



**Barcelona
Supercomputing
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Centro Nacional de Supercomputación



Inter-annual evaluation of the Spanish Air Quality Forecast System CALIOPE: 2010-2014

Gustavo Arévalo & José M. Baldasano

7th International Workshop on
Air Quality Forecasting Research



Sponsored by

NOAA, Environment Canada & the World Meteorological Organization



A very common question regarding the models in general and air quality models in particular, is as follows:

- How well the model is performing?
- Are the results have been evaluated??

 This work pretend to answer these questions, but also evaluate how continuous improvement processes have influenced the operation of CALIOPE Air Quality Forecasting System

Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences

Naomi Oreskes,* Kristin Shrader-Frechette, Kenneth Belitz

Verification and validation of numerical models of natural systems is impossible. This is because natural systems are never closed and because model results are always non-unique. Models can be confirmed by the demonstration of agreement between observation and prediction, but confirmation is inherently partial. Complete confirmation is logically precluded by the fallacy of affirming the consequent and by incomplete access to natural phenomena. Models can only be evaluated in relative terms, and their predictive value is always open to question. The primary value of models is heuristic.

In recent years, there has been a dramatic increase in the use of numerical simulation models in the earth sciences as a means to evaluate large-scale or complex physical processes. In some cases, the predictions generated by these models are considered as a basis for public policy decisions: Global circulation models are being used to predict the behavior of the Earth's climate in response to increased CO₂ concentrations; resource estimation models are being used to predict petroleum reserves in ecologically sensitive areas; and hydrological and geochemical models are being used to predict the behavior of toxic and radioactive contaminants in proposed waste disposal sites. Government

Verification: The Problem of "Truth"

The word verify (from Latin, *verus*, meaning true) means an assertion or establishment of truth (9). To say that a model is verified is to say that its truth has been demonstrated, which implies its reliability as a basis for decision-making. However, it is impossible to demonstrate the truth of any proposition, except in a closed system. This conclusion derives directly from the laws of symbolic logic. Given a proposition of the form "p" entails "q," we know that if "p" is true, then "q" is true if and only if the system that this formalism represents is closed.

puter program may be verifiable (12). Mathematical components are subject to verification because they are part of closed systems that include claims that are always true as a function of the meanings assigned to the specific symbols used to express them (13). However, the models that use these components are never closed systems. One reason they are never closed is that models require input parameters that are incompletely known. For example, hydrogeological models require distributed parameters such as hydraulic conductivity, porosity, storage coefficient, and dispersivity, which are always characterized by incomplete data sets. Geochemical models require thermodynamic and kinetic data that are incompletely or only approximately known. Incompleteness is also introduced when continuum theory is used to represent natural systems. Continuum mechanics necessarily entails a loss of information at the scale lower than the averaging scale. For example, the Darcian velocity of a porous medium is never identical to the velocity structure at the pore scale. Finer scale structure

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Institut
Cardiff

Dr. Jos
USAF Hqs
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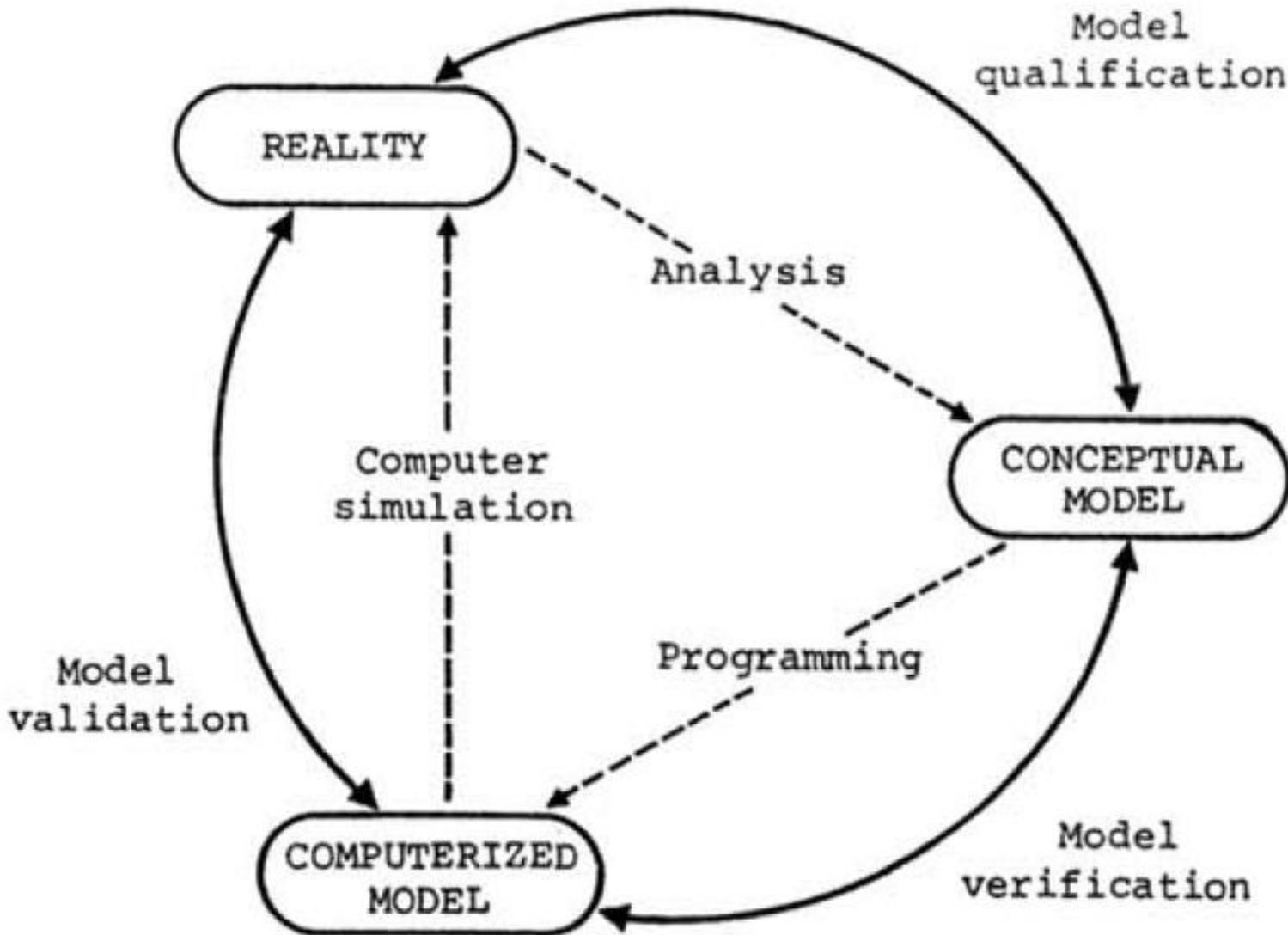
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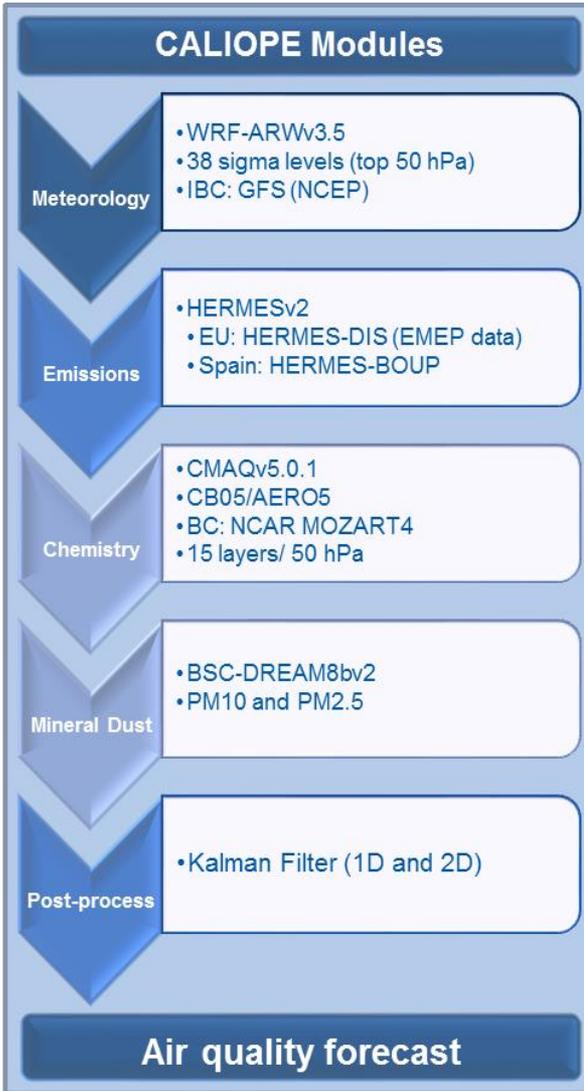
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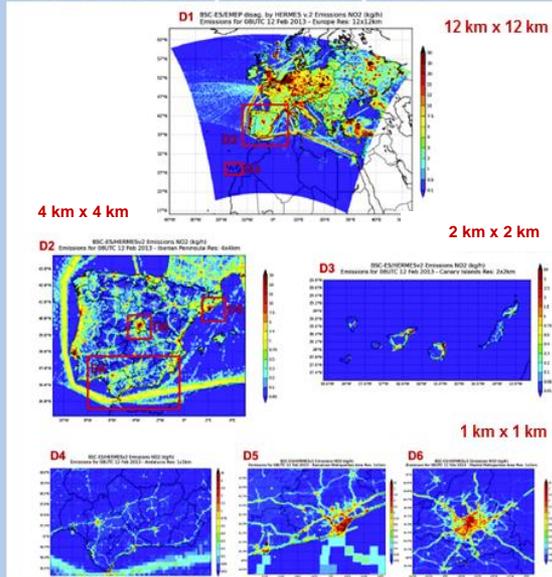


The CALIOPE air quality forecast system



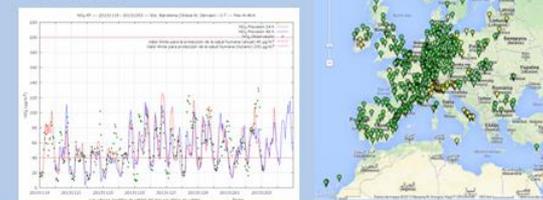
Forecast 48h

- Maps (AQ concentration, emis, meteo)
- AQ index / Population exposed



Forecast Evaluation (NRT)

- AQ monitoring network
- Satellite



Difusion

- Web (www.bsc.es/caliope)
- Smart phone app

Sistema CALIOPE
Pronóstico de la Calidad del Aire

CALIOPE
Pronóstico de la Calidad del Aire

Barcelona (Ciutatella) 10 - 10m

O₃ Buena

NO₂ Buena

SO₂ Buena

PM₁₀ Buena

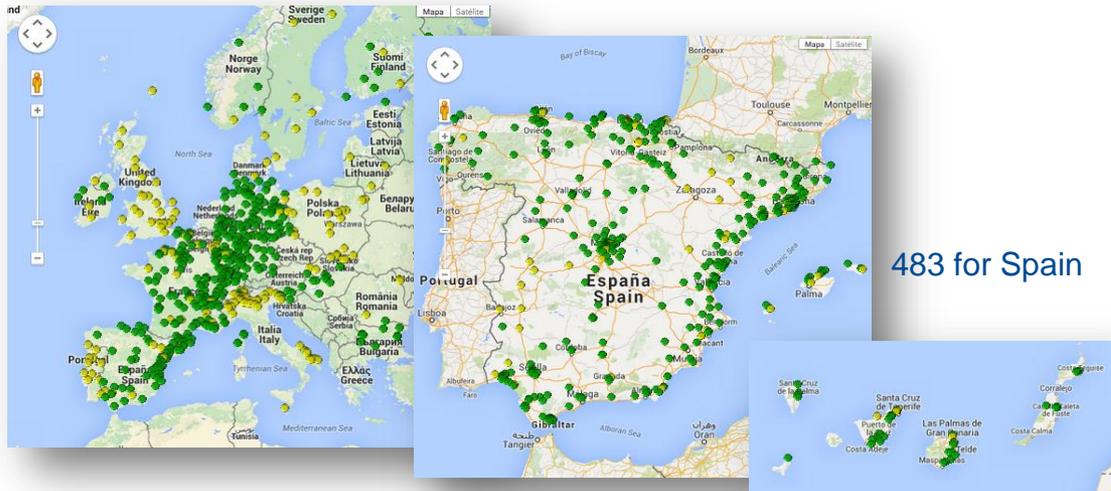
PM_{2.5} Buena

Ver en mapa

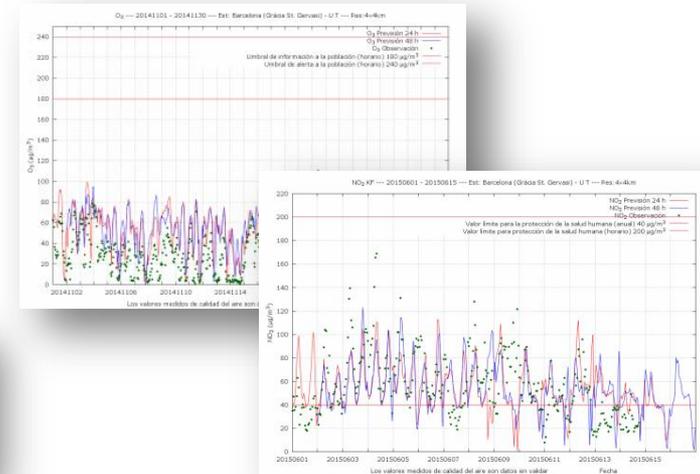
ANDROID APP ON Google play Available on the App Store

