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BAP IMPACT ASSESMENT USING A MODIFIED VERSION OF CMAQ MODEL OVER ZARAGOZA (SPAIN)

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INTRODUCTION

- BaP is a PAH. One of the most toxic pollutants, produced by incomplete combustion. Directive 2004/107/CE of the European Union establishes a limit of 1 ng/m3 of BaP

- OBJECTIVE: Estimate the BaP concentrations in the atmosphere by using last generation of air quality dispersion models with the inclusion of the transport, scavenging and deposition processes for the BaP.

- Two important process have been modeled:
  - Aerosol-gas partitioning phenomenon
  - Degradation of the particulated BaP by the ozone.

- Experiment: Simulations on an area of Zaragoza (Spain) during 12 weeks (11 weeks from 2010 and 1 from 2011) corresponding to the field campaign

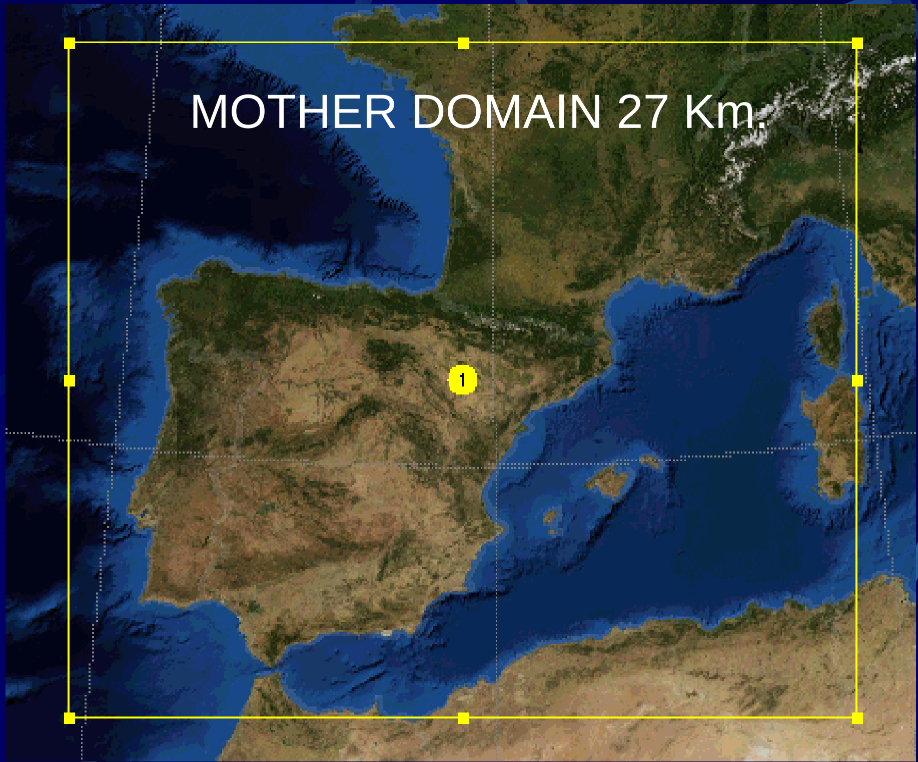
INTRODUCTION

- The new model has been validated using measurements from a PAH field campaign developed by ICB-CSIC (Zaragoza)

- 32 air quality (NO_2, O_3, SO_2, PM_{10},..) stations (26 from Aragon air quality network and 6 from Zaragoza air quality network) – with hourly standard average data -, and 1 DAILY AVERAGED BaP station.

- Model Simulations are performed in groups of 8 days (1 day spin off + 7 days)

DOMAINS

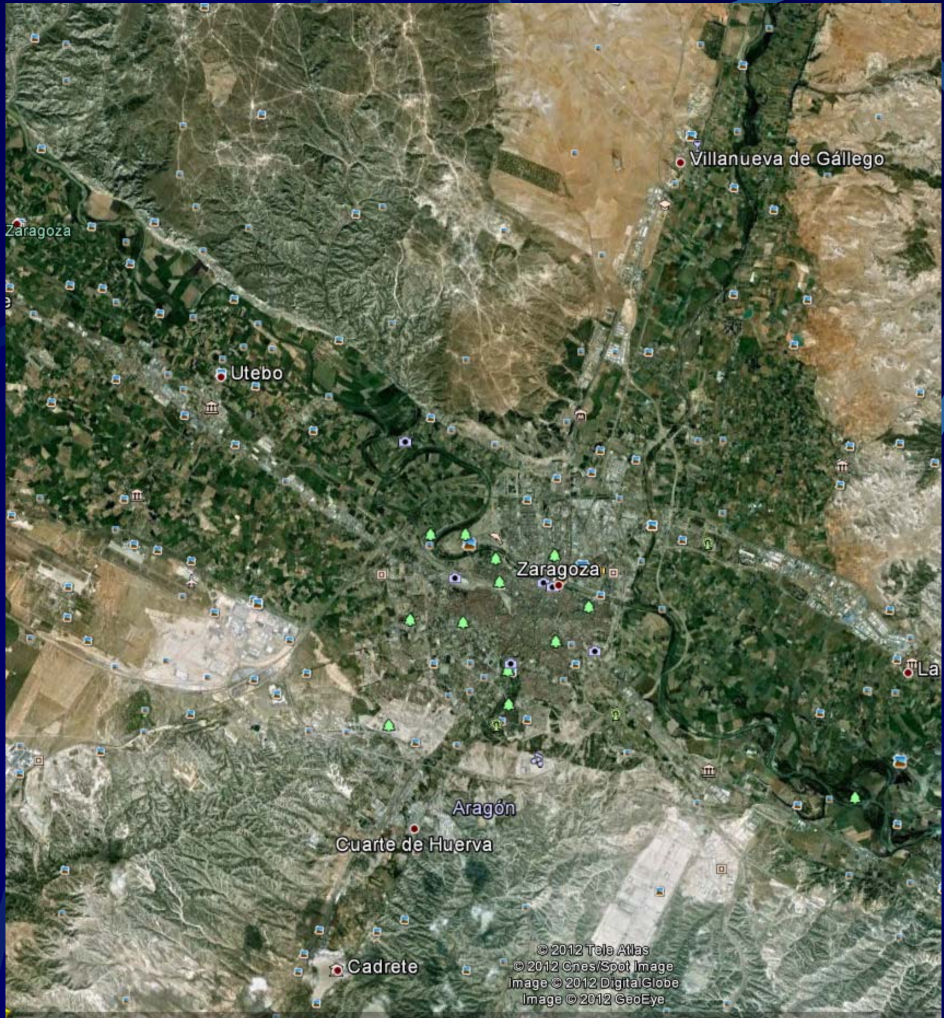


- Central point Lat: 41.69N Lon: 0.89W. Lambert Conformal Conic Projection

- Vertical resolution: 23 levels up to 100 mb.

- Mother domain: 27 Km spatial resolution and 67 * 55 grid cells

DOMAINS



1 km nesting level domain

3 NESTING LEVEL DOMAINS

Nesting domains:

- 9 Km spatial resolution 49*49 grid cells
- 3 Km spatial resolution 31*37 grid cells
- 1 Km spatial resolution 28*28 grid cells

- Meteorological global model data: GFS

- Two way meteorological nesting approach

MODELS

• **WRF meteorological model:** 3-D non-hydrostatic prognostic model that simulates mesoscale atmospheric circulations. WRF was developed at the National Center for Atmospheric Research (NCAR) and University Corporation for Atmospheric Research (UCAR). Version 3.3.1 (**September 2011)**

• **CMAQ air quality model:** Chemical transport model CMAQ (Community Multiscale Air Quality Modeling System) (EPA). CMAQ modeling system has been designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. CMAQ doesn´t support BaP modelling. Version 4.7.1 (June 2010)

• MCIP Meteorology-Chemistry Interface Processor Version 3.6 (June 2010)

MODELS

-Physics Options used in WRF:

• Cumulus Parameterization:

*GRELL-DEVENYI ENSEMBLE SCHEME (*Grell, G. A., and D. Devenyi, 2002: A generalized approach to parameterizing convection combining ensemble and data assimilation techniques. Geophys. Res. Lett., 29(14), Article 1693.)

