

# **WG1. Benchmarking DELTA-Tool**

## **Application on Portugal**

Alexandra Monteiro. Ana Isabel Miranda  
Diogo Lopes. Helena Martins. Isabel Ribeiro

# DELTA-Tool applications

DELTA-Tool has been used for model evaluation with the purposes of:



- Long-term air quality assessment purposes
- Operational forecast
- Specific air pollution research studies



over Portugal and urban areas (Porto & Lisbon)

# Our DELTA-Tool experience

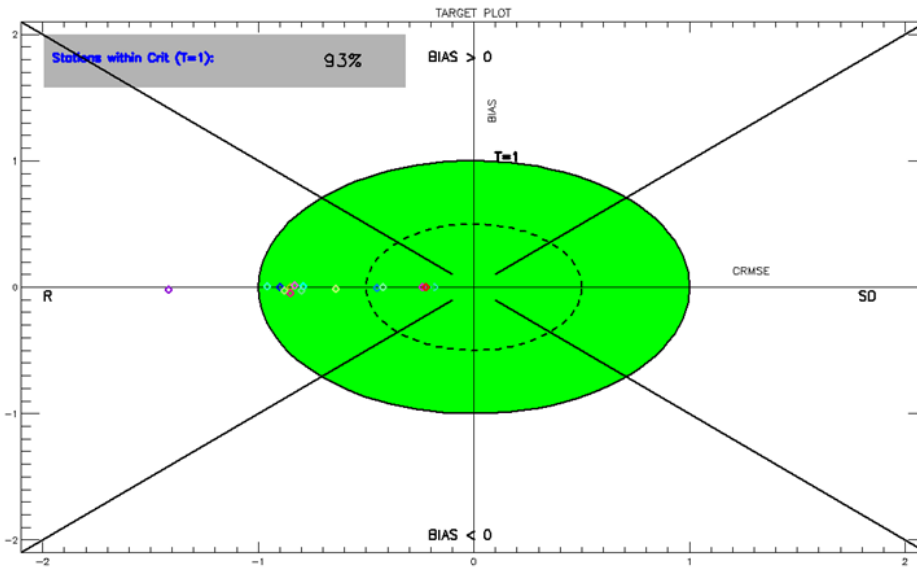
Official reports for Environmental Protection Agency



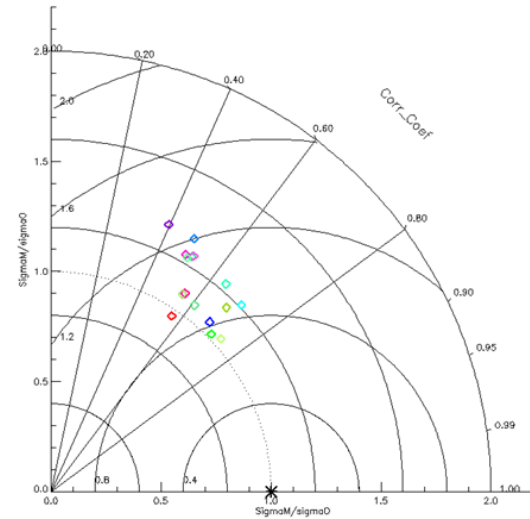
The performance of the air quality modelling system (for both assessment and forecast purposes) is evaluated using DELTA-Tool

# Some results – NO<sub>2</sub>

(a)

