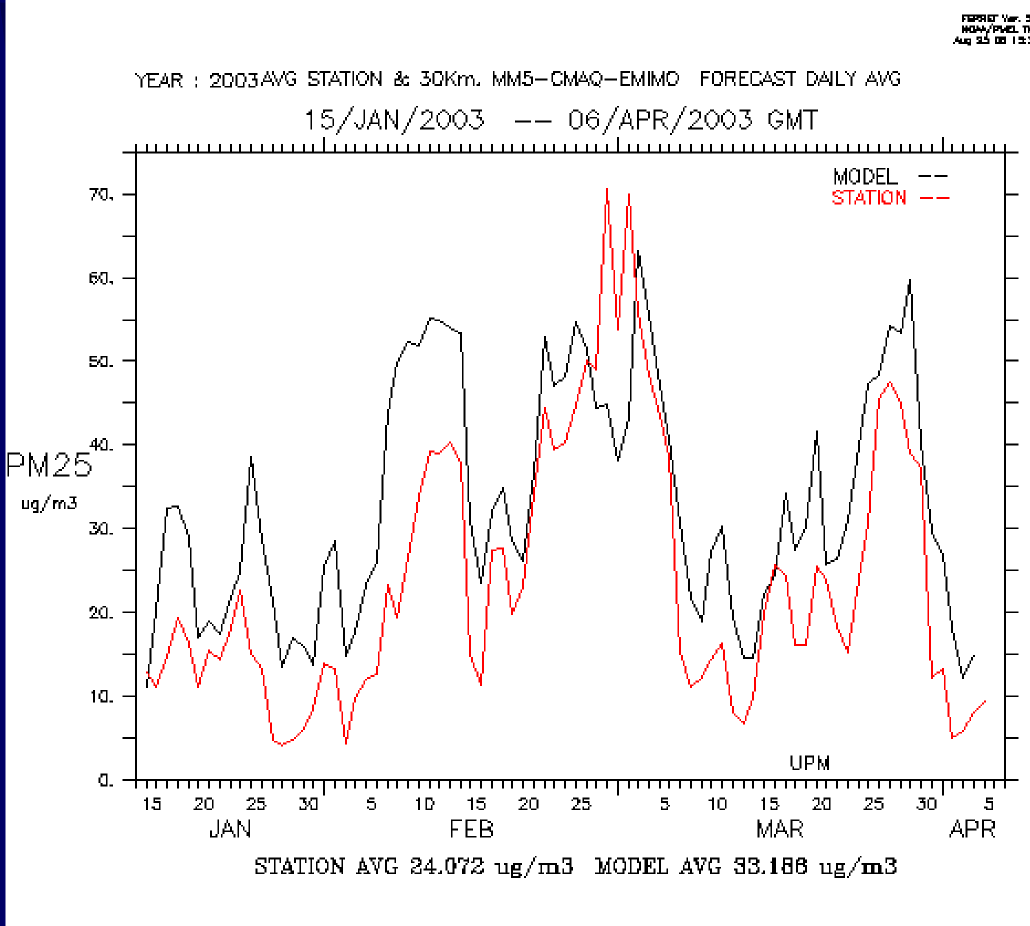


VERSION 2

WRF/CHEM
30 KM SP. RES.
GERMANY
JAN-APR, 2003
TNO 15 KM EMISSIONS
CAFÉ-DELTA TIME EMISS. PROFILES.
EDGAR EMISS.