• PBL Scheme and Diffusion:

Yonsei University (*YSU) PBL* (Hong, S.-Y., Dudhia, J., 2003. Testing of a new non-local boundary layer vertical diffusion scheme in numerical weather prediction applications. In: Proceedings of the 16th Conference on Numerical Weather Prediction, Seattle, WA.)

• Explicit Moisture Scheme :

LIN et al.SCHEME microphysics (Lin, Y.L., R. D. Farley, and H. D. Orville, 1983: Bulk parameterization of the snow field in a cloud model. J. Appl. Meteor., 22, 1065-1092)

MODELS

-Physics Options used in WRF-UHI:

•Radiation Schemes:

Rapid Radiative Transfer Model (RRTM) longwave radiation *(E.J. Mlawer, S.J. Taubman, P.D. Brown, M.J. Iacono and S.A. Clough, Radiative transfer for inhomogeneous atmospheres: RRTM, a validated correlated-k model for the longwave, J. Geophys. Res. 102 (D14) (1997), pp. 16663–16682*)

Simple cloud-interactive shortwave radiation scheme Dudhia radiation (Dudhia, Numerical study of convection observed during the winter monsoon experiment using a mesoscale two-dimensional Model, *J. Atmos. Sci.* 46 (1989), pp. 3077–3107)

MODELS

-**CCTM Options in CMAQ**

- Advection scheme: global mass-conserving scheme (Yamartino 1993)Yamartino, R. J., 1993: Nonnegative, conserved scalar transport using grid-cell-centered, spectrally constrained Blackman cubics for applications on a variable-thickness mesh. *Mon. Wea.Rev.* 121, 753-763.

- Vertical Difussion: Asymmetric Convective Model (ACM2) (Pleim and Chang, 1992) Pleim, J.E. and J. Chang, 1992: A non-local closure model for vertical mixing in the convective boundary layer. *Atmos. Envi*., 26A, 965-981.

- CB05 chemical mechanism (Yarwood et al. 2005). G. Yarwood, S. Rao, M. Yocke and G. Whitten, Updates to the Carbon Bond Chemical Mechanism: CB05 Final report to the US EPA, RT-0400675

- Euler Backward Solver (EBI) solver (Hertel et al. 1993) O. Hertel, R. Berkowicz, J. Christensen and Ø Hov, Test of two numerical schemes for use in atmospheric transport-chemistry models, *Atmospheric Environment* 27 (1993), pp. 2591–2611

- CMAQ Aerosol : The 5rd generation modal CMAQ aerosol model.

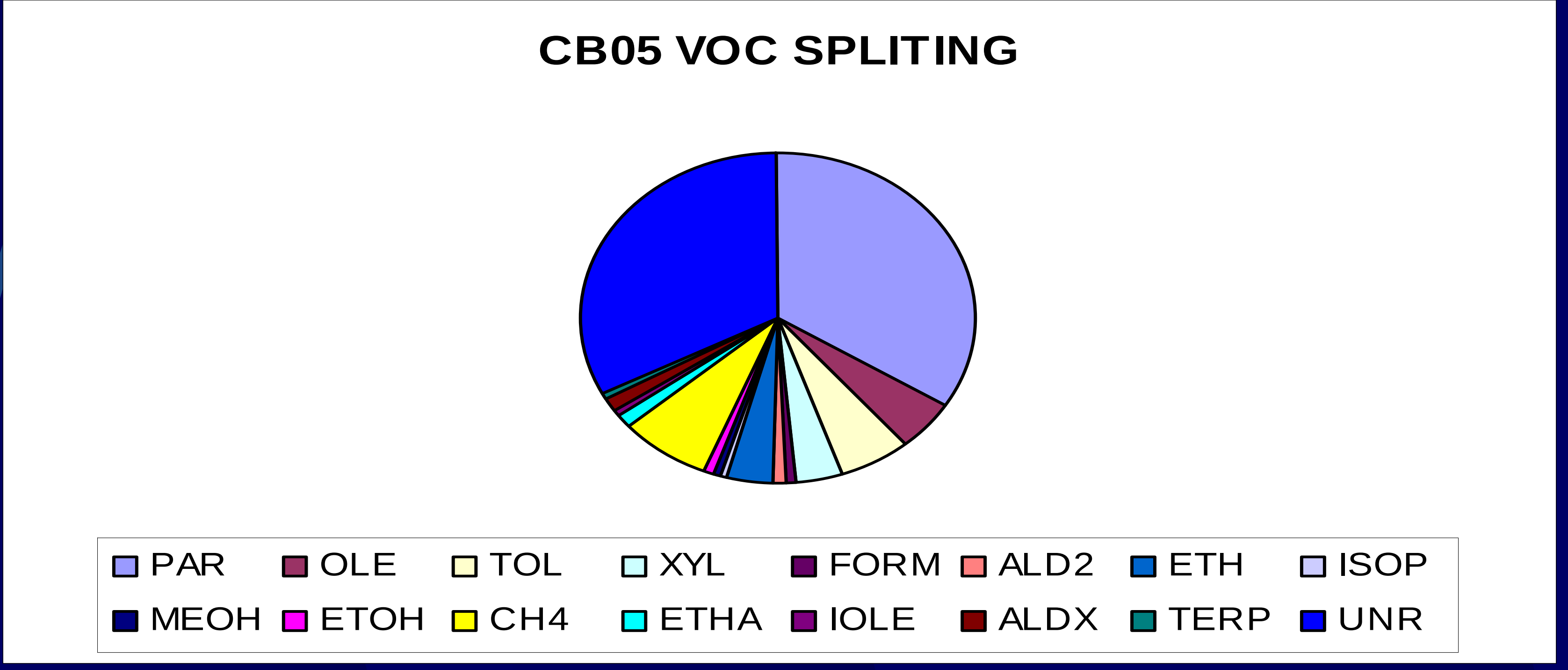
EMISSIONS

- Annual European emission inventory 7Km. Resolution (TNO)
- Main pollutants: SO2,NOx,CO,VOC,NH3,PM10,PM25
- Snap activities (S1-S10)
- BaP emission from EMEP Global inventory (0.5 resolution)
- Projection to Lambert Conformal Conic domain. EMEP/TNO grid TO Lamber Conformal Conic (EMIMO-UPM): EMEP interpolation routine updated by UPM
- European Temporal Profiles (country, activities)
- Biogenic emission (ISOP) : CMAQ (BIOMI-UPM)
- VOC splitting EMIMO to CB05
- Top-Down approach based on surrogates