Daily forecast evaluation for meteorology and air quality

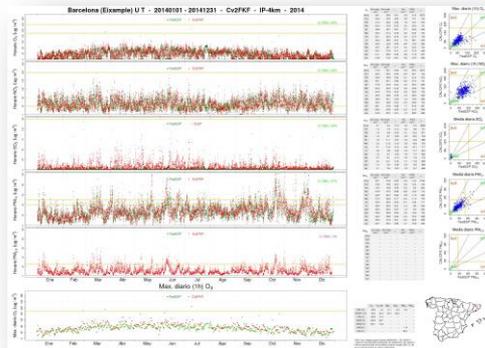
Air quality stations (971)



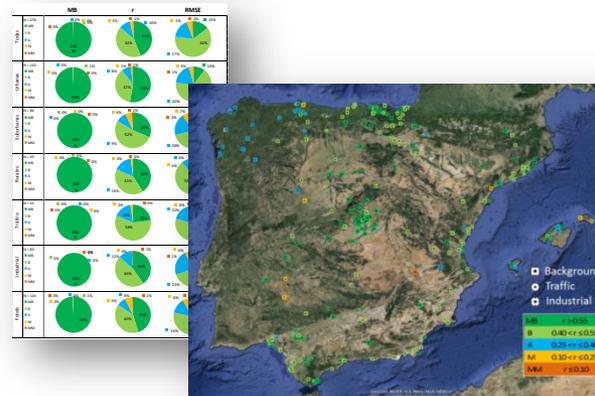
Daily Near Real Time evaluation O_3 , NO_2 , SO_2 , PM_{10} and $PM_{2.5}$



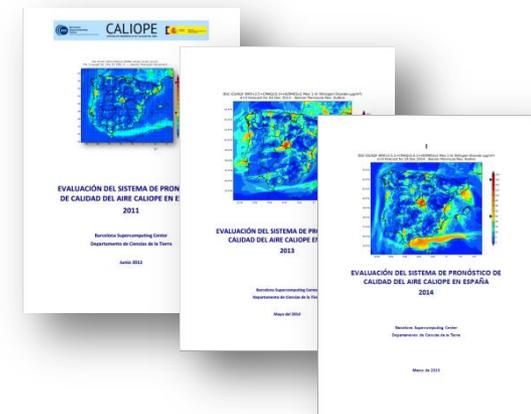
Accumulated Near Real Time evaluation sheet by station



Annual evaluation by air quality stations



Yearly annual evaluation report



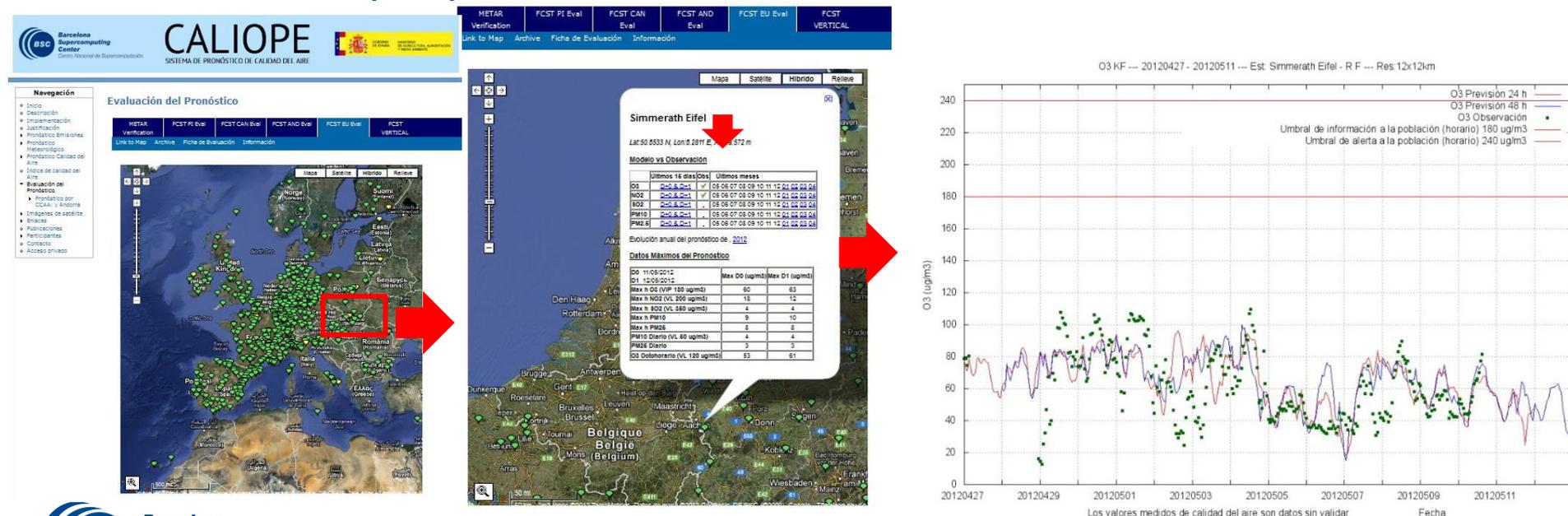
Confidence on the CALIOPE AQF system

(Baldasano et al, 2008)

1. Peer Review Publications:

Domain	Reference
Europe	Pay <i>et al</i> (2010, 2012a)
	Basart <i>et al</i> (2012) Schap <i>et al.</i> (2014)
	Baldasano <i>et al</i> (2008, 2011)
Spain	Pay <i>et al</i> (2011, 2012b, 2014)
	Borrego <i>et al</i> (2011) Sicardi <i>et al</i> (2012)
Barcelona & Madrid	Gonçalves <i>et al</i> (2009) Soret <i>et al.</i> (2011)
Cataluña (NE Spain)	Jiménez <i>et al</i> (2008) Aguilera <i>et al</i> (2013)

2. Near-Real Time (NRT) evaluation:



Main changes implemented into the CALIOPE System (2007–2014)



CALIOPE version	Date	Meteo	Emissions*		Boundary conditions	Chemical	Dust	Kalman Filter*	
			UE	IP				UE	IP
Cv1-fcst	Since 2007-06	WRF-ARW v2.2.1		HERMES-2004 (EMEP, 2004)	Syntheticals (6)		DREAM		
	Since 2009-06		HERMES-2004 (EMEP, 2004)	HERMES-2004 (EMEP, 2004)	LMDz-INCA daily				
Cv2-fcst	Since 2011-02-11	WRF-ARW v3.0.1.1			LMDz-INCA monthly average 2004	CMAQ v4.5	BSC-DREAM8b	-	NO ₂ , PM ₁₀ and PM _{2.5} (for O ₃ since 15-jun-2010)
	Since 2011-02-28			HERMES_DIS v.2.0 EMEP (2008)					
	Since 2011-05-03	WRF-ARW v3.2.1	HERMES-2004+ EMEP (2008)						
	Since 2012-03-12			HERMES_DIS v2.1 EMEP (2009)					
	Since 2012-06-22	WRF-ARW v3.3.1	HERMES-2004+ EMEP (2009) MEGAN included	HERMES_DIS v2.1 EMEP (2009) MEGAN included					
Cv3-fcst	Since 2012-08-14		HERMESv2 + EMEP (2009)		NCAR MOZART-4/GEOS-5 (6h)	CMAQ v5.0.1	BSC-DREAM8b v2	O ₃ , NO ₂ , PM ₁₀ and PM _{2.5}	
	Since 2012-09-17	WRF-ARW v3.5							
	Desde 2013-02-08	WRF-ARW v3.2.1	HERMESv2 + EMEP (2009)						
	Since 2013-08-30								
	Since 2014-03-14	WRF-ARW v3.5	HERMESv2 + EMEP (2011)			CMAQ v5.0.2			
	Since 2014-10-22	WRF-ARW v3.5.1							

2009

- ✓ WRF upgrade
- ✓ BCON LMDZ-INCA (daily)

2011

- ✓ WRF upgrade
- ✓ HERMES_DISv2 and EMEP update 2008
- ✓ BCON LMDZ-INCA monthly avg 2004
- ✓ KF IP incorporation

2012

- ✓ WRF upgrade
- ✓ EMEP update 2009
- ✓ BSC-DREAM8b upgrade
- ✓ HERMESv2 major upgrade (methodology and databases) and MEGAN inclusion
- ✓ CMAQ major upgrade (CB5 instead CB4 and AERO 5 instead AERO 4)
- ✓ KF EU incorporation



Main changes implemented into the CALIOPE System (2007–2014)



CALIOPE version	Date	Meteo	Emissions*		Boundary conditions	Chemical	Dust	Kalman Filter*	
			UE	IP				UE	IP
Cv1-fcst	Since 2007-06	WRF-ARW v2.2.1		HERMES-2004 (EMEP, 2004)	Syntheticals (6)		DREAM		
	Since 2009-06		HERMES-2004 (EMEP, 2004)	HERMES-2004 (EMEP, 2004)	LMDz-INCA daily				
Cv2-fcst	Since 2011-02-11	WRF-ARW v3.0.1.1			LMDz-INCA monthly average 2004	CMAQ v4.5	BSC-DREAM8b		NO ₂ , PM ₁₀ and PM _{2.5} (for O ₃ since 15-jun-2010)
	Since 2011-02-28								
	Since 2011-05-03	WRF-ARW v3.2.1	HERMES-2004+ EMEP (2008)	HERMES_DIS v.2.0 EMEP (2008)					
	Since 2012-03-12								
	Since 2012-06-22	WRF-ARW v3.3.1	HERMES-2004+ EMEP (2009) MEGAN included	HERMES_DIS v2.1 EMEP (2009) MEGAN included					
	Since 2012-08-14								
Cv3-fcst	Since 2012-09-17	WRF-ARW v3.5	HERMESv2 + EMEP (2009)		NCAR MOZART-4/GEOS-5 (6h)	CMAQ v5.0.1	BSC-DREAM8b v2	O ₃ , NO ₂ , PM ₁₀ and PM _{2.5}	
	Desde 2013-02-08	WRF-ARW v3.2.1							
	Since 2013-08-30								
	Since 2014-03-14	WRF-ARW v3.5	HERMESv2 + EMEP (2011)						
	Since 2014-10-22	WRF-ARW v3.5.1							

2013

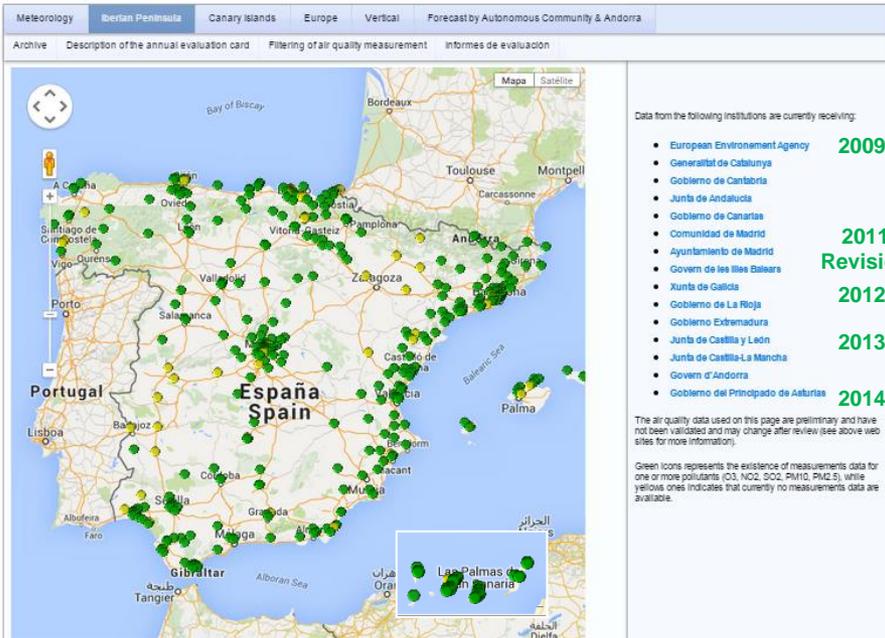
- ✓ WRF upgrade
- ✓ BCON MOZART 4/ GEOS-5 (6h) from NCARG

Machine upgrade

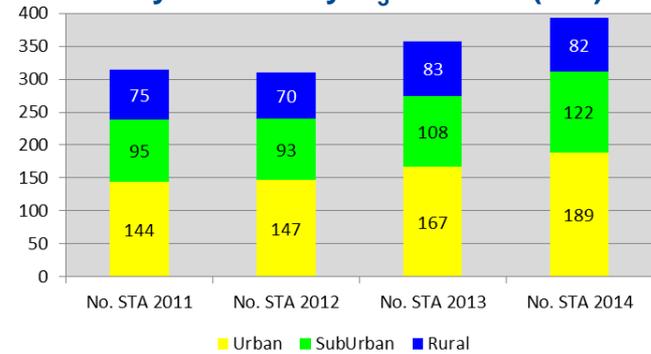
2014

- ✓ WRF upgrade + USGS land uses default database, changed by CORINE Land Cover v16 + SRTM (90m) default terrain, changed by Digital Elevation Database v4.1 from NASA
- ✓ EMEP update
- ✓ CMAQ upgraded and In-line plume rise calculation

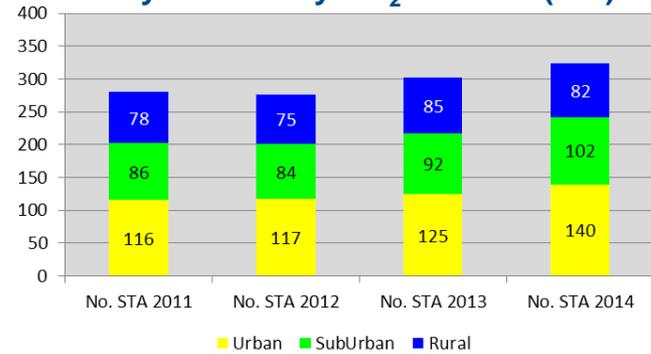
Observation data sources



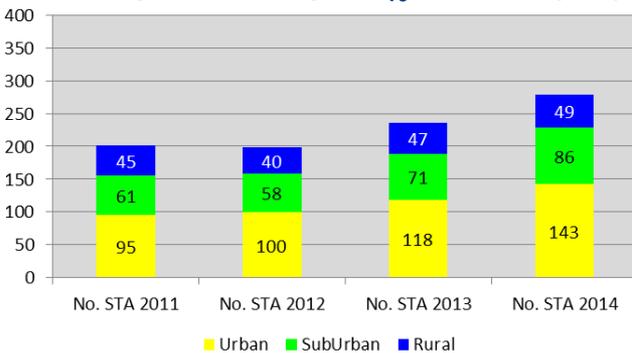
Yearly availability O₃ stations (No.)