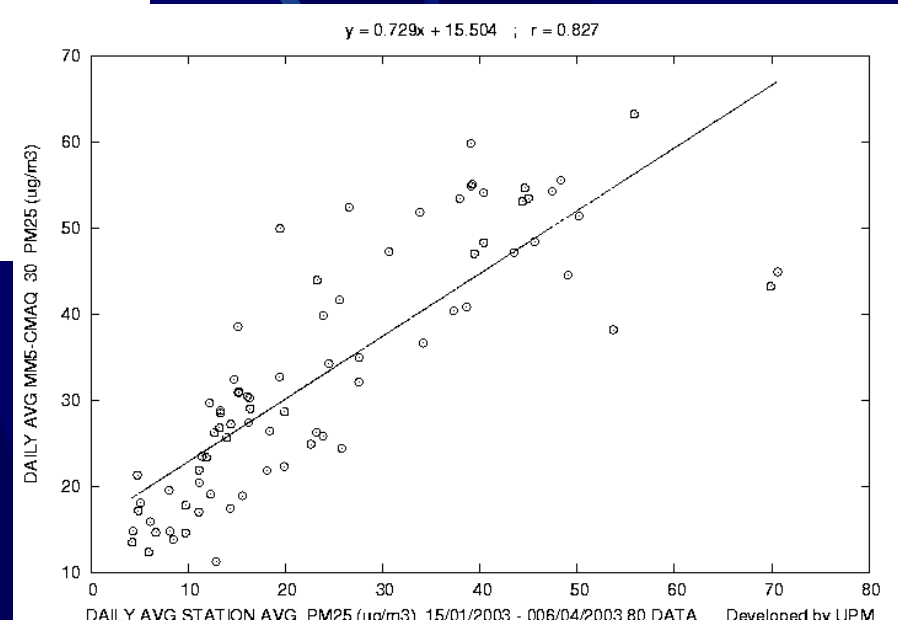


PM10 DAILY AVERAGES AND STATION AVERAGES

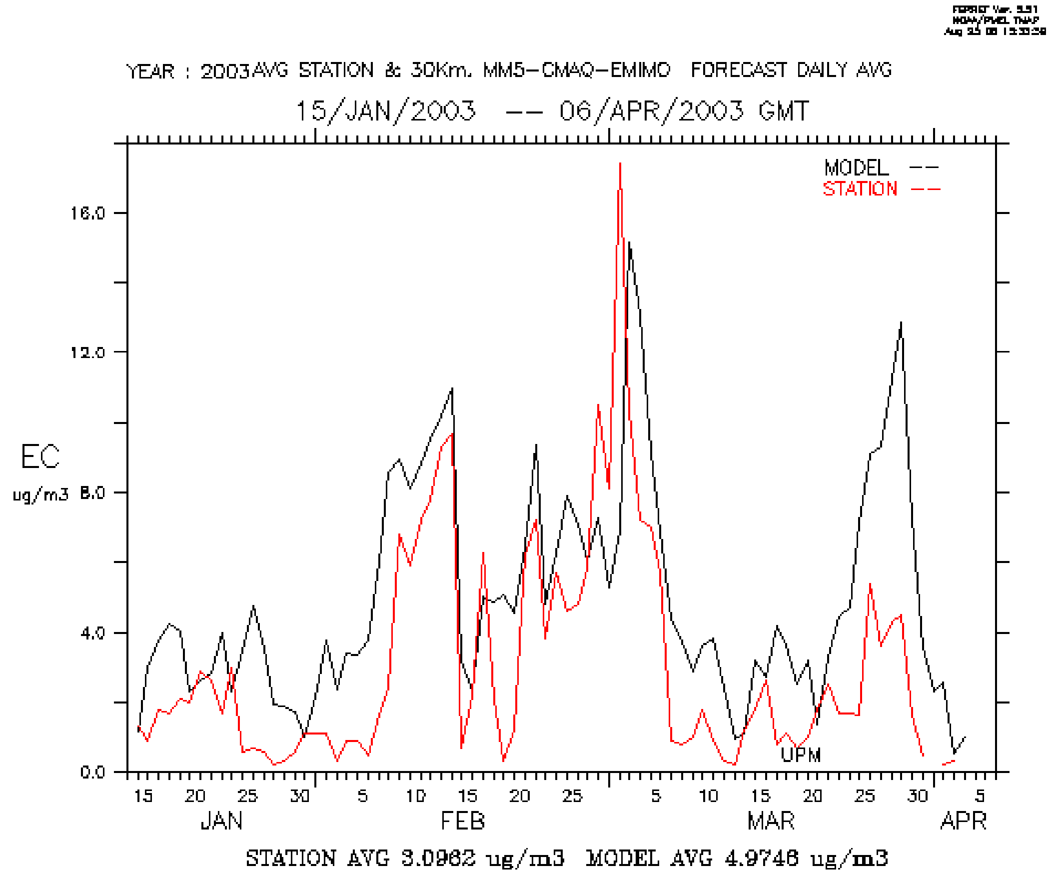


VERSION 2

WRF/CHEM
30 KM SP. RES.
GERMANY
JAN-APR, 2003
TNO 15 KM EMISSIONS
CAFÉ-DELTA TIME EMISS. PROFILES.
EDGAR EMISS.

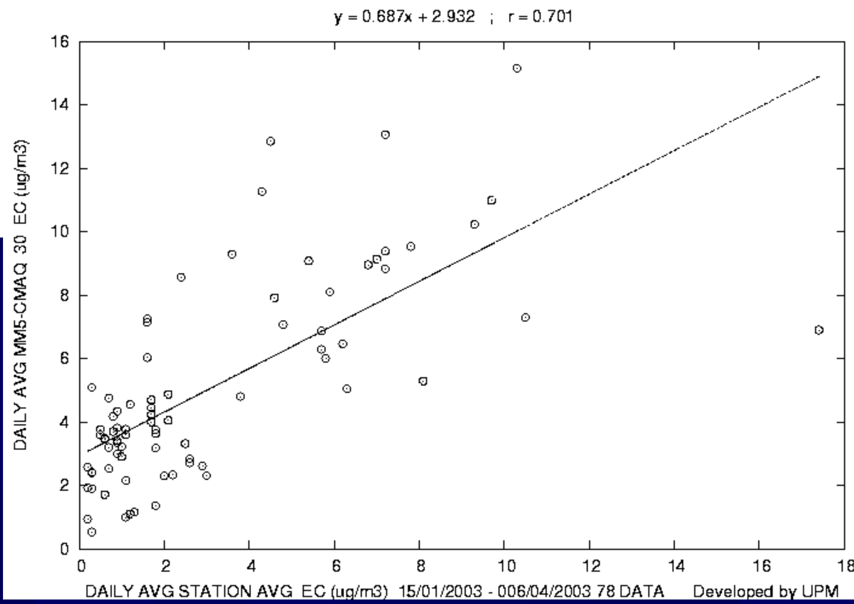


PM2.5 DAILY AVERAGES AND STATION AVERAGES



VERSION 2

WRF/CHEM
30 KM SP. RES.
GERMANY
JAN-APR, 2003
TNO 15 KM EMISSIONS
CAFÉ-DELTA TIME EMISS. PROFILES.
EDGAR EMISS.



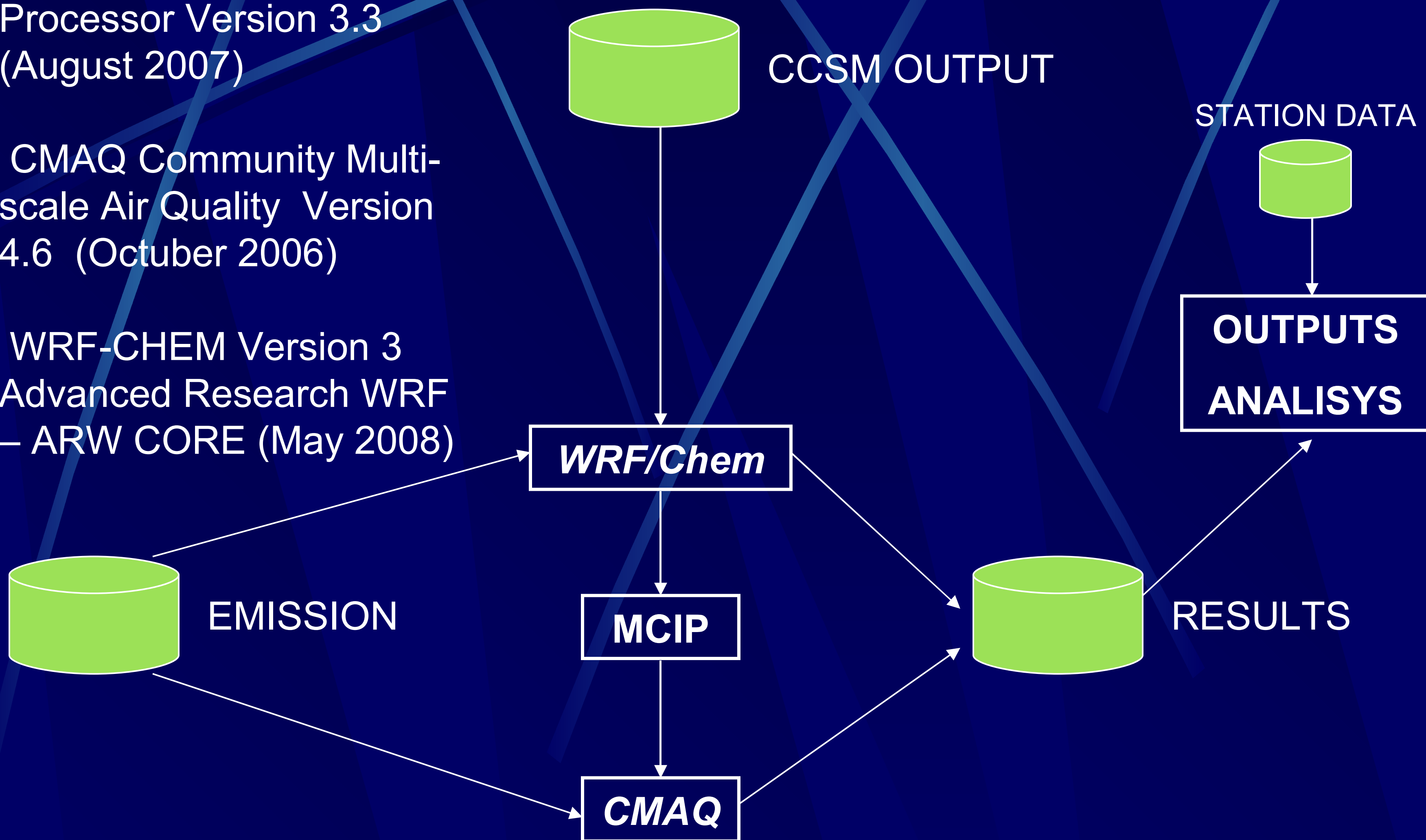
EC DAILY AVERAGES AND STATION AVERAGES

WRF/Chem & CMAQ SYSTEM

MCIP Meteorology-Chemistry Interface Processor Version 3.3 (August 2007)