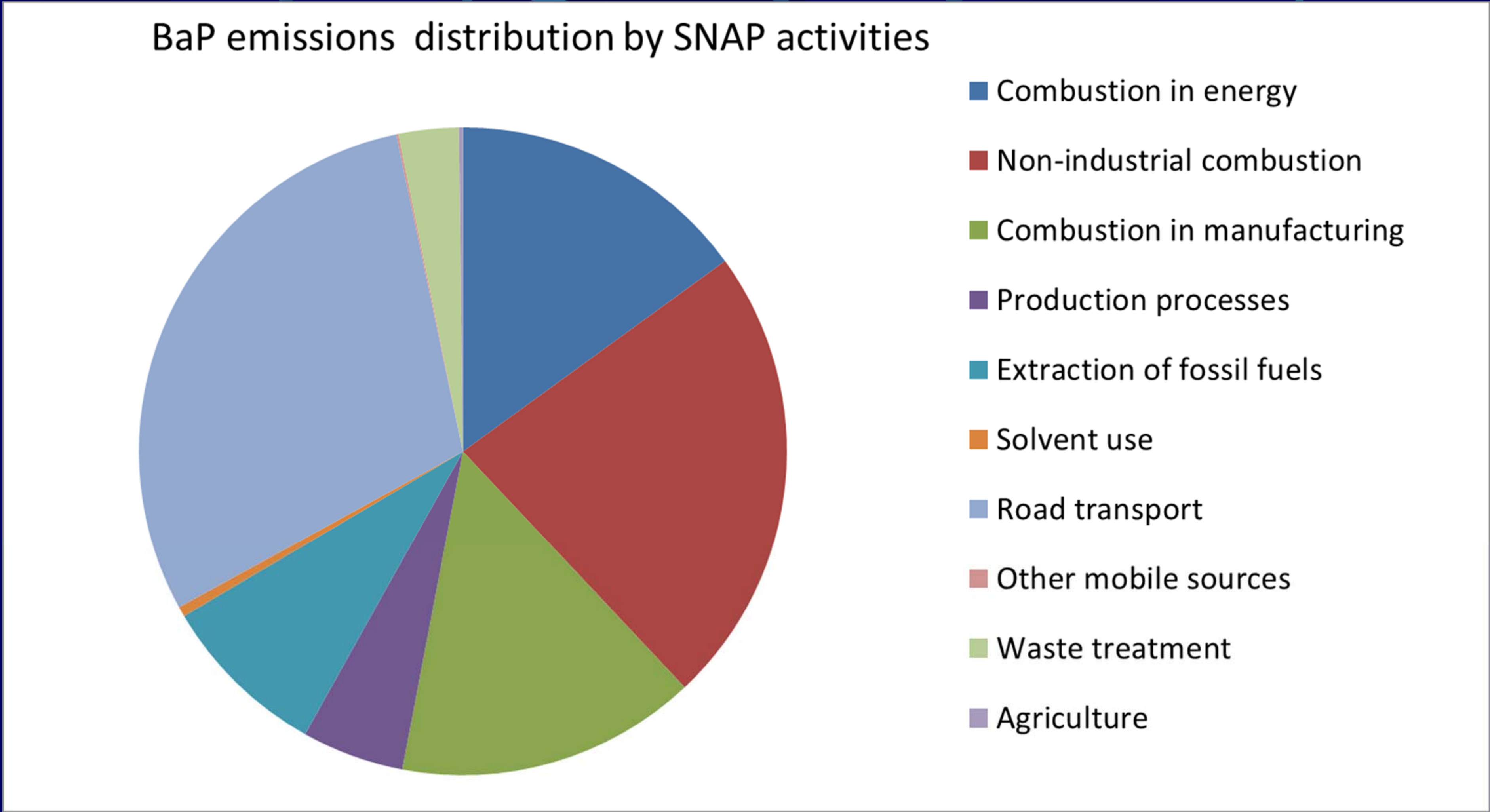
EMISSIONS

* SPECIATE Version 4.0 (January 18, 2007):
  . 1594 compounds
  . VOC-to-TOG Conversion Factors

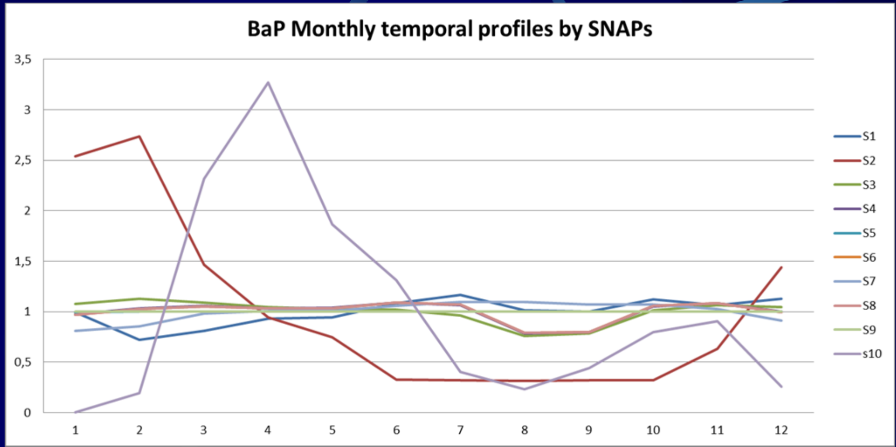
* Lumping VOC : EMITDB – Carter (*Development of an Improved Chemical Speciation Database for Processing Emissions of Volatile Organic Compounds for Air Quality Models*)

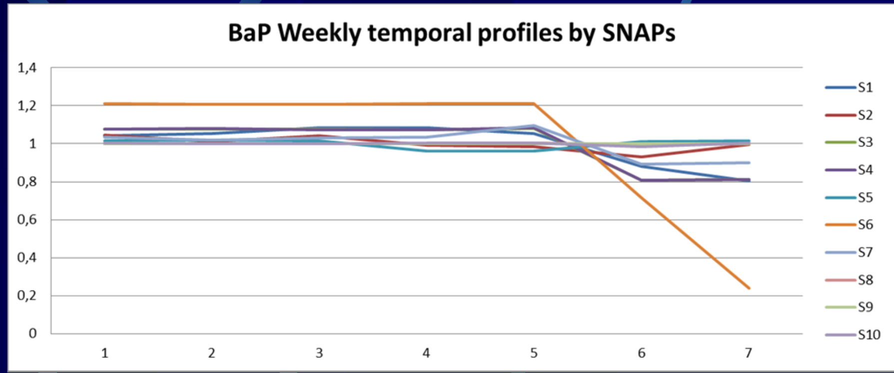


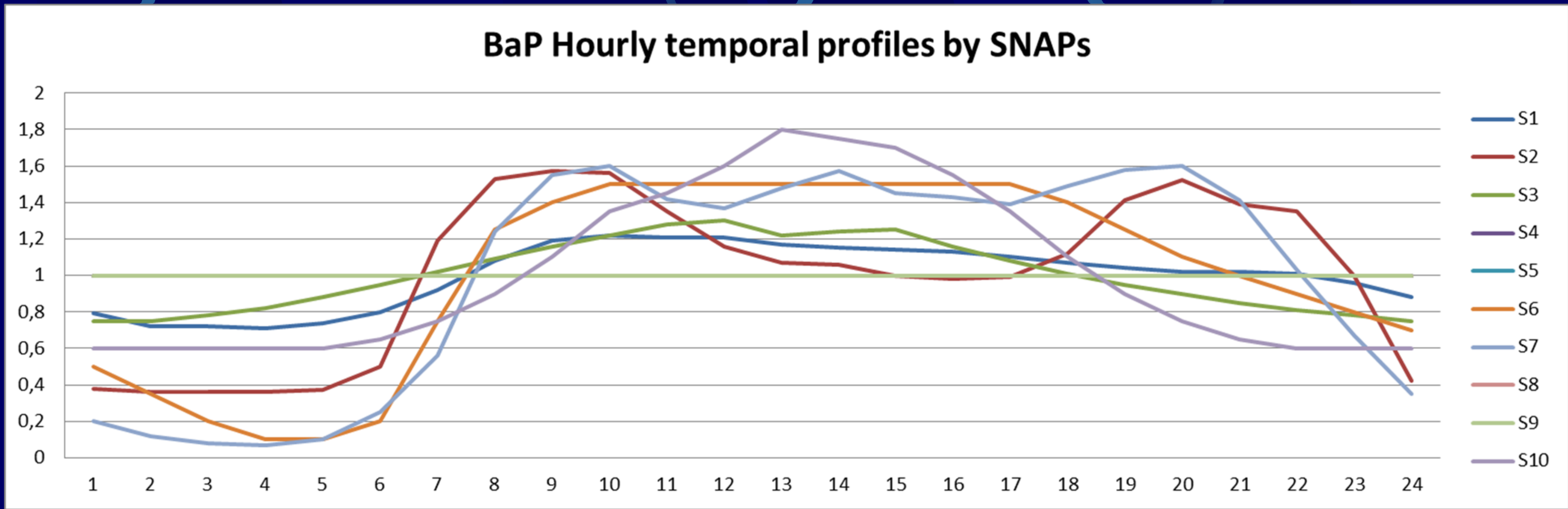
EMISSIONS


BaP emissions distribution by SNAP activities
Combustion in energy
Non-industrial combustion
Combustion in manufacturing
Production processes
Extraction of fossil fuels
Solvent use
Road transport
Other mobile sources
Waste treatment
Agriculture

