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Uncertainty mapping for air quality modelling and data assimilation

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6th Framework Programme- Policy oriented Research Priority 8.1 Topic 1.5 Task 2

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Introduction

Sources of uncertainty

Uncertainty parameters

Uncertainty mapping

Conclusions

Introduction

Aim, background and applications

Sources of uncertainty

Uncertainty parameters

Model error

Probability distribution functions

Standard deviation and bias

Uncertainty mapping

Spatial distribution of model error

Indicative uncertainty

Uncertainty related to input data

Using variance from spatial statistics

Uncertainty in exceedances

Accounting for temporal covariance, Monte Carlo methods, probability of exceedance, uncertainty in data assimilation methods, etc…

Conclusions

Aim

Raise awareness and promote discussion on uncertainty mapping in air quality applications

Background

- **Based on discussions and developments during the FP6 project Air4EU (www.air4eu.nl)**
- **Discussions on uncertainty and its mapping can be found in a number of Air4EU case studies, recommendation documents and cross-cutting issue reports**
- **Uncertainty maps are presented on the Air4EU mapping tool (www.air4eumaps.info)**

Why use uncertainty maps?

- It is at the heart of the scientific method to express uncertainty in any result
- It is honest and transparent
- Provides information on model quality
- Better basis for decision making

Why do we NOT use uncertainty maps?

- Decision makers do not want to know about uncertainty
- There is not enough information for the uncertainty assessment
- It may reflect unfavourably on the models

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Sources of model uncertainty

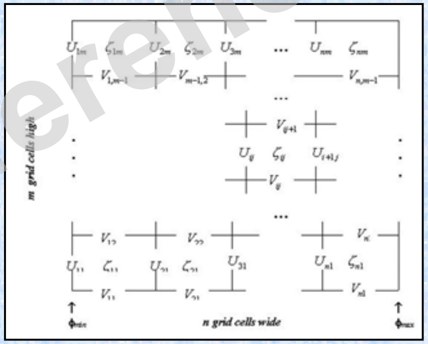
Model description

Model formulation

chemistry, dispersion, etc.

Numerical discretisation

numerical schemes, model resolution, etc.



Input data

Emissions

Meteorology

Boundary conditions

Surface, horizontal, etc.

Monitoring data

Data assimilation

Representativeness

Spatial representativeness

model resolution, subgrid variability

Temporal representativeness

stochastic processes

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Range of parameters for assessing model error

Mean absolute error	MAE
Mean square error	MSE
Normalised mean square error	NMSE
Root mean square error	RMSE
Relative percentile error	RPE (EU directives)
Bias	BIAS
Average normalised absolute bias	ANB
Fractional bias	FB
Correlation	R^2, r
Standard deviation	SD
Normalised standard deviation	NSD
Regression coefficients	slope, intercept
Index of agreement	D
Fraction of predictions …	FAC2

e.g. Chang and Hanna (2004), Borrego et al. (2007)