CMAQ Community Multi-scale Air Quality Version 4.6 (Octuber 2006)

WRF-CHEM Version 3 Advanced Research WRF – ARW CORE (May 2008)



CPU TIME & DISK SPACE

Time period: 10 YEARS & 64 PROCESSORS

SYSTEM	CPU TIME	DATA FULL 3D	DATA EXTRACT
WRF/Chem 50 Km.	130 DAYS	14 TB	245 GB
CMAQ 50 Km.	52 DAYS	8 TB	245 GB

EMISSION DATA

- TNO-UBA Emission Data:

  - SNAP Activities:

    1Energy sector, utilities, refinaries

    2Fossil fuels, small sources

    3Fossil fuels, industry

    4Process emissions

    5Mining

    6Solvent use, use of products

    7Road transport (SO_2 only)

    71Road transport gasoline 72Road transport diesel 73Road transport LPG

    741)Road transport non-exhaust (volatilization)

    752)Road transport non-exhaust (tire, break and road wear)

    8Non-road transport

    9Waste processing1

    10Agriculture

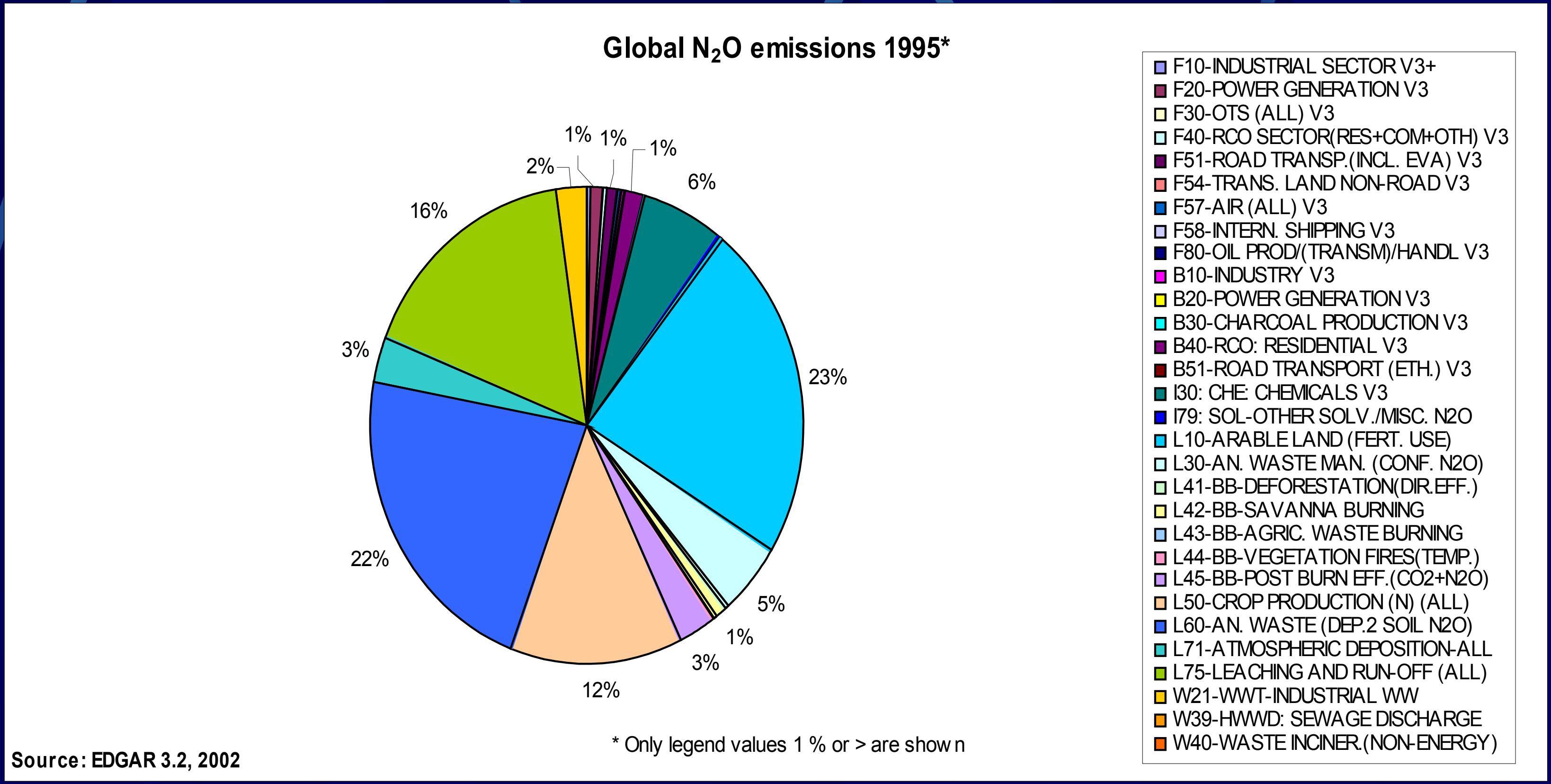
  - Geographic coordinates.

  - Cell Size is 1/4 degree by 1/8 degree

  - Pollutans: CH_4, CO, NH_3, NMVOC, NO_x, SO_2, PM_{10}, $PM_{2.5}$

EMISSION DATA

- Mother Domain include EDGAR (Emission Database for Global Atmospheric Research) :
  - * Geographic coordinates.
  - * Cell Size is 1 degree by 1 degree
  - * Pollutans: CO, NMVOC, NOx, SO2



