Optimizing initial values and emission factors on mesoscale air quality modelling using 4D-var data assimilation

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How can we improve air quality modelling predictions?

Objectives

- **Optimise chemical initial values** (background concentrations)
- **Optimise emission factors** – update emissions

This study needs…

- Assimilation of observed data (*in-situ* stations, satellites …)

4D-var data assimilation

Inverse modelling

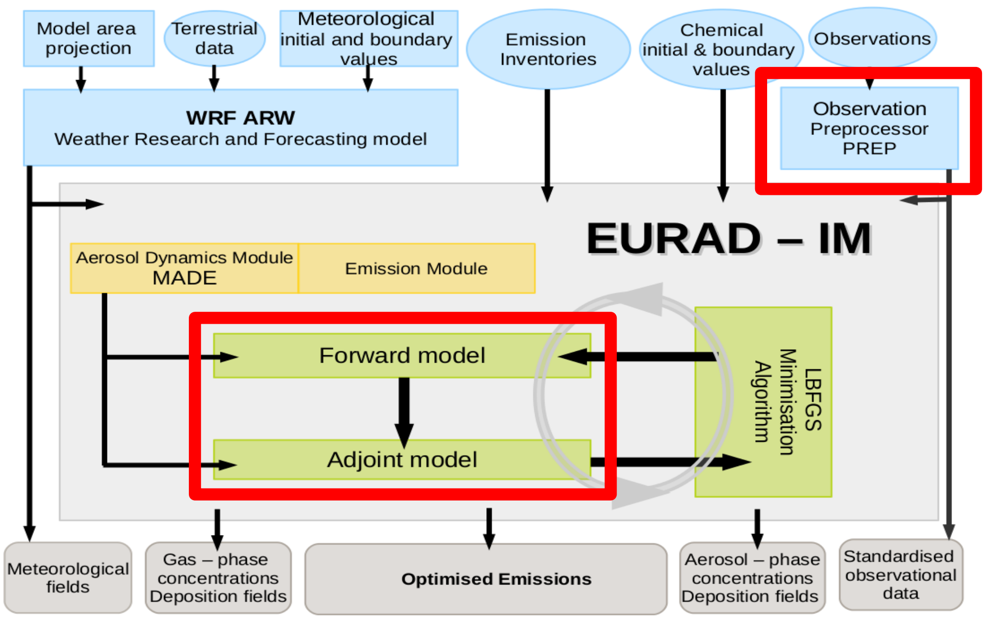
4D-var data assimilation – Inverse modelling techniques

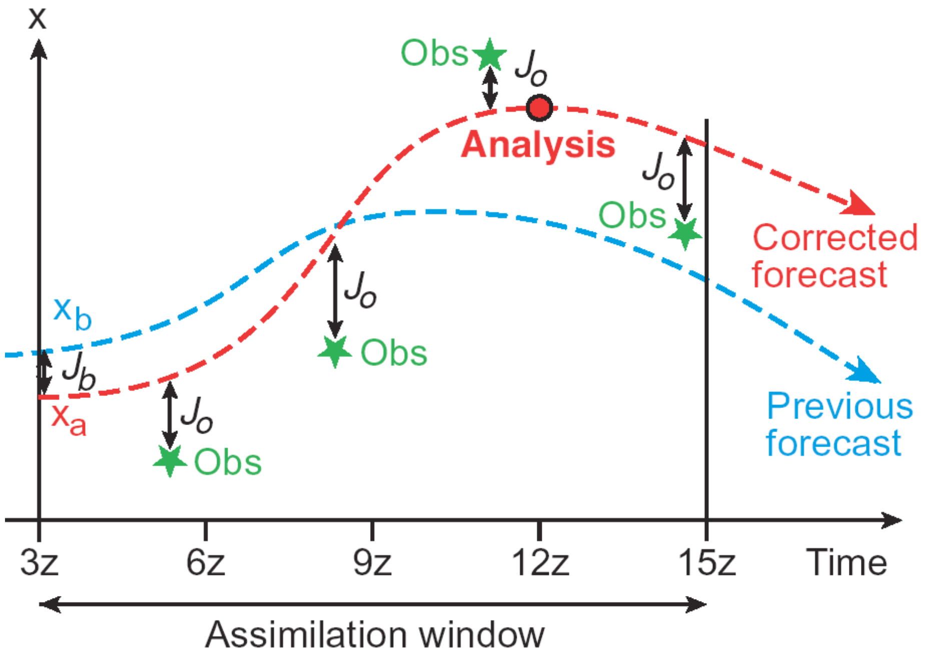
Definition

Data assimilation is an **analysis technique** in which the **observed information** is combined with physical and chemical knowledge of atmospheric processes encoded in the **numerical models**.

The **consistency of the system** is guaranteed by **the inverse simulation** of the emitted species and their products.

EURopean Air pollution Dispersion – Inverse Model





Cost function

Measures the distance between the model state – observations

– background

J_{iv} $\qquad$ J_{obs} $\qquad$ J_{ef}

$$J(x_o, e_o) = \frac{1}{2}[x_o - x_b]^T \mathbf{B}^{-1}[x_o - x_b] + \frac{1}{2}\sum_{i=0}^{N}\left([HM_i(x_o) - y_i]^T \mathbf{R}^{-1}[HM_i(x_o) - y_i]\right) + \frac{1}{2}[e_o - e_b]^T \mathbf{K}^{-1}[e_o - e_b]$$

Model state
X_0: analysis
X_b: 1st guess

Background Error Covariance Matrix

Model and Observational Operator

Observations Error Covariance Matrix

Emission Factor Error Covariance Matrix

To minimize!