Model error is an example of poor spatial sampling of the PDF

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Air4EU

Uncertainty parameters

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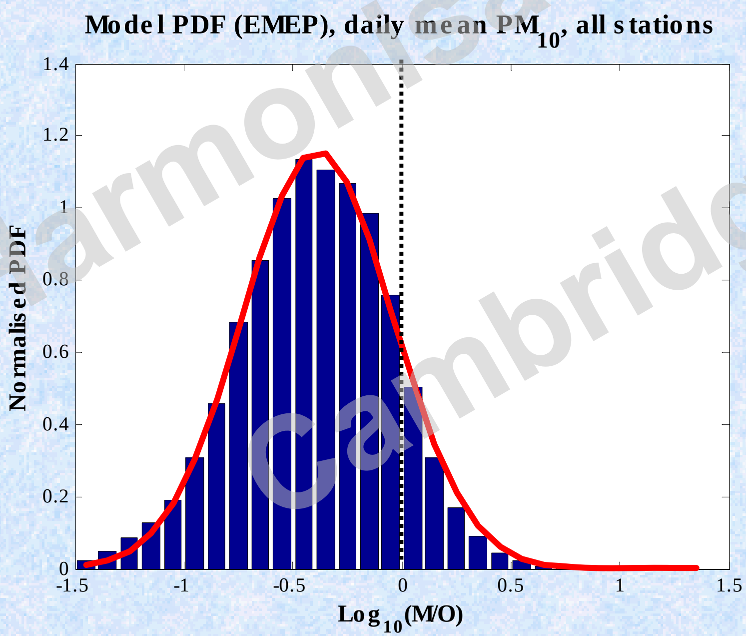
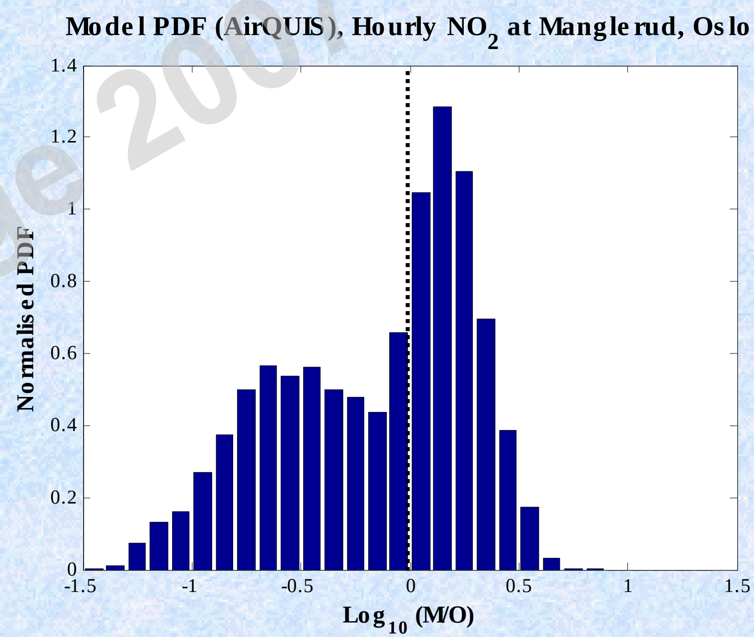
Probability distribution functions

- Are used in Bayesian approaches to uncertainty
- Describe the probable model result, given a ‘true’ or observed value (or visa versa)
- Contain all the uncertainty information
- Can be used to derive other statistical parameters



EMEP model PDF. Daily mean PM_{10} concentrations on the regional scale



AirQUIS model PDF. Hourly mean NO_2 concentrations at a traffic station

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Uncertainty parameters

The use of standard deviation (SD) and bias

- A PDF is not easy to show in map form, so …
- Use SD and bias to describe the normal PDF
- NOTE: PDFs in air quality tend to be log-normal rather than normal

Standard deviation is useful because…

- It can be statistically extracted from any sample
- It is similar to RMSE
- It can by calculated from ensemble methods
- It can be derived from spatial statistical methods such as kriging

Bias must be included

- Separately or implicitly through, e.g., RMSE
- If bias is known it should be removed

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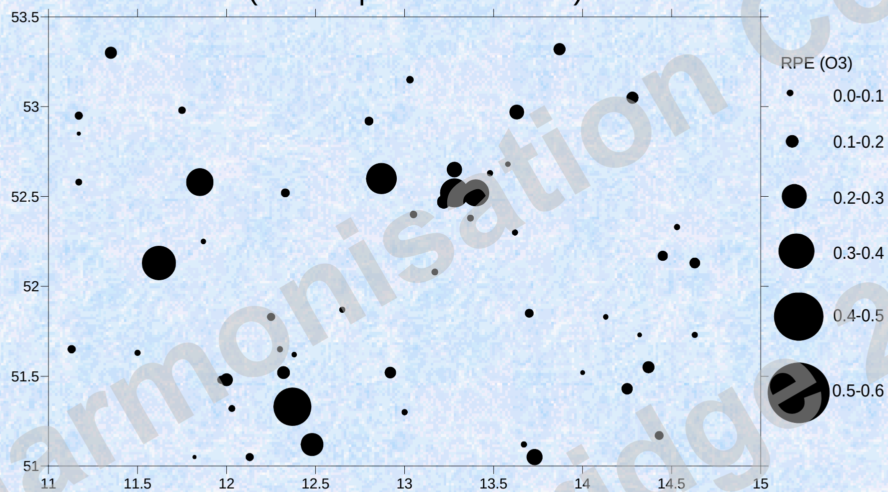
Example maps of model error, legislative applications

