Earth Sciences Department
Barcelona Supercomputing Center

DAURE 3rd scientific meeting

BSC-CNS Modeling results

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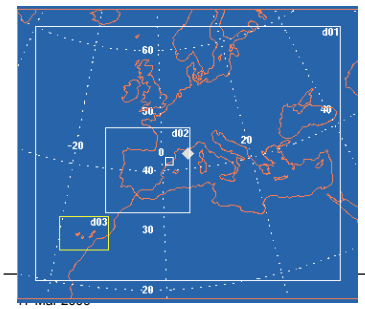
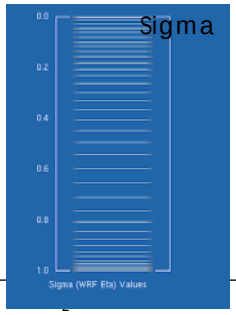
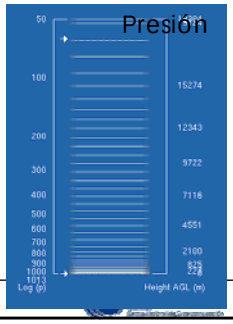
MODELING SYSTEM
WRF-ARW/HERMES/CMAQ/DREAM

- Domains:
  - D1 Europe: 480x400 at 12 km
  - D2 Iberian Peninsula: 399x399 at 4 km
- Vertical configuration
  - Meteorology: 38 sigma layers, top of the atmosphere at 50 hPa
  - Chemistry: 8 vertical layers
- Initial and boundary conditions: GFS 0.5ºx0.5º
- Emissions:
  - Europa: EMEP disaggregated
  - Iberian Península and Barcelona area: HERMES (España) + EMEP disaggregated (Portugal+Francia)







Working domain

Parámetros de definición de los dominios de trabajo

Dominio	Nº
D1	
D2	
Latitud central externo	
Longitud central externo	

Altura de los 38

Nº capa	N
38	
37	
36	
35	
34	
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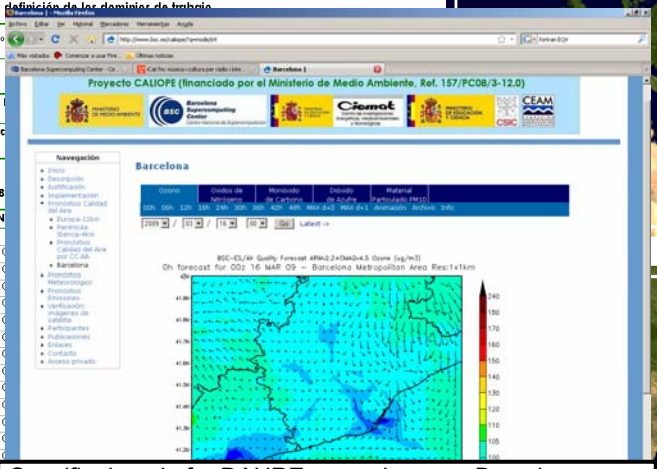
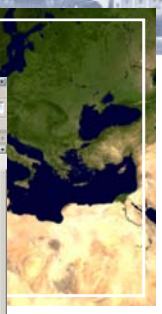




Specific domain for DAURE campaign over Barcelona geographical area at 1 km2 horizontal resolution

