Evaluation of the ETC/ACM AQ maps using Delta tool and few remarks to MQO

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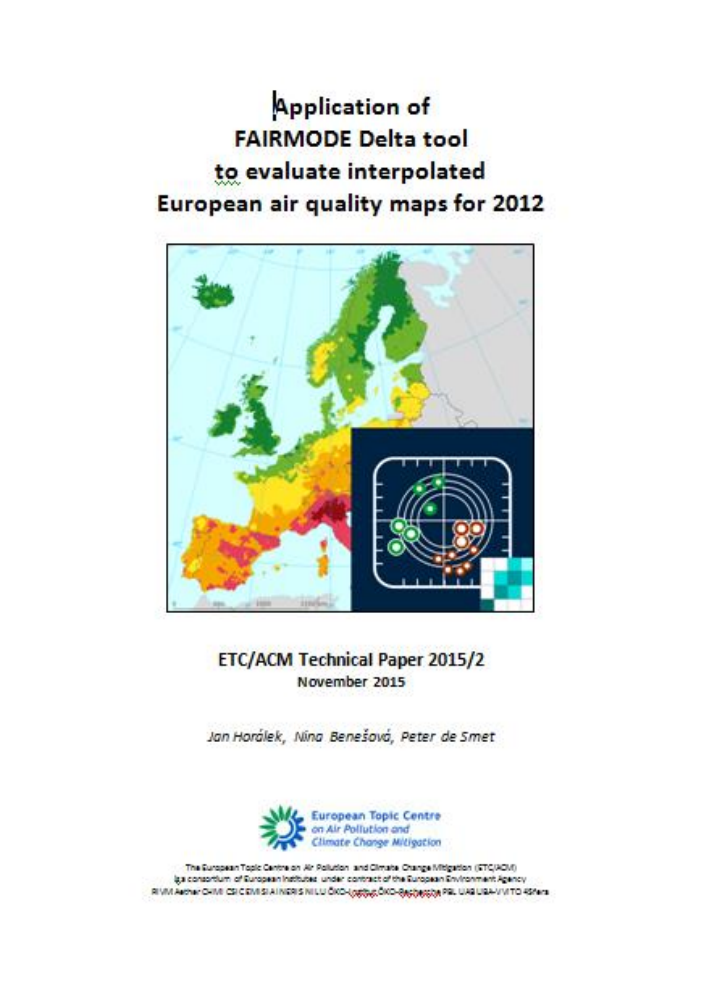
Presentation is based on

ETC/ACM Technical Paper 2015/2 „Application of FAIRMODE Delta tool to evaluate interpolated air quality maps for 2012“
acm.eionet.europa.eu/reports/

– based on Delta tool 5.0



Additionally, some results of Delta tool 5.3 will be presented.

1. Maps used in evaluation

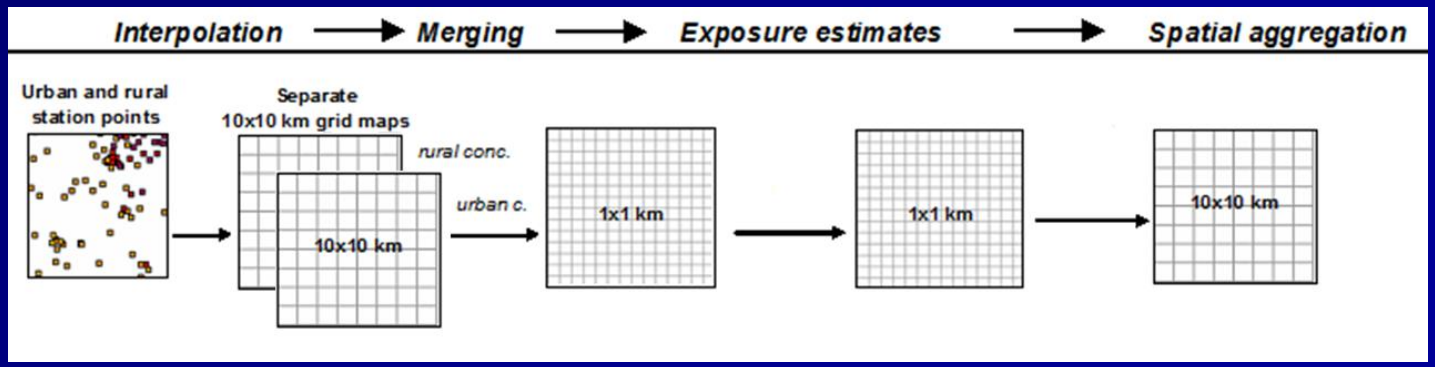
2. Delta tool, MQO and parameters used in

3. Evaluation by Delta tool and discussion

ETC/ACM mapping methodology

Regression – Interpolation – Merging Mapping

Linear regression model of monitoring data, CTM output and other supplementary data followed by ***interpolation of its residuals*** by kriging (so-called residual kriging).
Rural and urban background maps created separately (based on rural resp. urban/suburban background stations) are ***merged*** into the final maps using population density.



Analyzed maps

Final merged maps in 1x1 km resolution

PM_{10} – annual average for 2012
PM_{10} – 36th highest daily mean for 2012
$PM_{2.5}$ – annual average for 2012
O_3 – 26th highest daily maximum 8-hour mean for 2012

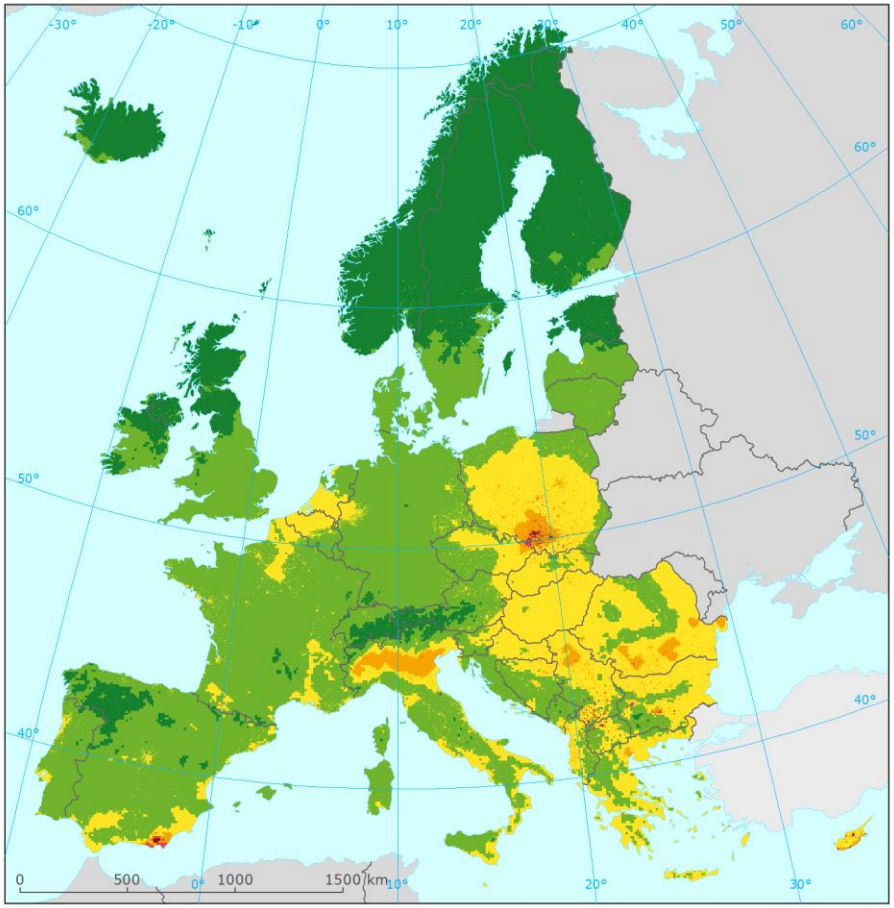
I.e.: two ***annual average*** maps, two ***percentile*** maps.

Two variants:

– maps created by full set of the stations (as routinely used)
evaluated by the same full set of the stations
– maps created by the MACC assimilation set of stations
evaluated by the MACC validation set of the stations

Analyzed maps

PM_{10} – annual average, 2012



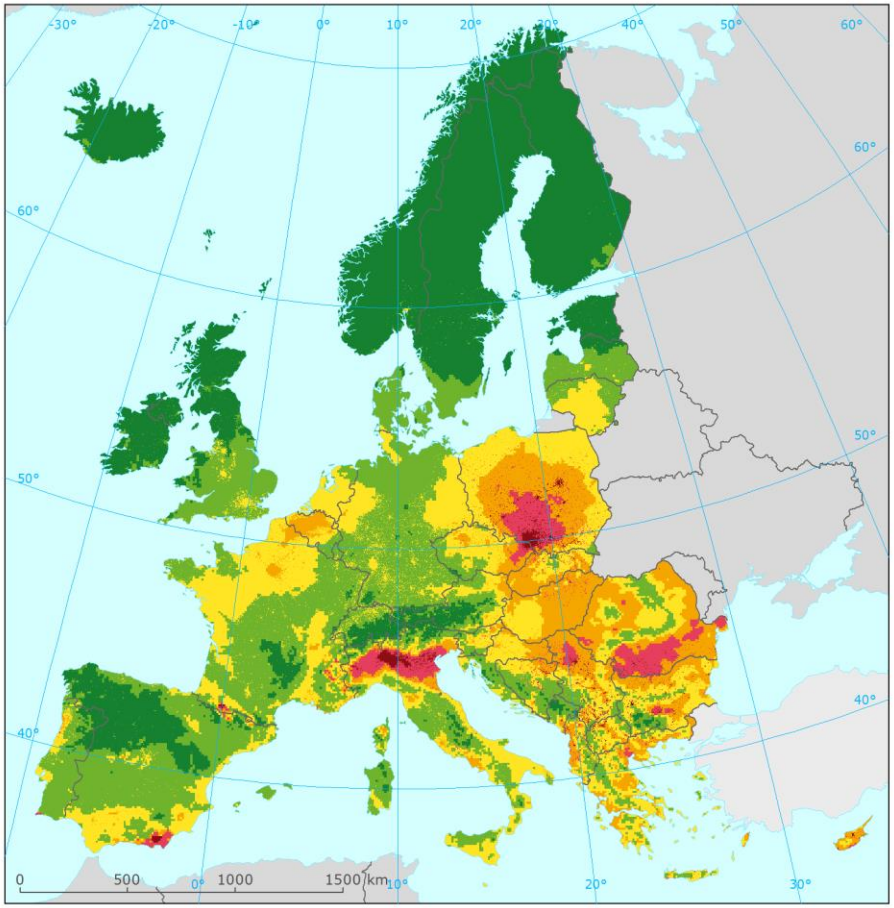
Particulate Matter (PM_{10})
Annual Average

Reference Year: 2012
Combined Rural and Urban Background Map
Resolution: 1x1 km

- ≤ 10 µg.m^{-3}
- 10 - 20 µg.m^{-3}
- 20 - 30 µg.m^{-3}
- 30 - 40 µg.m^{-3}
- 40 - 50 µg.m^{-3} (40 = LV)
- > 50 µg.m^{-3}
- outside data coverage
- poor data coverage