Spatial representation of RPE, Berlin O_3, REM-Calgrid model

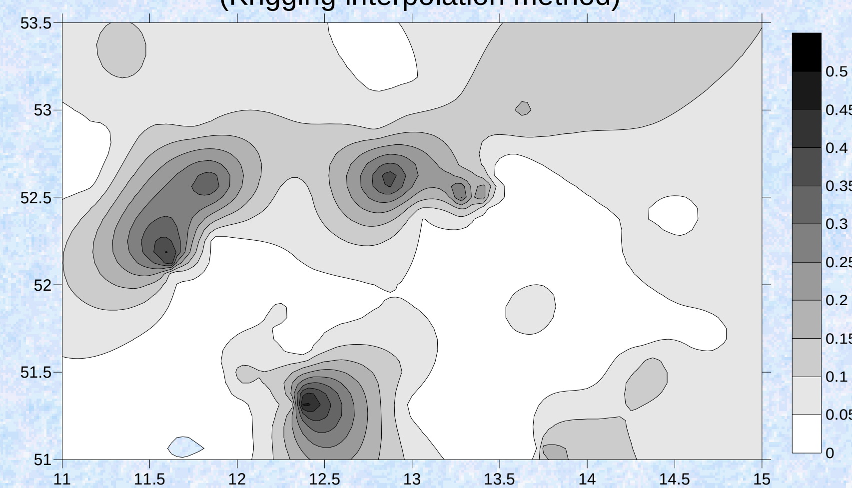
$$RPE = \frac{|O_P - M_P|}{O_P}$$

Spatial mapping of RPE for O3
(no interpolation method)



RPE represented by dot sizes

Spatial mapping of RPE for O3
(Kriging interpolation method)



RPE interpolated between points using kriging

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Uncertainty mapping

Indicative uncertainty

- **Presenting maps that are *indicative* of the standard deviation**
- **Generalised description of the standard deviation based on an absolute and a relative standard deviation**

$$\sigma_M(x,y) = \sqrt{\sigma_A^2 + \sigma_R^2 M(x,y)^2}$$

σ_R and σ_A can be calculated using:

Expert knowledge, e.g. σ_R = 25%

Normalised RMSE

$$\sigma_R = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(M_i - O_i)^2}}{\overline{M}}$$

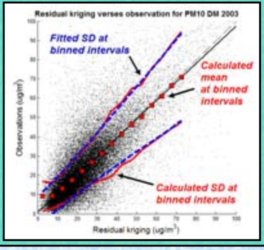
SD of the PDF

$$\sigma_R = 1 - \sqrt{\frac{1}{(n-1)}\sum_{i=1}^{n}\left(\frac{O_i}{M_i}\right)^2}$$

Prediction intervals

$$\sigma_M = t_{\alpha/2,n-2}\sqrt{\left[\frac{(n+1)}{n} + \frac{(M-\overline{M})^2}{\sigma_{MSD}^2}\right]\frac{\sum_{i=1}^{n}(O_i - M_i')^2}{(n-2)}}$$

Fits to scatter plots



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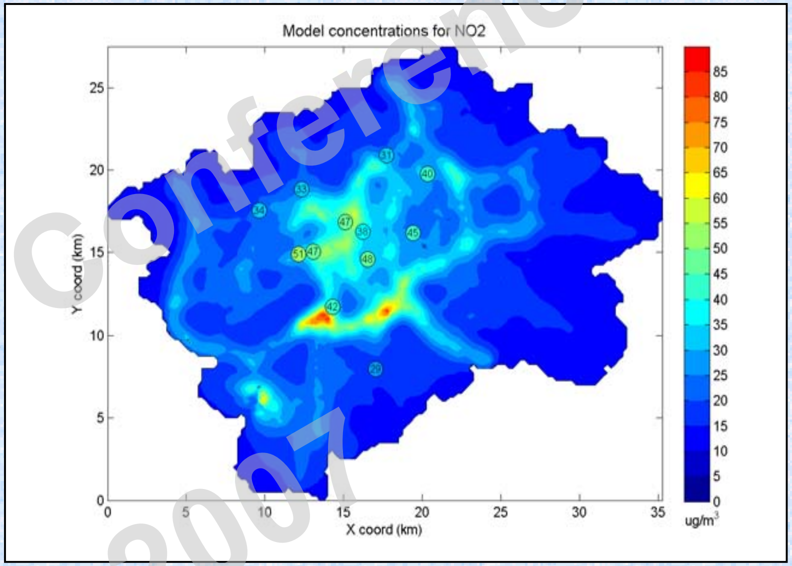
Example of an indicative uncertainty map