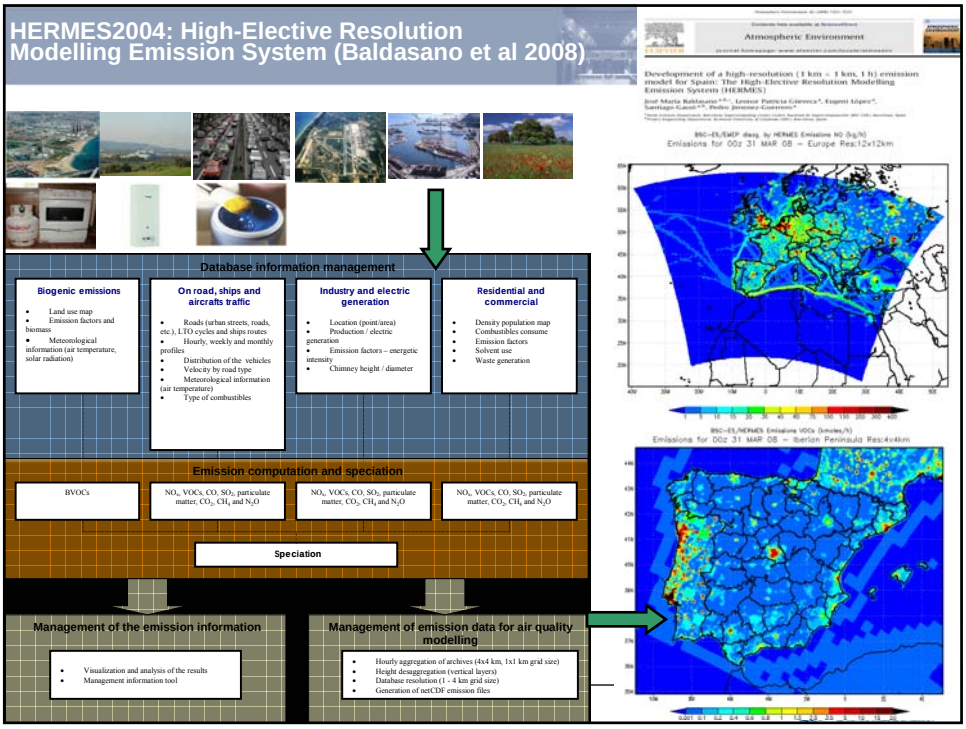
HERMES bottom-up emissions

http://www.bsc.es/caliope

Model configuration

Sistema CALIOPE - Península Ibérica		
Código simulación		Cv1PI-fcst
Fecha ejecución de la simulación		Desde 2007-06
Periodo simulación		Sistema operacional
Meteorología	**Modelo, versión**	WRF-ARW v2.2.1
	Nx,Ny,Nz,Res.Hor.	400,400,38,4km
	Parametrizaciones físicas: MP, CU, PBL, SF, LSM, SW, LW	WSM3, explicito, YSU, Monin-ObukovMM5, NoahLSM, Dudhia, RRTM
	IC-BC	NCEP/GFS 0.5ºx0.5º
	Varios	No 3-4DVAR
Emisiones	**Modelo, versión**	HERMES-2004
	Base datos (año)	HERMES + EMEP (2004)
	Varios	---
Química	**Modelo, versión**	CMAQ v4.5
	Nx,Ny,Nz,Res.Hor.	397,397,8,4km
	BC (layers)	Nested Cv1EU-fcst (8)
	Mecanismo químico	cb4-ae3-aq
	Mecanismo para partículas	AERO3
	Euler backward iterative solver	ebi-cb4
	Horiz./vert. advection scheme	Yamartino mass-conserving
	Vertical diffusion module	Eddy diffusivity theory
	Aerosol deposition velocity	aero-depv2 (2nd generation)
	Cloud module (convective mix.)	cloud-acm
	Dry deposition routine	Models-3 (Pleim)
	Varios	
Transporte polvo mineral	**Modelo, versión**	DREAM-8bin
	Varios	

HERMES2004: High-Elective Resolution Modelling Emission System (Baldasano et al 2008)



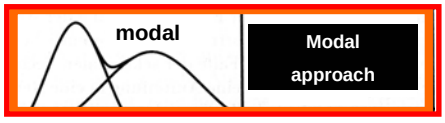
Model configuration

	Chemistry
CTM	CMAQ
Chemical mechanism	CBM-IV
Aerosol size distribution	Modal approach (3 modes)
Inorg. Aero. thermodinamic	ISORROPIA
SOA treatment	Empirical representation of SOA formation
	Natural dust transport
Dust condition	DREAM for Saharan dust outbreaks

	Meteorology
Meteorological driver	WRF
Dynamics	ARW
Microphysics	WSM-3 class
Radiation	RRTM, Dudhia scheme
PBL	YSU
Initialization and boundary conditions	NCEP/GFS analysis

Barcelona Domain	**1 km²**
Initialization	Nesting from Europe 4 km²
Vertical resolution	8
NX/NY(CMAQ)	147/147
Emission model	HERMES bottom-up
Boundary condition	Nesting from Spain 4 km²

Aerosol treatment:



Model treatment of PM

Especies químicas en fase aerosol consideradas en CMAQ (Binkowski and Roselle, 2003)