Analyzed maps

PM_{10} – 36th highest daily mean, 2012



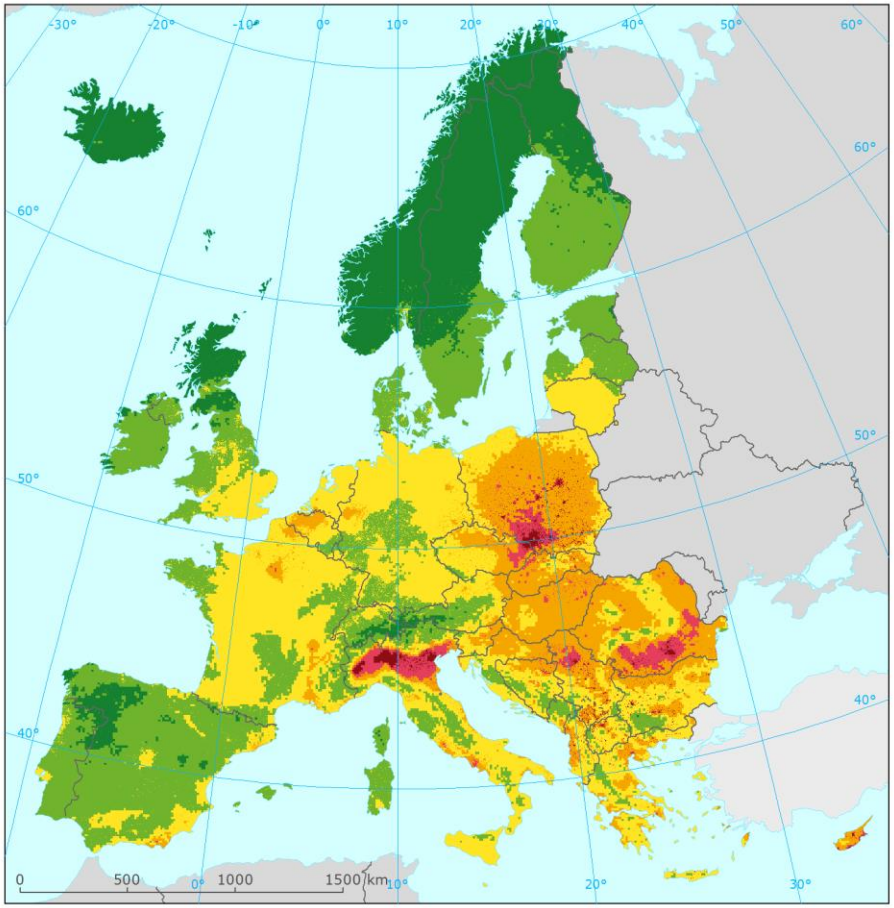
Particulate Matter (PM_{10})
36th Highest Daily Mean

Reference Year: 2012
Combined Rural and Urban Background Map
Resolution: 1x1 km

- ≤ 20 µg.m^{-3}
- 20 - 30 µg.m^{-3}
- 30 - 40 µg.m^{-3}
- 40 - 50 µg.m^{-3}
- 50 - 75 µg.m^{-3} (50 = LV)
- > 75 µg.m^{-3}
- outside data coverage
- poor data coverage

Analyzed maps

$PM_{2.5}$ – annual average, 2012



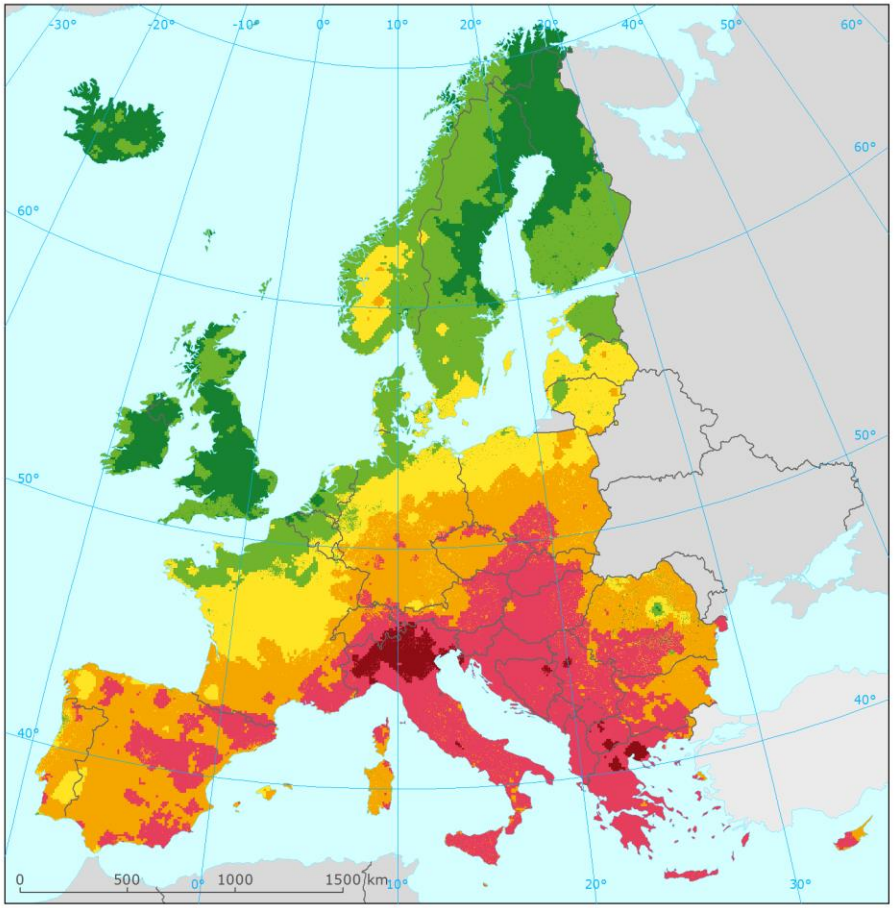
Fine Particulate Matter ($PM_{2.5}$)
Annual Average

Reference Year: 2012
Combined Rural and Urban Background Map
Resolution: 1x1 km

- ≤ 5 µg.m^{-3}
- 5 - 10 µg.m^{-3}
- 10 - 15 µg.m^{-3}
- 15 - 20 µg.m^{-3}
- 20 - 25 µg.m^{-3} (20 = LV_{2020})
- > 25 µg.m^{-3} (25 = TV, LV_{2015})
- outside data coverage
- poor data coverage

Analyzed maps

O_3 – 26th highest daily maximum 8-hour mean, 2012



Ozone – 26th Highest Daily Maximum 8-hour Mean

Reference Year: 2012
Combined Rural and Urban Background Map
Resolution: 1x1 km

- ≤ 90 µg.m^{-3}
- 90 - 100 µg.m^{-3}
- 100 - 110 µg.m^{-3}
- 110 - 120 µg.m^{-3}
- 120 - 140 µg.m^{-3} (120 = TV)
- > 140 µg.m^{-3}
- outside data coverage
- poor data coverage

Uncertainty estimates of analyzed maps

Using cross-validation

Map is calculated for every measurement point based on all available information except from the point in question.

Parameter	PM_{10} annual average				PM_{10}, 36th highest daily mean			
	Full set		Assimil. subset		Full set		Assimil. subset	
	Rural	Urban	Rural	Urban	Rural	Urban	Rural	Urban
RMSE [µg.m^{-3}]	3.8	6.1	4.4	7.4	7.7	11.9	8.7	14.9
Relative RMSE	21.4%	22.1%	25.0%	27.1%	24.5%	24.5%	27.5%	30.6%
Bias [µg.m^{-3}]	0.1	0.0	0.7	0.2	0.1	-0.1	1.0	-1.1

Parameter	$PM_{2.5}$ annual average				O_3, 26th highest daily max. 8h			
	Full set		Assimil. subset		Full set		Assimil. subset	
	Rural	Urban	Rural	Urban	Rural	Urb.	Rural	Urb.
RMSE [µg.m^{-3}]	3.0	3.3	3.3	3.3	8.5	9.1	8.5	9.2
Relative RMSE	24.9%	18.7%	27.1%	18.7%	7.4%	8.3%	7.5%	8.4%
Bias [µg.m^{-3}]	-0.4	0.1	-0.7	-0.5	0.2	-0.1	-0.1	0.2

1. Maps used in evaluation

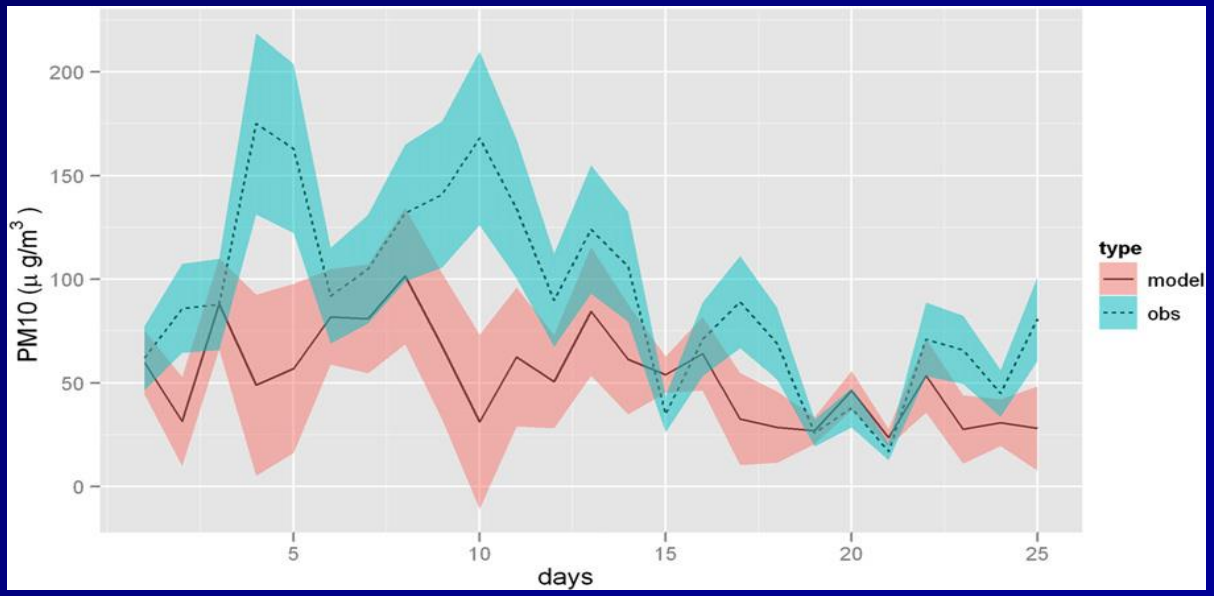
2. Delta tool, MQO and parameters used in

3. Evaluation by Delta tool and discussion

Delta tool and *MQO*

Delta tool applies the ***Model Quality Objective (MQO)***.

Basic concept of *MQO*: Model uncertainty should not exceed the measurement uncertainty.