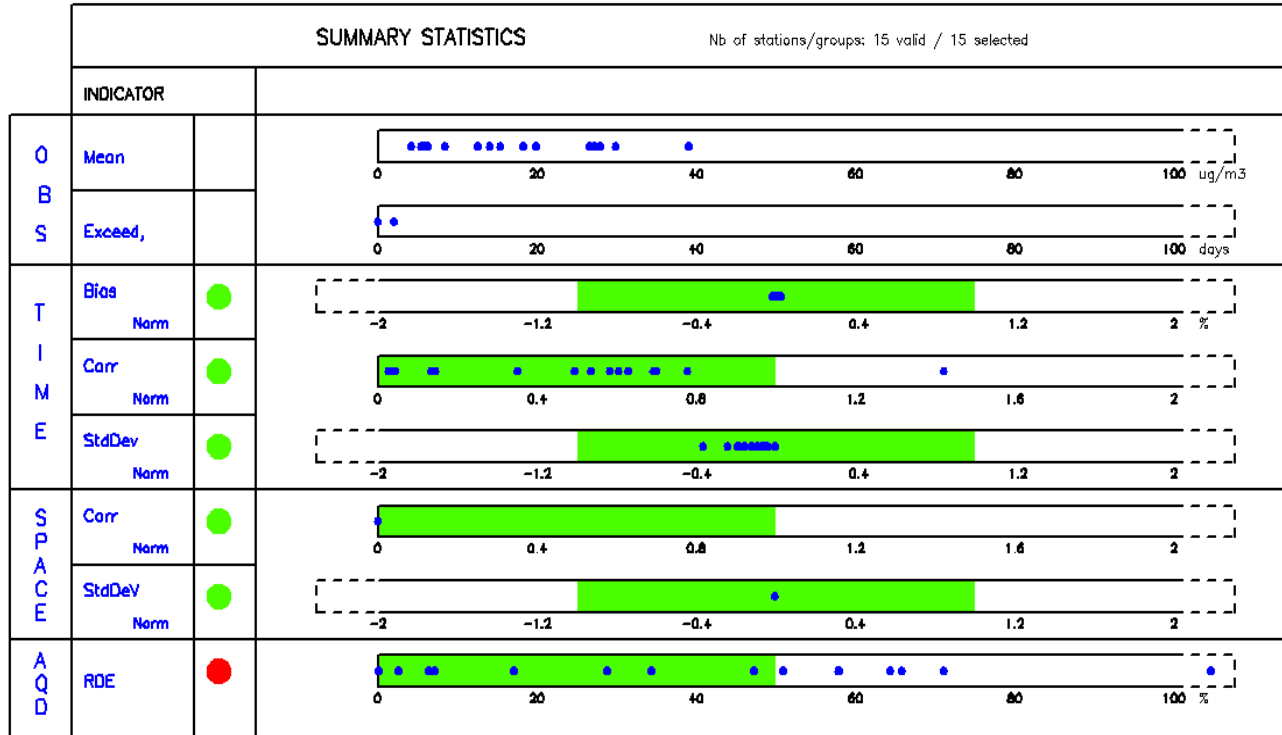


(b)



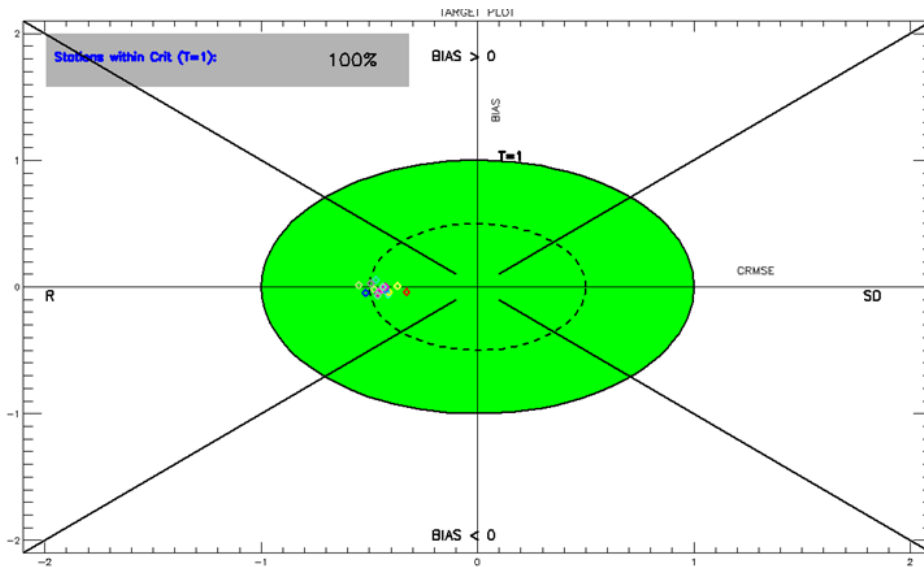
- |     |     |
|-----|-----|
| PMN | LOU |
| PFR | MEM |
| COM | ARC |
| OLD | CHA |
| SOB | FPD |
| ERV | ALV |
| FUN | TER |
| OU  |     |
| LAR |     |