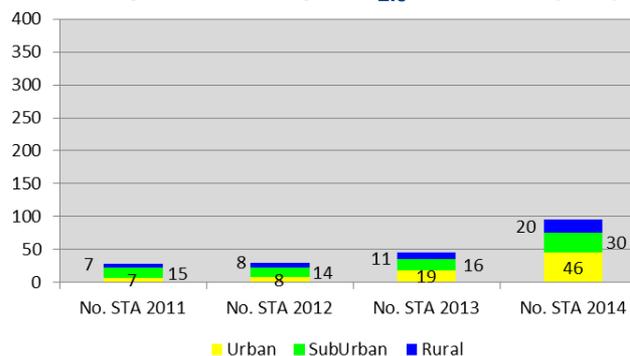
Yearly availability NO₂ stations (No.)



Yearly availability PM₁₀ stations (No.)



Yearly availability PM_{2.5} stations (No.)



From 2011 up to now

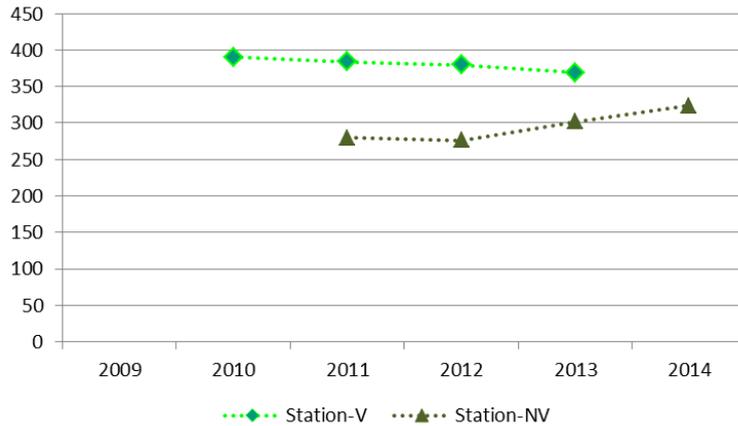
1.8 times more stations

4.1 times more observations

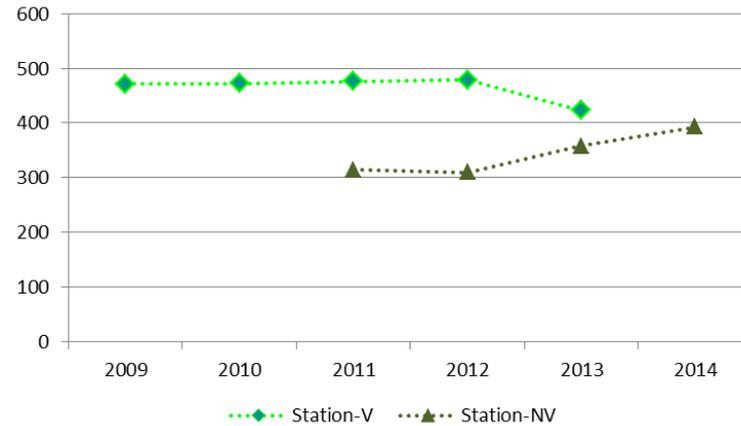
Number of stations by pollutant (validated and not validated)



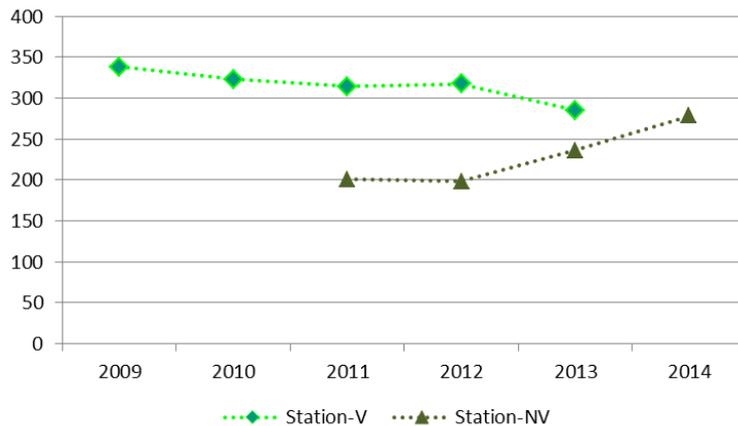
Number of stations for O₃



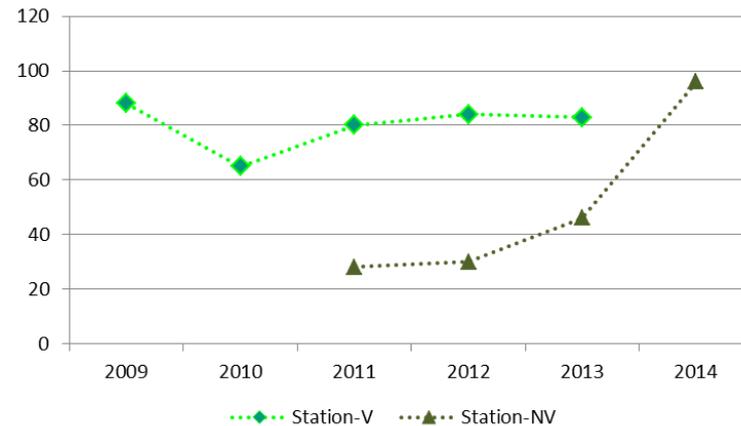
Number of stations for NO₂



Number of stations for PM₁₀



Number of stations for PM_{2.5}

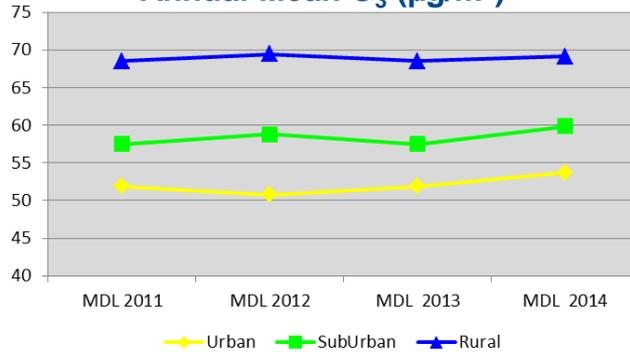


For the year 2013, not validated data are about to 80 – 85 % of the validated observation for O₃, NO₂ and PM₁₀ and about to 60% for the PM_{2.5}.

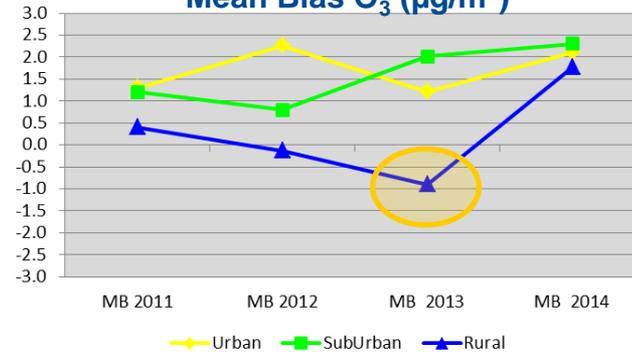
O₃ Annual average on hourly basis (KF)



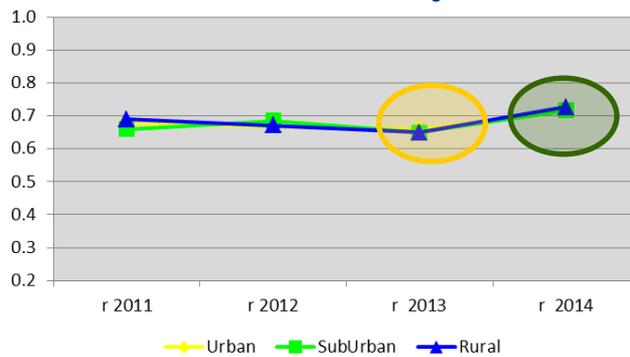
Annual Mean O₃ (µg/m³)



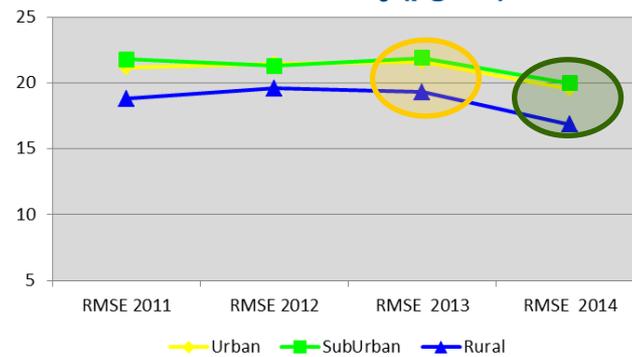
Mean Bias O₃ (µg/m³)



Correlation O₃



RMSE O₃ (µg/m³)



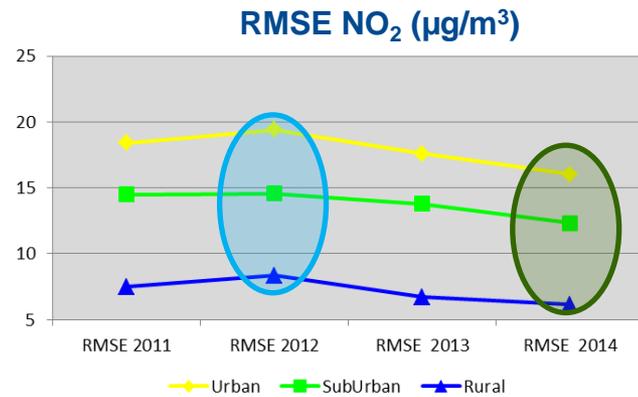
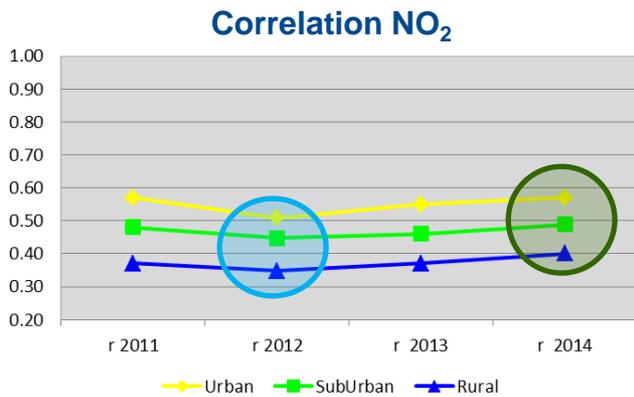
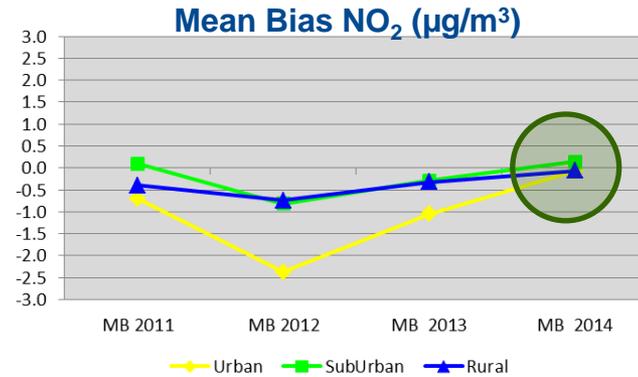
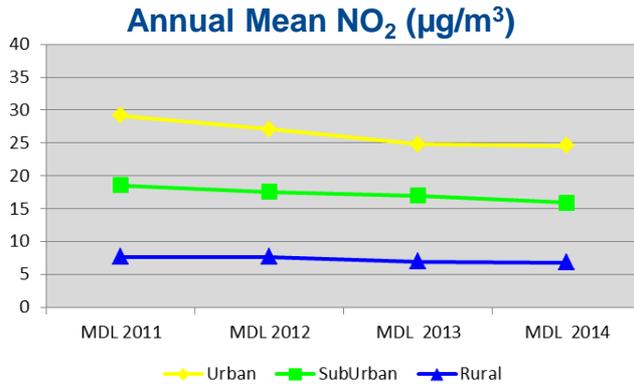
2013