EMISSIONS- BaP TEMPORAL PROFILES







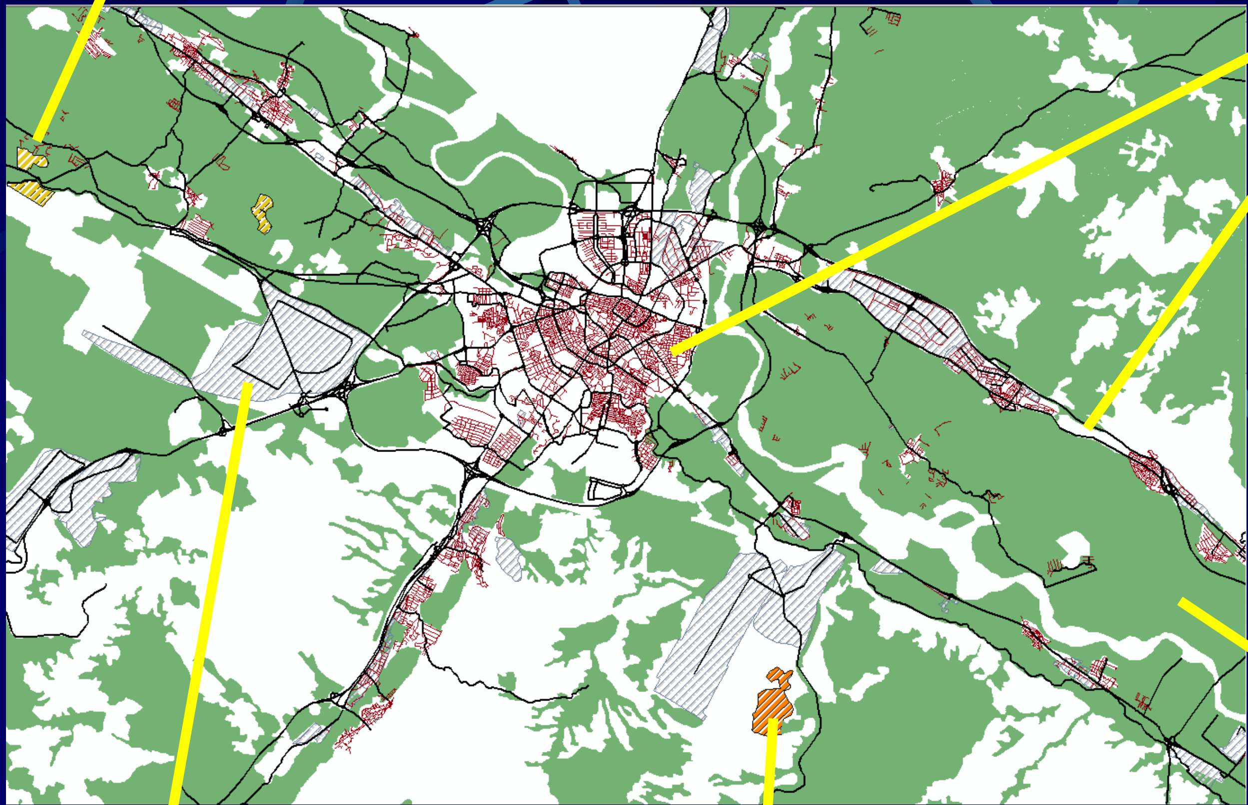
ADDITIONAL INPUT DATA

- High resolution topography.
- Corine Land Cover land uses. 100 m resolution
- Buildings location and hight by floors. Zaragoza/Huesca/Teruel
- Urban areas to the Aragon community
- Industrial area to the Aragon comunity.
- Roads to the Aragon comunity.
- Streets to Zaragoza/Huesca/Teruel cities

SURROGATES

SNAP 5 : Mineral extraction

SNAP 7,8 : Roads & Streets



SNAP 2: Buildings

SNAP 1,3,4,6 : Industrial areas

SNAP 9 : Waste treatment

SNAP 10 Agriculture

BaP CMAQ EXTENSION

- Add two new BaP species, aerosol (ABAP) and gas (SV-BAP) to simulate the transport, scavenging and deposition process. BaP in gas phase is treated as inert gas.

- BaP is emitted in particle phase, 99% accumulation mode (0.1 – 2.5 um) and 1% Aitken mode (< 0.1 um).

- Deposition and scavenging of the aerosol BaP is the same parameterizations as used for CMAQ organic aerosols.

- Deposition velocity of BaP gas is the same than used for the semi-volatil alkanes that is calculated by CMAQ.

BaP EXTENSION

- Absorptive mechanism plays the dominant role in the air affected by urban sources. New code has been added to calculate the partitioning of BaP between gas and particle mode. Based on the absorptive partitioning model of Pankov (1994) and Odum (1996).

- Reaction with ozone can be an important degradation pathway fo the particulate BaP in the atmosphere. Degradation of the aerosol BaP by the Ozone has been implemented into CMAQ based on Kwamena et al. 2004 .

AEROSOL – GAS PARTITIONING

$$C_{aer} = C_{tot} - C^{*}_{sat} \frac{C_{aer}/m}{Tot_{org}}$$

C_{aer} : Concentration in the particle phase

C_{tot} : Total concentration

C^{*}_{sat} : Saturation concentration

m : Molecular weight

Tot_{org} : Total abosorbing organic mass

AEROSOL – GAS PARTITIONING

$$C^*_{sat} = C_{sat} * T_{factor}$$

C_{sat} : BaP effective saturation concentration (5.4e-3 μ/m^3)

T_{factor} : Temperature dependence factor

$$T_{factor} = \frac{T^0}{T} e^{\left(\frac{\Delta H_{vap}}{R} \left(\frac{1}{T^o} - \frac{1}{T} \right) \right)}$$

T^0 : Reference temperature (298 ºK)

T : Air temperature

ΔH_{vap} : BaP Enthalpy of vaporization (116.7e3 J/mol)

R : Gas constant (8.314 J/mol ºK)

AEROSOL – GAS PARTITIONING

$$Tot_{org} = \sum_{j=1}^{n} \frac{C_{aer}}{m} + \frac{C_{init}}{m_{init}}$$

n: Number of compounds in the absorbing organic particle phase

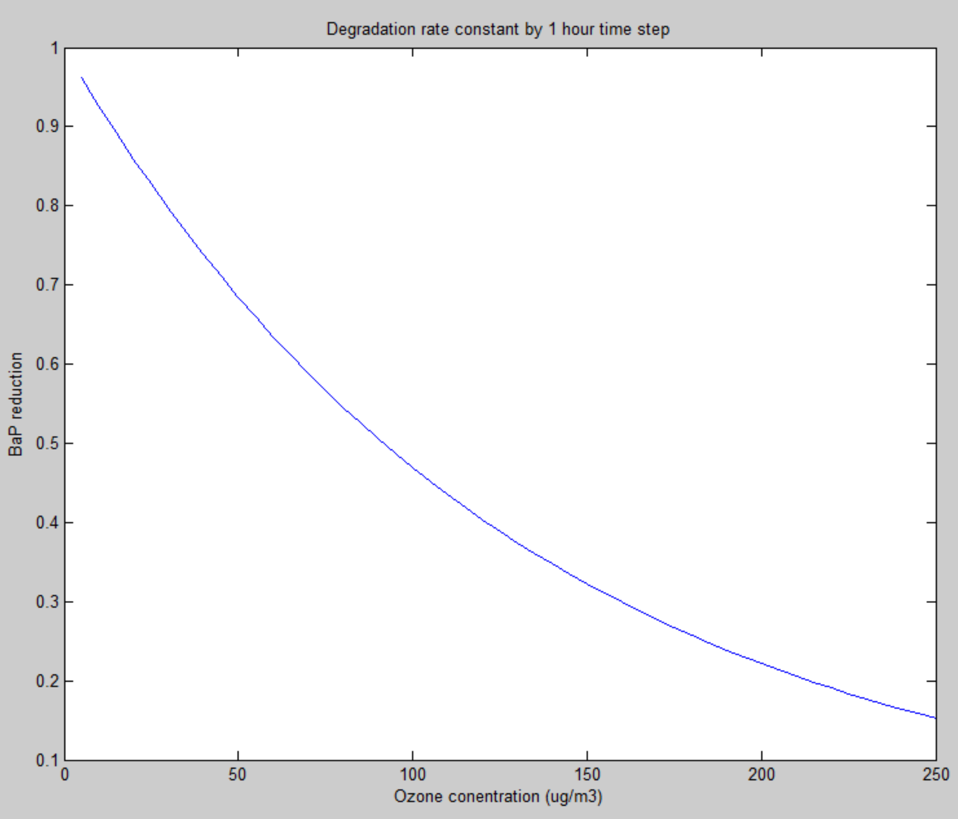
C_{init} : Represents any additional absorbing material in the particle phase

- The total absorbing organic mass (Totorg) is not known a priory in general, the set of nonlinear equations (j=1…n) is solved by an iteration method.