# Some results – NO<sub>2</sub>

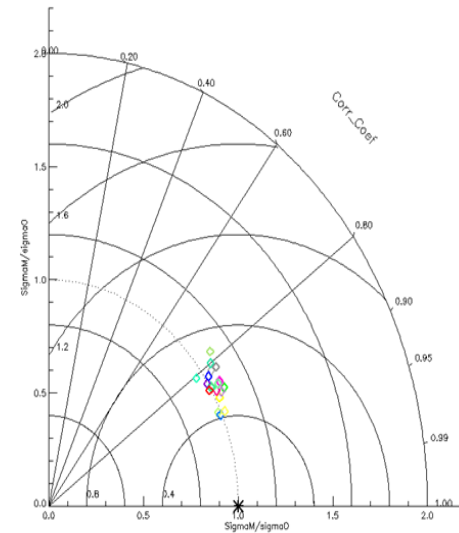


# Some results – O<sub>3</sub>

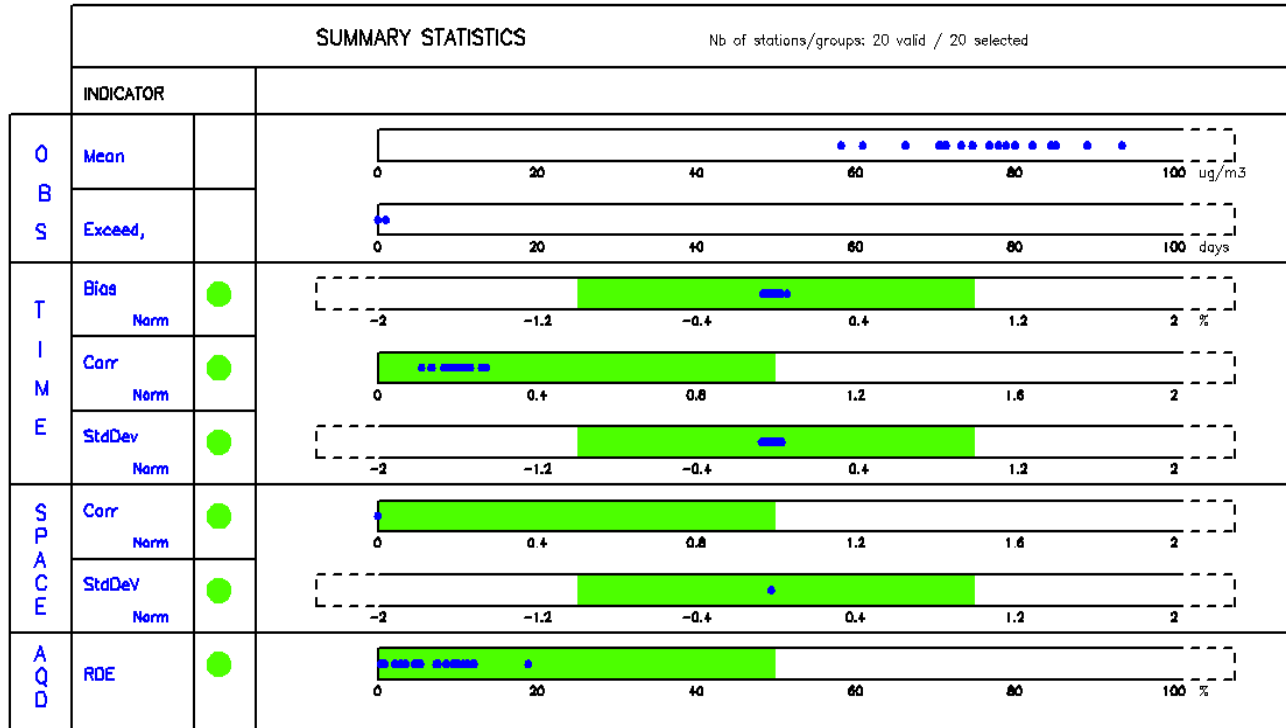
(a)



(b)