	Abbreviation	Description
{a1}	ASO4J	Accumulation mode sulfate mass
{a2}	ASO4I	Aitken mode sulfate mass
{a3}	ANH4J	Accumulation mode ammonium mass
{a4}	ANH4I	Aitken mode ammonium mass
{a5}	ANO3J	Accumulation mode nitrate mass
{a6}	ANO3I	Aitken mode aerosol nitrate mass
{a7}	AORGAJ	Accumulation mode anthropogenic secondary organic mass
{a8}	AORGAI	A
{a9}	AORGPAJ	A
{a10}	AORGPAI	A
{a11}	AORGBJ	A
{a12}	AORGBI	A
{a13}	AECJ	A
{a14}	AECI	A
{a15}	A25J	A anthropogenic mass
{a16}	A25I	Aitken mode unspecified anthropogenic mass
{a17}	ACORS	Coarse mode unspecified anthropogenic mass
{a18}	ASEAS	Coarse mode marine mass
{a19}	ASOIL	Coarse mode soil-derived mass
{a20}	NUMATKN	Aitken mode number
{a21}	NUMACC	Accumulation mode number
{a22}	NUMCOR	Coarse mode number
{a23}	SRFATKN	Aitken mode surface area
{a24}	SRFACC	Accumulation mode surface area
{a25}	AH2OJ	Accumulation mode water mass
{a26}	AH2OI	Aitken mode water mass

[a]Concentration units: mass [$\mu g\ m^{-3}$], number [m^{-3}].

NOT IMPLEMENTED IN CURRENT SIMULATIONS:
- → SSA
- → Mineral dust from European continent
- → Paved road emissions
- → Agriculture and livestock emissions

En CMAQ la fracción $PM_{2.5}$ está compuesta por las siguientes especies:

SO_4^{-2}: ASO4J + ASO4I
NO_3^-: ANO3J + ANO3I
AORGBJ+ AORGBI

ogénico a
n como:
A25J

lerada en CALIOPE tiene en cuenta aerosol *antropogénico* y *natural*, y se calcula a partir de los outputs de CMAQ + DREAM, respectivamente:

PM2.5: $SO_4^{2-} + NO_3^- + NH_4^+ + (EC+OC) + A25I + A25J + tmp1$
PM10: PM2.5+ACORS + tmp2

Provided Model Data

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#########################################################################
Abbreviation    Description
O3      Ozone
NO      Nitrogen monoxide
NO2     Nitrogen dioxide
SO2     Sulfur dioxide
CO      Carbon monoxide
TOL     Toluene
ISOP    Isoprene
TERP    Terpene
ALD2    High molecular weight aldehydes (RCHO, with R > H)
CRES    Cresol and higher molecular weight phenols
OLE     Olefinic carbon bond (alkene)
AS04I   Accumulation mode sulpfate mass
AS04J   Aitken mode sulfate mass
ANH4I   Accumulation mode ammonium mass
ANH4J   Aitken mode ammonium mass
ANO3I   Accumulation mode nitrate mass
ANO3J   Aitken mode nitrate mass
AORGAI  Accumulation mode anthropogenic secondary organic mass
AORGAJ  Aitken mode anthropogenic secondary organic mass
AORGPAI Accumulation mode primary organic mass
AORGPAJ Aitken mode primary organic mass
AORGBI  Accumulation mode secondary biogenic organic mass
AORGBJ  Aitken mode secondary biogenic organic mass
AECI    Accumulation mode elemental carbon mass
AECJ    Aitken mode elemental carbon mass
A25I    Accumulation mode unspecified anthropogenic mass
A25J    Aitken mode unspecified anthropogenic mass
ACORS   Coarse mode unspecified anthropogenic mass
NUMCOR  Coarse mode number
NUMATKN Aitken mode number
NUMACC  Coarse mode number
NH3     Ammonia (added after)
HNO3    Nitric acid (added after)
DREAM25 fine mineral dust mass (African continent)
DREAM10 coarse plus fine mineral dust mass (African continent)

#########################################################################
CMAQ model output species must be postprocessed in order to achieve compatibility with the observation species.
Below are some examples of observations and corresponding CMAQ output species:

Observation             CMAQ_output_species
PM2.5_sulfate           PM_sulfate=AS04I+AS04J
PM2.5_nitrate           PM_nitrate=ANO3I+ANO3J
PM2.5_ammonium          PM_ammonium=ANH4I+ANH4J
PM2.5_organic_aerosol   PM_organic_aerosol=AORGAI+AORGAJ+AORGPAI+AORGPAJ+AORGBI+AORGBJ
PM2.5_elemental_carbon  PM_elemental_carbon=AECI+AECJ
PM2.5_total_mass        PM2.5=AS04I+AS04J+ANO3I+ANO3J+NH4I+ANH4J+AORGAI+AORGAJ+AORGPAI+AORGPAJ+AORGBI+AORGBJ+AECI+AECJ+A25I+A25J+DREAM25
PM10_total_mass         PM10=PM2.5+ACORS+DREAM10
Particle number_2.5     NUMATKN + NUMACC