BECM for emission factors – K

Describes the emission rate covariances between emitted species at each location

$$K = G D^{1/2} D^{T/2} G$$

G: **Standard deviations** of the emission factors

Species	Standard deviations ($\delta \mathbf{u} = \ln f$)
SO_2	10.6
NH_3	10.6
NO	5.3
others	13.9

Personal communication with emission experts

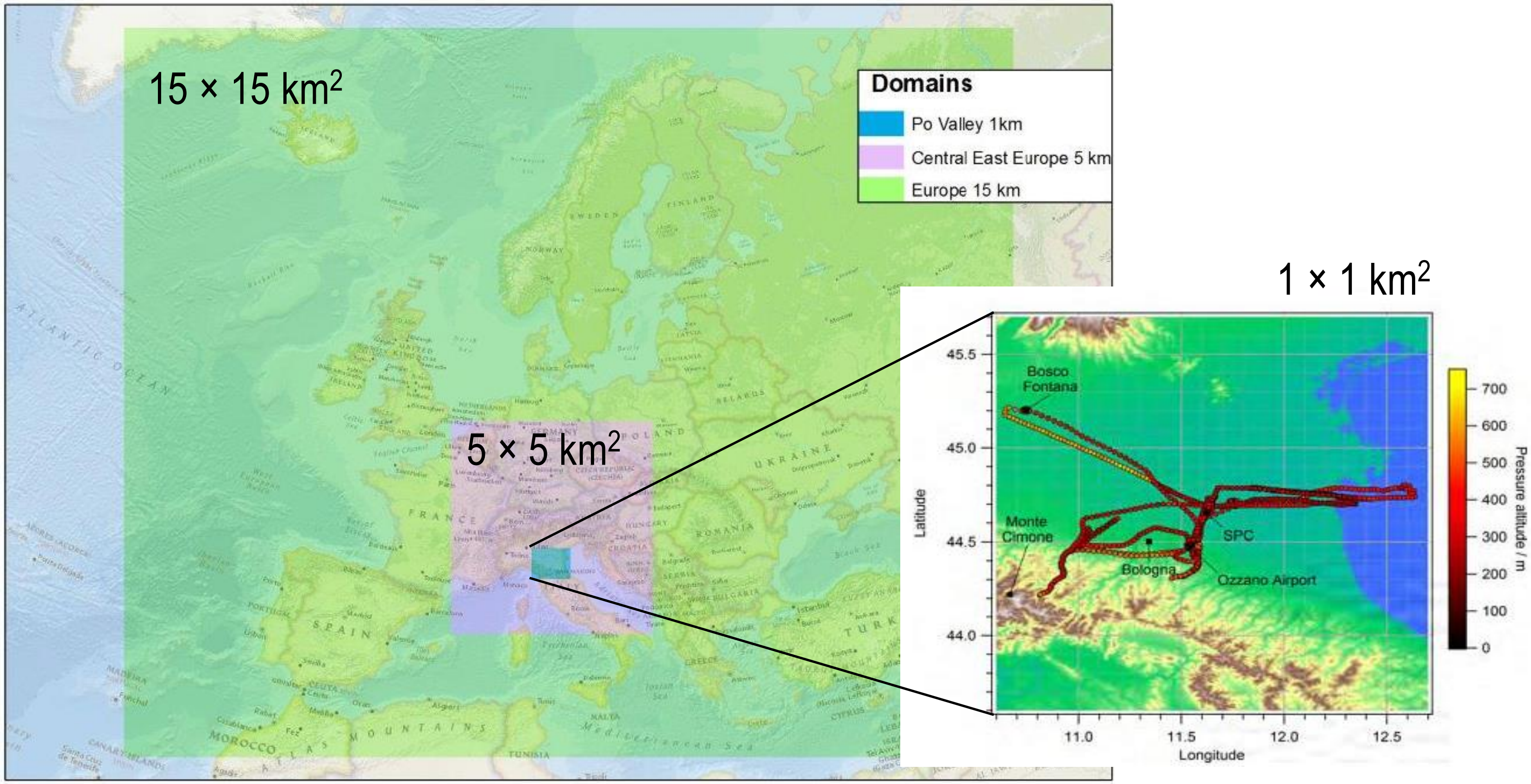
D : Background **correlations** of emitted species

	SO2	SO4	NO2	NO	ALD	HCHO	NH3	HC3	HC5	HC8	ETH	CO	ETE	OLT	OLI	TOL	XYL	KET	ISO	DIEN	ORA2	LIM	GLY	API
SO2	100	40	12	12	0.4	0.4	0.4	0.4	0.4	0.4	0.4	9	0.4	0.4	0.4	0.4	0.4	0.4	0	0.4	0.4	0	0.4	0
SO4		100	12	12	0.4	0.4	0.4	0.4	0.4	0.4	0.4	9	0.4	0.4	0.4	0.4	0.4	0.4	0	0.4	0.4	0	0.4	0
NO2			100	26	8	8	7	8	8	8	8	12	8	8	8	7	7	8	0.4	8	5	0.4	8	0.4
NO				100	8	8	7	8	8	8	8	12	8	8	8	7	7	8	0.4	8	5	0.4	8	0.4
ALD					100	26	5	6	6	6	6	5	10	6	6	5	5	26	0.3	6	5	0.3	26	0.3
HCHO						100	5	6	6	6	6	5	10	6	6	5	5	26	0.3	6	5	0.3	26	0.3
NH3							100	5	5	5	5	5	5	5	5	5	5	5	0.3	5	5	0.3	5	0.3
HC3								100	23	23	23	5	18	15	15	6	6	6	0.3	18	8	0.3	6	0.3
HC5									100	23	23	5	18	15	15	6	6	6	0.8	18	8	0.8	6	0.8
HC8										100	23	5	18	15	15	6	6	6	0.8	18	8	0.8	6	0.8
ETH											100	5	18	15	15	6	6	6	0.8	18	8	0.8	6	0.8
CO												100	6	5	5	5	5	5	0.3	5	5	0.3	5	0.3
ETE													100	23	23	6	6	10	1	18	5	1	10	1
OLT														100	27	5	5	6	15	5	10	15	6	15
OLI															100	5	5	6	15	5	10	15	6	15
TOL																100	24	5	0.3	5	5	0.3	5	0.3
XYL																	100	5	0.3	5	5	0.3	5	0.3
KET																		100	0.3	6	5	0.3	26	0.3
ISO																			100	0.8	18	40	0.4	40
DIEN																				100	5	15	6	15
ORA2																					100	15	5	15
LIM																						100	0.3	40
GLY																							100	0.3
API																								100