Source: Thunis et al. (2012)

Delta tool and *MQO*

According to the concept of MQO, the successful model should fulfill for 90% monitoring points the relation:

$$MQO = \frac{\sum_{i=1}^{N}(M_i - O_i)^2}{2\sum_{i=1}^{N}U(O_i)^2} \leq 1,$$

for time series

$$MQO = \frac{\left|\overline{M} - \overline{O}\right|}{2U(\overline{O})} = \frac{\left|bias\right|}{2U(\overline{O})} \leq 1,$$

for annual averages

$$MQO = \frac{\left|M_{perc} - O_{perc}\right|}{2U(O_{perc})} \leq 1,$$

for percentiles

where

O	is observation
M	is modelled value
U(O)	is expanded uncertainty of *O*

Measurement uncertainty is a key input to the MQO.

The requirement of 90% is motivated by AQD.

Measurement uncertainty expression

Approach applied in Delta – based on the assumption that the uncertainty of each measurement O_i is composed of a component proportional to the concentration level and a non-proportional component as in :

$$u^2(O_i) = u_p{}^2(O_i) + u_{np}{}^2(O_i) = (1-\alpha)(u_r^{RV} O_i)^2 + \alpha(u_r^{RV} RV)^2$$

where $u_p(O_i)$ is the proportional component of uncertainty
$u_{np}(O_i)$ is the non-proportional component of uncertainty
α is the non-proportional fraction of the uncertainty around RV
u_r^{RV} is the relative uncertainty around RV
RV is the reference value

Expanded uncertainty *U(Oi)* is calculated by expanding uncertainty *u(Oi)* by so-called coverage factor *k*, i.e.

$$U(O_i) = k\,u(O_i) = k u_r^{RV} \sqrt{(1-\alpha)\cdot O_i^2 + \alpha \cdot RV^2}$$

Measurement uncertainty – annual indicators

The uncertainty of the annual average concentration is expected to be reduced compared to $U(O_i)$. To cover this aspect, the proportional and non-proportional components of the uncertainty are divided by parameters N_p and N_{np}. Expanded uncertainty of the annual average of observations:

$$U(\overline{O}) = ku_r^{RV} \sqrt{\frac{(1-\alpha)}{N_p}\overline{O}^2 + \frac{\alpha \cdot RV^2}{N_{np}}}$$

The uncertainty for a percentile value is considered in the Delta tool just as the uncertainty of the observation value O_i corresponding to the relevant percentile. I.e. it is calculated simply as

$$U(O_i) = ku_r^{RV} \sqrt{(1-\alpha) \cdot O_i^2 + \alpha \cdot RV^2}$$

Measurement uncertainty expression

Parameters used in Delta 5.0 to calculate measurement uncertainty

Pollutant	Indicator	k	u_r^{RV}	RV	α	N_p	N_{pp}
PM_{10}	Annual average	2.00	0.140	50 µg.m^{-3}	0.018	40	1
	Percentile (a)	2.00	0.140	50 µg.m^{-3}	0.018	-	-
$PM_{2.5}$	Annual average	2.00	0.180	25 µg.m^{-3}	0.035 (b)	40	1
O_3	Percentile (a)	1.40	0.090	120 µg.m^{-3}	0.620	-	-

(a) For percentiles, parameters relevant for daily mean (PM_{10}), resp. 8-hour daily maximum (O_3) are used.
(b) In the Delta tool the value 0.035 is actually used, although in Thunis et al. (2015) the value 0.05 is given.

The *MQO* is highly sensitive to these parameter values.

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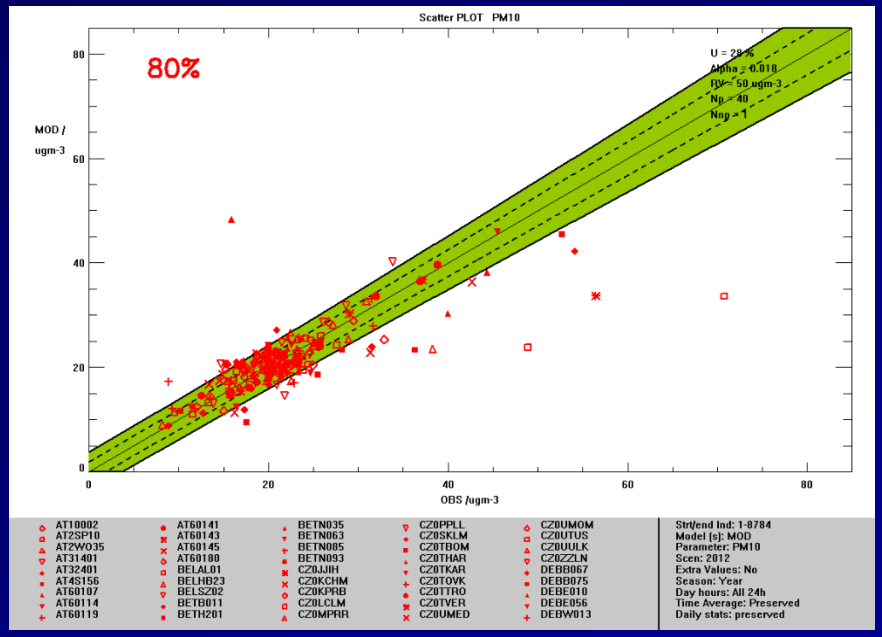
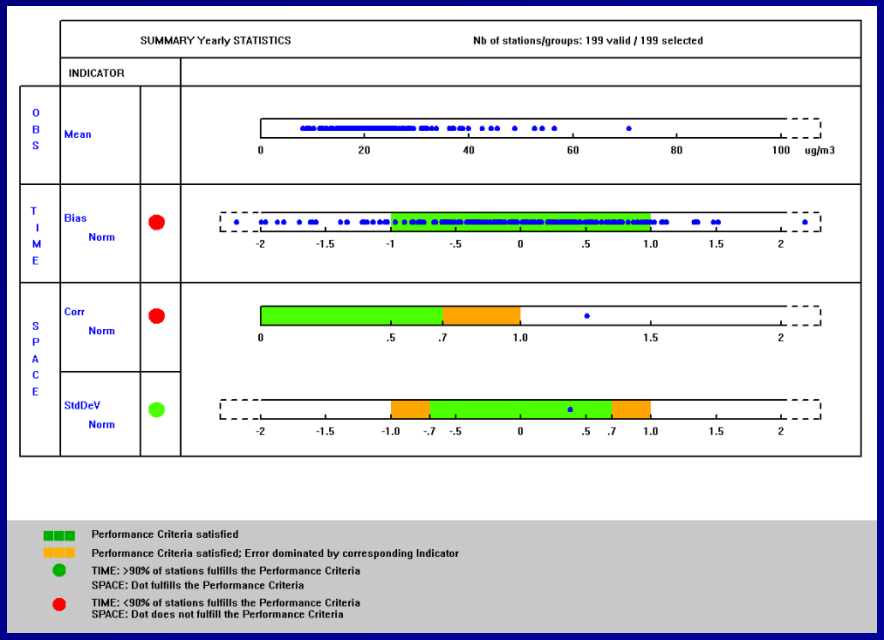
Evaluation using Delta tool 5.0

PM_{10} annual average, 2012

mapping using assimilation subset of the stations, against validation subset of the stations, all types

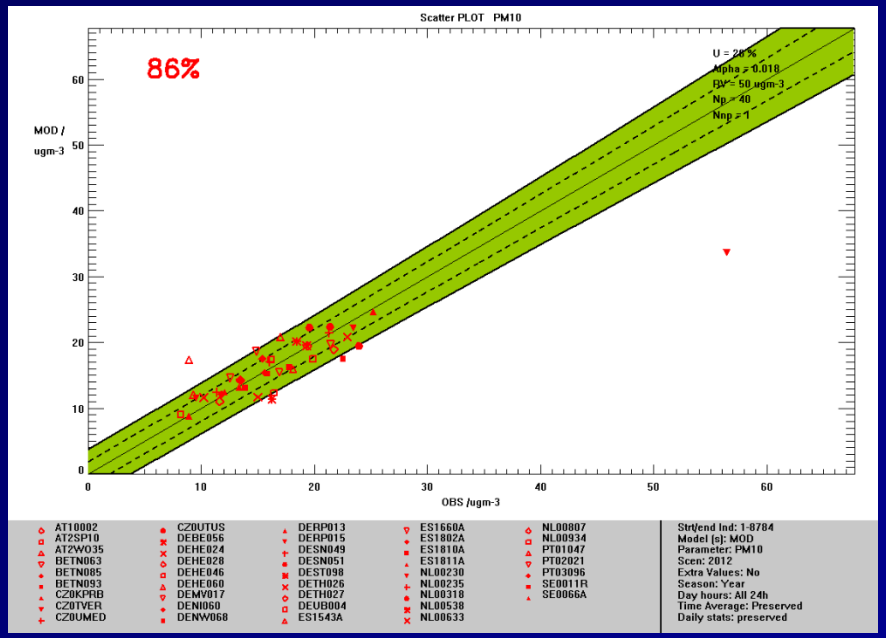


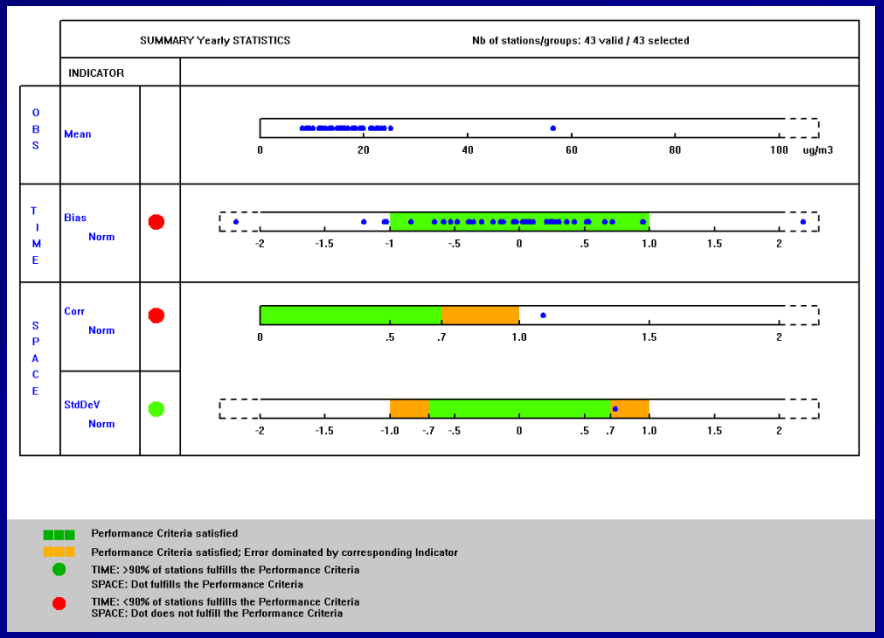


Evaluation using Delta tool 5.0

PM_{10} annual average, 2012

mapping using assimilation subset of the stations, against validation subset of the stations, rural background stations