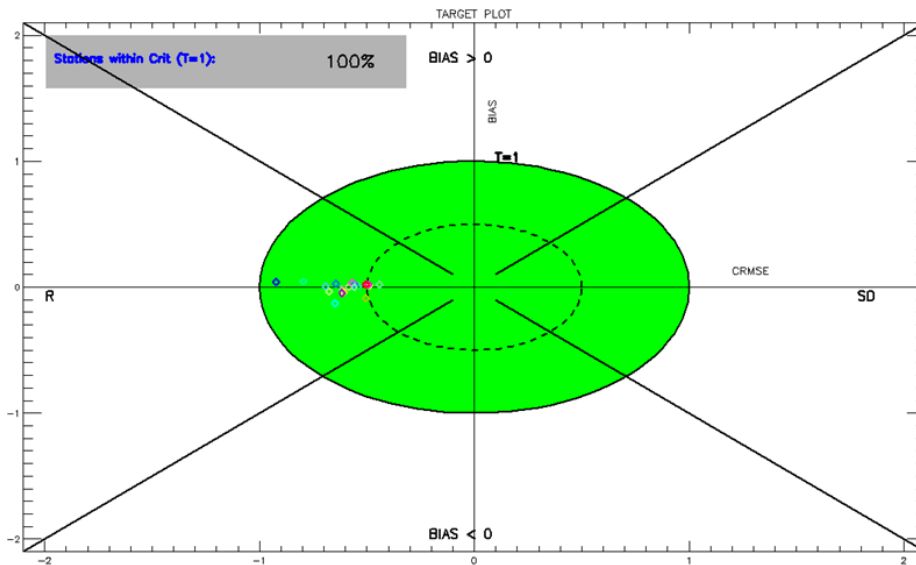
# Some results – O<sub>3</sub>



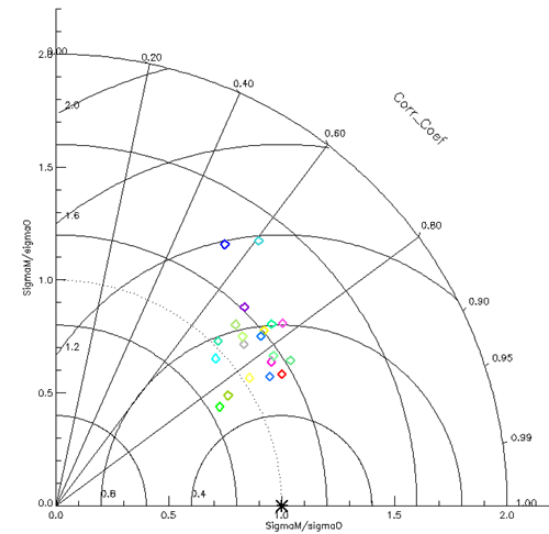
- MEC
- PFR
- OLO
- SOB
- CQI
- ILH
- ERV
- FUN
- MOV
- PP
- OLI
- LAR
- LOU
- MEM
- ARC
- CHA
- FPO
- ALV
- LNH
- TER

# Some results – PM10

(a)

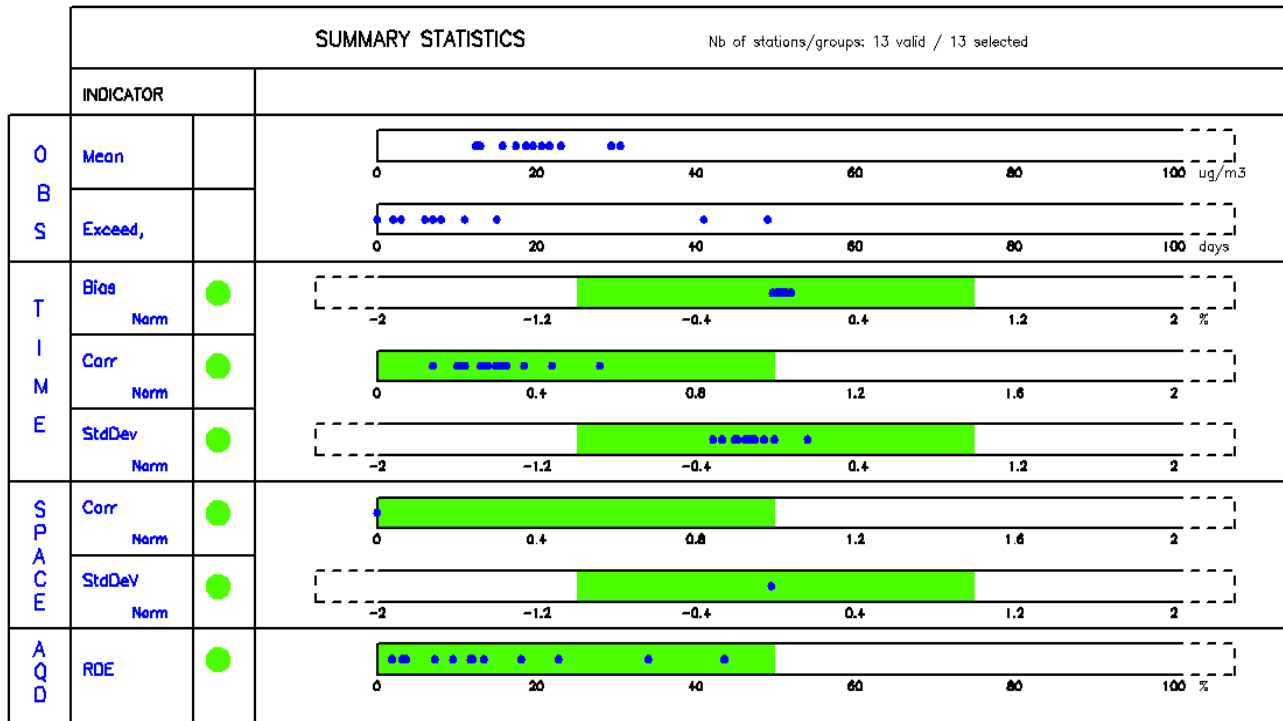


(b)