Prague, annual mean NO_2, ATEM model

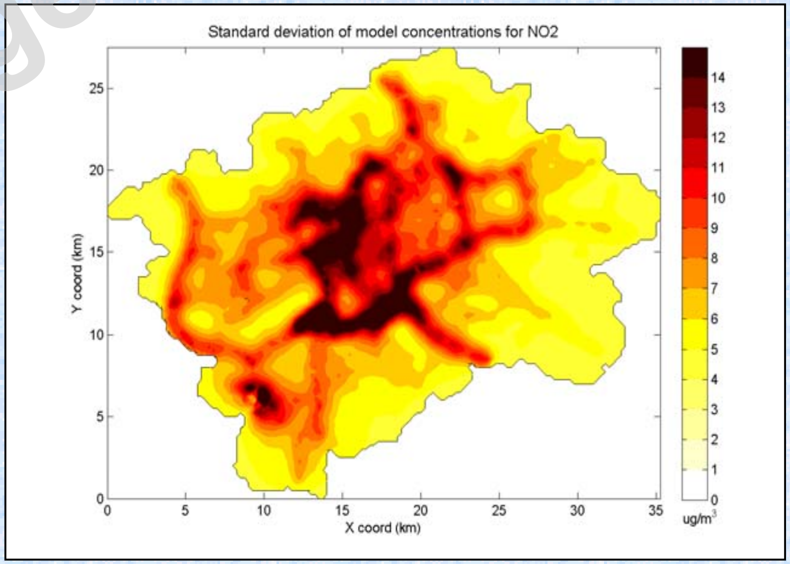
Based on normalised RMSE

σ_R = 27%

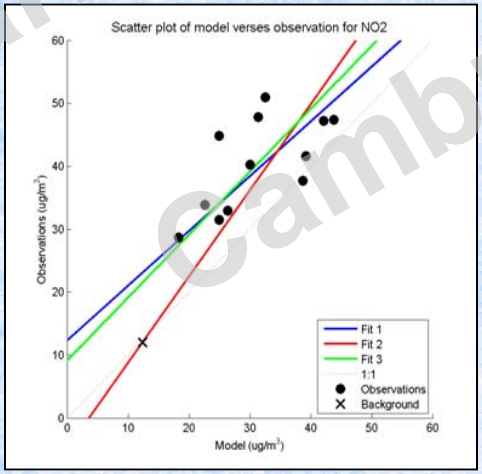
σ_A = 0



Model



Uncertainty



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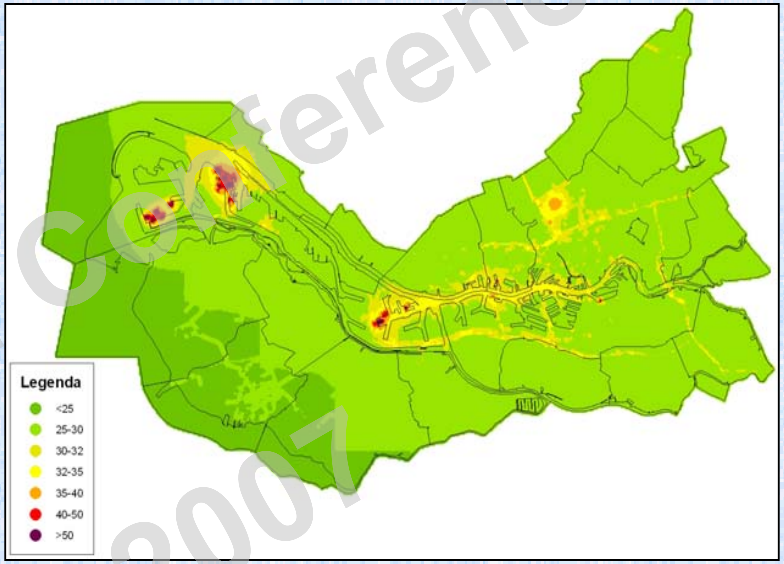
Uncertainty mapping