- ✓ WRF upgrade
- ✓ **BCON NCAR MOZART 4/ GEOS-5 (6h) in 20130830**

2014

- ✓ **WRF upgrade + USGS land uses default database, changed by CORINE Land Cover v16 + SRTM (90m) default terrain, changed by Digital Elevation Database v4.1 de la NASA**
- ✓ EMEP update
- ✓ CMAQ upgraded and In-line plume rise calculation

NO₂ Annual average on hourly basis (KF)



2012

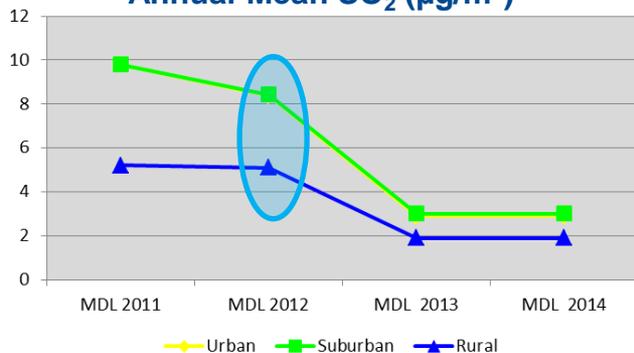
- ✓ WRF upgrade
- ✓ EMEP update 2009
- ✓ BSC-DREAM8b upgrade
- ✓ **HERMESv2 major upgrade (methodology and databases) and MEGAN inclusion**
- ✓ **CMAQv5.0 major upgrade (CB5 instead CB4 and AERO 5 instead AERO 4)**

2014

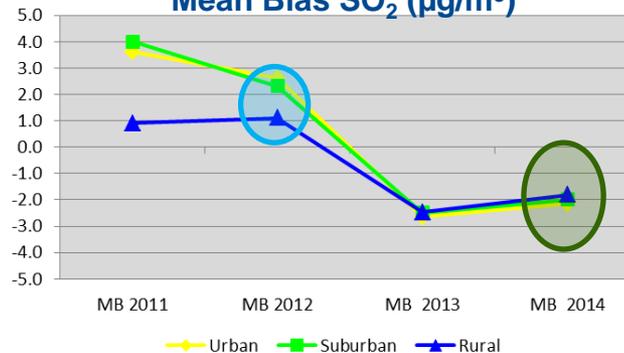
- ✓ **WRF upgrade + USGS land uses default database, changed by CORINE Land Cover v16 + SRTM (90m) default terrain, changed by Digital Elevation Database v4.1 from NASA**
- ✓ EMEP update
- ✓ CMAQ upgraded and In-line plume rise calculation

SO₂ Annual average on hourly basis

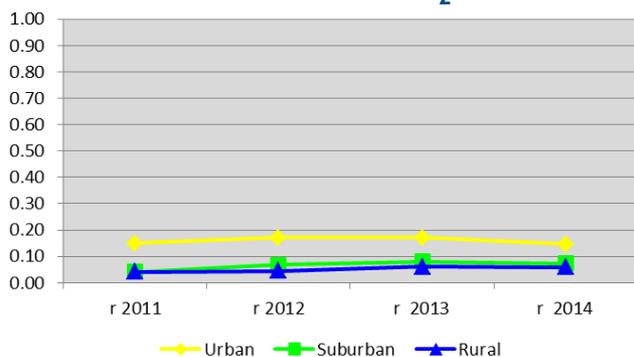
Annual Mean SO₂ (µg/m³)



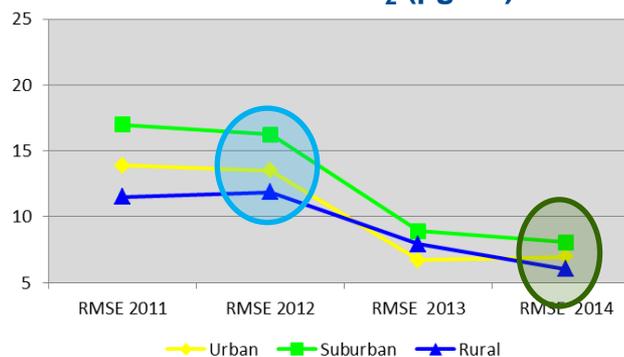
Mean Bias SO₂ (µg/m³)



Correlation SO₂



RMSE SO₂ (µg/m³)



2012

- ✓ WRF upgrade
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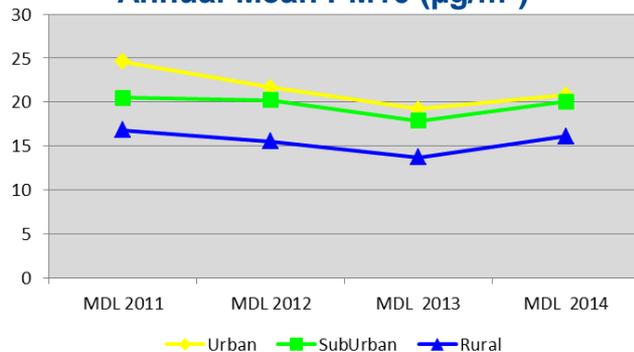
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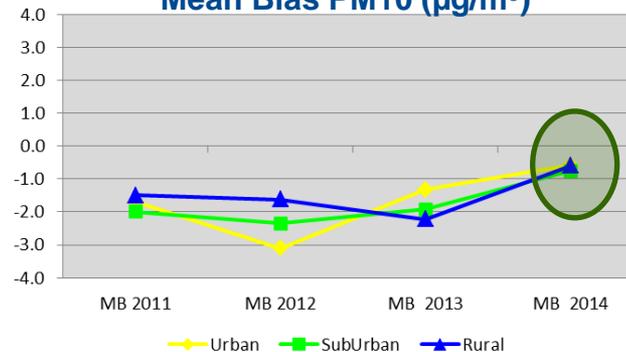
PM10 Annual average on hourly basis (KF)



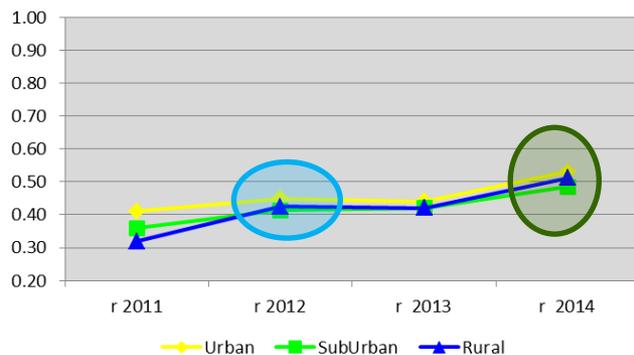
Annual Mean PM10 ($\mu\text{g}/\text{m}^3$)



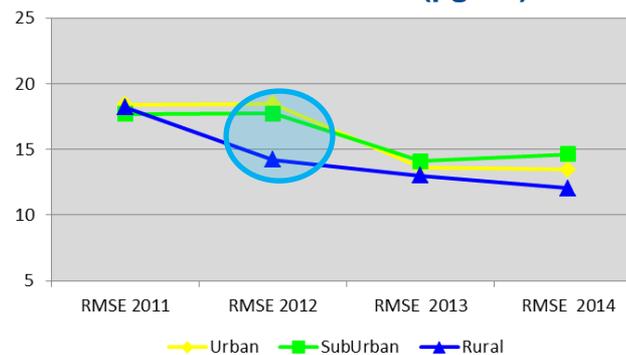
Mean Bias PM10 ($\mu\text{g}/\text{m}^3$)



Correlation PM10



RMSE PM10 ($\mu\text{g}/\text{m}^3$)



2012

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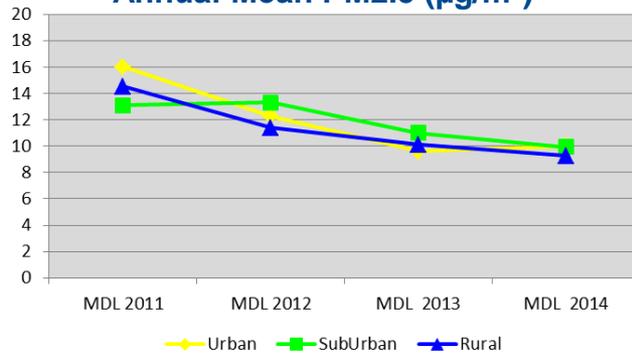
2014

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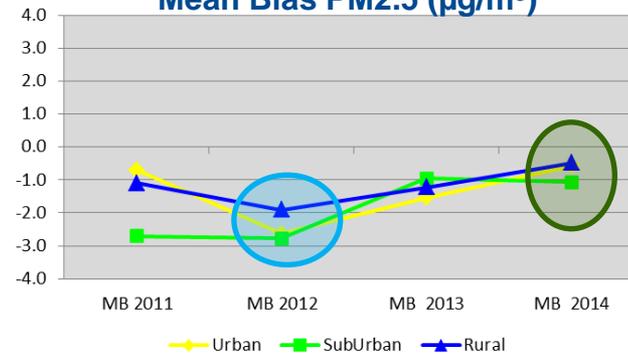
PM2.5 Annual average on hourly basis (KF)



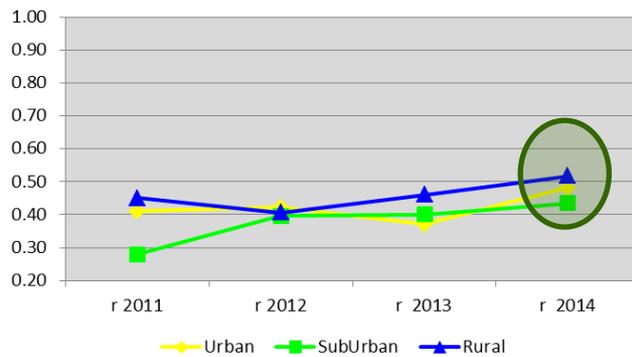
Annual Mean PM2.5 ($\mu\text{g}/\text{m}^3$)



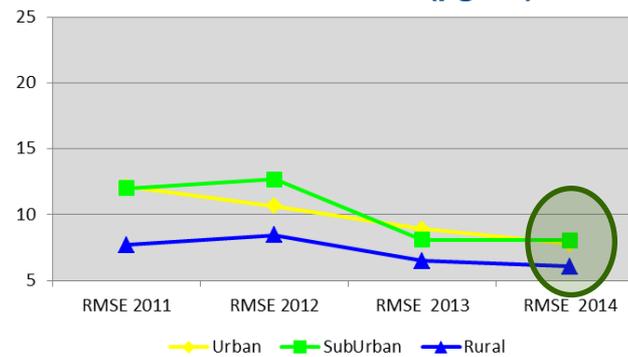
Mean Bias PM2.5 ($\mu\text{g}/\text{m}^3$)



Correlation PM2.5



RMSE PM2.5 ($\mu\text{g}/\text{m}^3$)



2012

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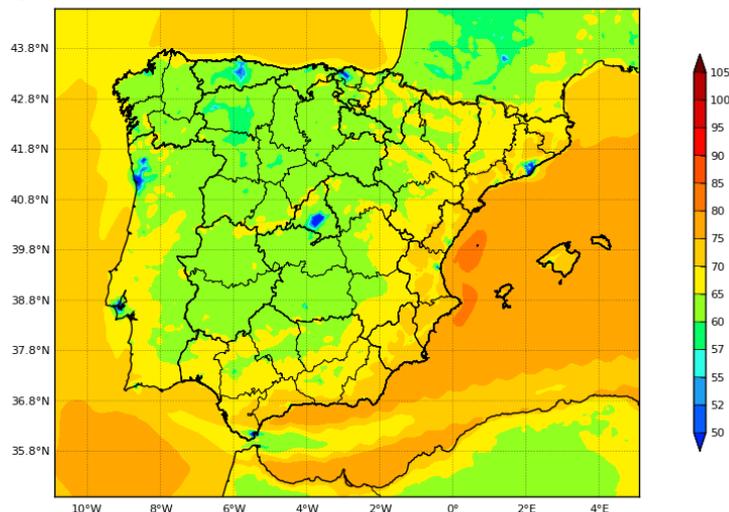


Comparison of the CALIOPE maps result for the Iberian Peninsula (2011- 2014)