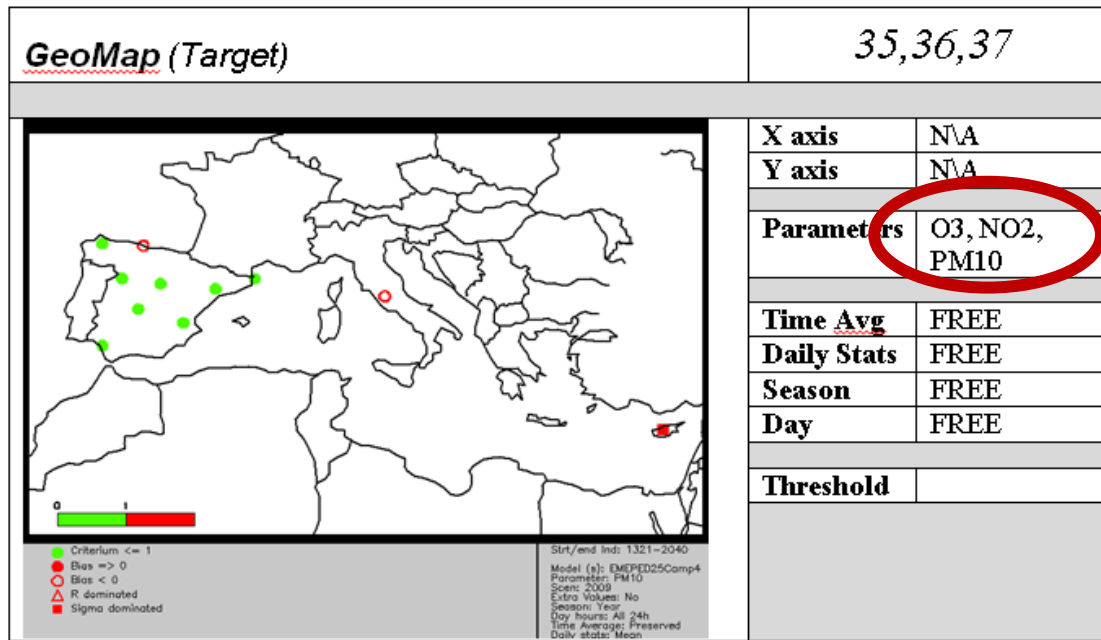


# Some results – PM10



- MEC
- OLD
- COI
- ILH
- ERV
- FUN
- FRN
- LAR
- MEM
- ARC
- CHA
- ALV
- TER

# 1<sup>st</sup> problem: number of pollutants



For when the other legislated pollutants?  
PM2.5; SO2; C6H6; ...

# What we do for the other pollutants...



Available online at [www.sciencedirect.com](http://www.sciencedirect.com)

ScienceDirect

Environment International 34 (2008) 613–620

ENVIRONMENT  
INTERNATIONAL

[www.elsevier.com/locate/entint](http://www.elsevier.com/locate/entint)

## Procedures for estimation of modelling uncertainty in air quality assessment

C. Borrego\*, A. Monteiro, J. Ferreira, A.I. Miranda, A.M. Costa, A.C. Carvalho, M. Lopes

*CESAM, Departamento de Ambiente e Ordenamento, Universidade de Aveiro, 3810-193 Aveiro, Portugal*

Available online 29 January 2008

### Abstract

The main objectives of this work focus, firstly, on a review of the current existent methodologies to estimate air quality modelling uncertainty, and, secondly, in the preparation of guidelines for modelling uncertainty estimation, which can be used by local and regional authorities responsible for air quality management. From the application exercise, it was concluded that it is possible to define a subset of statistical parameters able to reproduce the general uncertainties estimation. Concerning the quality indicators defined by EU directives, the results show that the legislated uncertainty estimation measures are ambiguous and inadequate in several aspects, mainly in what concerns the error measures for hourly and daily indicators based on the highest observed concentration. A relative error at the percentile correspondent to the allowed number of exceedances of the limit value was suggested and tested, showing that is a more robust and appropriate parameter for model performance evaluation.

© 2007 Elsevier Ltd. All rights reserved.