- The gas phase concentrations of the low volatility products have to exceed a threshold concentration before organic material can be transferred to the particle phase.

$$\sum_{i=1}^{n} \left(\frac{C_{gas,i}}{C^{*}_{sat,i}} \right) \geq 1$$

BaP particle degradation by Ozone



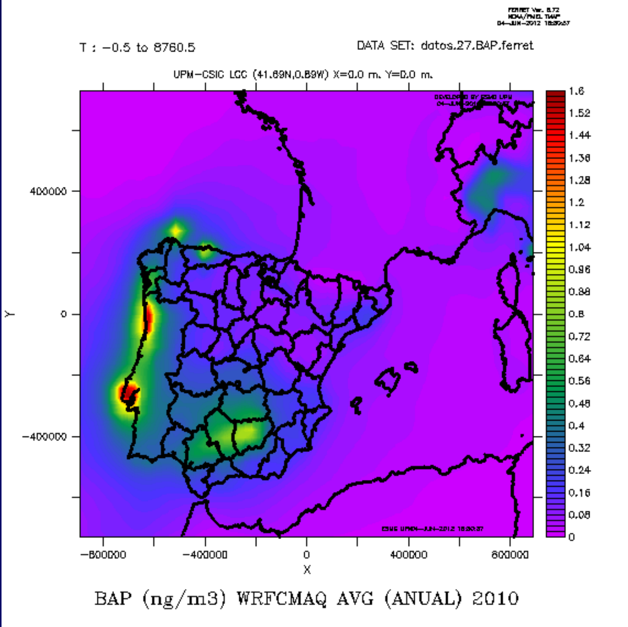
$$K = \frac{K_{\max} K_{O_3} [O_3]}{1 + K_{O_3} [O_3]}$$

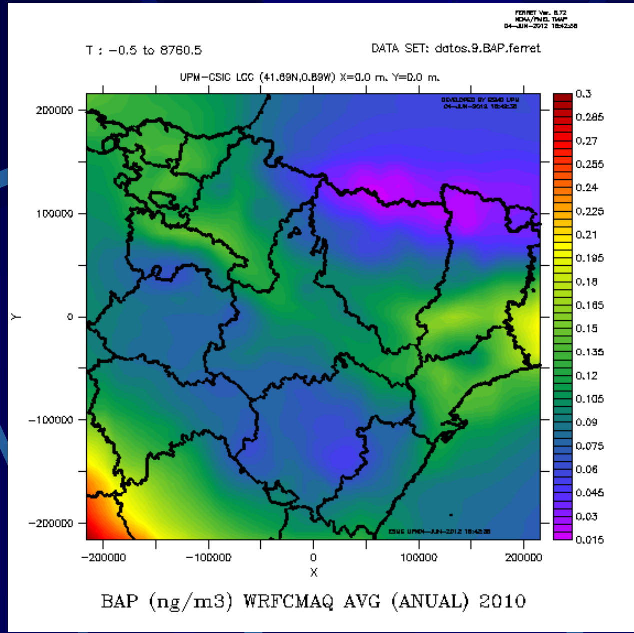
K : Degradation rate constant

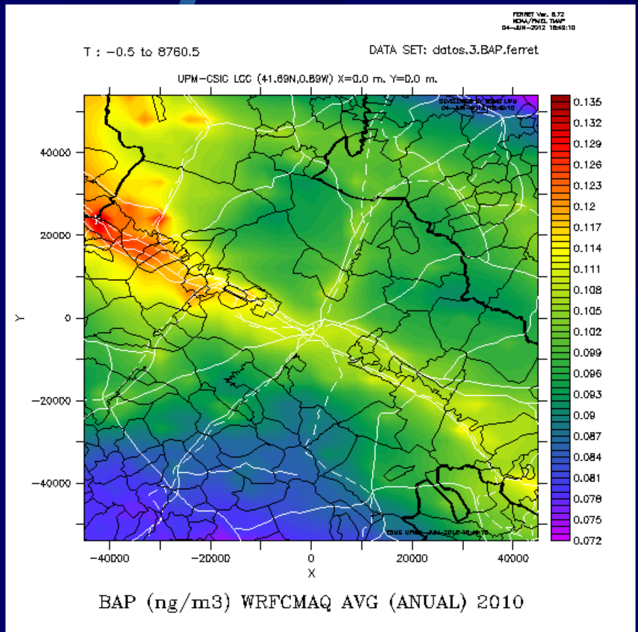
$K_{\max}$: Maximum rate coefficient (0.06 s^{-1})

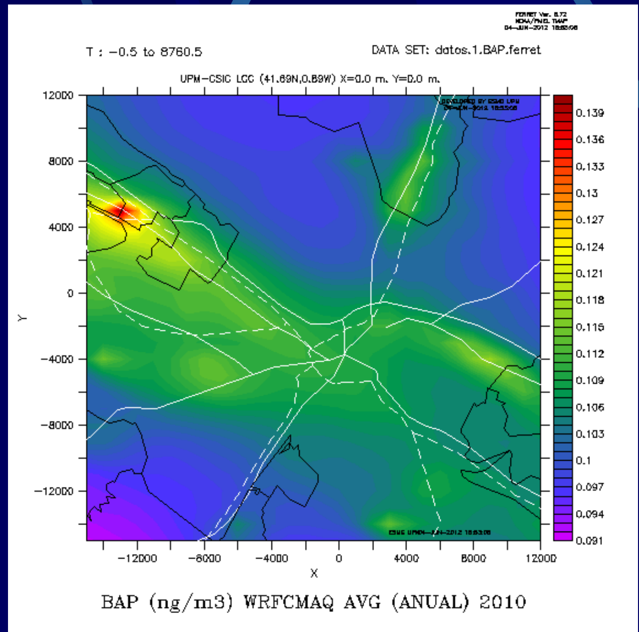
K_{O_3} : Ozone gas to surface equilibrium constant (0.028 $10^{-13} cm^3$)