>10% | >1% | < 1%

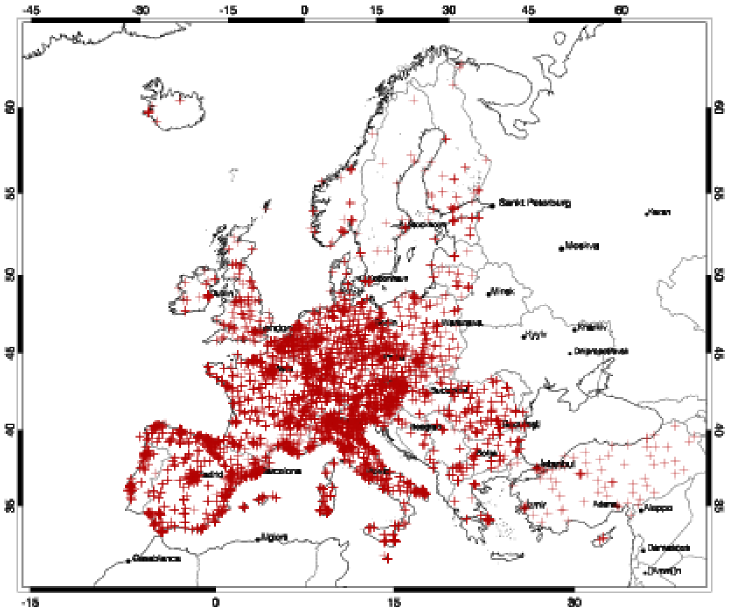
Case study

Case study: Po valley (10-12 . 07 . 2012)



EC FP7 PEGASOS campaings

Case study: observations



Ground stations observations

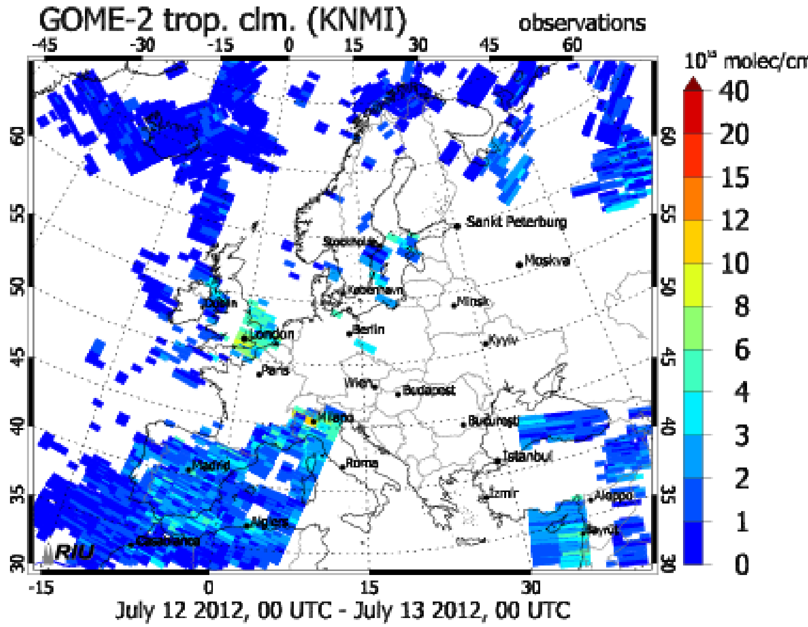
AirBase – the European air quality database (NO_2, O_3, CO and SO_2)

Satellite observations

GOME-2 (NO_2)

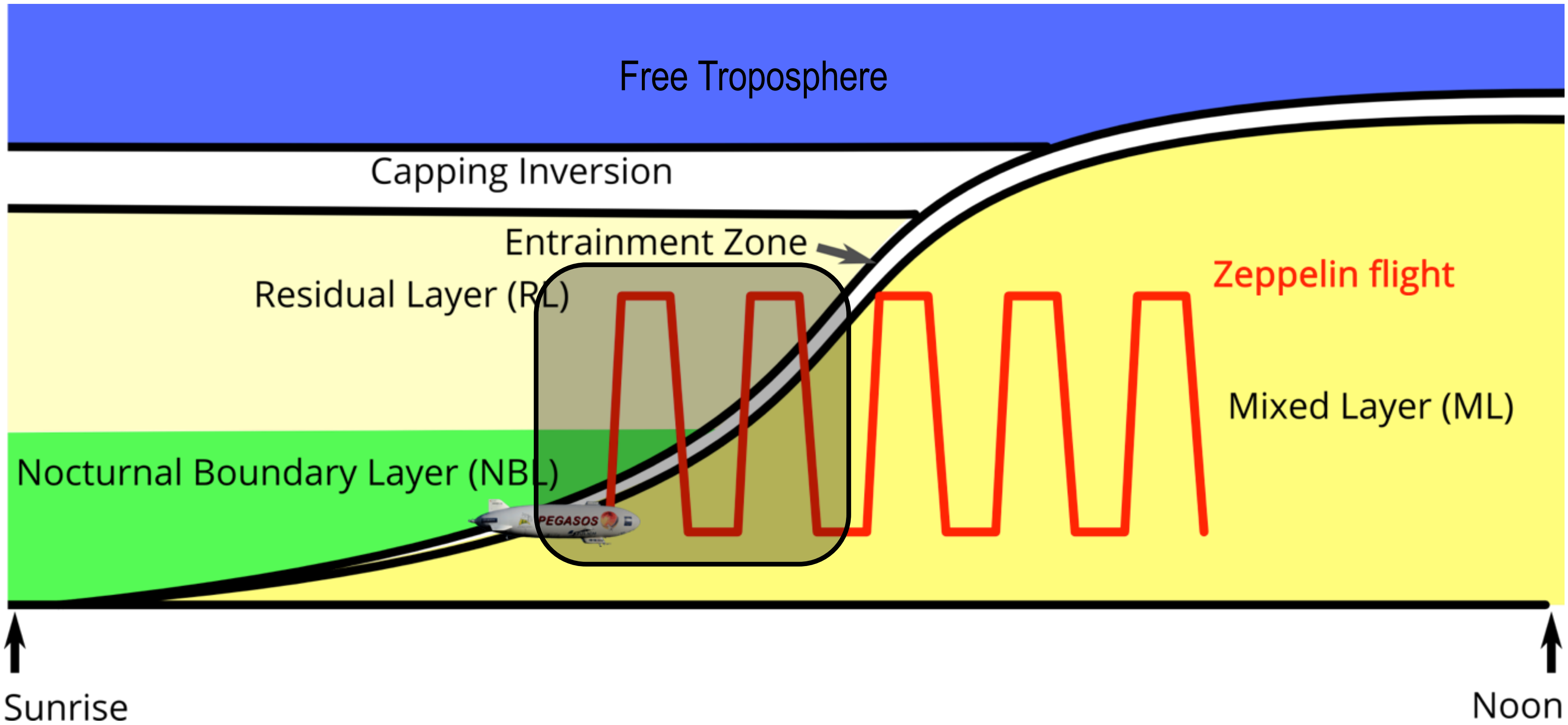
MOPPIT (CO, O_3)