Application for scenario prediction

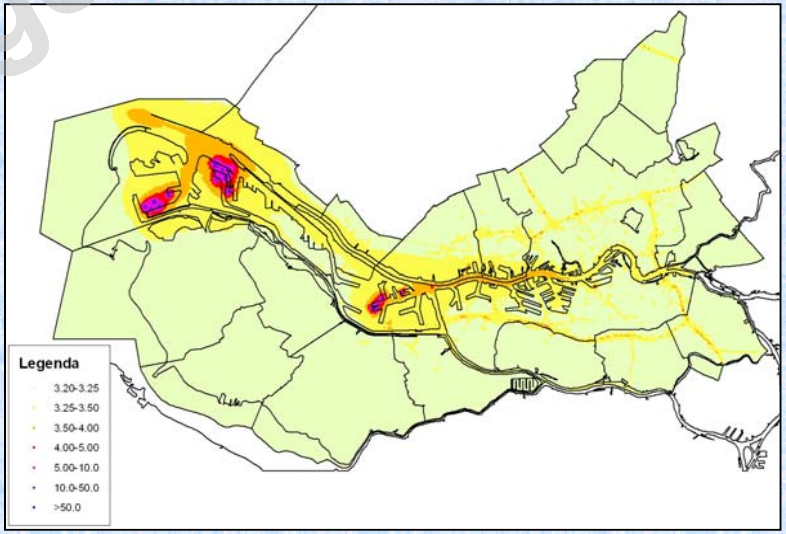
Predicted concentrations of PM_{10} for 2010 in Rotterdam, using the Urbis model



Model prediction

Expert assessment of emission uncertainty in the various source sectors

⇨Spatial map of the emission scenario uncertainty



Uncertainty due to emissions

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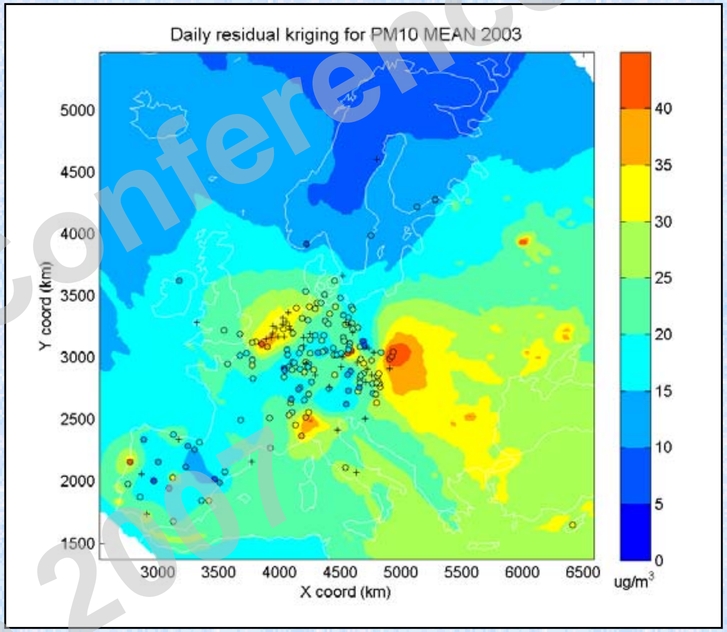
Spatial statistics

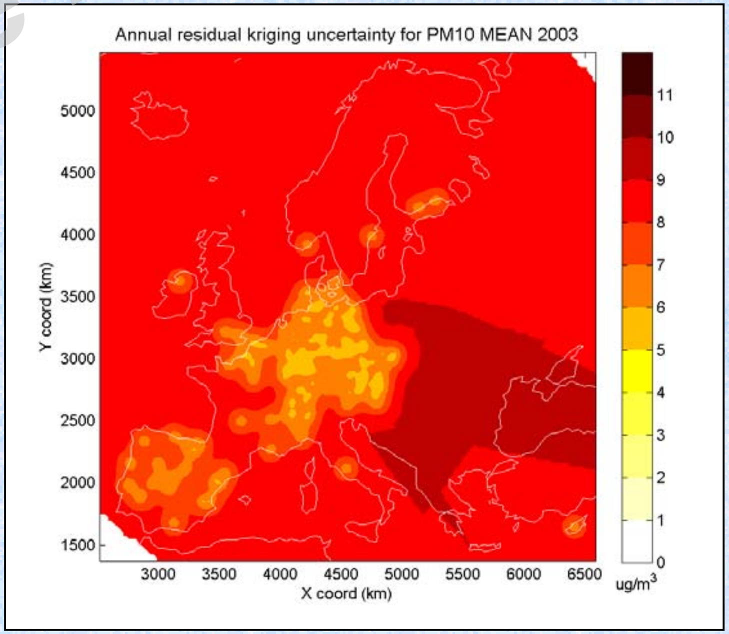
Maps may also be made using kriging, residual kriging or other statistical interpolation methods



Residual kriging of annual mean rural background PM_{10} using the EMEP model and Airbase stations