**Keywords:** Air quality; Modelling; Uncertainty; Quality indicators

## Statistical quality indicators for air quality model performance evaluation

Quality indicators	Formula	Range of acceptable values	Ideal value
Correlation coefficient	$r = \left[ \frac{\sum_{i=1}^N (C_{oi} - \bar{C}_o)(C_{pi} - \bar{C}_p)}{\sqrt{\sigma_o \sigma_p}} \right]$	0–1	1.0
Fractional bias	$FB = \frac{\bar{C}_o - \bar{C}_p}{0.5(\bar{C}_o + \bar{C}_p)}$	(-2)–2	0.0
Root mean squared error	$RMS = \sqrt{\frac{1}{N} \sum_{i=1}^N (C_{oi} - C_{pi})^2}$	n.a.	0.0
Normalized standard deviation	$NSD = \frac{\sigma_p}{\sigma_o}$	0–1	1.0
Normalized mean square error	$NMSE = \frac{(\bar{C}_o - \bar{C}_p)^2}{\bar{C}_o \bar{C}_p}$	n.a.	0.0
Average normalized absolute bias	$ANB = \left( \frac{ \bar{C}_o - \bar{C}_p }{\bar{C}_o} \right)$	n.a.	0.0
Geometric mean bias	$MG = \exp(\ln \bar{C}_o - \ln \bar{C}_p)$	>0.0	1.0
Geometric variance	$VG = \exp\left[ (\ln \bar{C}_o - \ln \bar{C}_p)^2 \right]$	>0.0	1.0
Fraction of predictions within a factor of 2 of observations	$\frac{C_p}{C_o}$	0.5–2	1.0
Index of agreement	$d = 1 - \frac{\sum_{i=1}^N (C_{pi} - C_{oi})^2}{\sum_{i=1}^N ( C_{pi} - \bar{C}_o  +  C_{oi} - \bar{C}_o )^2}$	0–1	1.0

n.a. — not applicable.

# What we do for the other pollutants...

Mean statistical parameters for PM2.5

Station	r	RMS	BIAS	FB	NSD	NMSE	ANB	MG	VG	d
	[-]	[ $\mu\text{g}\cdot\text{m}^{-3}$ ]	[ $\mu\text{g}\cdot\text{m}^{-3}$ ]	[-]	[-]	[-]	[-]	[ $\mu\text{g}\cdot\text{m}^{-3}$ ]	[ $\mu\text{g}\cdot\text{m}^{-3}$ ] <sup>2</sup>	[-]
CHA	0.71	4.93	-0.04	-0.01	1.05	0.44	0.49	0.98	1.00	0.83
ERV	0.72	10.79	-0.26	-0.02	1.13	0.52	0.72	0.99	1.00	0.84
FUN	0.69	3.97	0.13	0.03	0.88	0.57	0.66	0.95	1.00	0.82
LAR	0.69	8.06	-0.39	-0.04	1.19	0.76	0.67	0.96	1.00	0.81
MEM	0.71	5.05	-0.04	-0.01	1.02	0.54	0.66	0.98	1.00	0.83
MVE	0.35	20.66	-0.37	-0.04	0.74	5.03	0.92	0.95	1.00	0.52
OLI	0.61	8.71	-0.13	-0.01	1.09	0.46	0.55	1.00	1.00	0.77
OLO	0.75	2.64	0.07	0.02	0.96	0.48	0.54	1.00	1.00	0.86
PFR	0.64	6.93	0.08	0.01	0.90	1.53	0.87	0.92	1.01	0.78
SOB	0.71	4.90	-0.05	-0.01	1.12	0.52	0.54	1.02	1.00	0.84
TER	0.70	5.47	-0.09	-0.01	0.98	0.44	0.66	0.95	1.00	0.83
Mean	0.66	7.46	-0.10	-0.01	1.01	1.03	0.66	0.97	1.00	0.79

## Legend

r: Correlation coefficient  
RMS: Root mean squared error  
FB: Fractional bias  
NSD: Normalized standard deviation  
NMSE: Normalized mean square error  
ANB: Average normalized absolute bias  
MG: Geometric mean bias  
D: Index of agreement

# 2<sup>nd</sup> problem: legislation thresholds

Pollutant	Reference period	Legislation parameter	$\mu\text{g.m}^{-3}$
<b>SO<sub>2</sub></b>	1 hour	Limit value	350
	1 day	Limit value	125
	1 hour	Alert threshold	500
	Winter	Critical level	20
<b>NO<sub>2</sub></b>	1 hour	Limit value	200
	1 year	Limit value	40
	3 hours	Alert threshold	400
<b>NOx</b>	1 year	Critical level	30
<b>C<sub>6</sub>H<sub>6</sub></b>	1 year	Limit value	5
<b>CO</b>	8 hours	Limit value	10000
<b>PM10</b>	1 day	Limit value	50
	1 year	Limit value	40
<b>PM2,5</b>	1 year	VA: 25	25
<b>O<sub>3</sub></b>	8 hours	VA: 120	120
	1 hour	Information threshold	180
	1 hour	Alert threshold	240