Zeppelin data: NO_2, O_3, CO



NO_2 tropospheric column

Case study: Zeppelin NT flight pattern



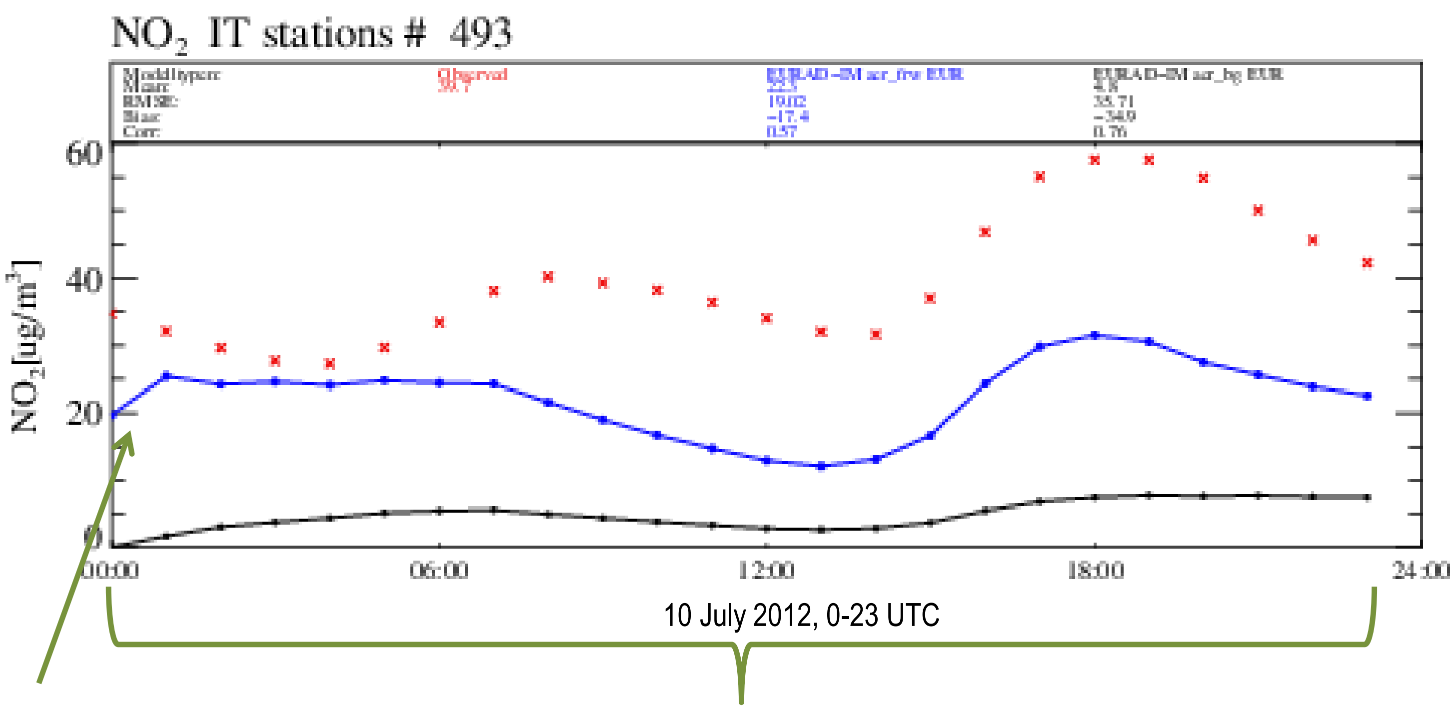
Adapted from Stull, 1988

How campaign data can indicate corrections to the model?

Case study: results (routinely observations)

European domain (15 km)

