

Uncertainties of monitoring and modelling

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European Project

The uncertainty concept is one of the crucial points of Quality Assurance/Quality Control procedures that should provide quantitative information about the monitoring/modelling precision, identifying the uncertainty sources and their potential reduction. The development of a consistent procedure for the uncertainty evaluation is still a challenge for the scientific community. Nevertheless, in the scope of the AIR4EU project, it was outlined a possible procedure for the correct estimation of uncertainties, at different levels of expertise and/or available data.

Monitoring

data quality objectives

Monitoring programme/ Monitoring objective	Compounds	Accuracy	Precision	Data time coverage
EUROAIRNET Mapping, comparability		≤10%	≤2 ppb	≥90%
EU Regulatory Monitoring Detect non-compliance with directives	SO ₂ , NO ₂ PM, Pb	15% 25%		90% annual -
EMEP Provide basis for control of models		15-25%		90% annual
WMO-GAW Detect trends over short term (5 years)	Examples: O ₃ NO ₂ PM _{2.5}	15% or 3 ppb 20% or 50 ppt 0.05+5% M	10% or 1 ppb 10% or 25 ppt 10%	80% monthly - 90% monthly

recommendations

Basic requirements

Report data and associated uncertainty for compliance assessment of EU Directives.

Best practice recommendations

Establishment of a QA/QC plan based on EUROAIRNET recommendations. Dissemination of report data and associated uncertainty along with the QA/QC plan.

Scientific recommendations

Clear statement of the data quality objectives and an adequate documented QA/QC plan formulation and implementation.

Modelling

step 1 uncertainty according to the EU directives

EU Directives establish requirements for air quality modeling as a measure of modeling results acceptability:

"maximum deviation of the measured and calculated values, over the period for calculating the appropriate threshold, without taking into account the timing of the events"

$$RME = \frac{\max(C_{o,p} - C_{p,p})}{C_{o,\max}(C_{o,p} - C_{p,p})}$$

Pollutant	Quality Indicator	Quality Objective	Directive
SO ₂ , NO ₂ , NO _x	Hourly mean	50-60%	1999/30/EC
	Daily mean	50%	
	Annual mean	30%	
PM, Pb	Annual mean	50%	2000/69/EC
	8-hour mean	50%	
CO	Annual mean	50%	2000/69/EC
Benzene	Annual mean	50%	2002/03/EC
	8-hour daily mean	50%	
Ozone	8-hour daily mean	50%	2002/03/EC
	1-hour average	50%	

an alternative model error measure is...

concentration relative error at the percentile (p) corresponding to the allowed number of exceedances of the limit value normalized by the observation

$$RPE = \frac{C_{o,p} - C_{p,p}}{C_{o,p}} \cdot p$$

- 1) more robust (uses the percentile instead of the maximum value)
- 2) evaluates model performance in the high concentration ranges
- 3) direct link to the EU Directives, since the model uncertainty is examined in the concentration range of the limit values

recommendations

Basic requirements I

Presentation of a qualitative (e.g., graphical) and a quantitative (e.g., statistical) analysis of model results against measured values from the air quality network. For the application of the Quality Objectives of the Air Quality Framework Directive it is recommended to use the alternative model error Relative Percentile Error (RPE) when dealing with percentiles. For annual means, both RPE and RME (relative maximum error) are compatible for annual means and should be applied in that context.

step 2 total model uncertainty

"the computation of the total uncertainty induced in the output by quantified uncertainty in the inputs and model, and the attributes of the relative importance of the input uncertainties in terms of their contributions."



How to estimate Total Model Uncertainty? statistical analysis

Quality indicators	Formula	Ideal value
Correlation coefficient	$r = \frac{\sum (C_{o,i} - \bar{C}_o)(C_{p,i} - \bar{C}_p)}{\sqrt{\sum (C_{o,i} - \bar{C}_o)^2 \sum (C_{p,i} - \bar{C}_p)^2}}$	1.0
Fractional bias	$Fb = \frac{C_o - C_p}{C_o}$	0.0
Root mean squared error	$RMS = \sqrt{\sum (C_{o,i} - C_{p,i})^2}$	0.0
Normalized standard deviation	$NSD = \frac{RMS}{C_o}$	1.0
Normalized mean square error	$NMSE = \frac{C_o - C_p}{C_o}$	0.0
Average normalized absolute bias	$ANAB = \frac{ C_o - C_p }{C_o}$	1.0
Geometric mean bias	$MG = \exp(\ln(C_o - \ln C_p))$	1.0
Geometric variance	$VG = \exp(\ln(C_o - \ln C_p)^2)$	1.0
Fraction of predictions within a factor of 2 of observations	$0.5 \leq \frac{C_p}{C_o} \leq 2.0$	1.0

Quality indicators	EPA	Acceptable values
Normalized accuracy of the maximum 1h concentration unpaired in space and time	$E = \frac{1}{N} \sum \frac{C_o - C_p}{C_o}$	± 15-20%
Normalized bias test	$A_b = 100 \left(\frac{C_o - C_p}{C_o} \right)$	± 0.05-0.15
Gross error of all pairs Co > 60 ppb	$D = \frac{1}{N} \sum \frac{C_o - C_p}{C_o}$	± 30-35%

C_o and C_p are the concentration observed and predicted

recommendations

Basic requirements II

For the estimation of the Total Model Uncertainty it is recommended to use the following statistical parameters: correlation coefficient, fractional bias and normalized standard deviation.

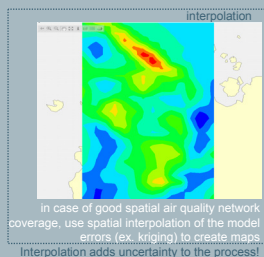
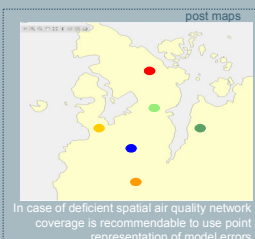
Best practice recommendations

Stochastic variability to investigate the contribution of the different components of total model uncertainty. It is recommended to filter out stochastic processes from the monitoring data based on spectral analysis and the quantification of model uncertainty without the influence of stochastic variations.

Scientific recommendations

Analysis of intrinsic model uncertainty to perform a sensitivity analysis and/or model intercomparison to evaluate the different model modules to determine intrinsic model uncertainty (ex. Monte Carlo approach).

step 3 uncertainty mapping



Suggestion of parameters to be represented for directive purposes
 RPE for daily/hourly averages
 RME for annual averages
 also
 NMSE Normalised Mean Square Error
 Fb Fractional Bias

recommendations

Basic requirements

When there is limited information concerning the model error, then mapping of uncertainty can be carried out by a 'best estimate', based on other information available. This should be applied to the assessment map as a relative uncertainty. When more information is available concerning the model error, then the RMSE of the RME and RPE from these sites can be used as indicative of the uncertainty. Regression relations between model concentrations and model types are more indicative of the spatial variation than direct spatial interpolation of the error. The applicability of interpolation of RME or RPE can also be assessed through cross-validation.

Best practice recommendations

If both urban and local scale models exist then spatial distribution of model uncertainty should include the individual uncertainties of the models and their contribution to the total model uncertainty. If data assimilation techniques are used and provided uncertainty estimates, then the variance or standard deviations should be used to map uncertainty.

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