$[O_3]$: Ozone conentratrion







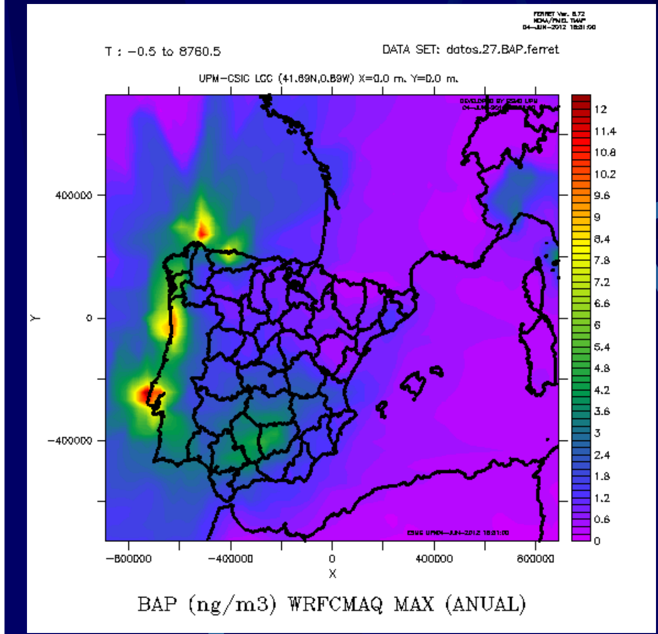


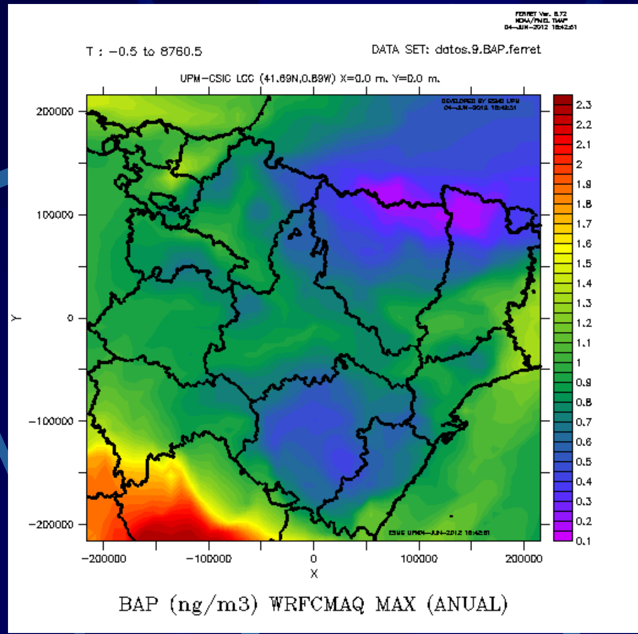
Surface results

BaP annual average (12 weeks)

One week per month

27,9,3,1 Km. Spatial resolution

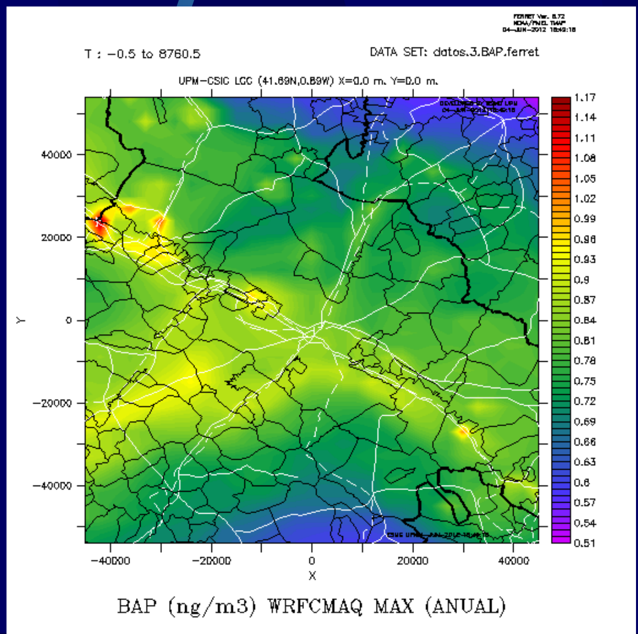


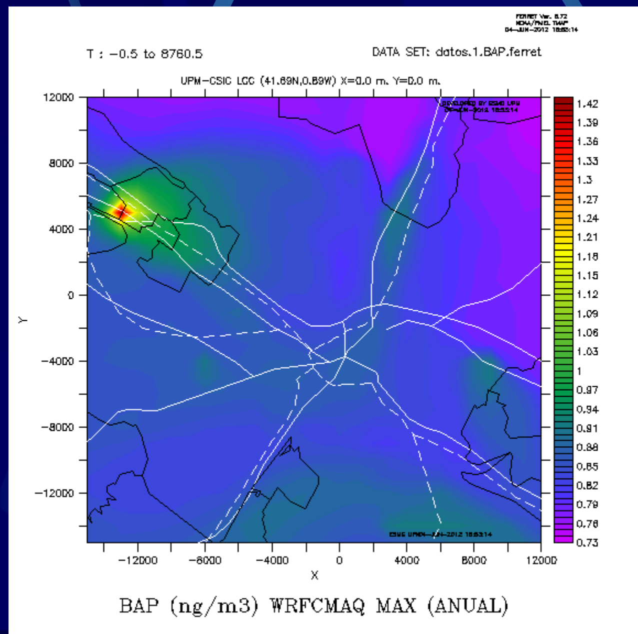


Surface results

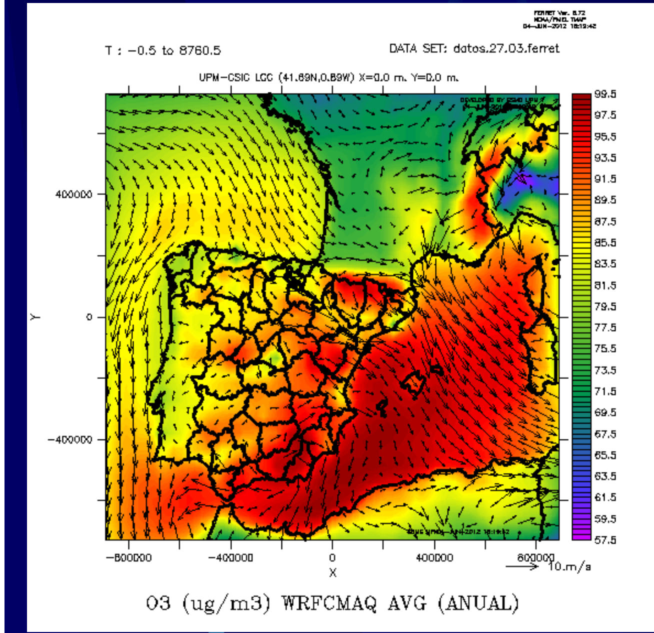
BaP annual maximum (12 weeks)