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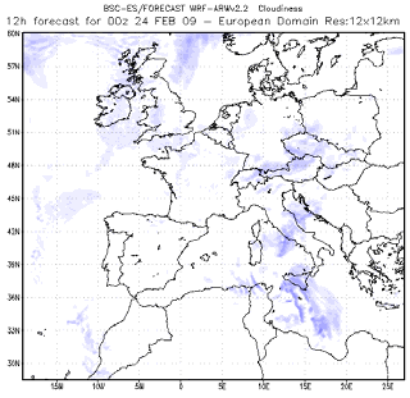
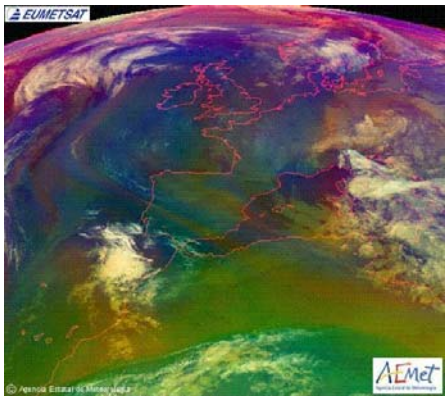
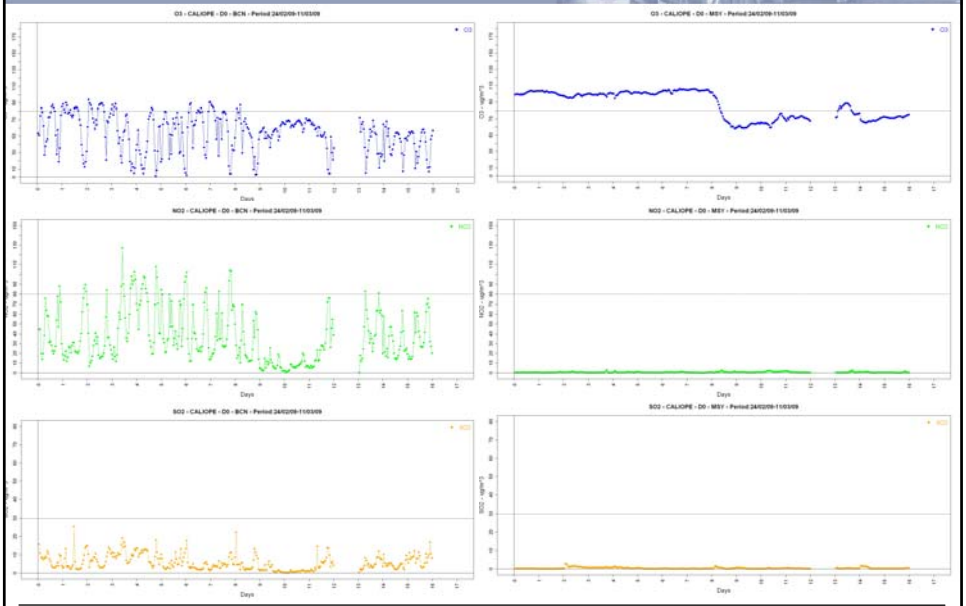
Plus meteorological results:
-2m Temperature
-2m Mixing ratio
-10m wind speed
-10m wind direction
-Surface pressure