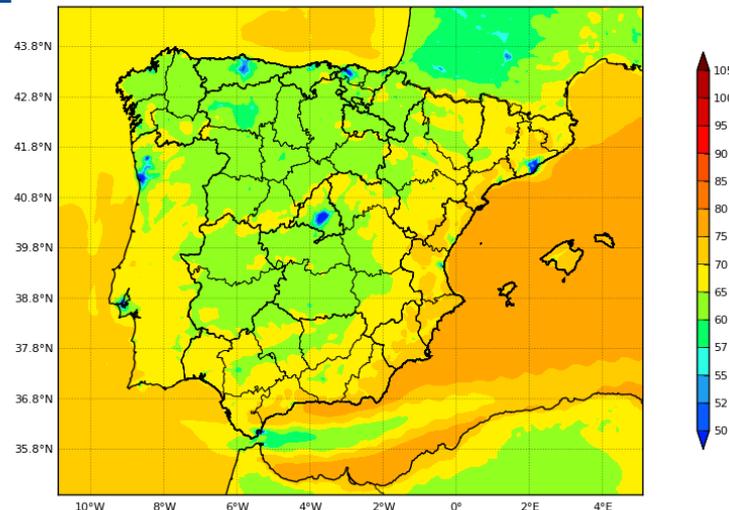
O₃ from April to September mean on hourly basis



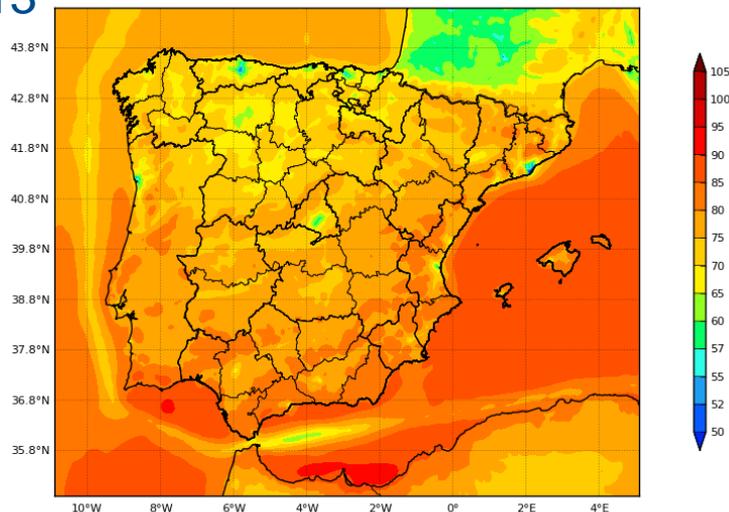
2011 BSC-ES/AQF WRF v3.2 + CMAQv 4.5 + HERMES Apr-Sept Ozone ($\mu\text{g}/\text{m}^3$)
Forecast - 2011 - Iberian Peninsula Res: 4x4km



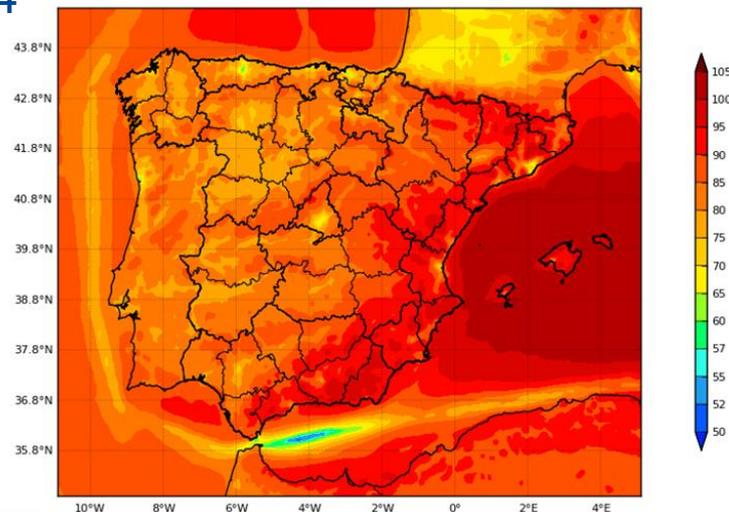
2012 BSC-ES/AQF WRFv3.5 + CMAQv5.0 + HERMESv2 Apr-Sept Ozone ($\mu\text{g}/\text{m}^3$)
Forecast - 2012 - Iberian Peninsula Res: 4x4km



2013 BSC-ES/AQF WRFv3.5 + CMAQv5.0 + HERMESv2 Apr-Sept Ozone ($\mu\text{g}/\text{m}^3$)
Forecast - 2013 - Iberian Peninsula Res: 4x4km



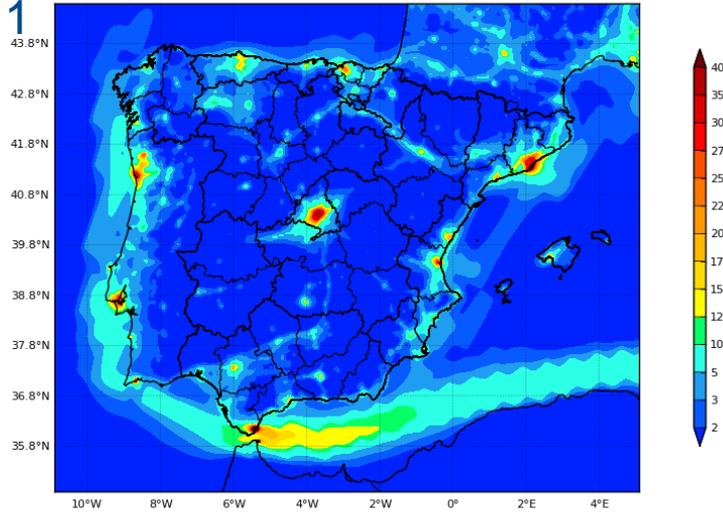
2014 BSC-ES/AQF WRFv3.5 + CMAQv5.0 + HERMESv2 April-September Ozone ($\mu\text{g}/\text{m}^3$)
Cv3F-2014 - Iberian Peninsula Res: 4x4km



NO₂ Annual mean on hourly basis

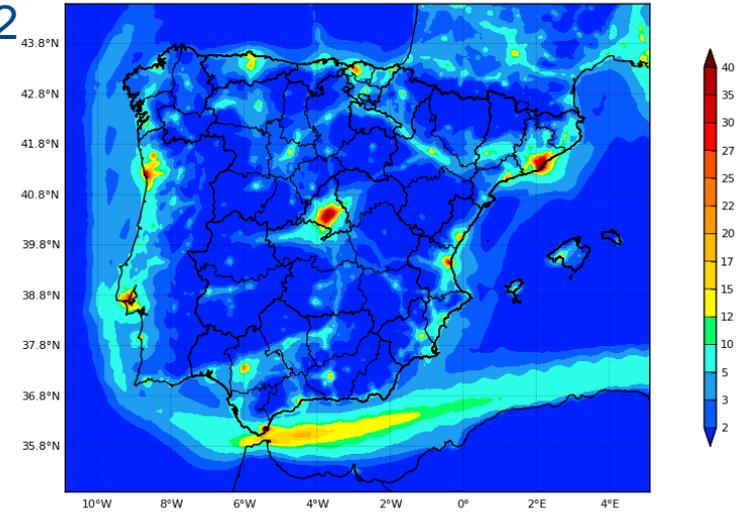
BSC-ES/AQF WRF v3.2 + CMAQ v4.5.1 + HERMES Annual Nitrogen Dioxide ($\mu\text{g}/\text{m}^3$)
Forecast - 2011 - Iberian Peninsula Res: 4x4km

2011



BSC-ES/AQF WRFv3.5 + CMAQv5.0 + HERMESv2 Annual Nitrogen Dioxide ($\mu\text{g}/\text{m}^3$)
Forecast - 2012 - Iberian Peninsula Res: 4x4km

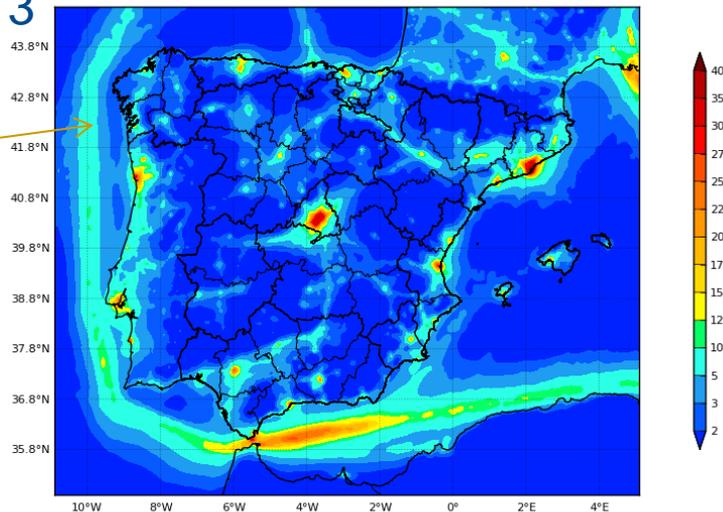
2012



BSC-ES/AQF WRFv3.5 + CMAQv5.0 + HERMESv2 Annual Nitrogen Dioxide ($\mu\text{g}/\text{m}^3$)
Forecast - 2013 - Iberian Peninsula Res: 4x4km

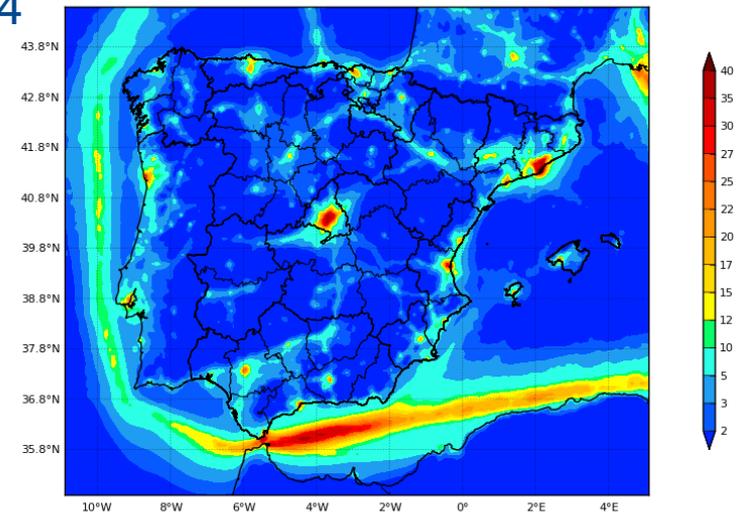
2013

Better emissions definition



BSC-ES/AQF WRFv3.5 + CMAQv5.0 + HERMESv2 Annual Nitrogen Dioxide ($\mu\text{g}/\text{m}^3$)
Cv3F-2014 - Iberian Peninsula Res: 4x4km

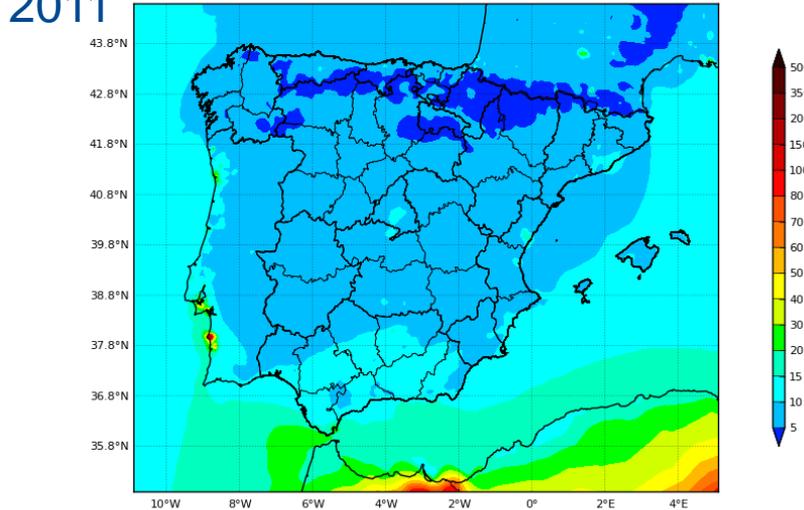
2014



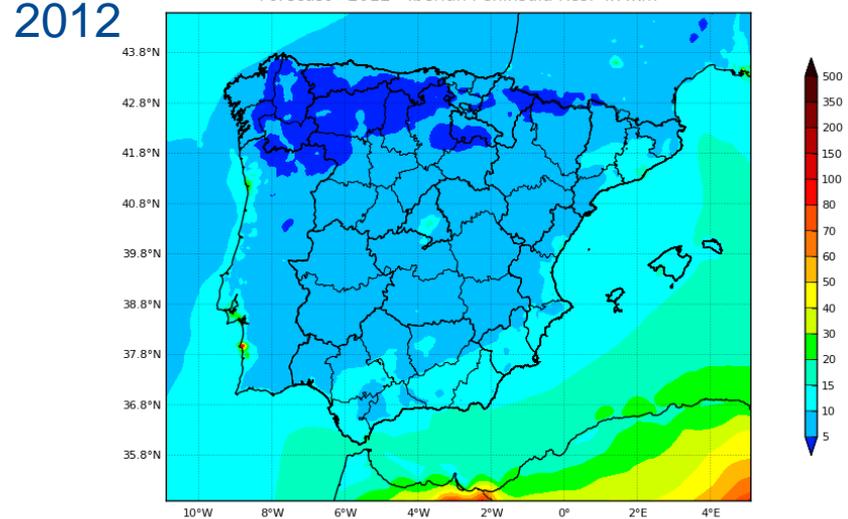
PM10 Annual mean on hourly basis



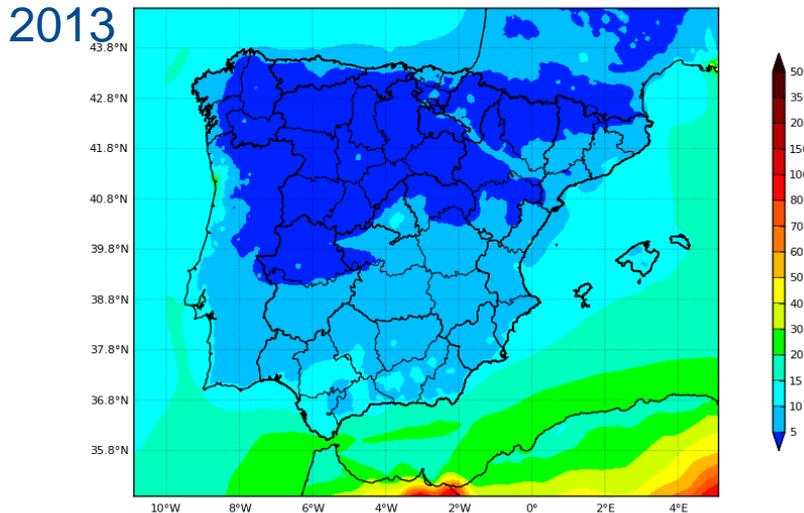
2011
BSC-ES/AQF WRF v3.2+CMAQ v4.5+HERMES¹+BSC-DREAM8b
Forecast - 2011 - Iberian Peninsula Res: 4x4km
Annual PM10 ($\mu\text{g}/\text{m}^3$)