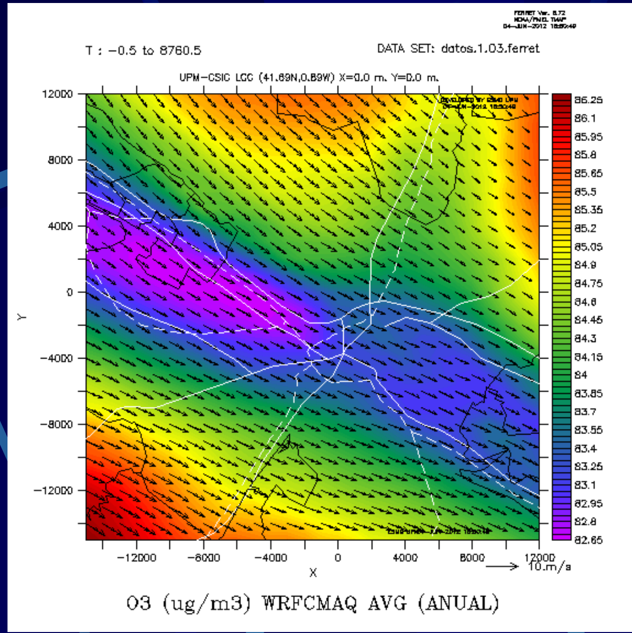
One week per month

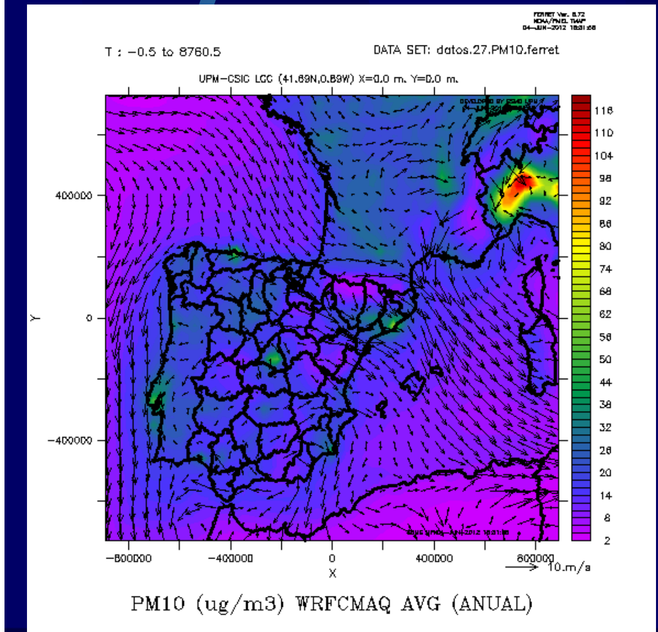


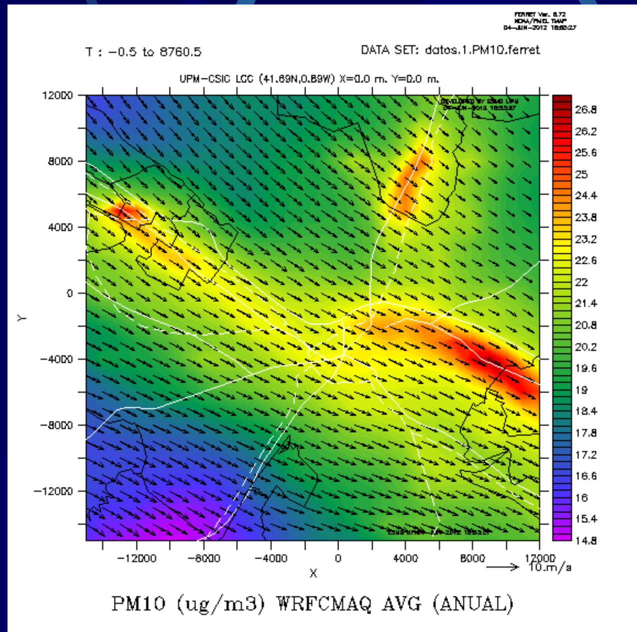


27,9,3,1 Km. Spatial resolution









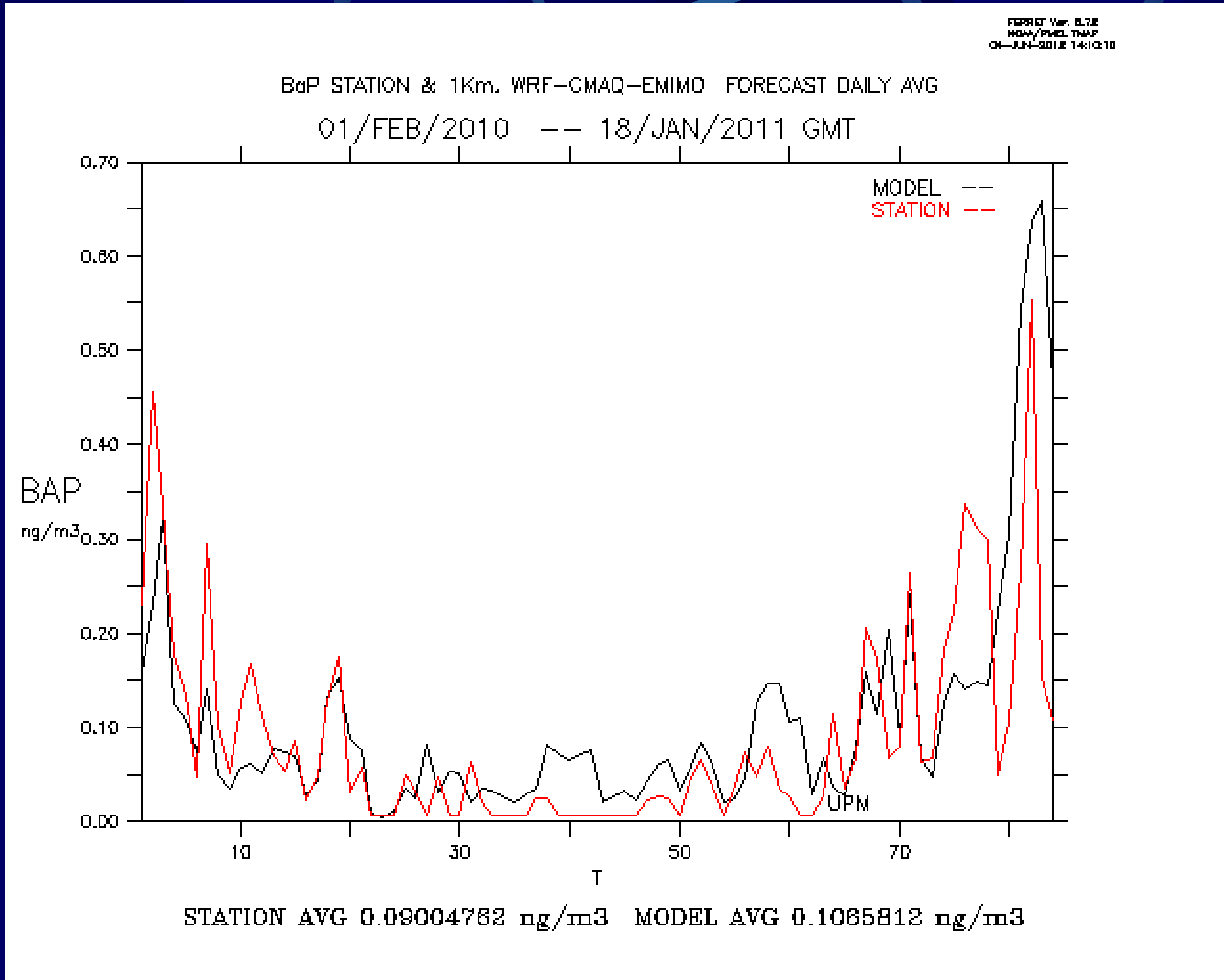
Surface results & winds

O3 annual average (12 weeks)