EMISSION DATA

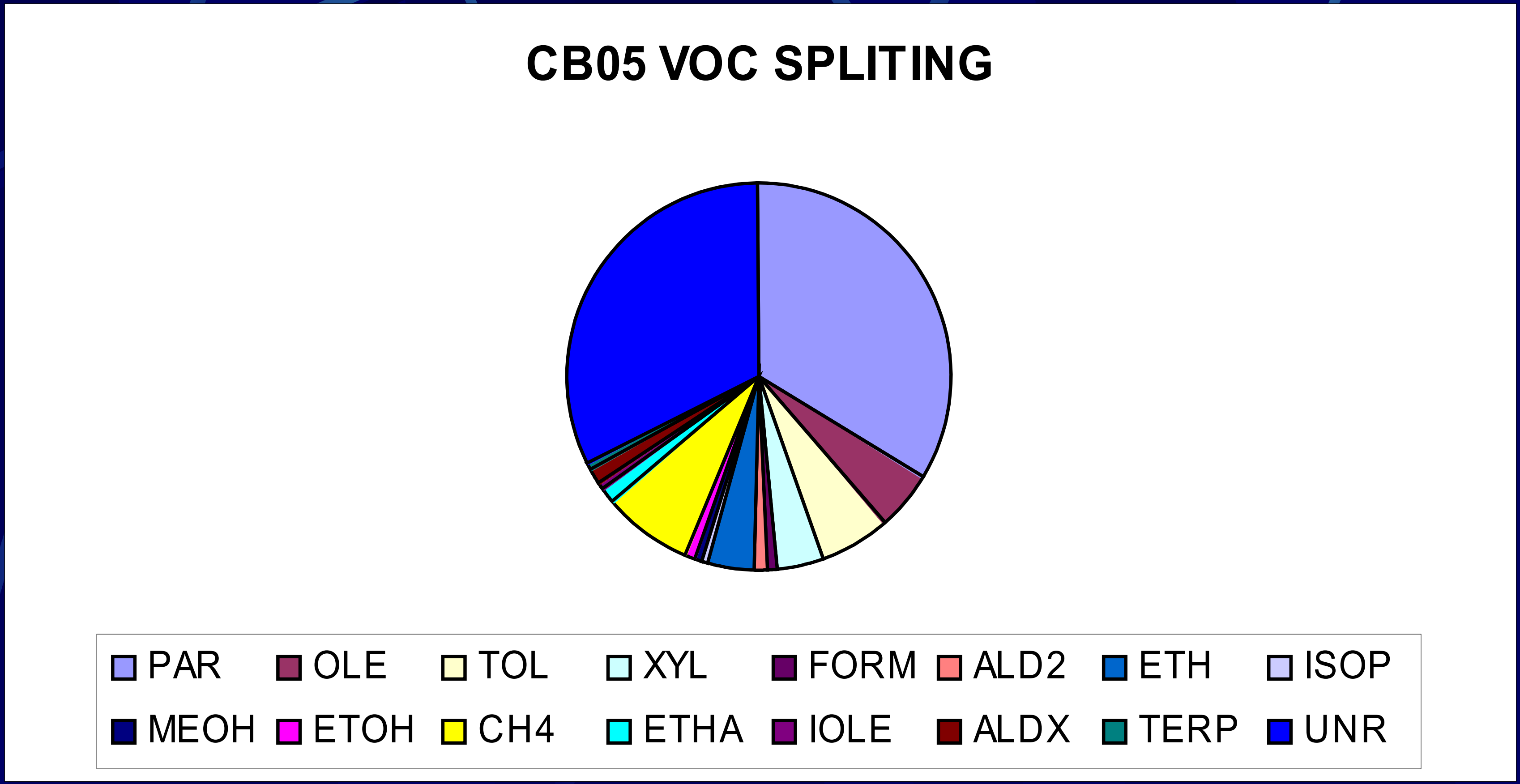
-Geographic coordinates TO Lamber Conformal Conic CMAQ grid:

* EMEP interpolation routine updated by UPM.

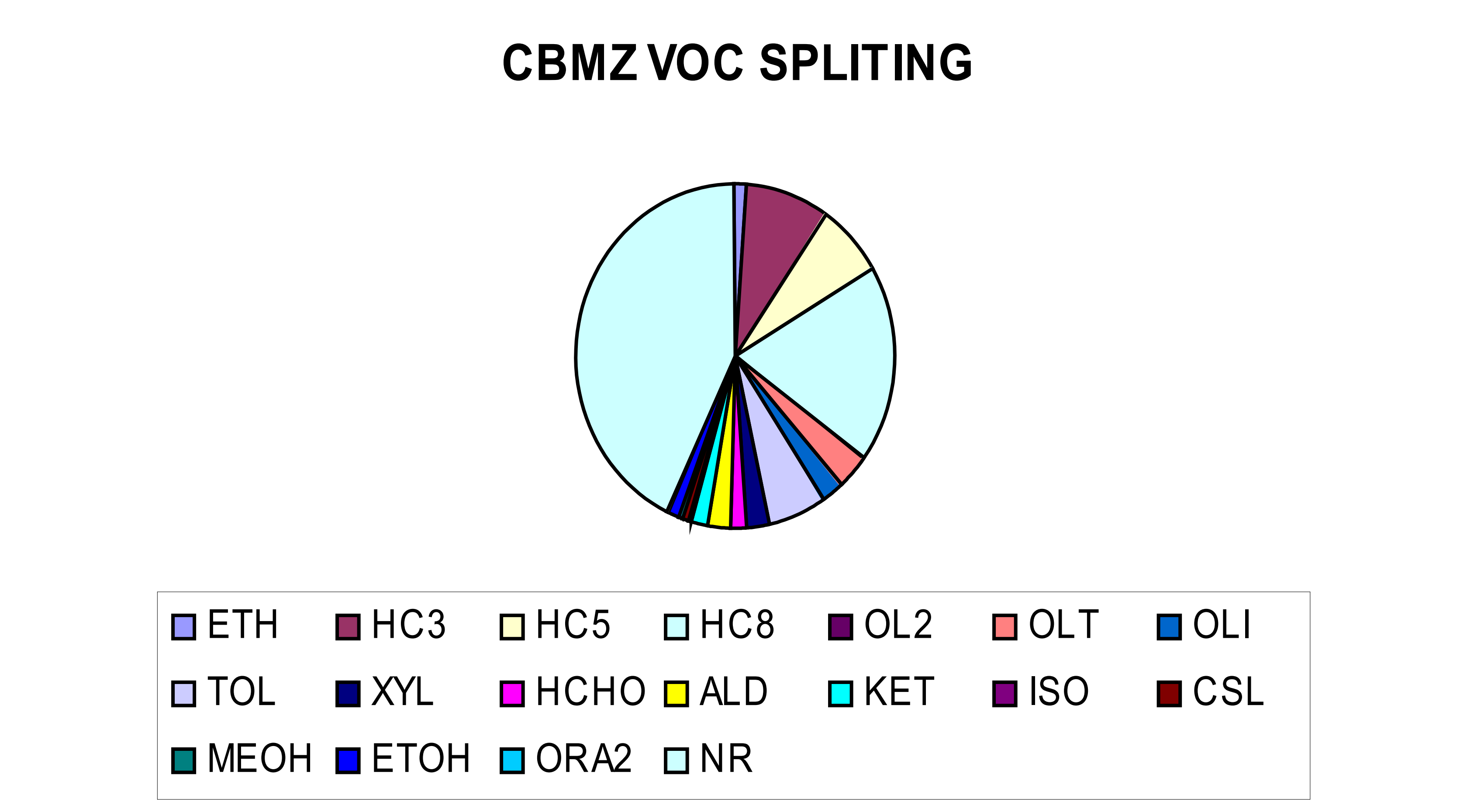
-Time distribution of EURODELTA

- VOC SPLITING:
  * SPECIATE Version 4.0 (January 18, 2007):
    . 1594 compounds
    . VOC-to-TOG Conversion Factors
  * Lumping VOC :
    . EMITDB – Carter (*Development of an Improved Chemical Speciation Database for Processing Emissions of Volatile Organic Compounds for Air Quality Models*)