Period: 24/02/2009 – 11/03/2009

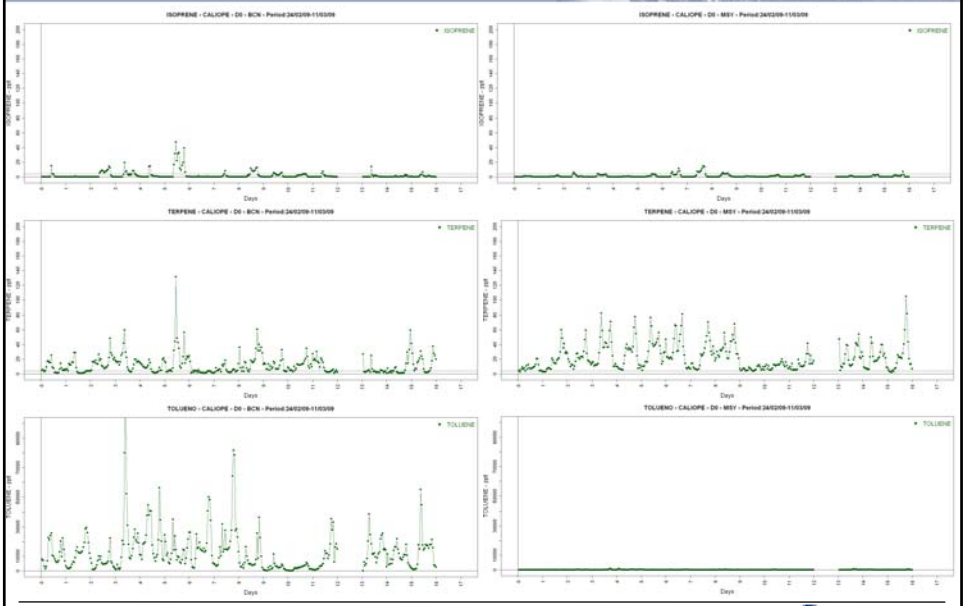




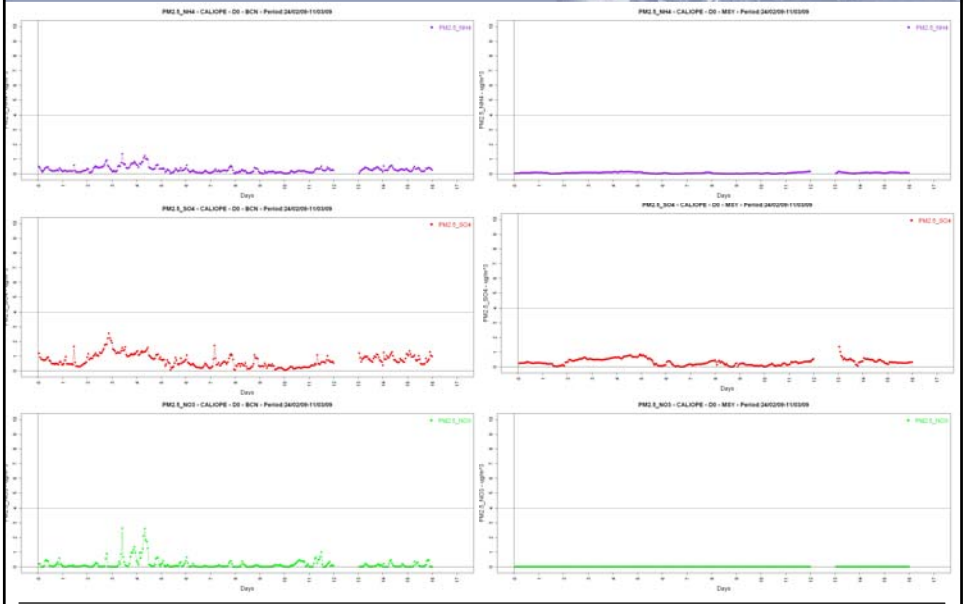
MODEL RESULTS: 24/02/2009 – 11/03/2009
O_3 – NO_2 – SO_2



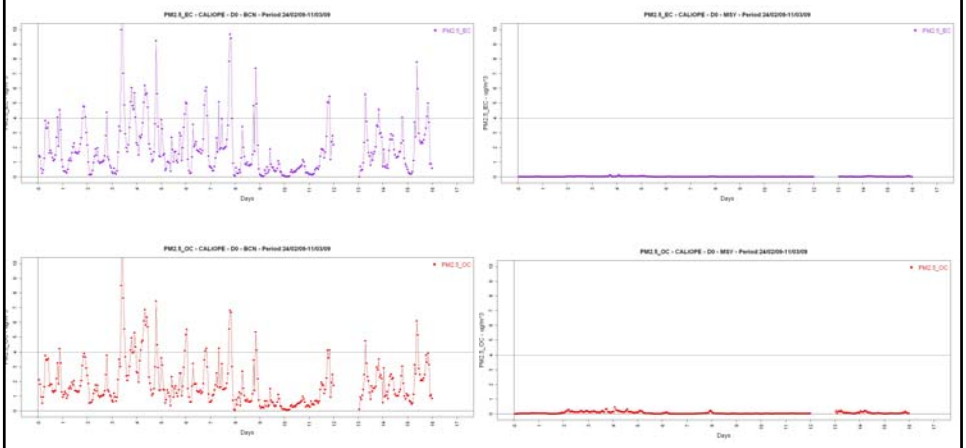
MODEL RESULTS: 24/02/2009 – 11/03/2009
Isoprene – Terpene - Toluene



MODEL RESULTS: 24/02/2009 – 11/03/2009
Ammonium – Sulphate - Nitrate



MODEL RESULTS: 24/02/2009 – 11/03/2009
Elemental carbon (EC) – Organic carbon (OC)



Model Evaluation References

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Thank you