****** In situ non-assimilated observations
------- Background (ref.run)
------- Analysis



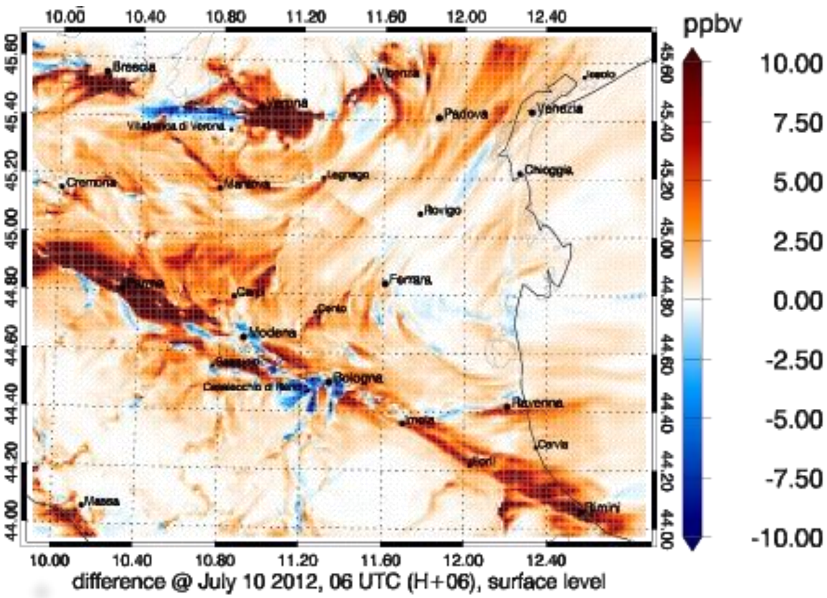
IV optimization

EF optimization

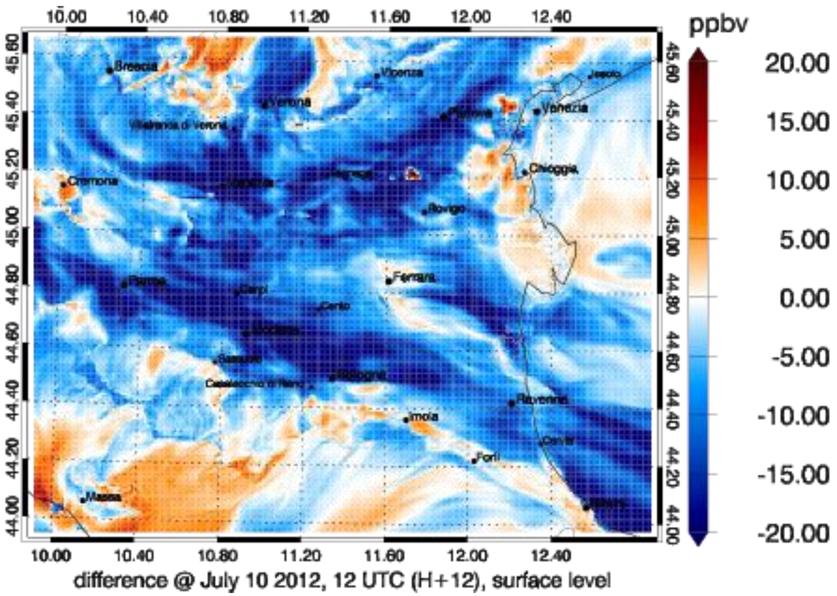
Case study: results (routinely observations)

Δ (analysis – background)

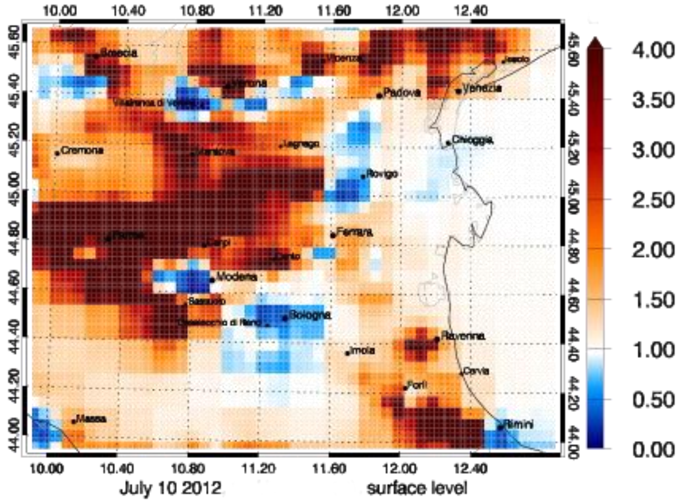
NO$_2$



O$_3$



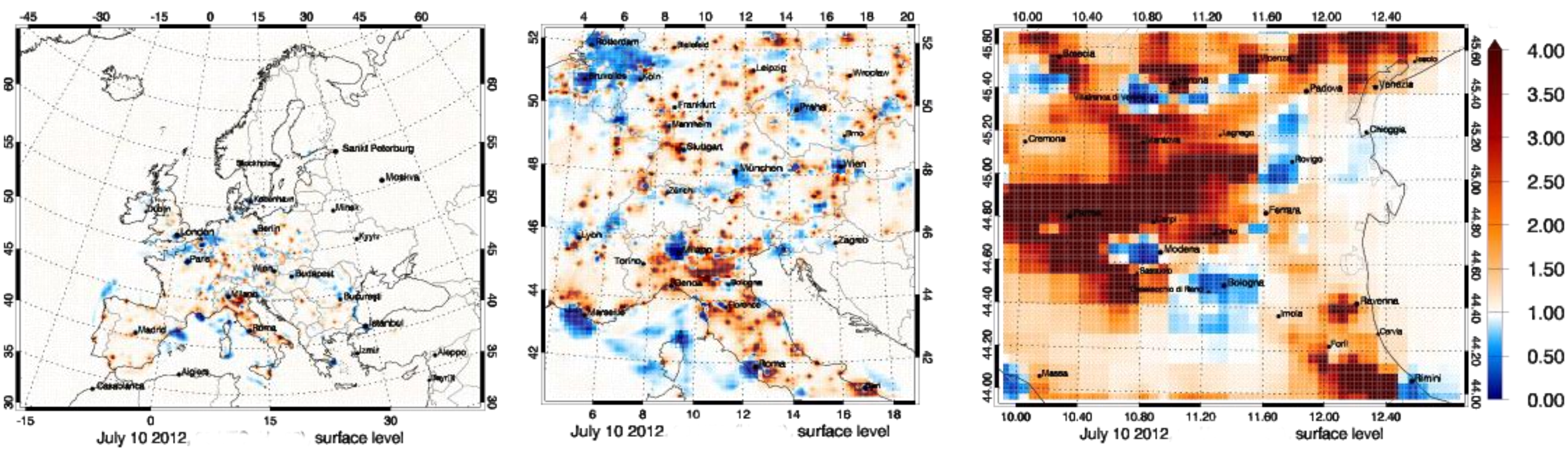
Emission factors corrections (NO)