2012
BSC-ES/AQF WRFv3.5+CMAQv5.0+HERMESv2+BSC-DREAM8b v2.0 Annual PM10 ($\mu\text{g}/\text{m}^3$)
Forecast - 2012 - Iberian Peninsula Res: 4x4km



2013
BSC-ES/AQF WRFv3.5+CMAQv5.0+HERMESv2+BSC-DREAM8b v2.0 Annual PM10 ($\mu\text{g}/\text{m}^3$)
Forecast - 2013 - Iberian Peninsula Res: 4x4km



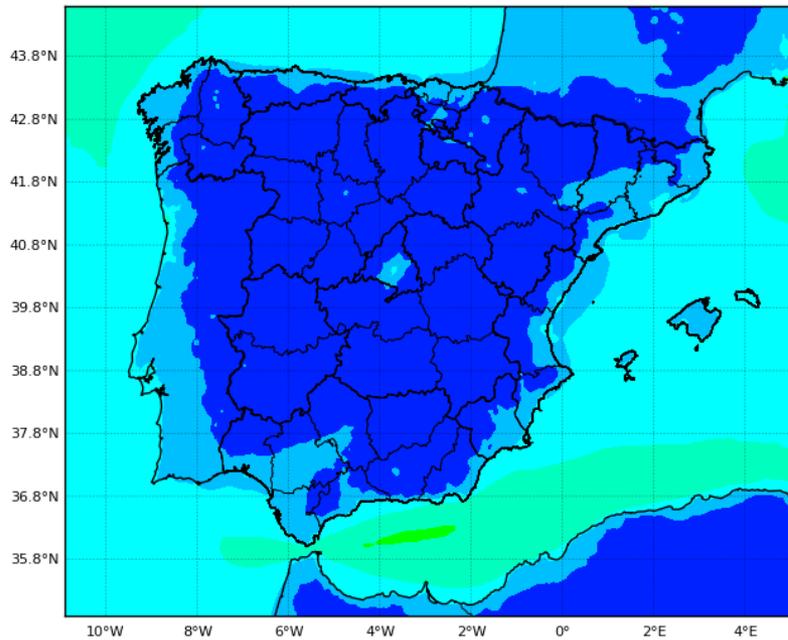
2014
BSC-ES/AQF WRFv3.5+CMAQv5.0+HERMESv2+BSC-DREAM8b v2.0 Annual PM10 ($\mu\text{g}/\text{m}^3$)
Cv3F-2014 - Iberian Peninsula Res: 4x4km



PM10 by model contribution



BSC-ES/AQF WRFv3.5+CMAQv5.0+HERMESv2 Annual PM10 ($\mu\text{g}/\text{m}^3$)
Cv3F-2014 - Iberian Peninsula Res: 4x4km



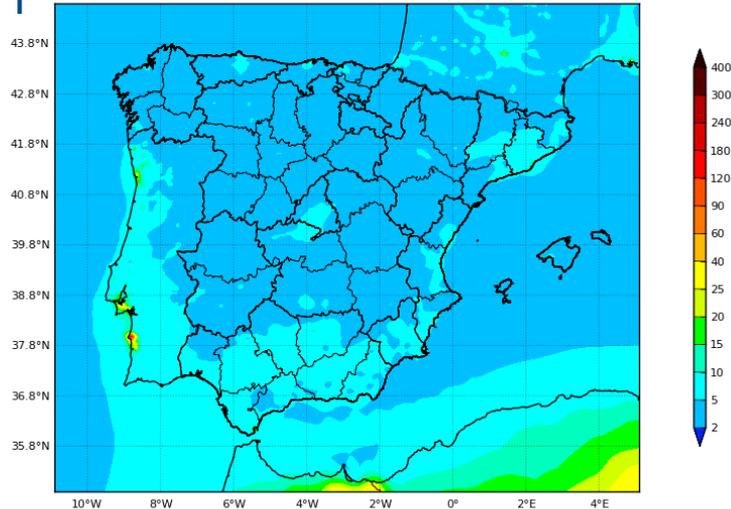
BSC-ES/AQF WRFv3.5+CMAQv5.0+HERMESv2+BSC-DREAM8b v2.0 Annual PM10 ($\mu\text{g}/\text{m}^3$)
Cv3F-2014 - Iberian Peninsula Res: 4x4km



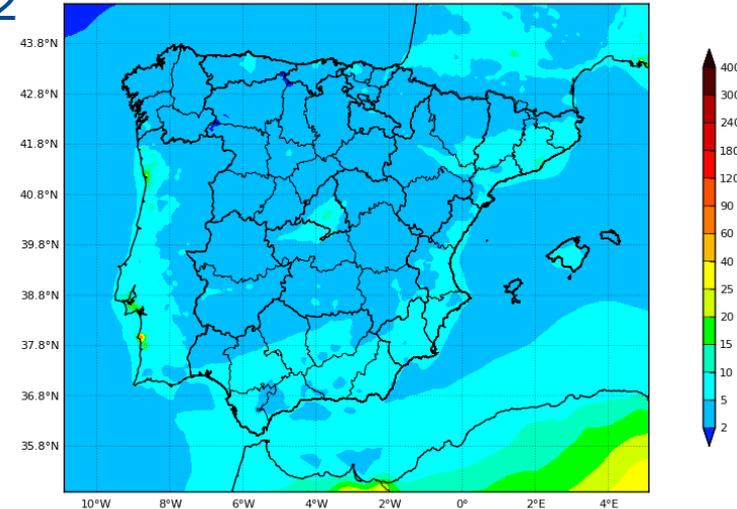
PM2.5 Annual mean on hourly basis



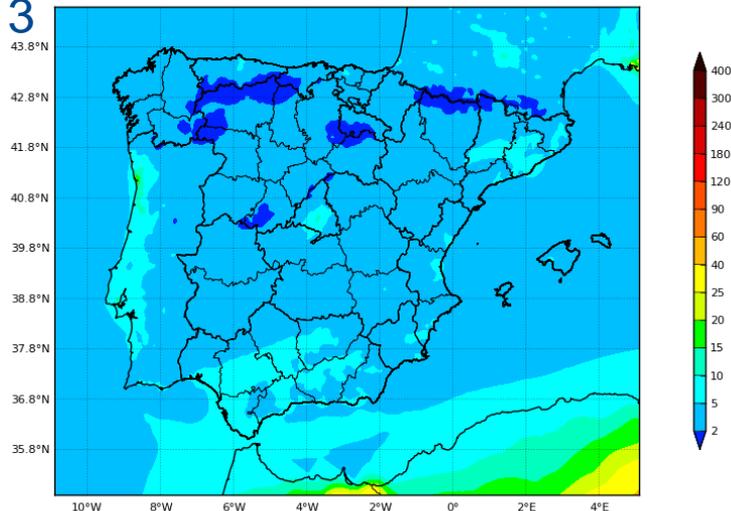
2011
BSC-ES/AQF WRFv3.5+CM_v3.2.0+HER_4.5iv2+BSC-I_EAM8b v2.0 Annual PM25 ($\mu\text{g}/\text{m}^3$)
Forecast - 2011 - Iberian Peninsula Res: 4x4km



2012
BSC-ES/AQF WRFv3.5+CMAQv5.0+HERMESv2+BSC-DREAM8b v2.0 Annual PM25 ($\mu\text{g}/\text{m}^3$)
Forecast - 2012 - Iberian Peninsula Res: 4x4km



2013
BSC-ES/AQF WRFv3.5+CMAQv5.0+HERMESv2+BSC-DREAM8b v2.0 Annual PM25 ($\mu\text{g}/\text{m}^3$)
Forecast - 2013 - Iberian Peninsula Res: 4x4km



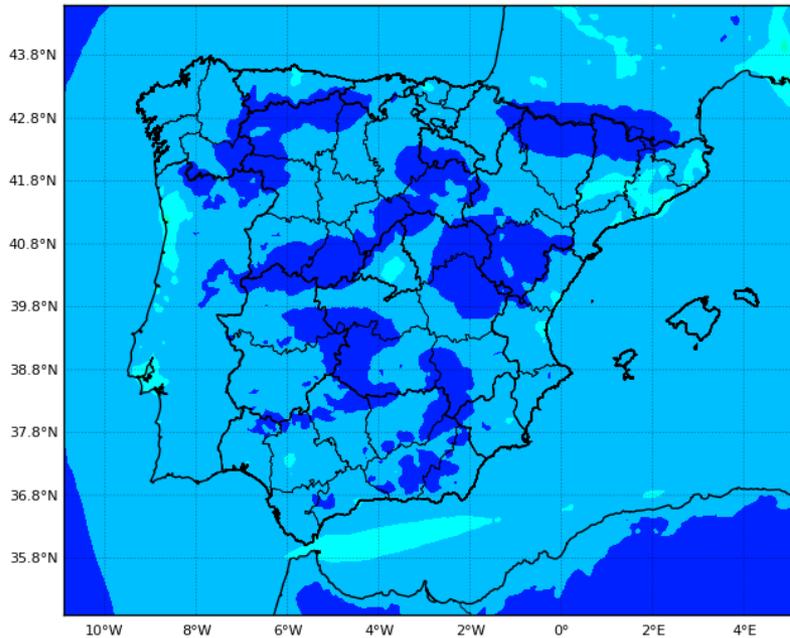
2014
BSC-ES/AQF WRFv3.5+CMAQv5.0+HERMESv2+BSC-DREAM8b v2.0 Annual PM25 ($\mu\text{g}/\text{m}^3$)
Cv3F-2014 - Iberian Peninsula Res: 4x4km



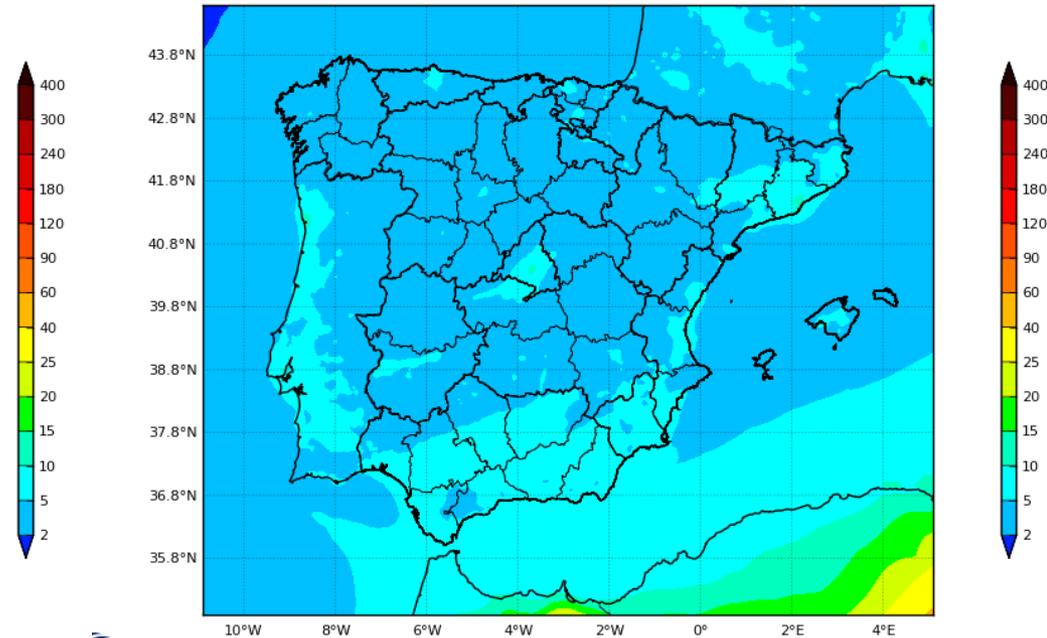
PM2.5 by model contribution



BSC-ES/AQF WRFv3.5+CMAQv5.0+HERMESv2 Annual PM25 ($\mu\text{g}/\text{m}^3$)
Cv3F-2014 - Iberian Peninsula Res: 4x4km