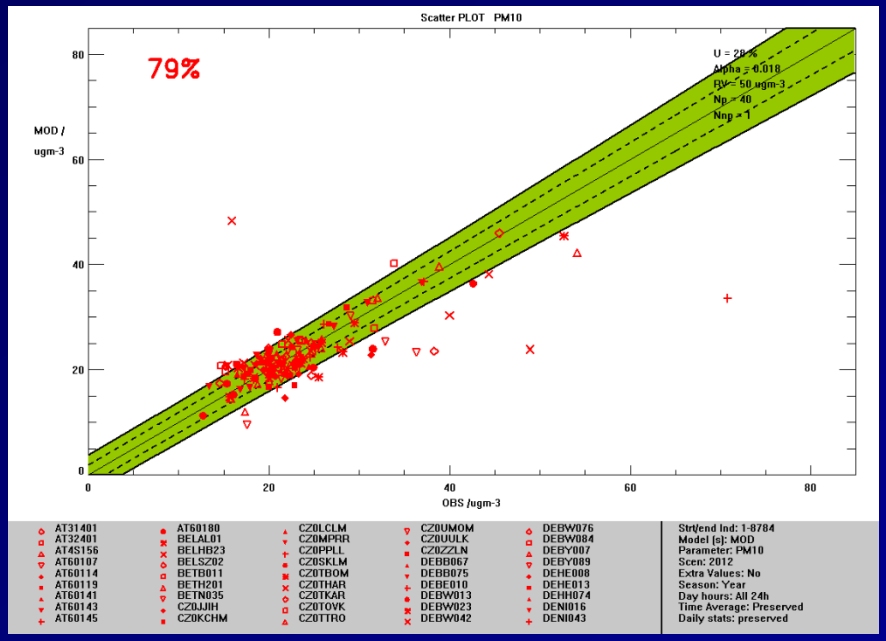


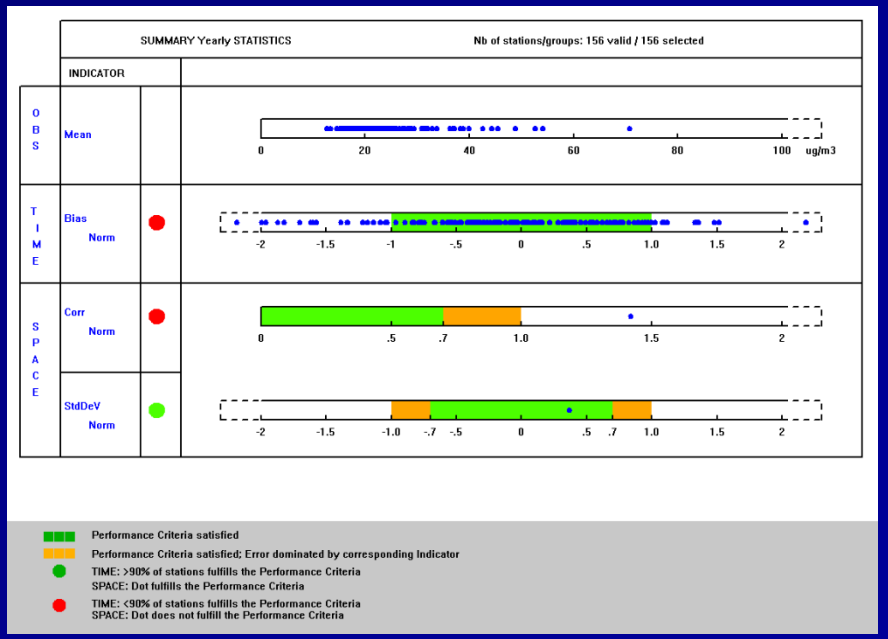


Evaluation using Delta tool 5.0

PM_{10} annual average, 2012

mapping using assimilation subset of the stations, against the validation subset, urban/suburb. background stations

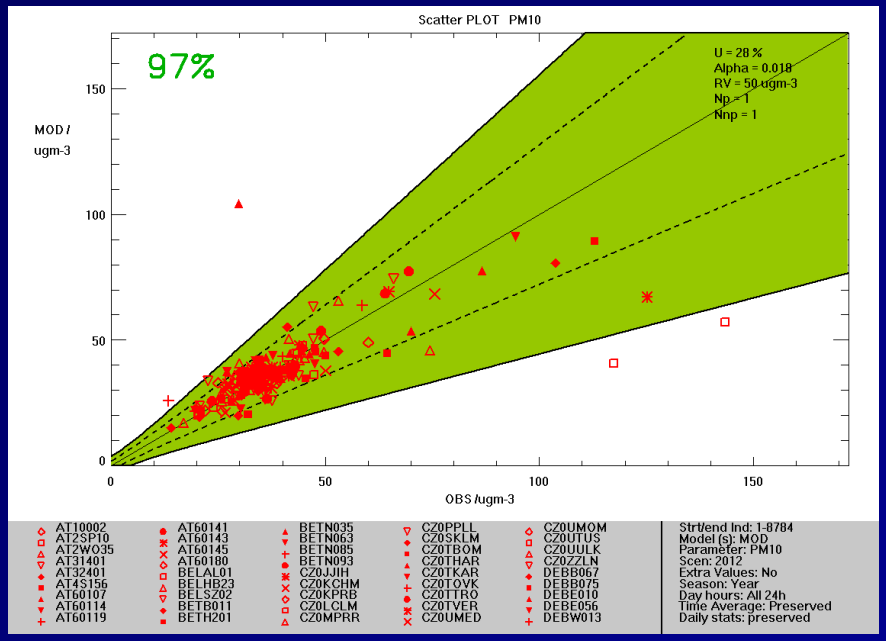


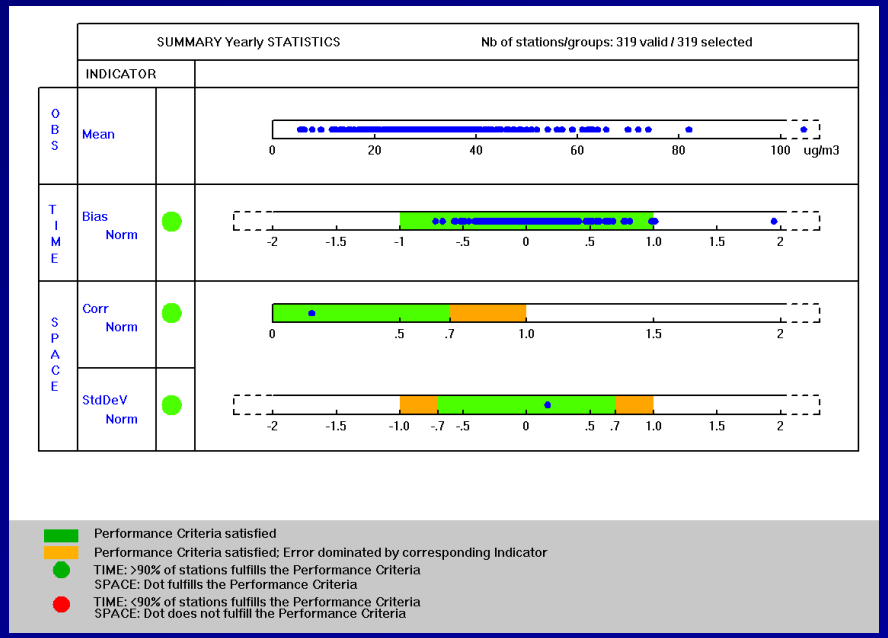


Evaluation using Delta tool 5.0

PM_{10} – 36th highest daily mean, 2012

mapping using assimilation subset of the stations, against validation subset of the stations, all types

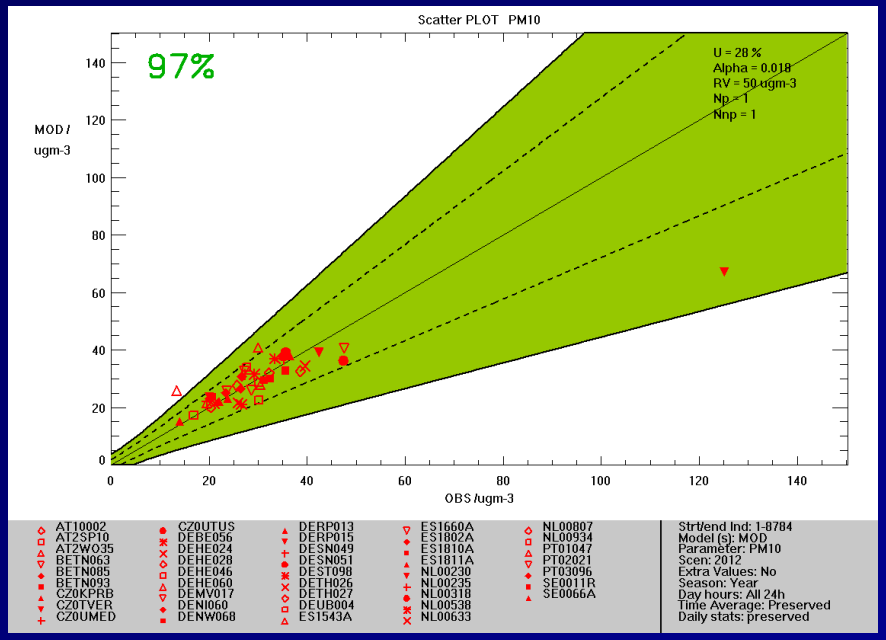


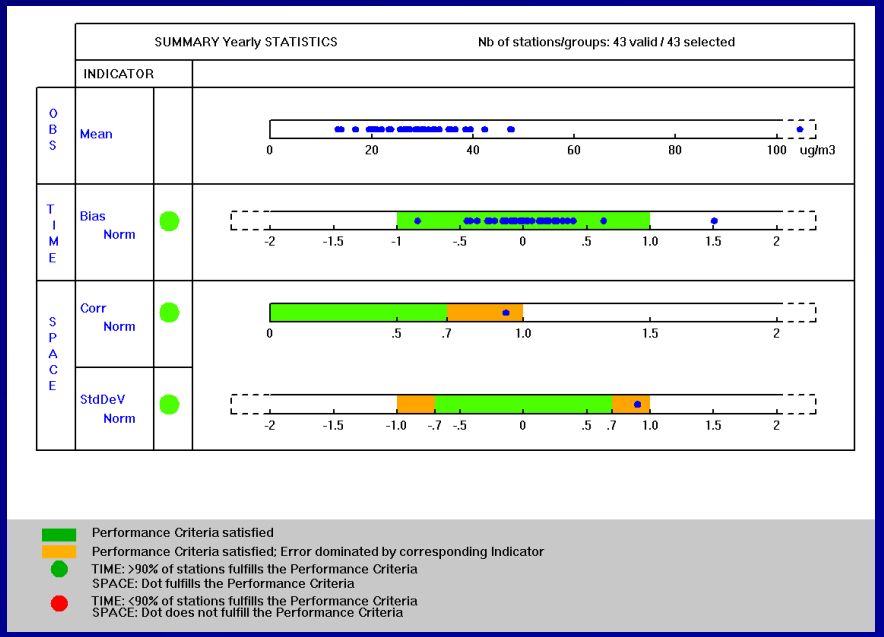


Evaluation using Delta tool 5.0

PM_{10} – 36th highest daily mean, 2012

mapping using assimilation subset of the stations, against validation subset of the stations, rural background stations