# Legislated thresholds

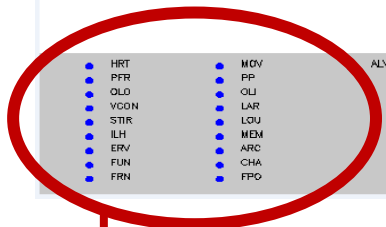
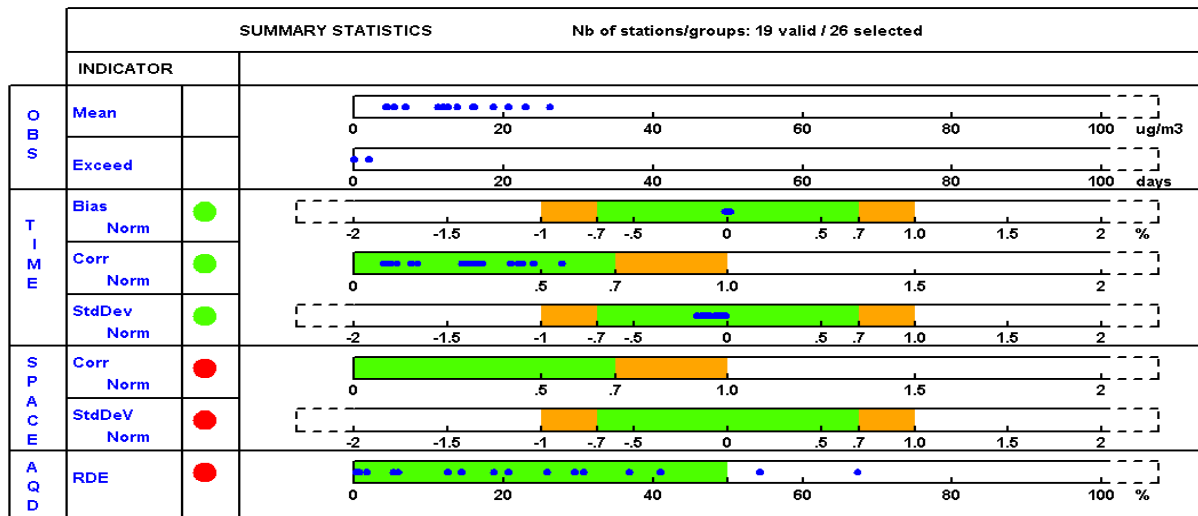
<p>● Criterion <math>\leq 1</math> ● Bias <math>\Rightarrow 0</math> ○ Bias <math>&lt; 0</math> △ R dominated ■ Sigma dominated</p>	<p>Start/end Ind: 1321-2040 Model (s): EMEP025Camp4 Parameter: PM10 Scen: 2009 Extra Values: No Season: Year Day hours: All 24h Time Average: Preserved Daily state: Mean</p>	
<p><b>Description</b></p>	<p><u>GeoMap map showing the locations of the selected stations, together with the Target value for O3 (8hr mean), hourly NO2, daily PM10, hourly WS and TEMP. Colors indicate whether or not the uncertainty criterium is satisfied yes or no; and if not satisfied the location in the target (Bias <math>&gt;0</math>, Bias <math>&lt;0</math>, Correlation dominated or NMSD dominated</u></p>	



There are other legislated parameters that are not included like:

- Information and alert thresholds for O3
- Annual average PM10
- Annual average NO2
- ...

# 2<sup>nd</sup> problem: identification of stations/regions with model deficiencies



Not legible (and as it is. the legend is not necessary!)  
 Maybe using different symbols. similar to the target plot  
 At least to be possible to identify the stations out of criteria

Minor notes  
about our use of DELTA-Tool



# Preparation of cdf file

The manual do not explain how to build the cdf file...  
Maybe some information/help can be given

The screenshot shows a software window titled "DELTATOOL\_MODcsv2cdf \*\*\* VERSION 1.1". The interface is divided into two main sections. On the left, there are several input fields and buttons. At the top left, "HOME\_DIR =" is followed by a text box containing "C:\deltatool\". Below this is a "ReadInfo >>" button. A large rectangular box contains a group of input fields: "STARTUP\_FILE =", "INIT\_RUN =", "END\_RUN =", "INPUT\_DIR =", "FILE\_ID =", "IN\_FILE =", "OUTPUT\_DIR =", "MODEL/OUTPUT =", and "OUT\_FILE =", each followed by an empty text box. Below this group is a "SaveInfo" button followed by "in File" and a text box containing "InfoMODcsv2cdf.txt". At the bottom left, there is a "Progress" label followed by a horizontal progress bar. At the very bottom, there are three buttons: "HELP", "GO", and "EXIT". On the right side of the window, there is a large empty area labeled "COMMENTS" at the top right.