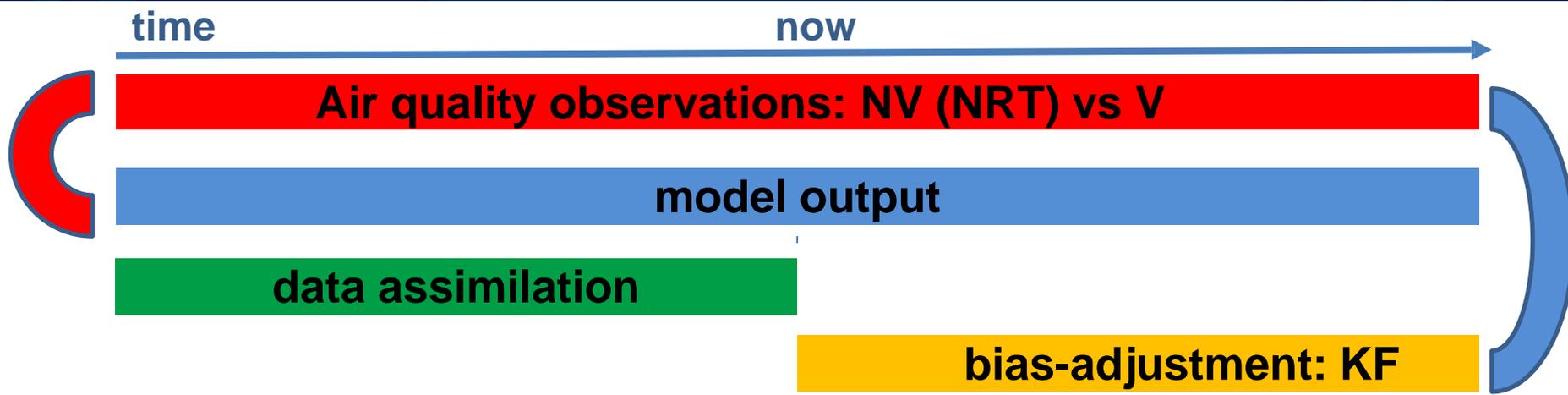


BSC-ES/AQF WRFv3.5+CMAQv5.0+HERMESv2+BSC-DREAM8b v2.0 Annual PM25 ($\mu\text{g}/\text{m}^3$)
Cv3F-2014 - Iberian Peninsula Res: 4x4km



**Evaluation of the CALIOPE results
with and without Kalman Filter (KF)
respect
to the use not validated (NV) or validated observations (V)**

On the usage of observations



 Barcelona Supercomputing Center <small>Centro Nacional de Supercomputación</small> Earth Sciences Department	Working document CALIOPE system	Date:
		Pág.: 1 de 7
		Códe:
Data base filtering of air quality measurement		

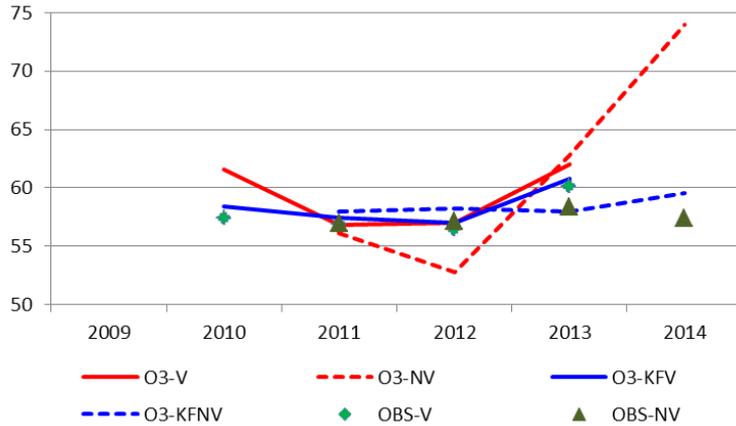
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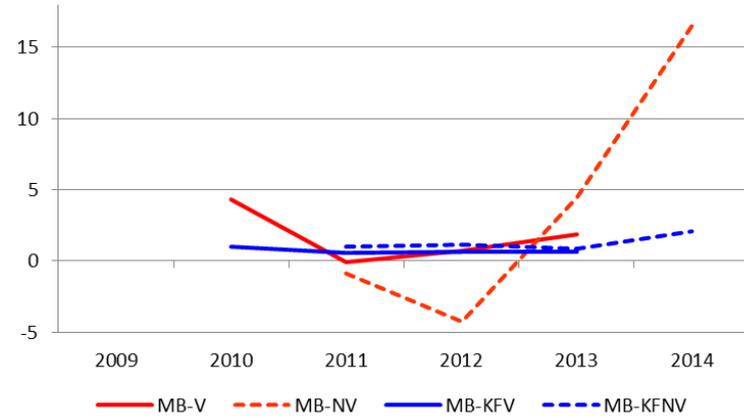
O₃ Annual average on hourly basis



Annual mean O₃ (µg/m³)

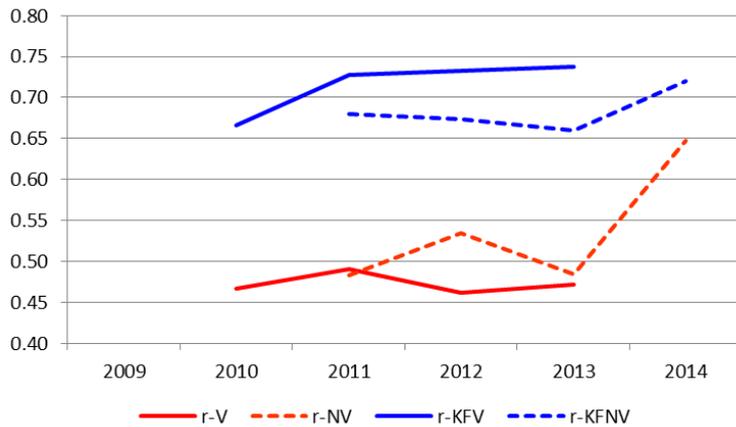


Annual Mean Bias O₃ (µg/m³)

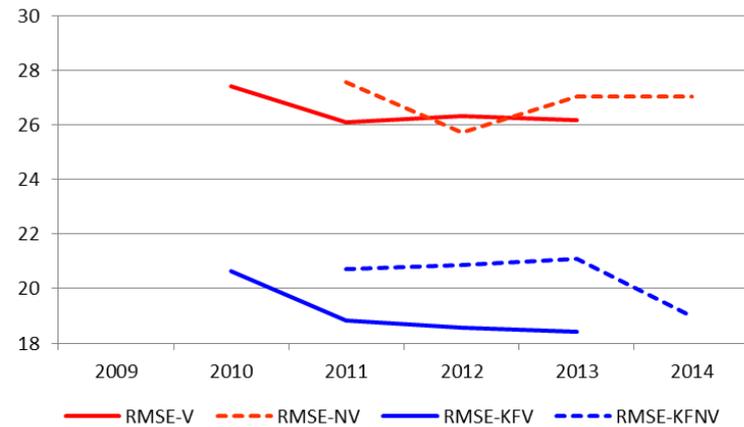


Observations: ◆ OBS-V: Validated
▲ OBS-NV: Not Validated

Annual correlation O₃



Annual Run Mean Square Error O₃ (µg/m³)



— O3-V: Model evaluated with *validated* observations
- - - O3-NV: Model evaluated with *not validated* observations

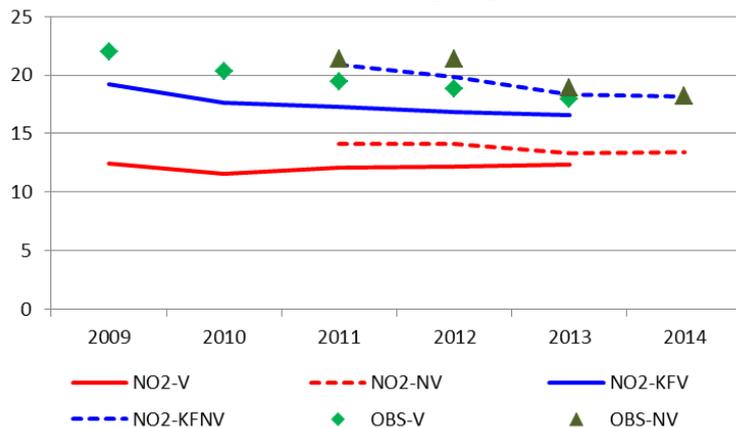
— O3-KFV: KF evaluated with *validated* observations
- - - O3-KFNV: KF evaluated with *not validated* observations

For the validated observations with KF the MB is reduced in average ~60%, the correlation is improved in ~50% and the RMSE is reduced in ~50%

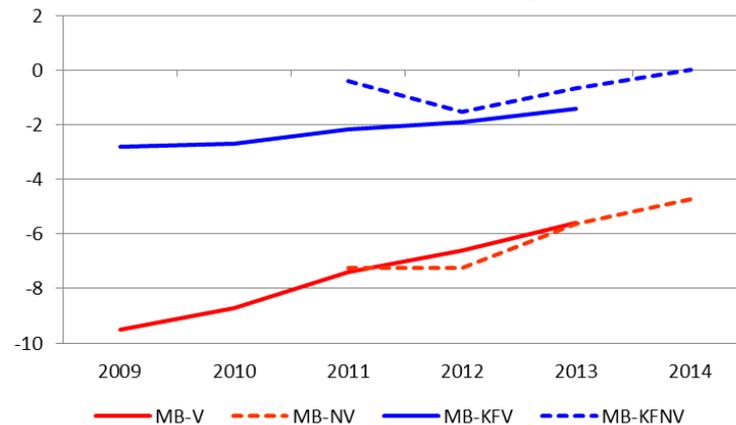
NO₂ Annual average on hourly basis



Annual mean NO₂ (µg/m³)

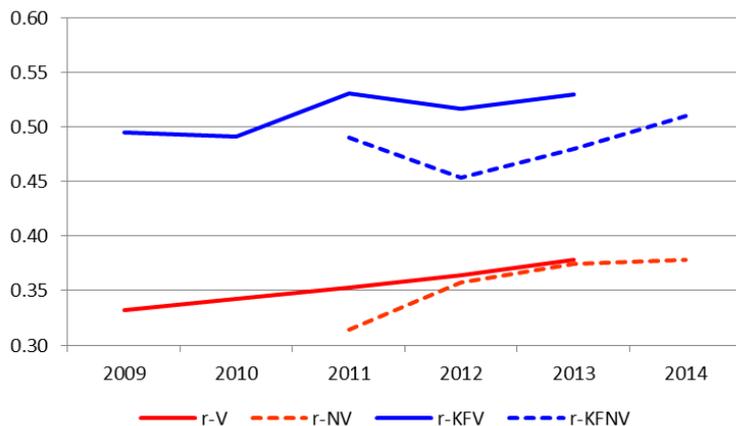


Annual Mean Bias NO₂ (µg/m³)

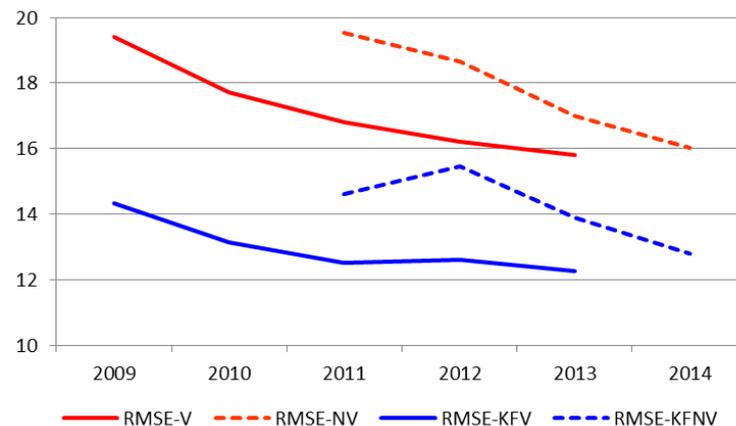


Observations: ◆ OBS-V: Validated
▲ OBS-NV: Not Validated

Annual correlation NO₂



Annual Run Mean Square Error NO₂ (µg/m³)



— O3-V: Model evaluated with validated observations
- - - O3-NV: Model evaluated with not validated observations

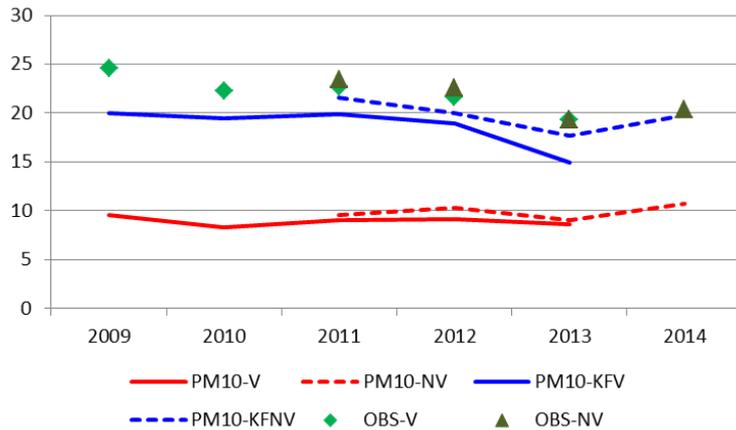
— O3-KFV: KF evaluated with validated observations
- - - O3-KFNV: KF evaluated with not validated observations