VOC SPLITING

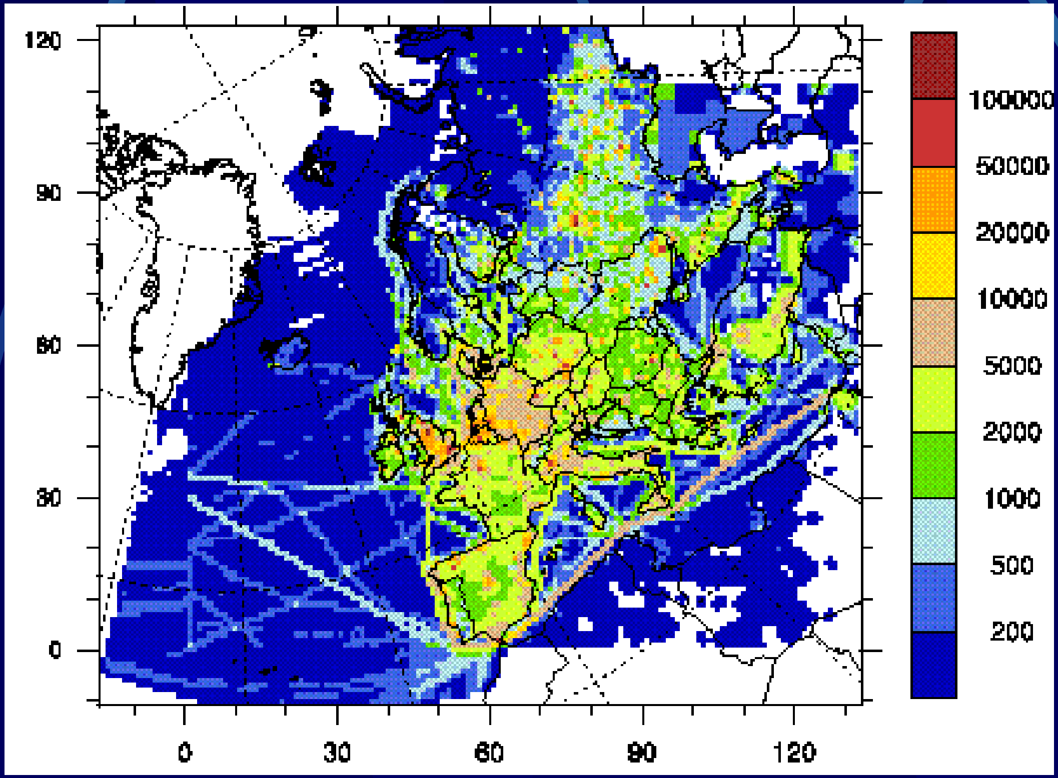


VOC SPLITING



EMISSION DATA YEARLY PROFILE

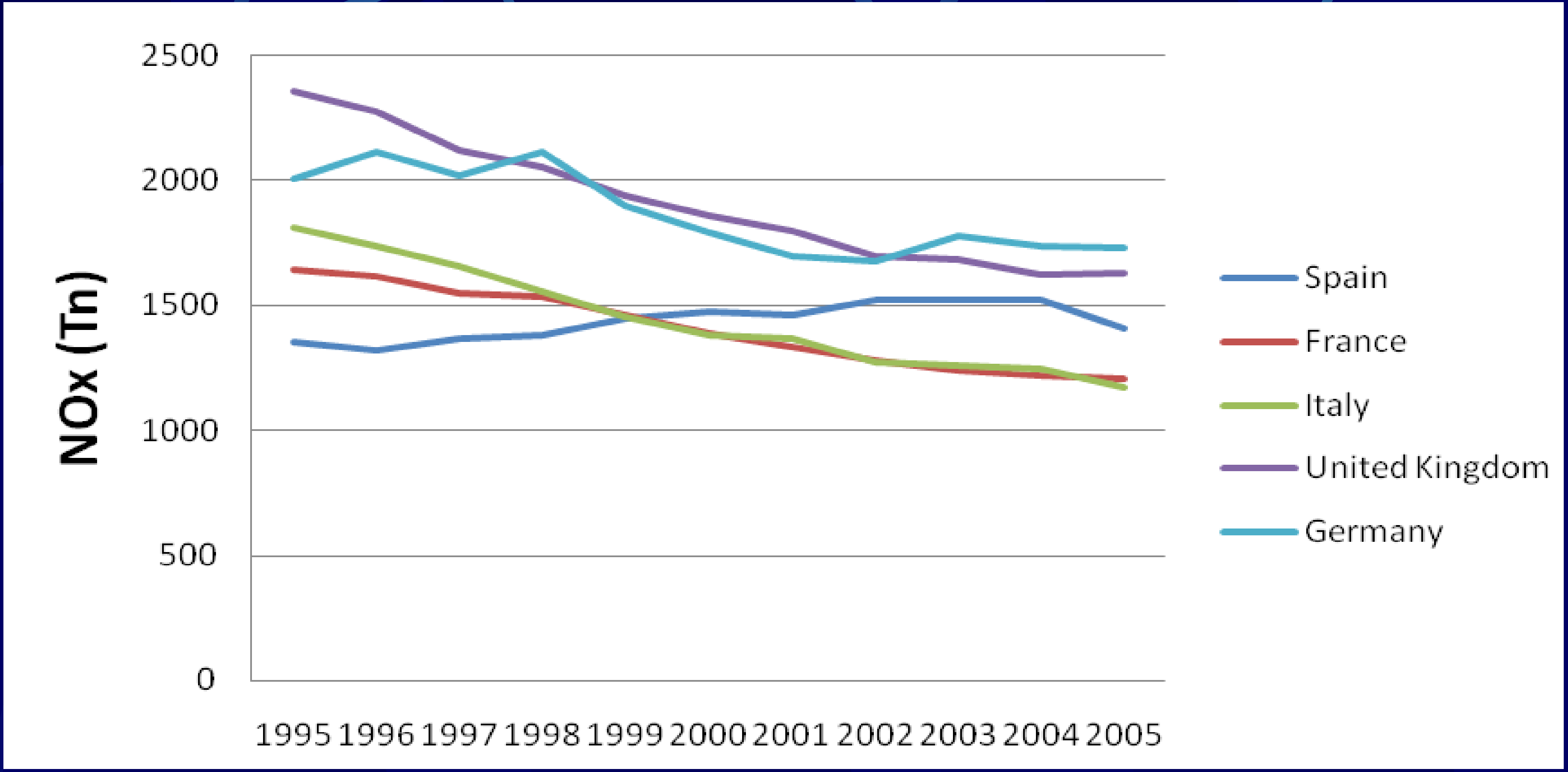
- DATA BY YEAR (1995-2005), SNAP ACTIVITY, COUNTRY AND POLLUTANT
- REFERENCE YEAR 2003
- BASED ON : EMEP ACTIVITY DATA AND EMISSION DATABASE