Allows the update of emission inventories

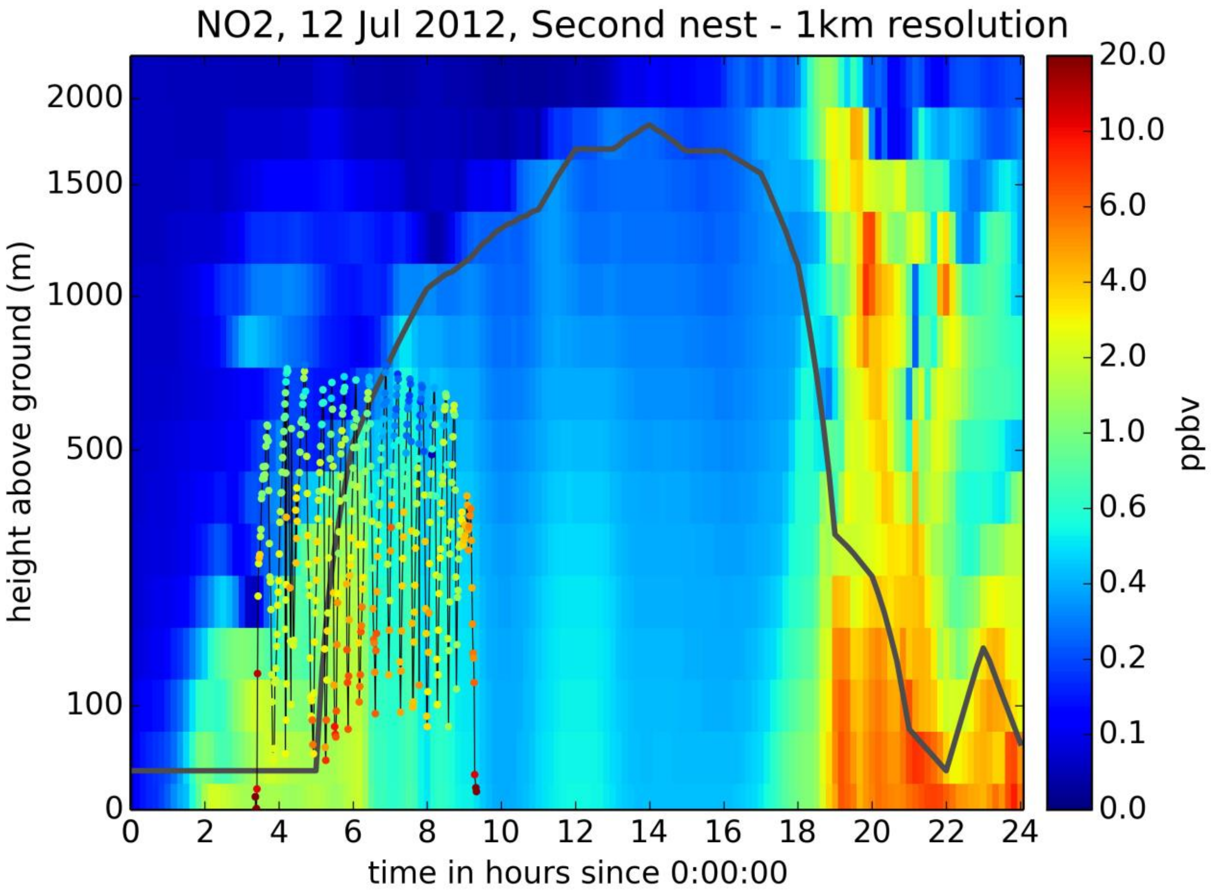
Case study: results (routinely observations)

Emission factors corrections (NO)



4D-var in high resolved grids identify emission patterns

Case study: results (assimilation of Zeppelin campaign)



Hovmøeller plot

Resolution: 1 x 1 km^2

10 min

- In the mixed layer, the observed NO_2 **concentrations are higher** than the analysed ones, up to 300-400 m. (may be due to problems of PBL height simulation – WRF parameterization)
- Analysis (background colour) **match** with the airborne data in upper altitudes (500-700m) until around 8:00, as well as at close to 300 m until 6:00.

Aerosols


Po Valley (Feb. 2015)

Optimization of:

Initial values

Emission factors (under development)

Aerosols – initial values optimization

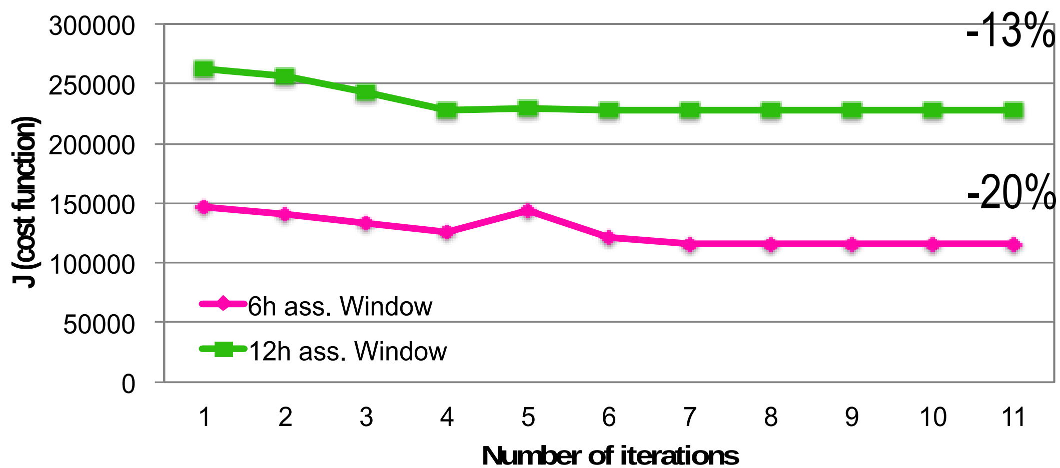
European domain (15×15km^2)