One week per month

PM 27,1 Km. Spatial resolution

VALIDATION

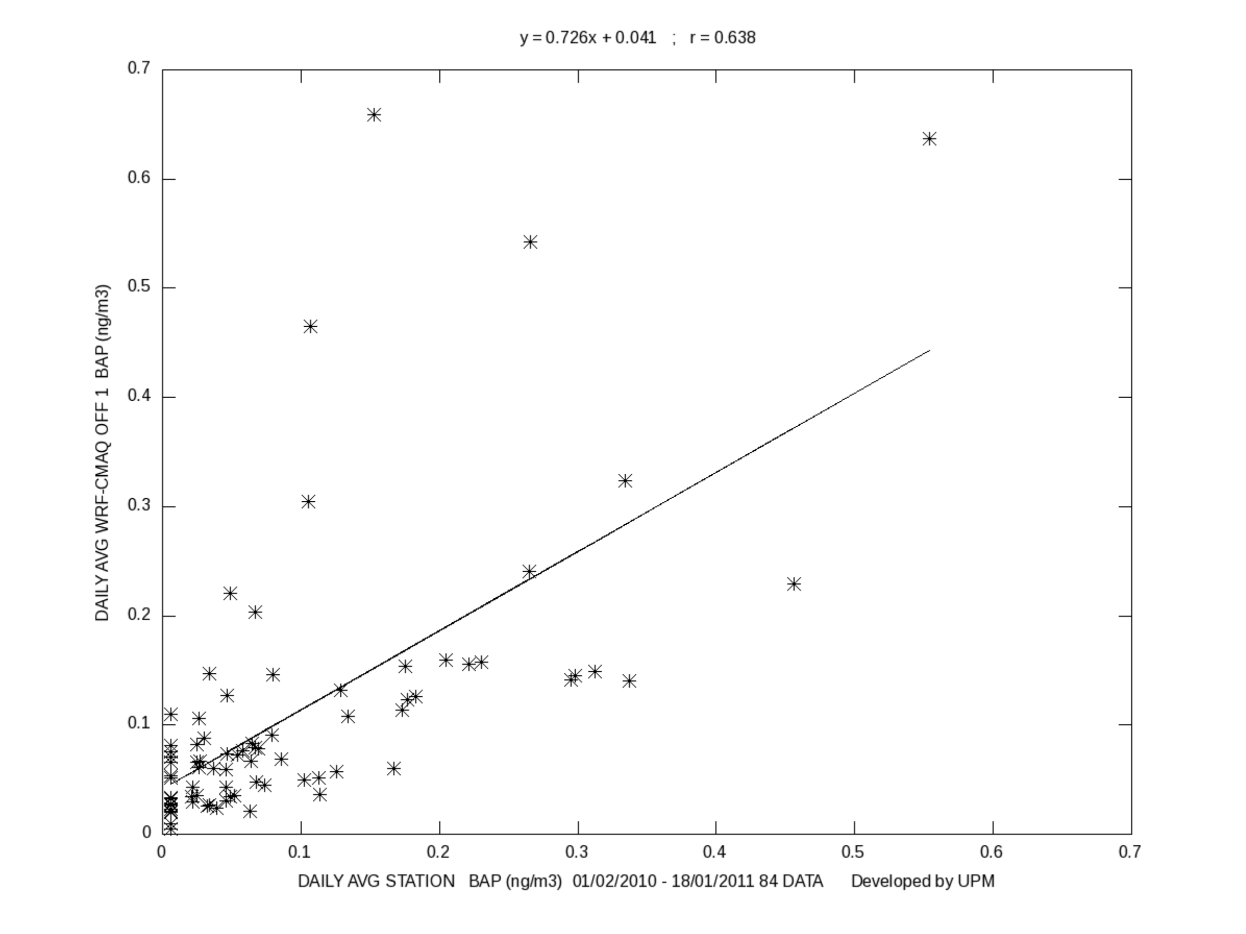


Surface results
1Km resolution
&
Monitoring station

BaP station

Daily average
12 weeks
(One week per month)

VALIDATION



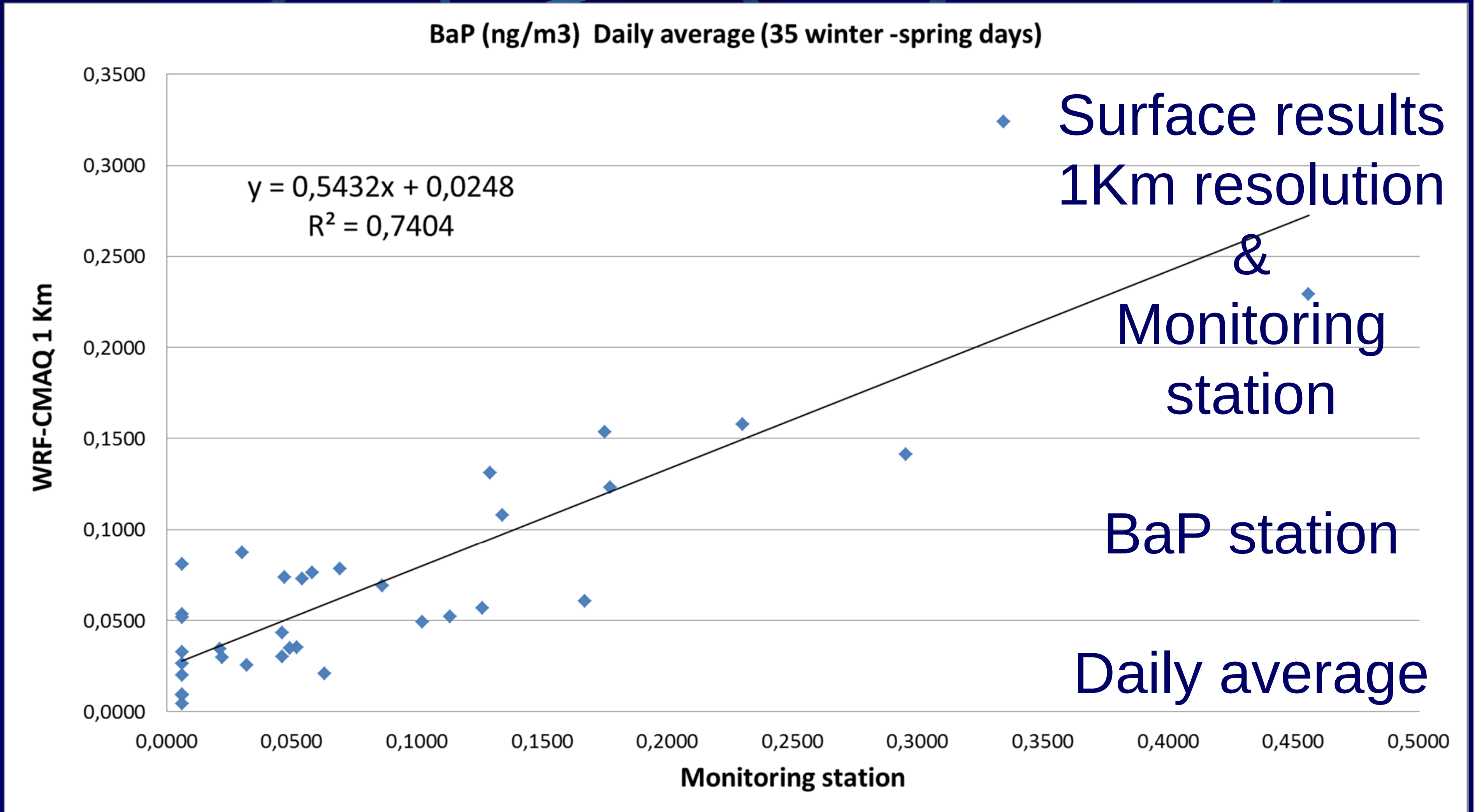
Surface results
1Km resolution
&
Monitoring
station

BaP station

Daily average
12 weeks
(1 week per month)

	1 KM	3 KM	9 KM	27 KM	N
R	0.638	0.632	0.629	0.632	84 data

VALIDATION



Surface results 1Km resolution & Monitoring station

BaP station

Daily average

CONCLUSIONS

- We have added the ability to simulate the atmospheric behavior of BaP to CMAQ. This includes the addition of two processes: gas/particle partitioning and degradation by ozone. Other aspect such as transport and diffusion is developed using de CMAQ framework. Also the CMAQ aerosol module provides the necessary aerosol parameters to the gas/particle partitioning model.

- WRF-CMAQ modeling system, which has been extended to simulate BaP concentrations, can be used to get the spatial and temporal distribution of BaP concentrations across large areas domain and to also assess the impact of different emissions reduction strategies. The EU target value for BaP of ambient air (1 ng/m3) is exceeding over area close to a mineral extraction zone. Finally the results from the modeling can be used to assess the possible health impacts of BaP concentrations above the EU target value.

- Meteorological model WRF and dispersion model CMAQ are well validated modeling tools, the BaP extension has been validated using monitored data at an urban site.

CONCLUSIONS

- The agreement is generally satisfactory, the best results are observed in winter period, which is the most important for the BaP concentrations. The model validation shows the BaP extension performance is correct over the modeled area. The BaP concentrations agree well with the observations, particularly very high B(a)P peaks are resolved by the extended model.

The modeling system reproduces the degree of seasonality of the BaP, with higher concentrations in the winter months. This is particularly prevalent at urban locations, where domestic combustion is the major source. In the rest of areas, for example industrial zones, concentrations are affected by other meteorological parameters, temperature, boundary layer, wind speed and direction…

The uncertainties in the emission of BaP cover the difference between the model and measured results in the cases where the model disagrees with the observations. In future works, we will try reduce the uncertainties of the emission, adding more detailed information to the emission model EMIMO. One of the biggest difficulties for modeling the concentrations is the uncertainty is their emissions and this remains the most important obstacle to the validation of the model.

CONCLUSIONS

- It was not possible to make BaP hourly validation because hourly measurements are not available. In the future a bigger evaluation task will be developed, with hourly data and more monitoring locations.

Acknowledgements

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