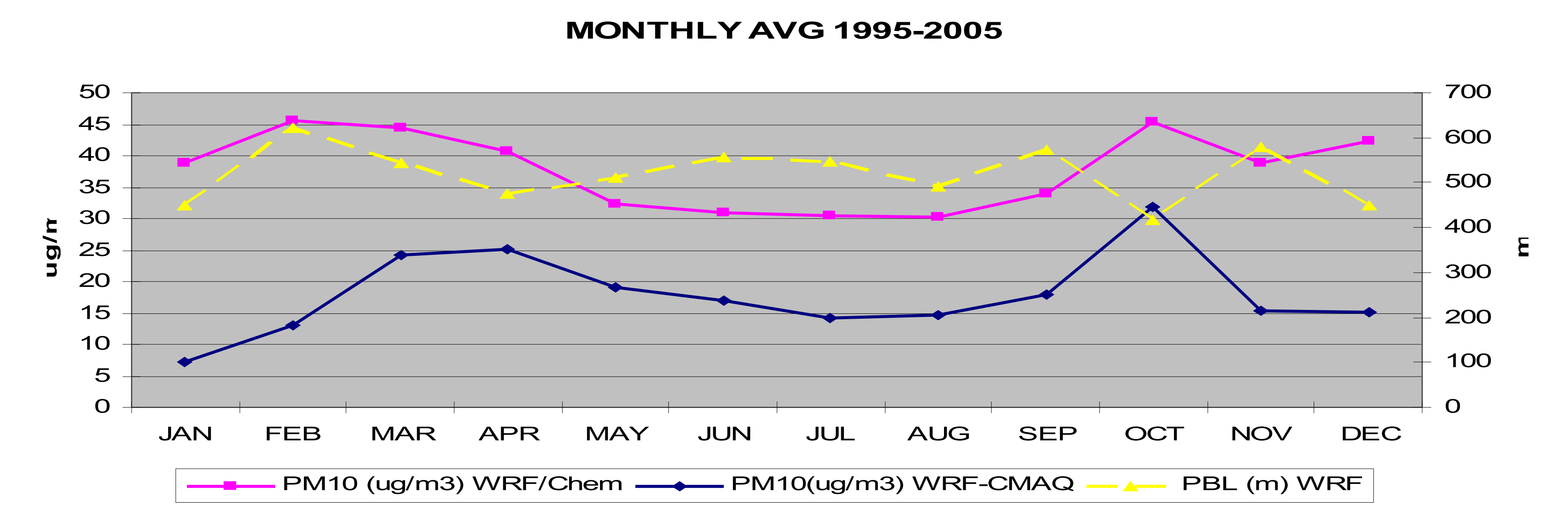


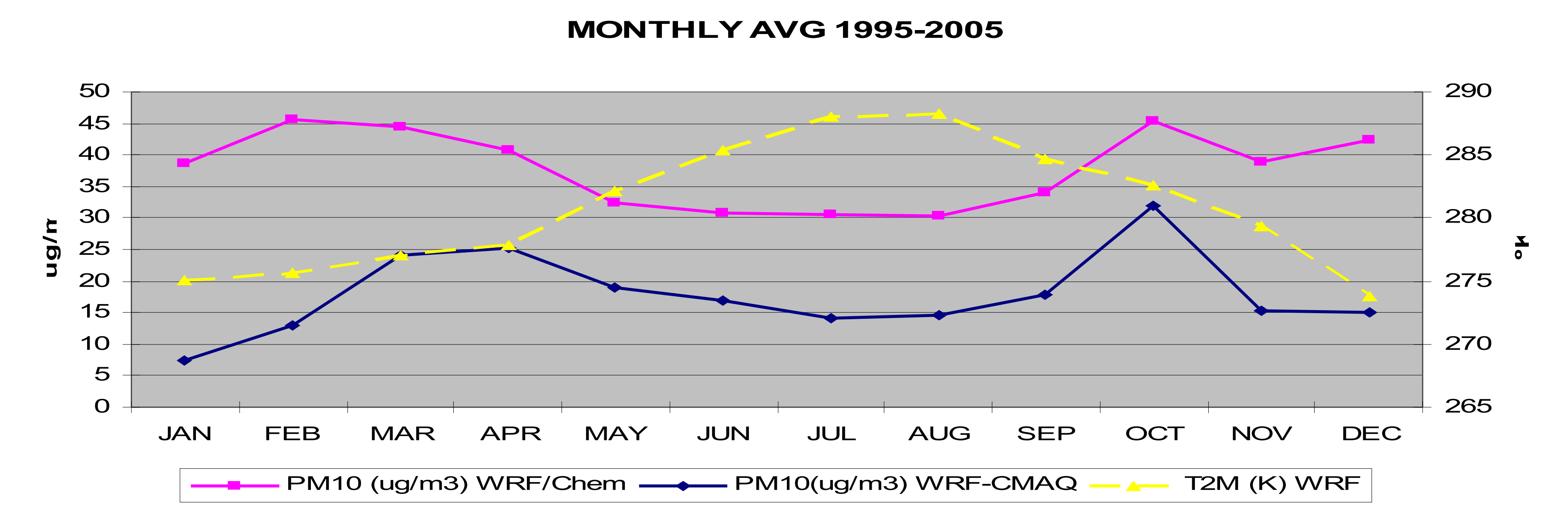
NOx (Tn)
EMISSION
2003

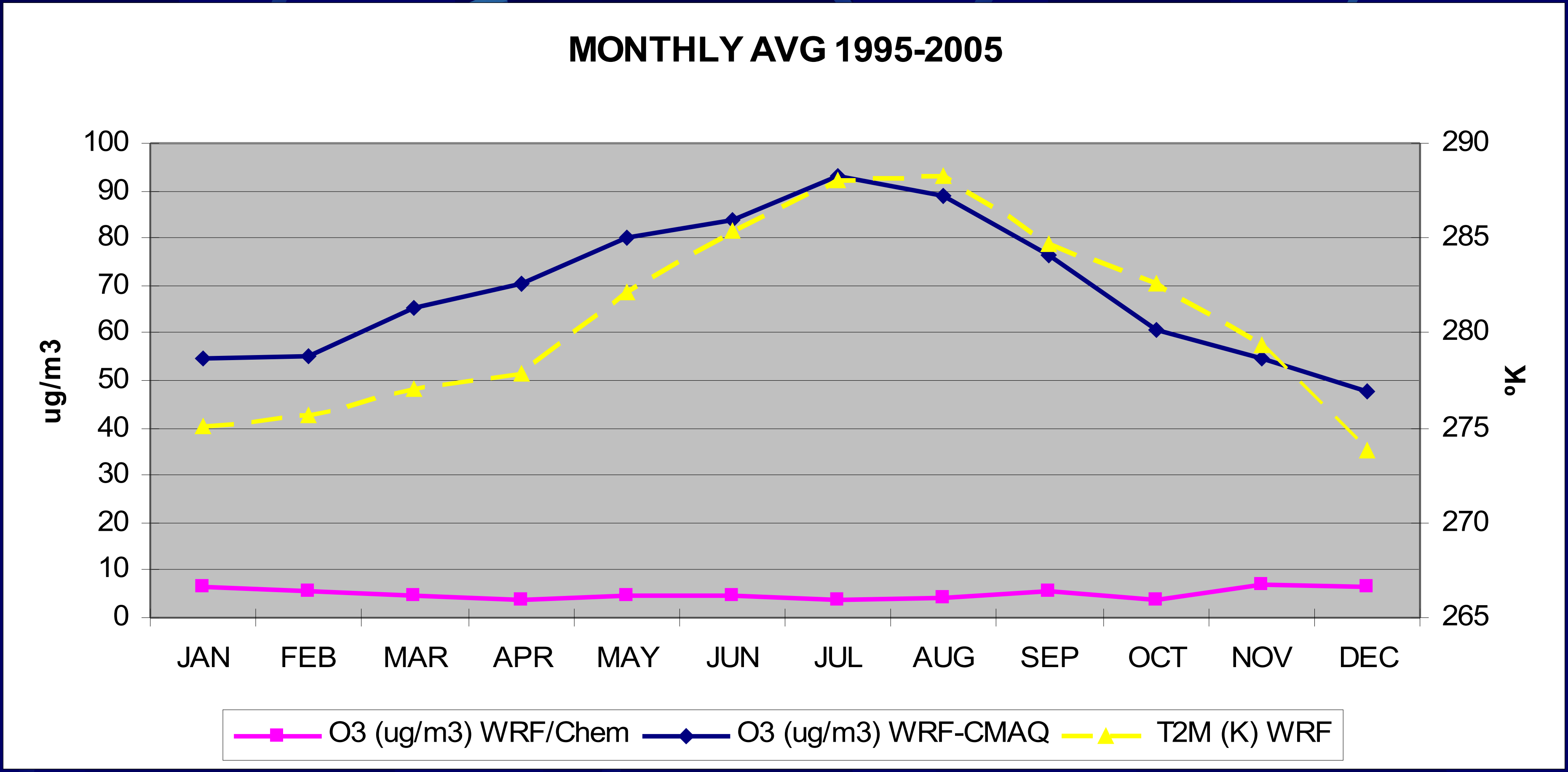
EMISSION DATA YEARLY EVOLUTION

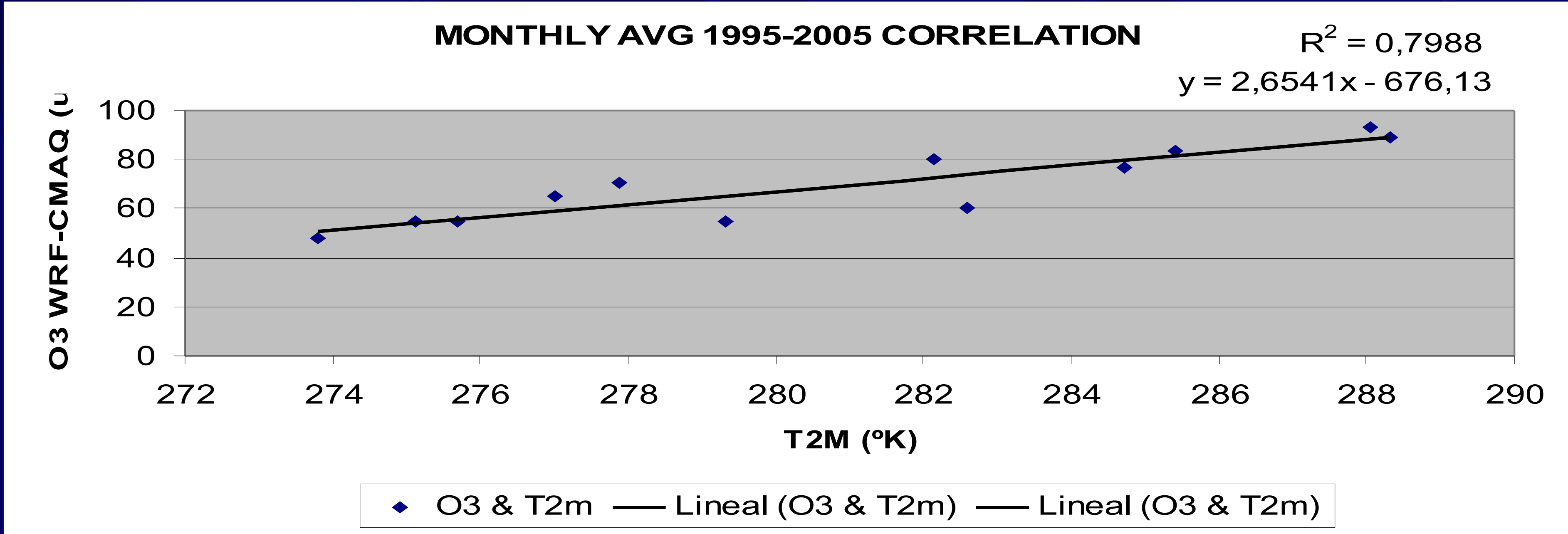
NOx (Tn) EMISSION 1995-2005

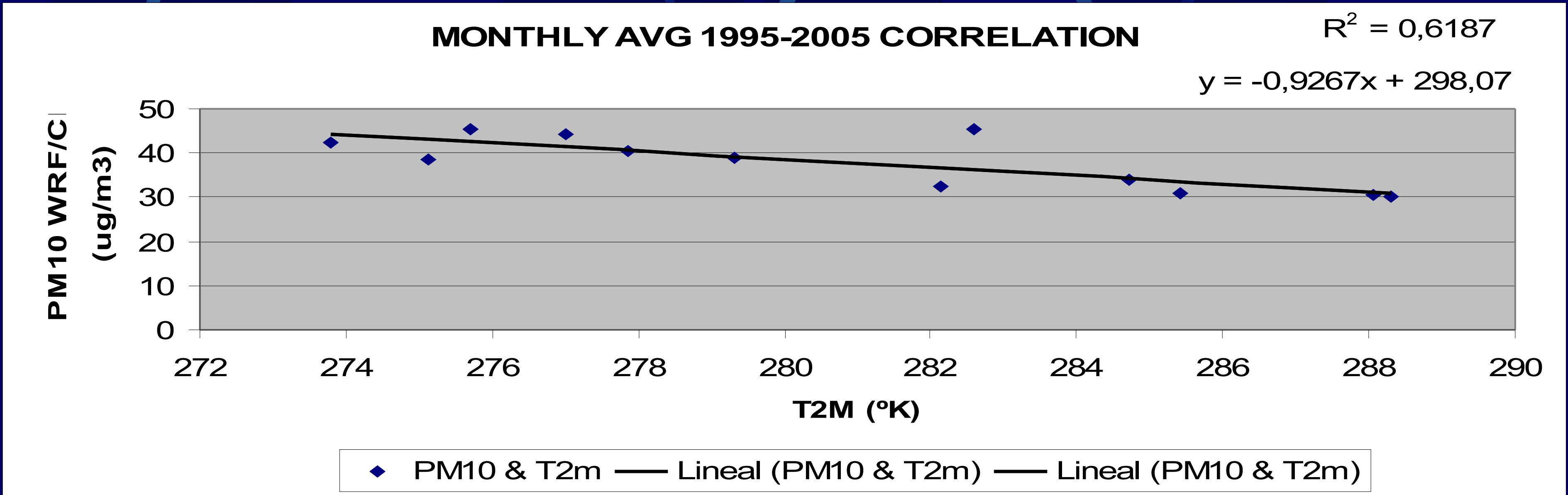


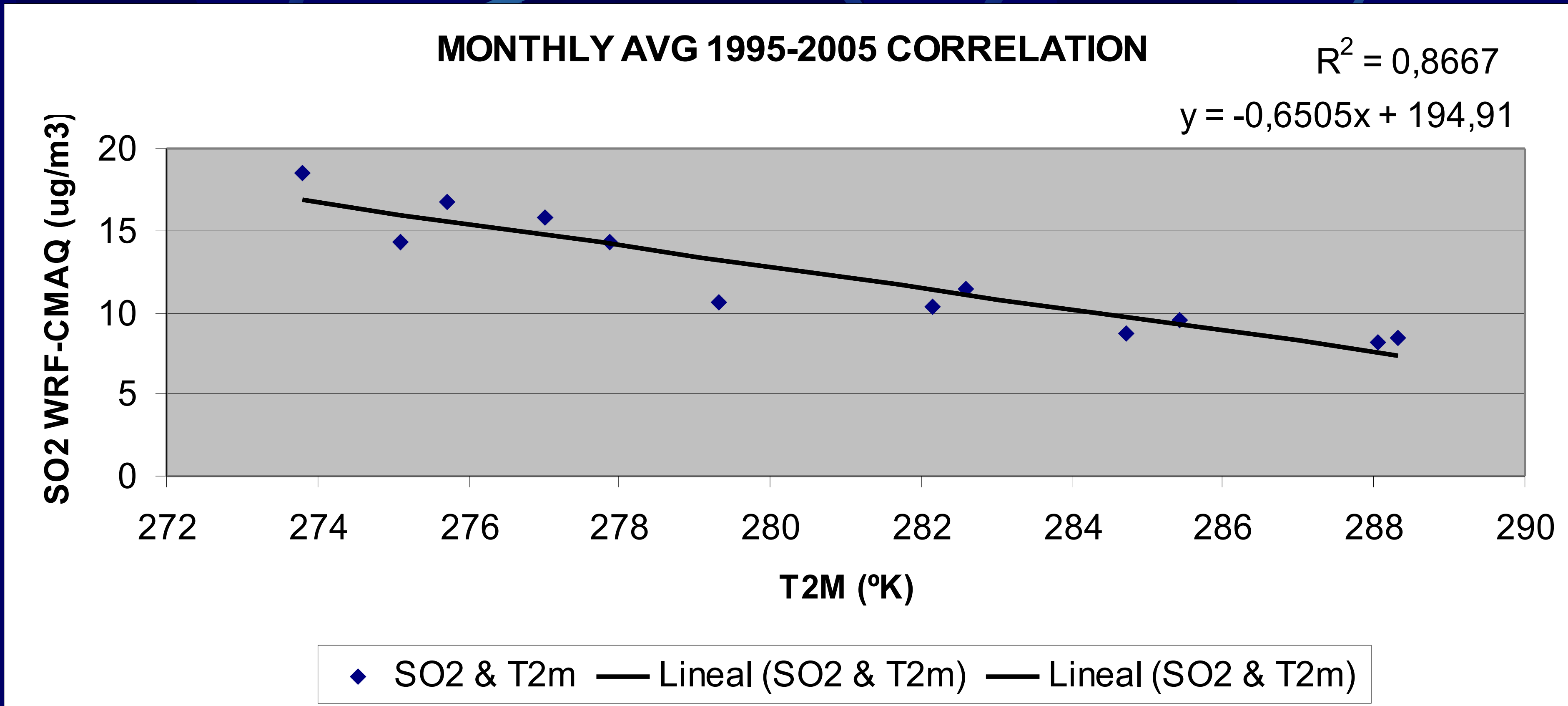

MONTHLY AVG 1995-2005
ug/m
m
50
45
40
35
30
25
20
15
10
5
0
700
600
500
400
300
200
100
0
JAN FEB MAR APR MAY JUN JUL AUG SEP OCT NOV DEC
PM10 (ug/m3) WRF/Chem
PM10(ug/m3) WRF-CMAQ
PBL (m) WRF


MONTHLY AVG 1995-2005
ug/m
ºK
50
45
40
35
30
25
20
15
10
5
0
290
285
280
275
270
265
JAN FEB MAR APR MAY JUN JUL AUG SEP OCT NOV DEC
PM10 (ug/m3) WRF/Chem
PM10(ug/m3) WRF-CMAQ
T2M (K) WRF


MONTHLY AVG 1995-2005
ug/m3
ºK
100
90
80
70
60
50
40
30
20
10
0
290
285
280
275
270
265
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC
O3 (ug/m3) WRF/Chem
O3 (ug/m3) WRF-CMAQ
T2M (K) WRF


MONTHLY AVG 1995-2005 CORRELATION