SD is calculated in these methods using the kriging variance

$$\sigma_M(x,y) = \sqrt{Var(x,y)}$$



Uncertainty map

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Uncertainty in exceedances

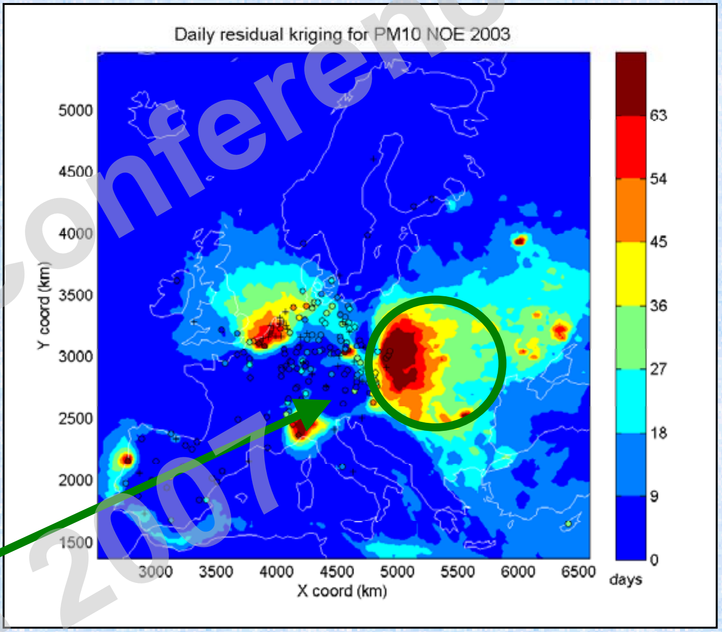
Use daily mean uncertainty

⇨ probability of exceedance

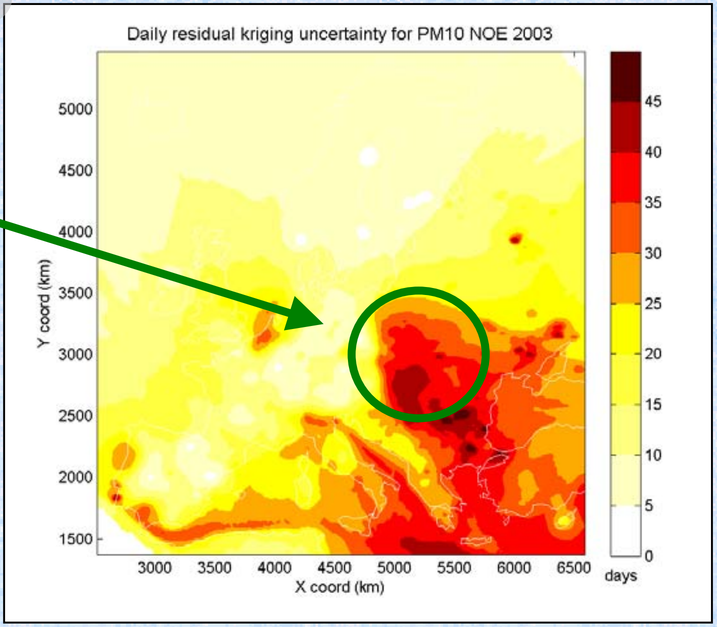
Use the annual mean uncertainty

⇨ spatial representativeness bias

Calculate the uncertainty in the number of exceedance days



Large number of exceedance days (> 60 days)



Large uncertainty in the areas removed from observations (SD > 35 days)

Number of exceedances, and related uncertainty, of the daily mean EU limit for PM_{10} rural background only

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Conclusions

General comments

- There is currently no established methodology, parameter or presentation method for communicating uncertainty
- It will be necessary to have a common parameter(s) for representing uncertainty if it is to be useful for intercomparison purposes
- Different mapping methods use different methodologies for uncertainty assessment

Recommendations

- Spatial interpolation of model error is not recommended
- Some indication of the uncertainty must always be given, preferably as maps but otherwise as a single value
- Present assessment maps with a contour or colour selection that is indicative of the uncertainty
- Bias should be removed from maps when it is known

Future challenges

- **Convincing air quality modellers to include uncertainty in their maps**
  - How many presentations of maps at this conference will include uncertainty?
- **Establishing homogenous and accepted methodologies for determining and presenting spatial uncertainty**
- **Increase cooperation between atmospheric modellers and spatial statistical groups**
- **Inclusion of uncertainty in the entire process, from emissions to risk assessment**
  - e.g. EU projects HEIMTSA and INTERESSE
- **Convince decision makers that they should want to know about uncertainty**
- **Reformulation of directives and other legislation to properly include aspects of uncertainty**

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