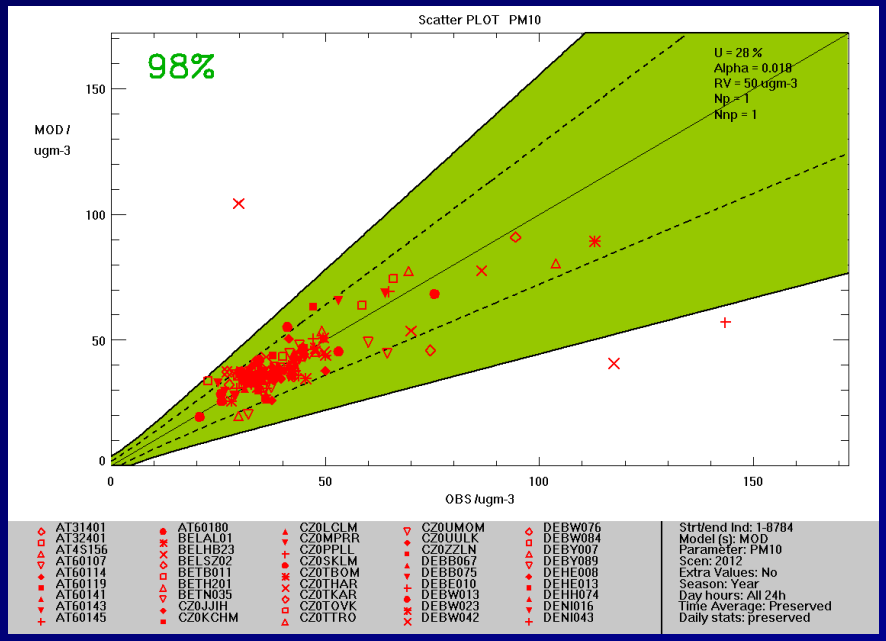


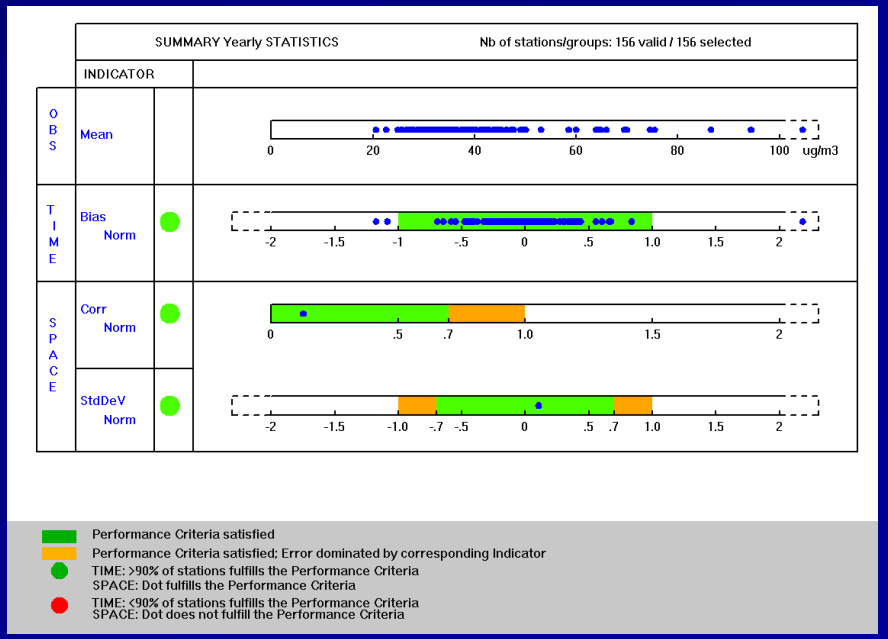


Evaluation using Delta tool 5.0

PM_{10} – 36th highest daily mean, 2012

mapping using assimilation subset of the stations, against the validation subset, urban/suburb. background stations

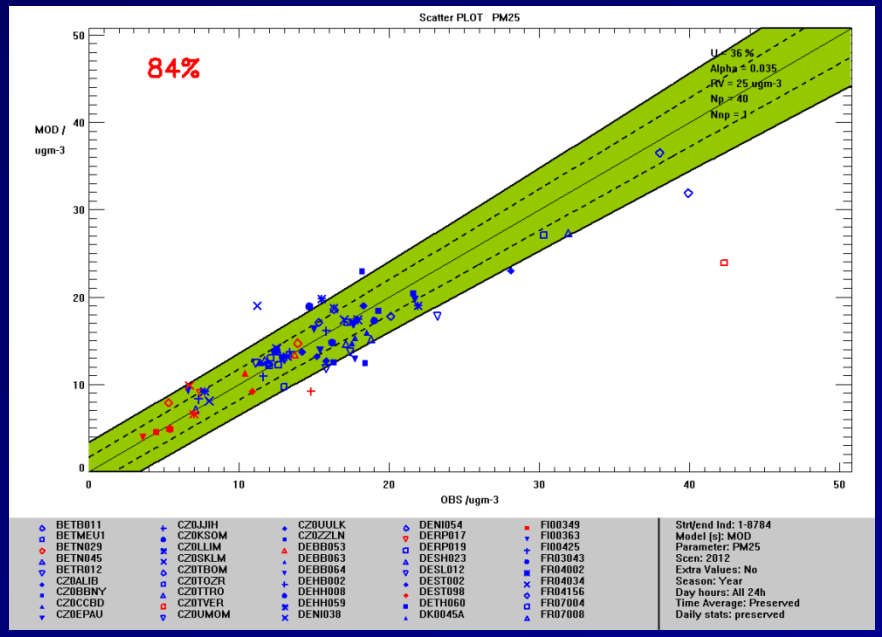


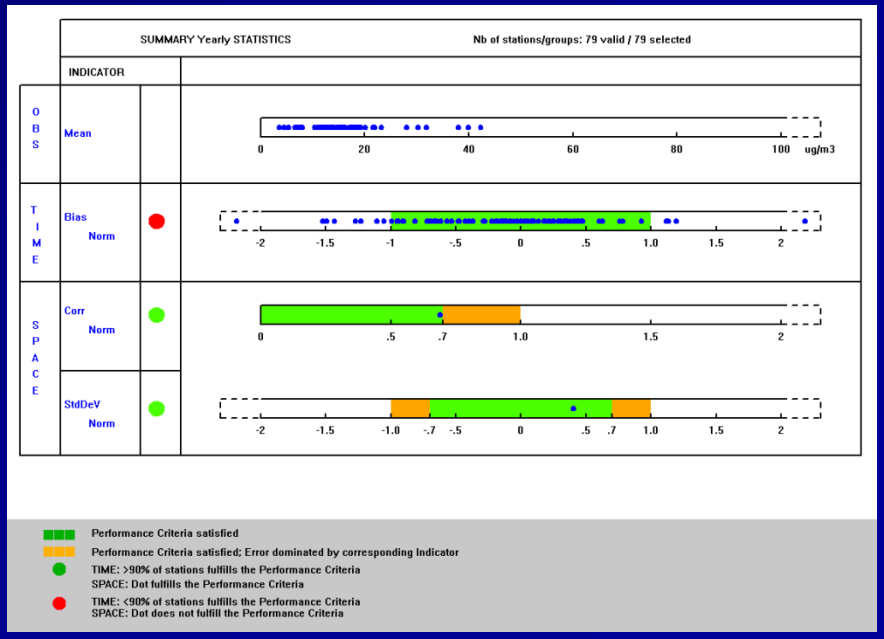


Evaluation using Delta tool 5.0

$PM_{2.5}$ annual average, 2012

mapping using assimilation subset of the stations, against validation subset of the stations, all types

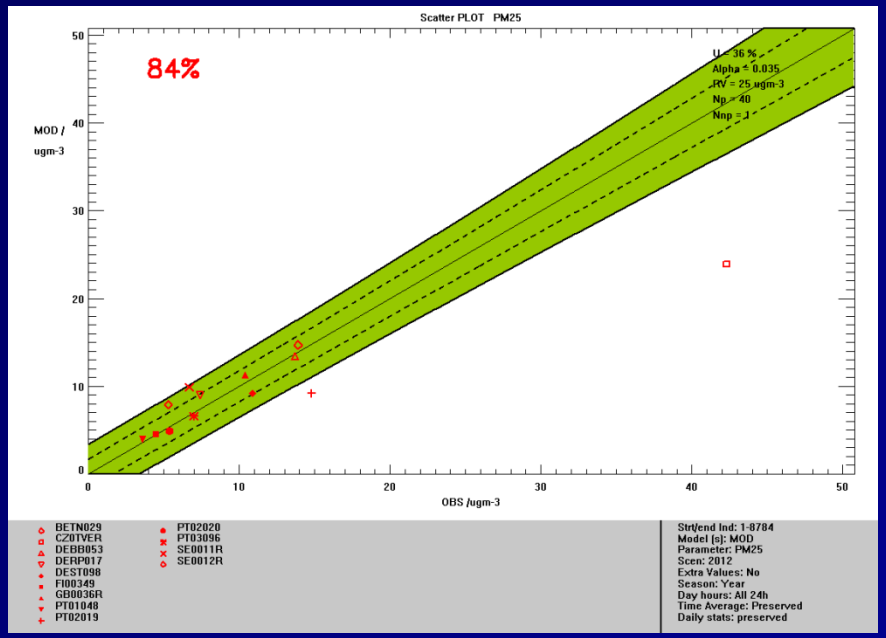


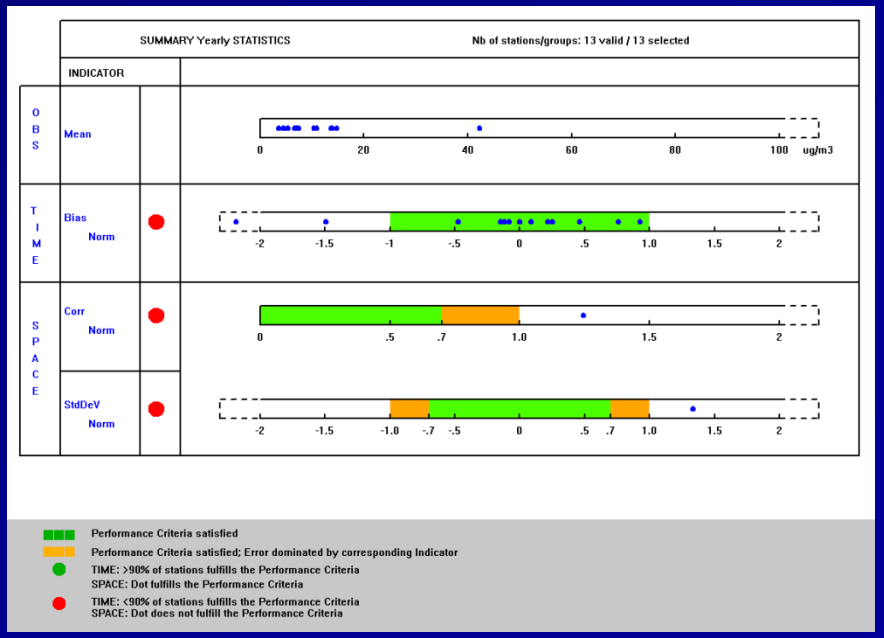


Evaluation using Delta tool 5.0

$PM_{2.5}$ annual average, 2012

mapping using assimilation subset of the stations, against validation subset of the stations, rural background stations