# Bisextile years

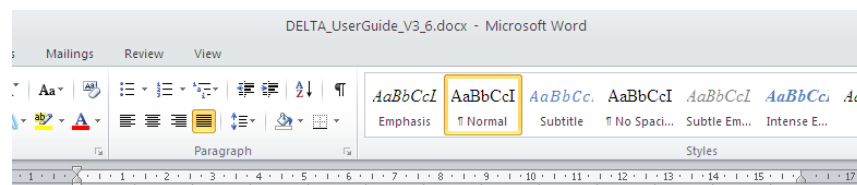
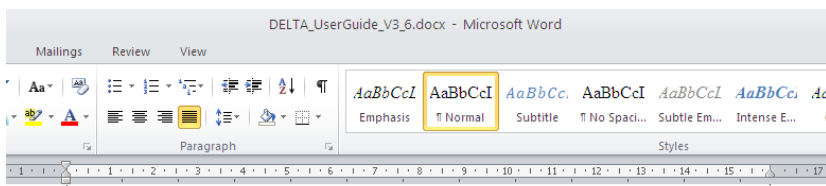
DELTA-TOOL manual

“Year: year of interest (for bisextile years **only first 8760** data are considered)”



Not only that: the year have also to be other  
Don't work with bisextile years identification

# Just some notes about the User's Guide



## DELTA Version 3.6 User's Guide

### Contributors

**P. Thunis, A. Pederzoli, E. Georgieva,  
C. Cuvelier, D. Pernigotti, B. Degraeuwe**

Joint Research Centre, Ispra

24 April 2014

The date is updated each time  
the document is accessed

### 1. Introduction

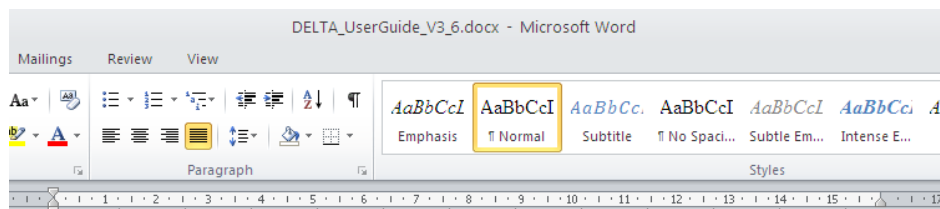
This document describes version 3.5 of the DELTA tool. This tool is an IDL-based evaluation software which includes the main assets of the EuroDelta, CityDelta, and POMI tools (Cuvelier et al. 2007; Thunis et al. 2007). It allows the user to perform rapid diagnostics of air quality and meteorological model performances. Although DELTA focuses on the air pollutants mentioned in the Air Quality Directive 2008 (AQD) it can be used for other variables as well. As it works on the comparison of time series at specific locations it addresses all relevant spatial scales (from local to regional). Some material about DELTA has been already presented in different documents:

**METHOD2012:** *Performance criteria to evaluate air quality modeling applications*, P. Thunis, A. Pederzoli, D. Pernigotti. *Atmospheric Environment*, Volume 59, November 2012, Pages 476-482

**UNCERT2012:** Set of 3 papers:

- *Performance criteria to evaluate air quality modeling applications*, P. Thunis, A. Pederzoli, D. Pernigotti. *Atmospheric Environment*, Volume 59, November 2012, Pages 476-482
- *Model quality objectives based on measurement uncertainty: Part I: Ozone*, P. Thunis, D. Pernigotti and M. Gerboles. 2012, *Atmospheric Environment*, Volume 79, November 2013, Pages 861-868
- *Model quality objectives based on measurement uncertainty: Part II: PM10 and NO2*. D. Pernigotti, P. Thunis, M. Gerboles and C. Belis, *Atmospheric Environment*, Volume 79, November 2013, Pages 869-878

# Just some notes about the User's Guide



details are provided in METHOD2012 and UNCERT2012 regarding the link between the confidence levels associated to the measurements and model results on one hand and the confidence level associated to the modeled-to-measured differences as used in the MQO (see Eq. 1).

For model producing annual averages, the uncertainty is expressed as :

$$U(\bar{O}) = k u_r^{RV} \sqrt{\frac{(1-\alpha)}{N_p} \bar{O}^2 + \frac{\alpha * RV^2}{N_{np}}} \quad (12)$$

where  $N_p$  and  $N_{np}$  are used for annual averages only and account for the compensation of errors due to random noise and other factors like periodic re-calibration of the instruments.

→ Formulas are missing

The following values have been proposed for hourly/daily values