$R^2 = 0,7988$
y = 2,6541x - 676,13
O3 WRF-CMAQ (u
100
80
60
40
20
0
272
274
276
278
280
282
284
286
288
290
T2M (ºK)
O3 & T2m
Lineal (O3 & T2m)
Lineal (O3 & T2m)


MONTHLY AVG 1995-2005 CORRELATION
$R^2 = 0,6187$
y = -0,9267x + 298,07
PM10 WRF/C
(ug/m3)
50
40
30
20
10
0
272
274
276
278
280
282
284
286
288
290
T2M (ºK)
PM10 & T2m
Lineal (PM10 & T2m)
Lineal (PM10 & T2m)


MONTHLY AVG 1995-2005 CORRELATION
R2 = 0,8667
y = -0,6505x + 194,91
SO2 WRF-CMAQ (ug/m3)
20
15
10
5
0
272
274
276
278
280
282
284
286
288
290
T2M (ºK)
SO2 & T2m
Lineal (SO2 & T2m)
Lineal (SO2 & T2m)

CONCLUSIONS

1. The results show a good agreeement between observed and modelled meteorological variables – with CCSM3 global climate model.
3. The architecture configuration seems to play a good role and the BC’s and IC’s provided to WRF/CHEM and WRF-CMAQ are considered to be good.
5. The 10 year monthly averaged values are compared for PM10 modelled concentrations from WRF/CHEM and WRF-CMAQ with Planetary Boundary Layer Height (PBL) and 2 m temperature.
8. PBL and PM10 values compare in anti-cyclic phase for monthly values, 2m temperature and PM10 values compare also in anti-cyclic phase for yearly values and finally O3 values obtained with WRF/CHEM compare poorly with those obtained with WRF-CMAQ (phase chemistry is not activated).
12. The WRF-CMAQ O3 values compare good with observations (R2=0.57) but the WRF/CHEM compare poorly with the observations (R2=0.05) (phase chemistry is not activated).
15. 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 is very poor.
18. 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.

ACKNOWLEDGEMENTS

1. We would like to thank Dr. Georg Grell and Dr. Steven Peckham for the WRF/CHEM model and support.

2. We would like to thank US EPA for CMAQ model

3. Thanks to PSU/NCAR for MM5 model

4. Thanks to NCAR for the CCSM3 code