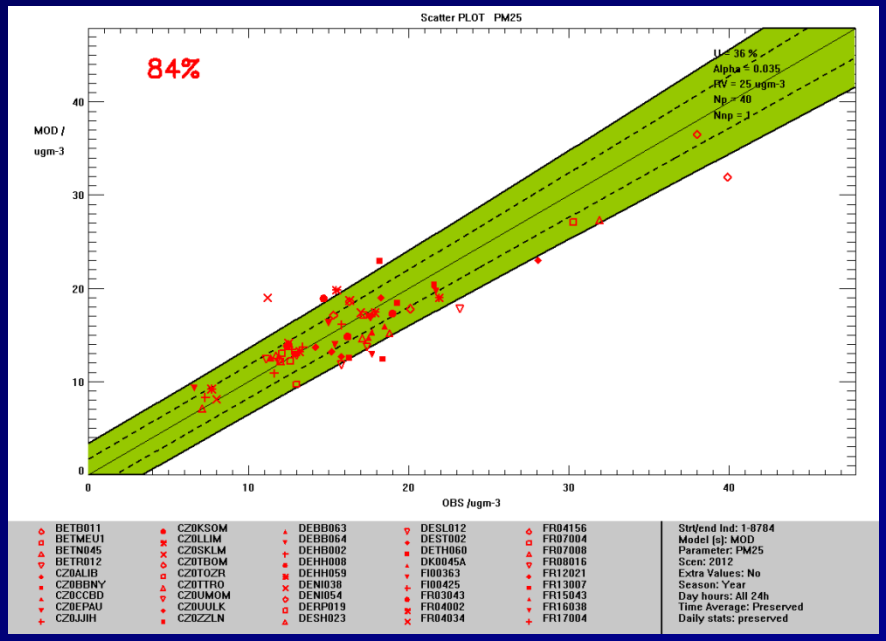


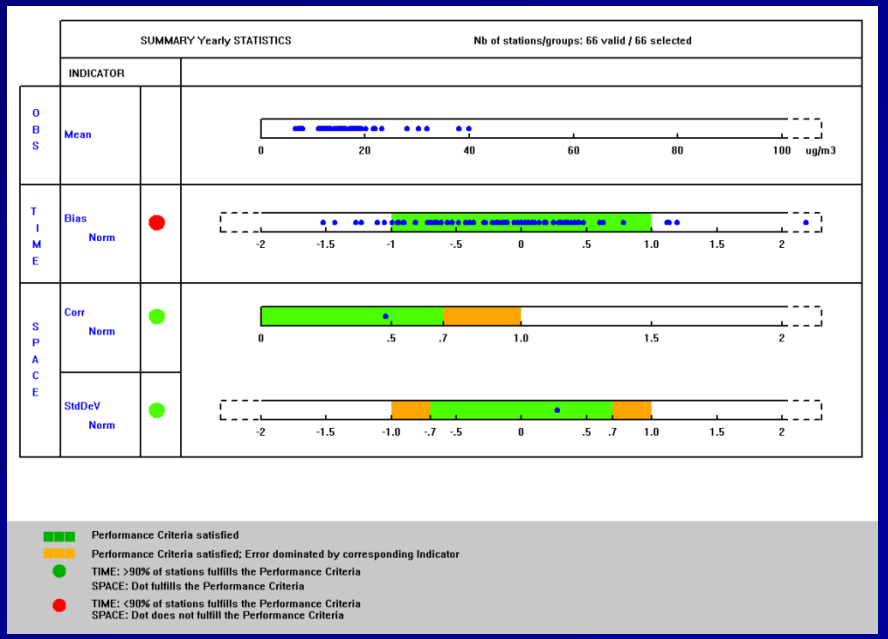


Evaluation using Delta tool 5.0

$PM_{2.5}$ annual average, 2012

mapping using assimilation subset of the stations, against the validation subset, urban/suburb. background stations

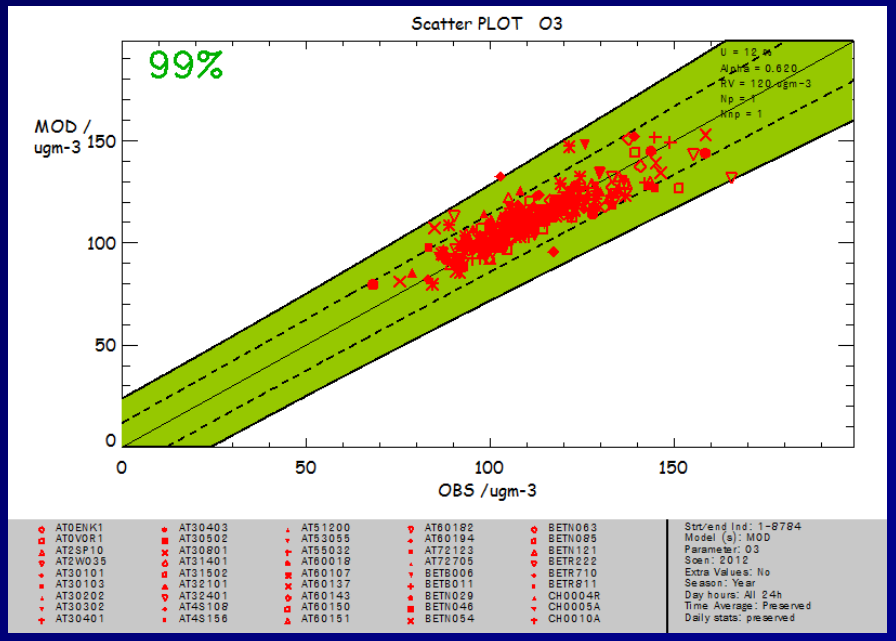


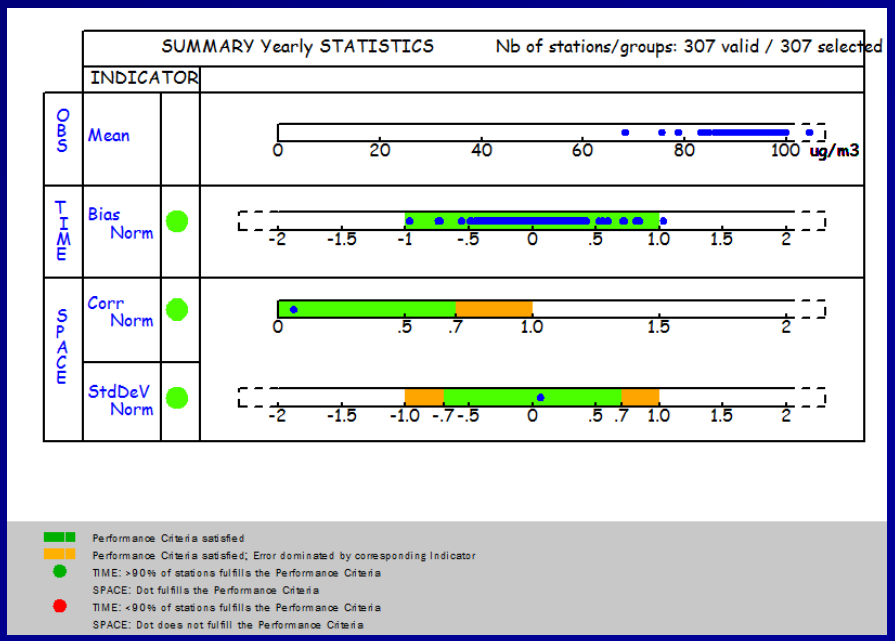


Evaluation using Delta tool 5.0

Ozone, 26th highest daily max. 8-hourly daily mean, 2012

mapping using assimilation subset of the stations, against validation subset of the stations, all types

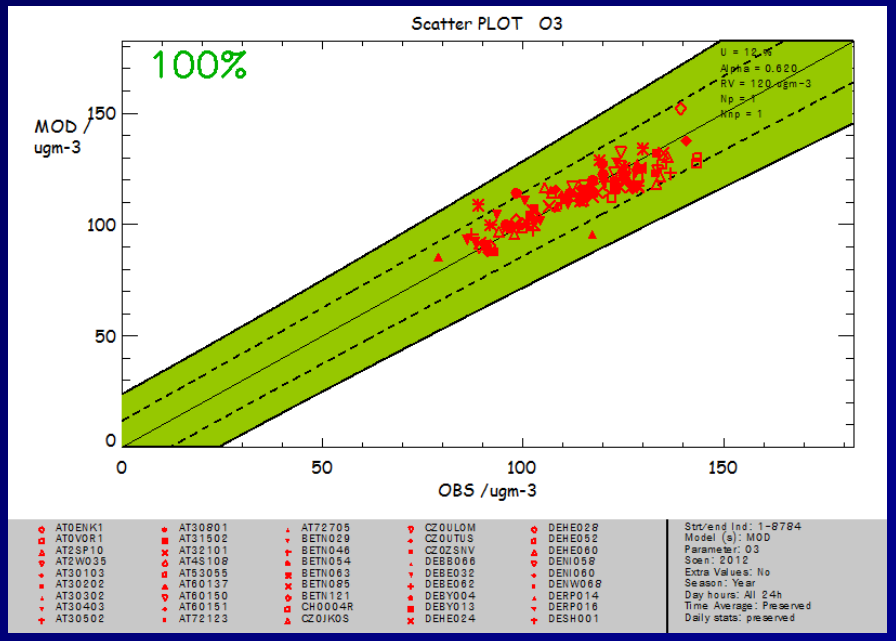


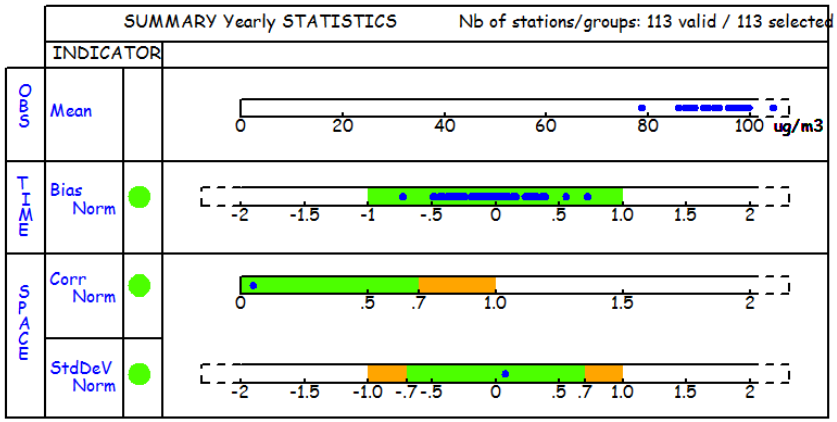


Evaluation using Delta tool 5.0

Ozone, 26th highest daily max. 8-hourly daily mean, 2012

mapping using assimilation subset of the stations, against validation subset of the stations, rural background stations