For the validated observations with KF the MB is reduced in average ~71%, the correlation is improved in ~43% and the RMSE is reduced in ~24%

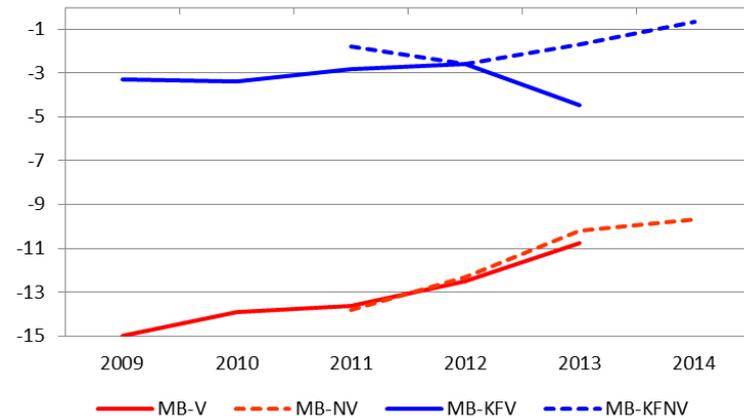
PM10 Annual average on hourly basis



Annual mean PM10 ($\mu\text{g}/\text{m}^3$)

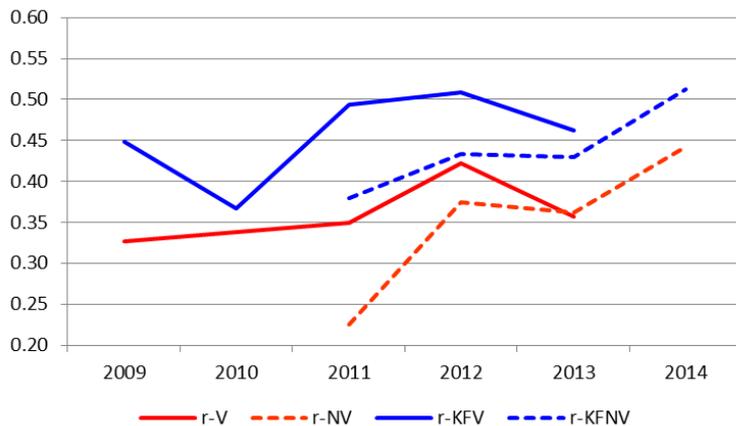


Annual Mean Bias PM10 ($\mu\text{g}/\text{m}^3$)

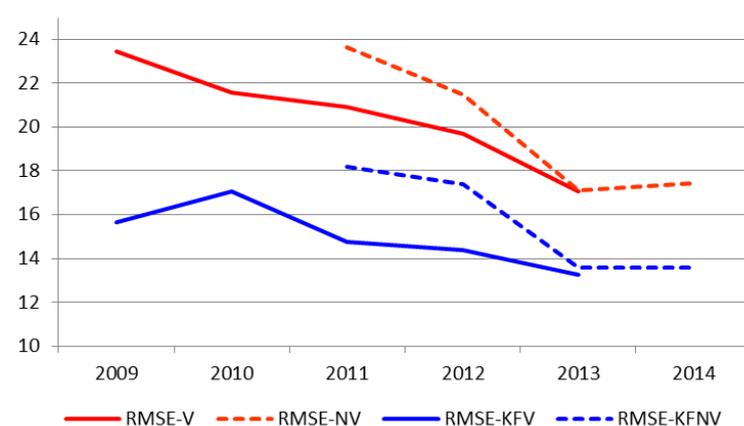


Observations: ◆ OBS-V: Validated
▲ OBS-NV: Not Validated

Annual correlation PM10



Annual Run Mean Square Error PM10 ($\mu\text{g}/\text{m}^3$)



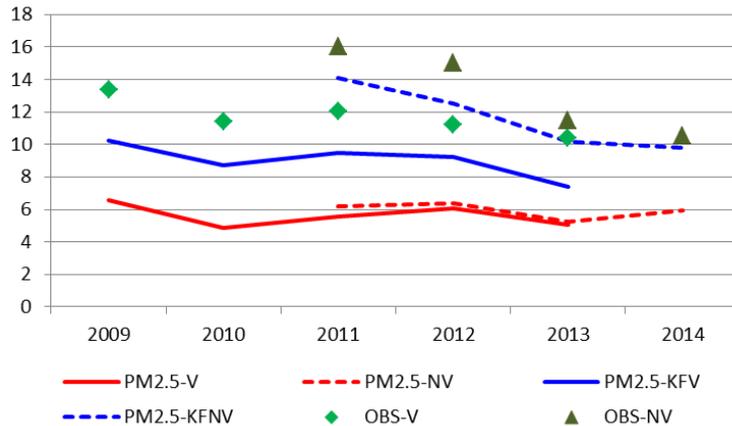
— O3-V: Model evaluated with validated observations
- - - O3-NV: Model evaluated with not validated observations

— O3-KFV: KF evaluated with validated observations
- - - O3-KFNV: KF evaluated with not validated observations

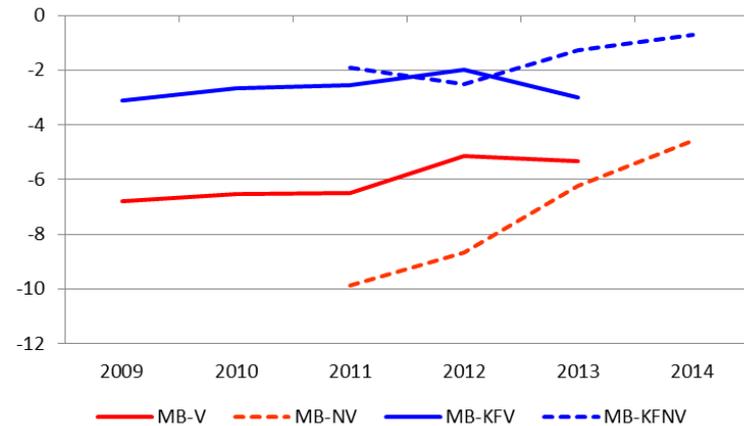
For the validated observations with KF the MB is reduced in average ~74%, the correlation is improved in ~24% and the RMSE is reduced in ~25%

PM2.5 Annual average on hourly basis

Annual mean PM2.5 ($\mu\text{g}/\text{m}^3$)

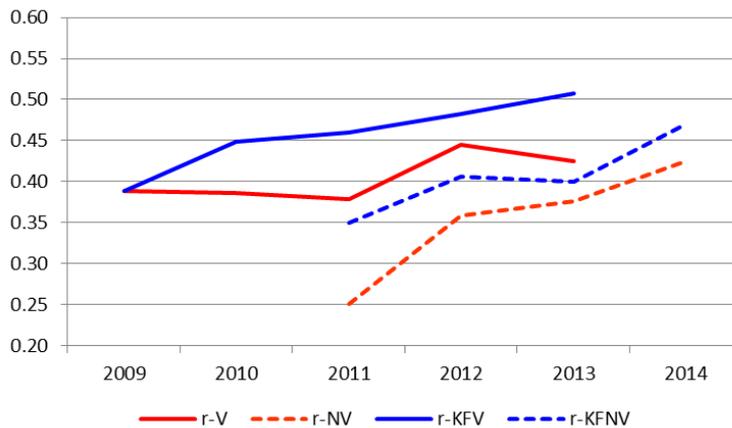


Annual Mean Bias PM2.5 ($\mu\text{g}/\text{m}^3$)

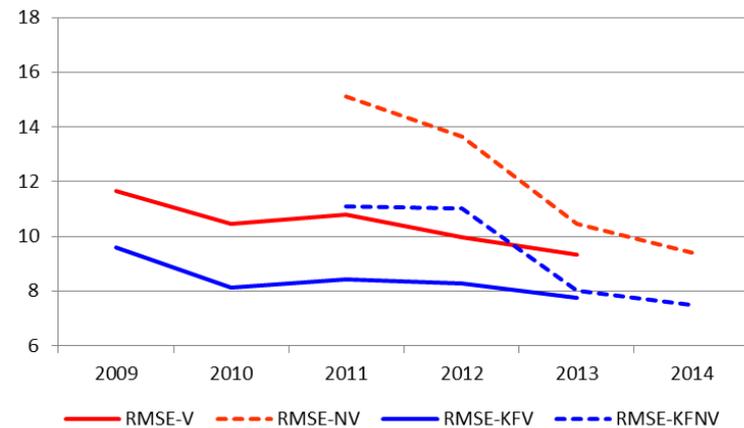


Observations: ◆ OBS-V: Validated
▲ OBS-NV: Not Validated

Annual correlation PM2.5



Annual Run Mean Square Error PM2.5 ($\mu\text{g}/\text{m}^3$)



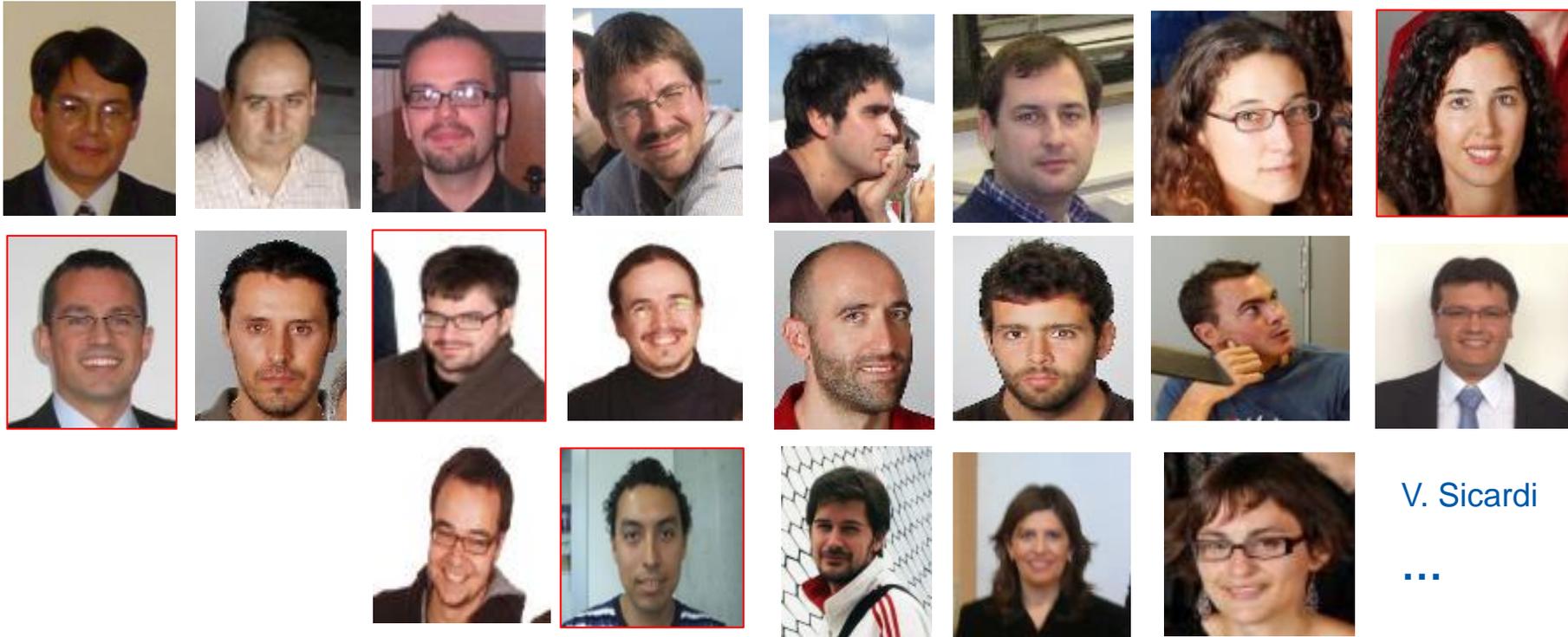
— O3-V: Model evaluated with validated observations
- - - O3-NV: Model evaluated with not validated observations

— O3-KFV: KF evaluated with validated observations
- - - O3-KFNV: KF evaluated with not validated observations

For the validated observations with KF the MB is reduced in average ~56%, the correlation is improved in ~16% and the RMSE is reduced in ~20%

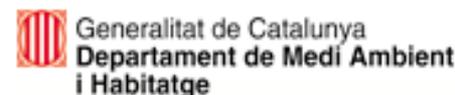
- The KF post-process has contributed to improving significantly the air quality forecast results for O_3 , NO_2 , PM_{10} and $PM_{2.5}$.
- MB and RMSE were reduced after the application of KF: between 50-75% and 20-30%, respectively; and r has increased for all pollutants: O_3 : 51%, NO_2 : 43%, PM_{10} : 25% and $PM_{2.5}$: 16%.
- O_3 skills are difficult to improve because depend strongly of the boundary conditions and the nocturnal chemistry.
- NO_2 skills are improved, especially the r and RMSE; the MB has also improved due to improved levels.
- PM_{10} and $PM_{2.5}$ have about the same behavior of the NO_2 , the r and RMSE have improved, but the mean of the model is roughly constant.
- The use of validated observations (no NRT) improve the statistical skills.

CALIOPE AQFS team (2006-2014) and institutional support



V. Sicardi

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Thanks for your attention

jose.baldasano@bsc.es