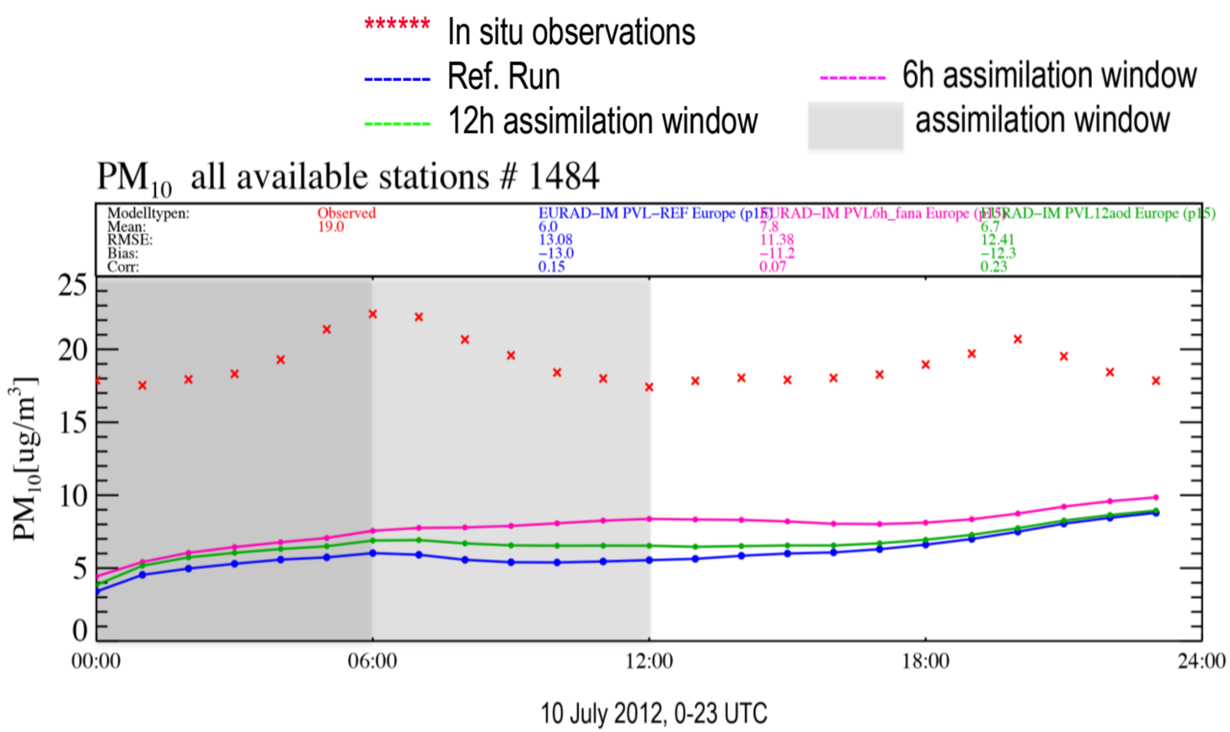
Observations:

Ground stations (PM10, PM2.5, NO_2, NH_3, O_3, CO, SO_2)

Assimilation window:

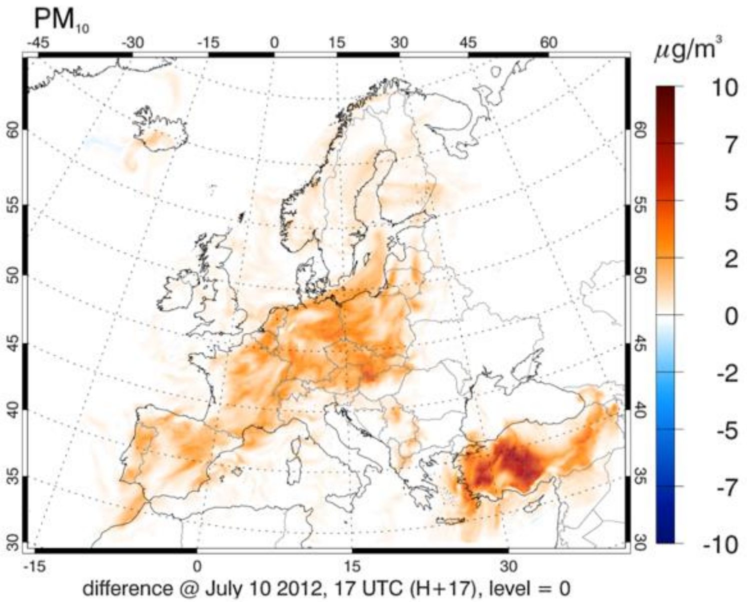
6 and 12h

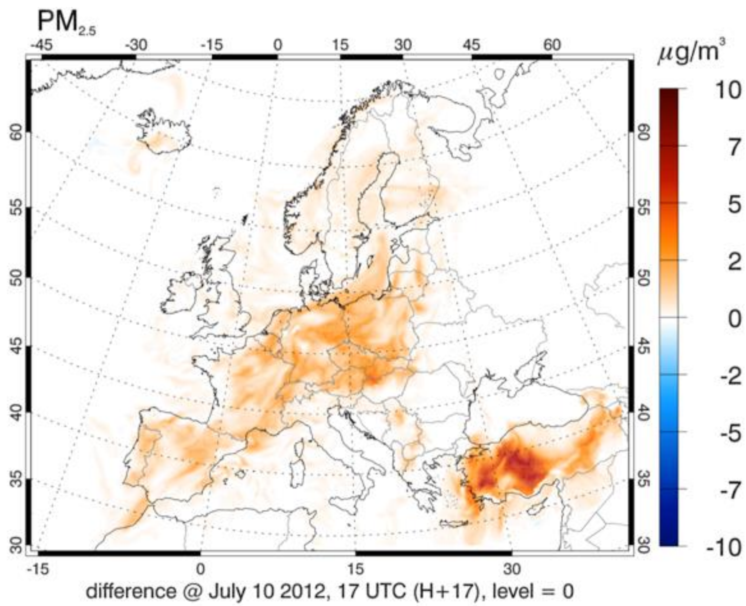


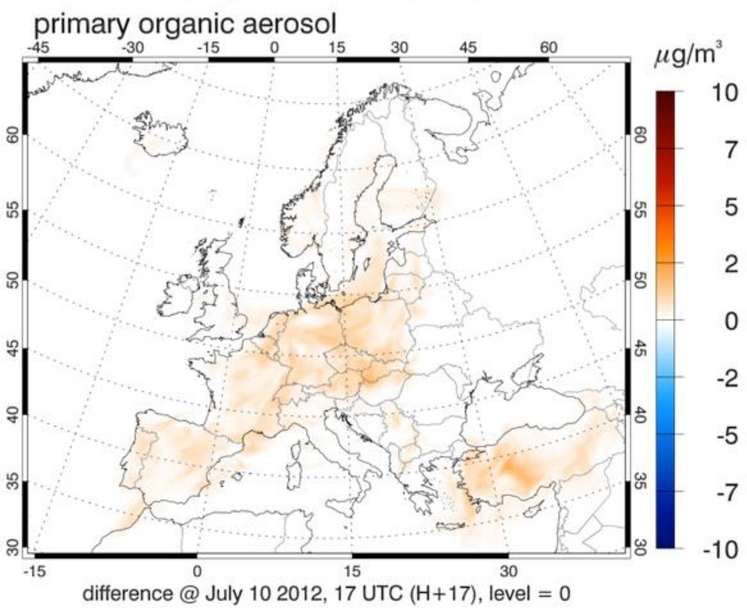


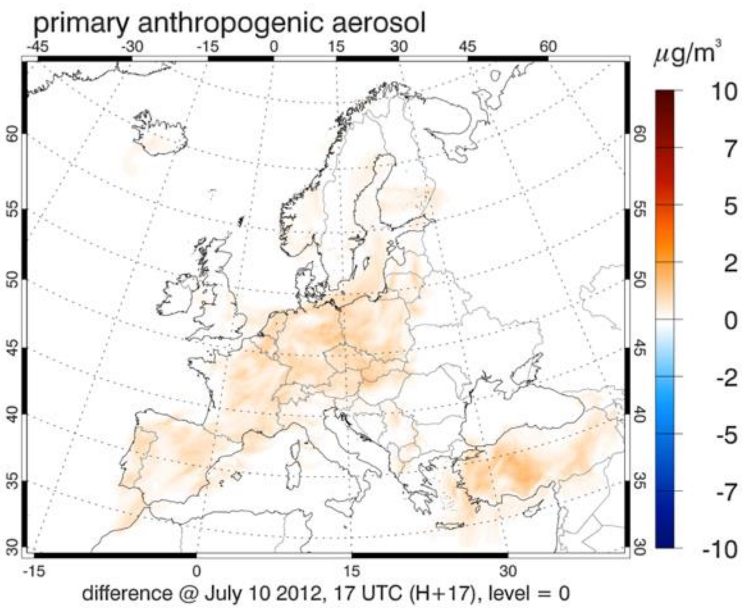
Aerosols – initial values

Δ = analysis – background



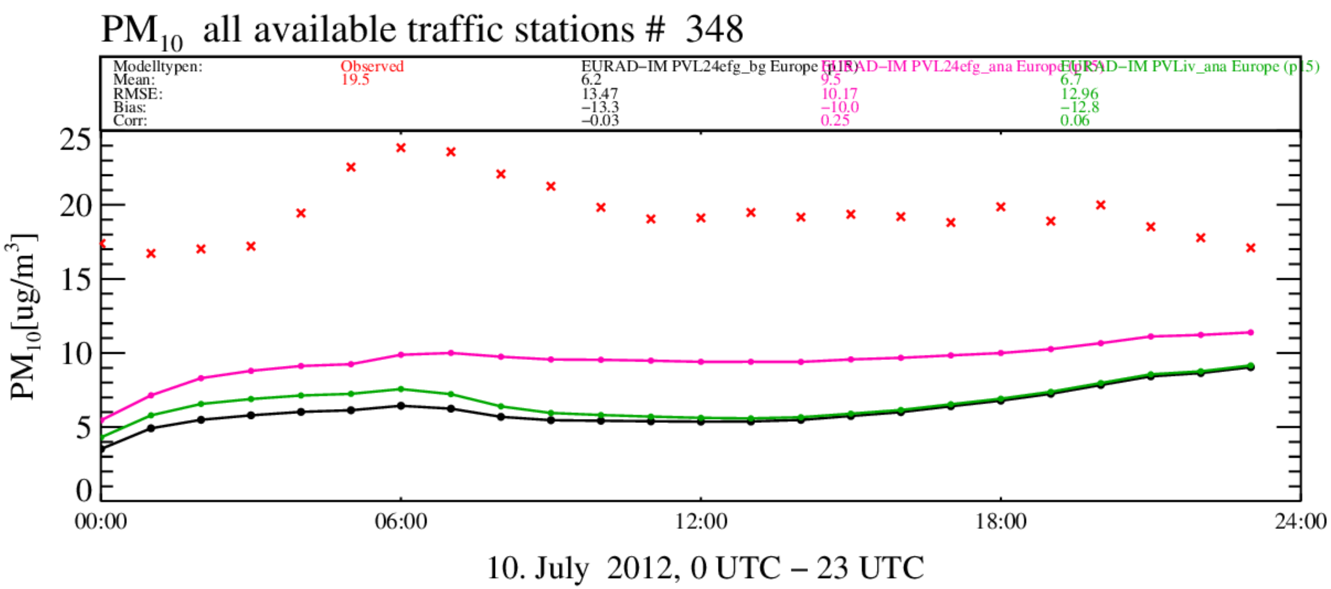






Aerosols – initial values optimization + gas phase

****** In situ observations
------- Background (1st guess)
------- Optimal IV aerosol (6h AW)
------- Optimal IV aerosol + (IV+EF) gas-phase (24h AW)



- $IV_{aerosol}$ + $(IV+EF)_{gas\text{-}phase}$ improved the model results (RMSE decreased ~ 5 $\mu g.m^{-3}$)
- EF optimization for aerosols is the key to assume daily profile of aerosol concentrations

Aerosol – EF optimization

Work in progress...

$$J(x_o, e_o) = \frac{1}{2}[x_o - x_b]^T \mathbf{B}^{-1}[x_o - x_b] + \frac{1}{2}\sum_{i=0}^{N}\left([HM_i(x_o) - y_i]^T \mathbf{R}^{-1}[HM_i(x_o) - y_i]\right) + \frac{1}{2}[e_o - e_b]^T \mathbf{K}^{-1}[e_o - e_b]$$

~10 routines were changed

4 new routines (adjoint model)

	VORGPAJ	VORGPAI	VECJ	VECI	VP25AJ	VP25AI	VANTHA	VSEASAJ	VSEAS	VSOILA
VORGPAJ	100	80	23	23	70	70	70	0	0	0
VORGPAI		100	23	23	70	70	70	0	0	0
VECJ			100	80	70	70	70	0	0	0
VECI				100	70	70	70	0	0	0
VP25AJ					100	80	70	12	12	12
VP25AI						100	70	12	12	12
VANHA							100	12	12	12
VSEASAJ								100	80	0
VSEAS									100	0
VSOILA										100

Background correlation matrix for EF

Final remarks

- Assimilation of emitted species and their products (space and time)
  – good performance
- Join optimisation of IV and EF to improve AQ predictions
- Application in high resolved grids (up to 1×1 km^2)
- **Contribute to correct emission inventories**

Thanks for your attention!