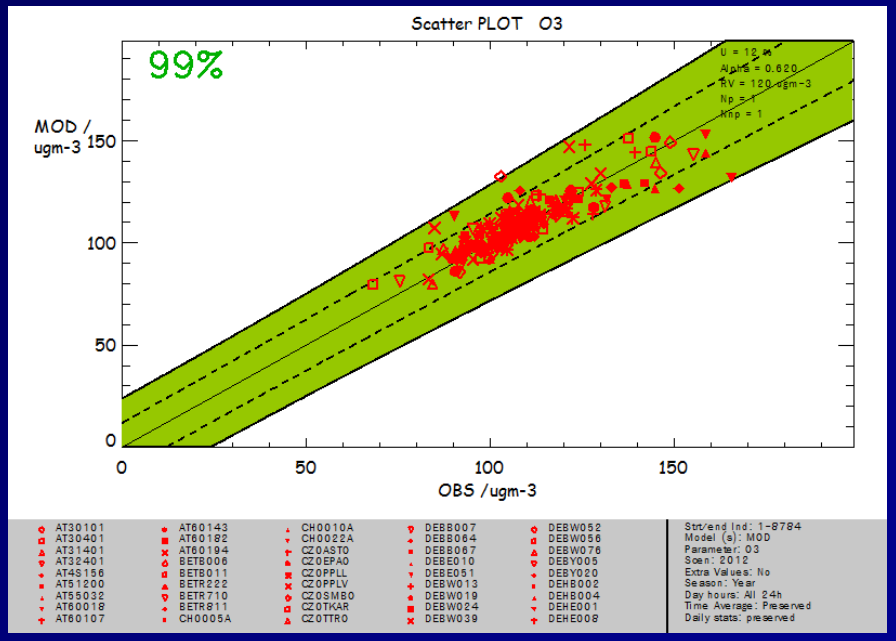


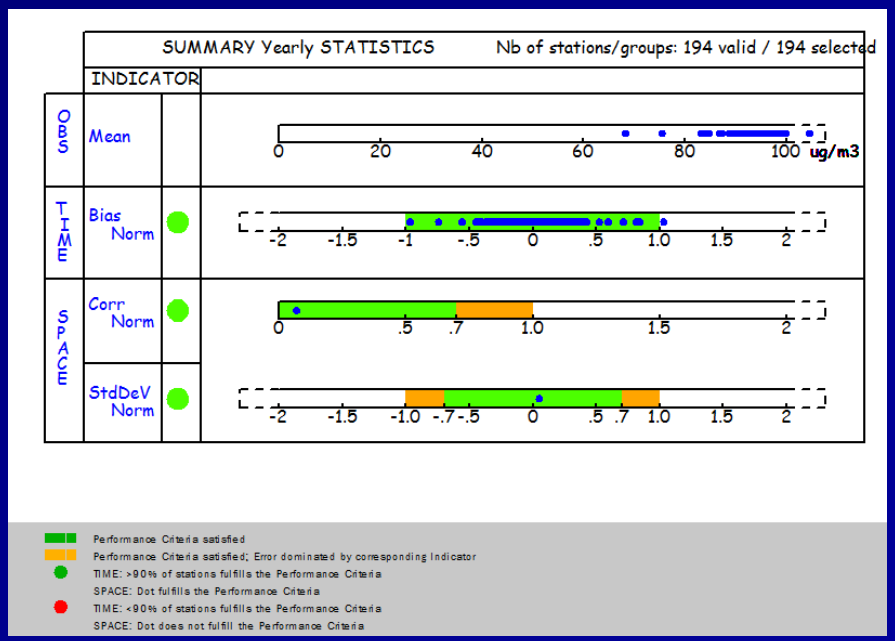


Evaluation using Delta tool 5.0

Ozone, 26th highest daily max. 8-hourly daily mean, 2012

mapping using assimilation subset of the stations, against the validation subset, urban/suburb. background stations





Evaluation using Delta tool 5.0

Summary results

Pollutant and indicator	Type of stations used for evaluation	Map based on full station set and evaluated by the same set			Map based on assimilation subset evaluated by validation subset		
		MQO criterion	Performance criteria		*MQO* criterion	Performance criteria	
			Corr.	St. dev.		Corr.	St. dev.
PM_{10} annual average	Rural background	92%	+	+	86%	- (a)	+
	Urban/suburb. b.	85%	+	+	79%	-	+
	All	87%	+	+	80%	-	+
PM_{10} 36th highest daily mean	Rural background	99%	+	+	97%	+	+
	Urban/suburb. b.	99%	+	+	98%	+	+
	All	99%	+	+	97%	+	+
$PM_{2.5}$ annual average	Rural background	94%	+	+	84%	-	-
	Urban/suburb. b.	90%	+	+	84%	+	+
	All	91%	+	+	84%	+	+
Ozone 26th highest d. max. 8-h.	Rural background	100%	+	+	100%	+	+
	Urban/suburb. b.	98%	+	+	98%	+	+
	All	99%	+	+	99%	+	+

(a) If calculated outside the Delta software according to Equation 2.9, the correlation criterion is fulfilled.

Discussion points

MQO used in the Delta tool is stricter than the requirements for models under AQ Directive.

(i) *MQO*: model uncertainty should not exceed the measurement uncertainty; *AQD*: model uncertainty can be higher that the measurement uncertainty – 50% modelling uncertainty vs. 25% resp. 15% measurement uncertainty.

(ii) The modelling uncertainty is defined in the AQD as the maximum deviation of the measured and calculated concentration levels for 90% of individual monitoring points.

Next to this, the values of the measurement uncertainty used in the Delta tool for PM_{10} and $PM_{2.5}$ are based on the reference gravimetric method which is many times lower than the uncertainty of the beta ray method

Discussion points

Output of the Delta tool is very sensitive to the monitoring uncertainty used.

Delta 5.0 gives highly different results for the annual averages and for percentiles (i.e. x-th highest values). Reason: large difference in the measurement uncertainty set for annual averages and for percentiles. Measurement uncertainty of the percentile value is considered as an uncertainty of the corresponding daily value, although this is not fully correct.

(If X is the P-th percentile and U is the uncertainty of X, the value $X+U$ perhaps is no longer the P-th percentile.)

Update in Delta 5.3

$$MQI = \frac{|\bar{O} - \bar{M}|}{\beta U_{95}(\bar{O})} \leq 1$$

Parameters used in Delta 5.3 to calculate measurement uncertainty

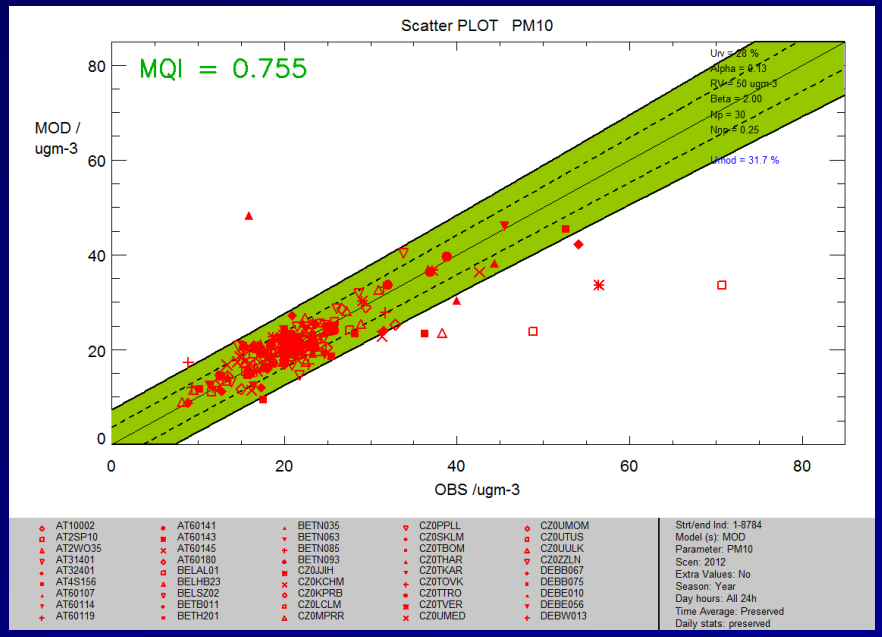
Pollutant	Indicator	β	$k.u_r^{RV}$	RV	α	N_p	N_{np}
PM_{10}	Annual average	2.00	0.280	50 µg.m^{-3}	0.13	30	0.25
$PM_{2.5}$	Annual average	2.00	0.360	25 µg.m^{-3}	0.13	30	0.25

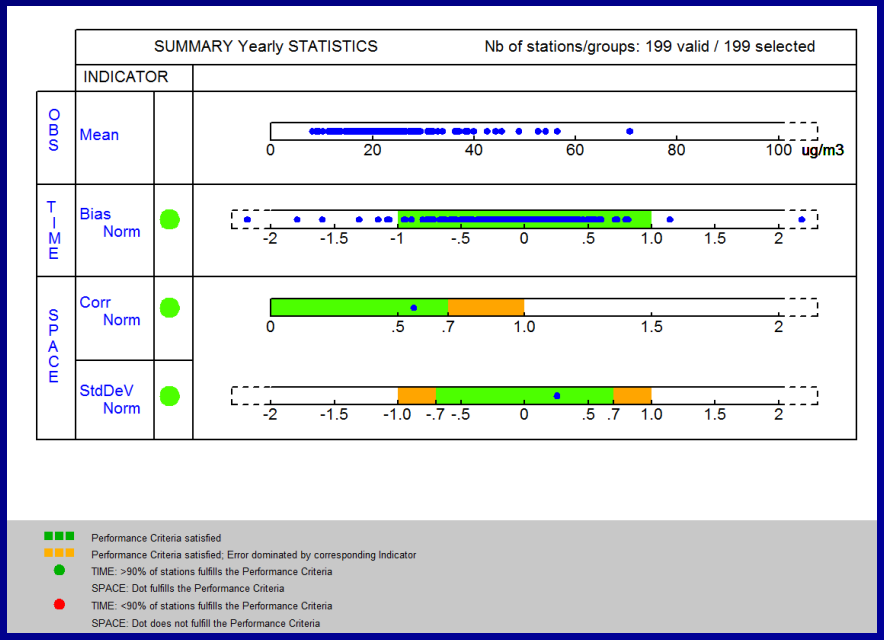
The *MQI* and thus MQO highly sensitive to these values.

Evaluation using Delta tool 5.3

PM_{10} annual average, 2012

mapping using assimilation subset of the stations, against validation subset of the stations, all types

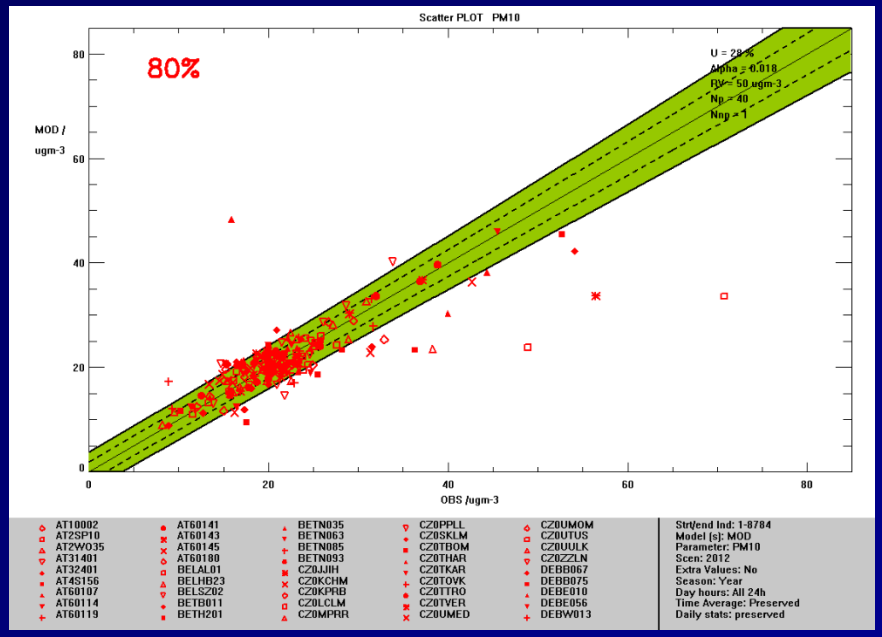


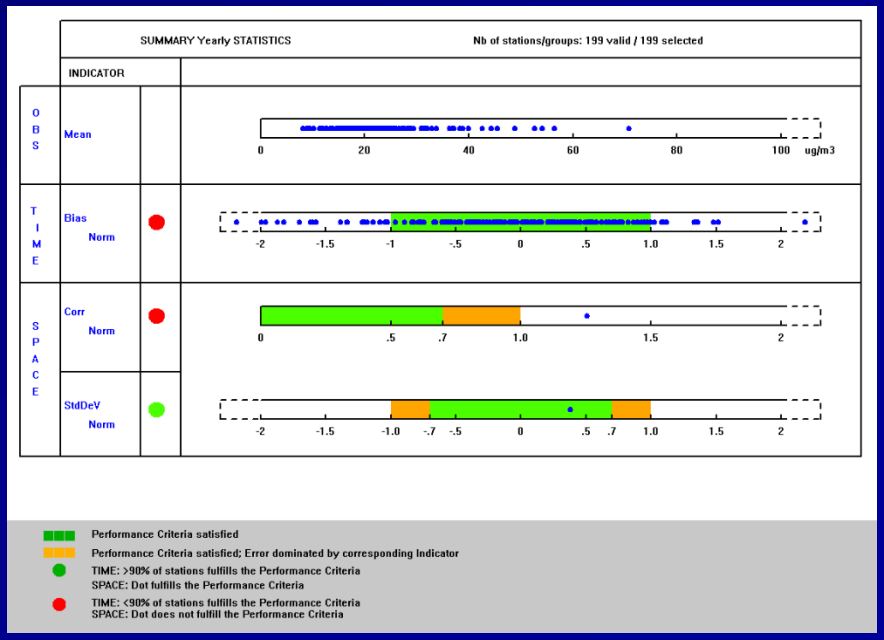


Evaluation using Delta tool 5.0

PM_{10} annual average, 2012

mapping using assimilation subset of the stations, against validation subset of the stations, all types

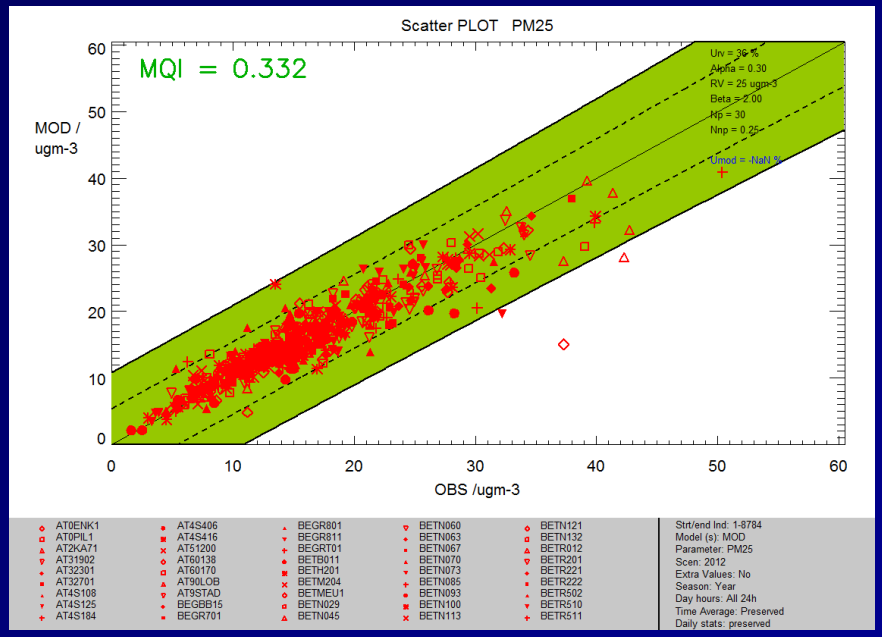


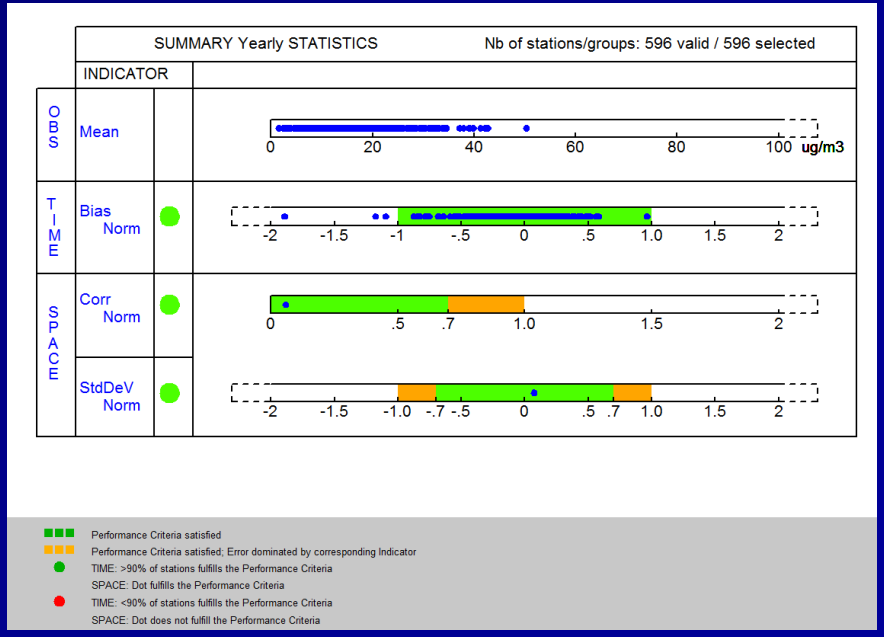


Evaluation using Delta tool 5.3

$PM_{2.5}$ annual average, 2012

mapping using full set of the stations, against all staions of this full set

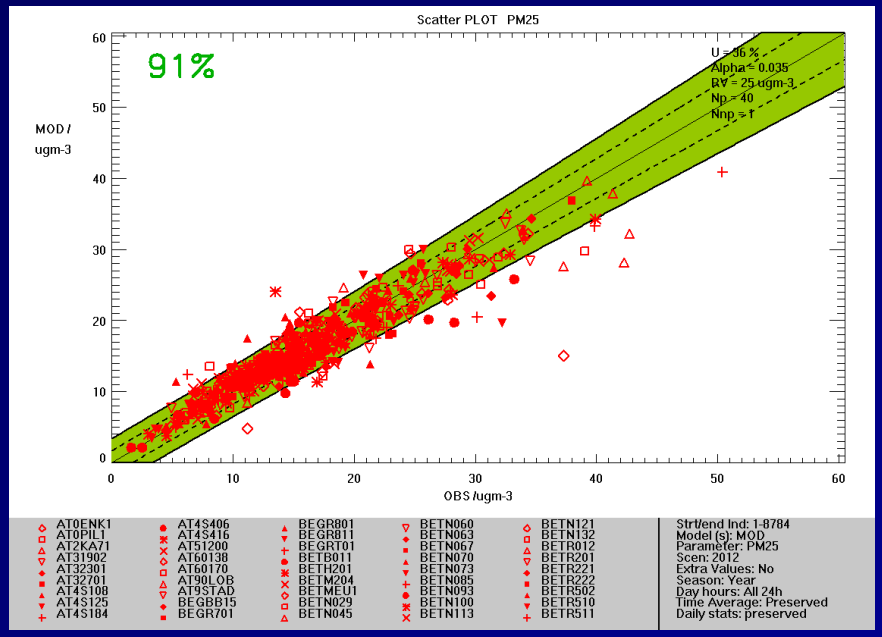


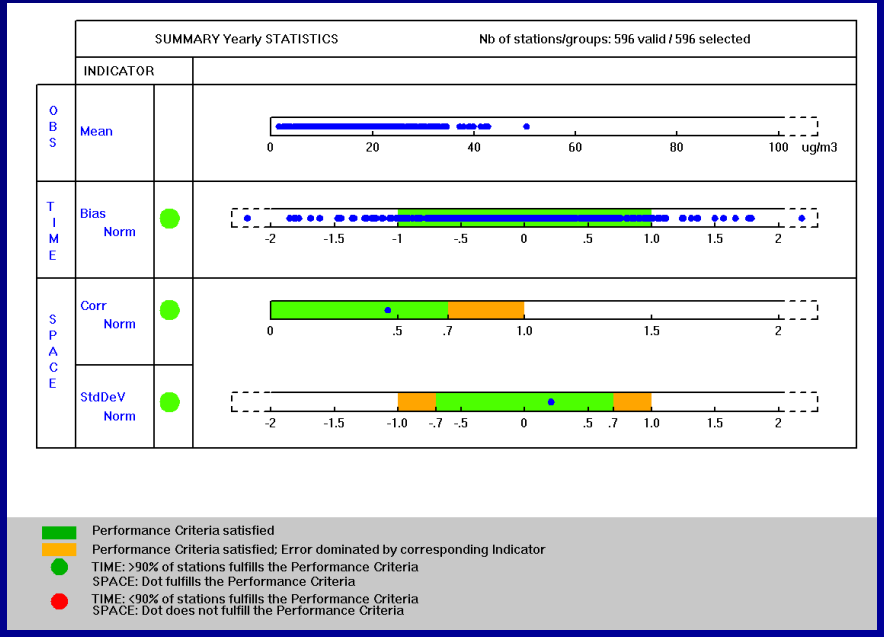


Evaluation using Delta tool 5.0

$PM_{2.5}$ annual average, 2012

mapping using full set of the stations, against all staions of this full set





Thank you for your attention.