

# Air4EU

**Air Quality Assessment for Europe: from local to continental scale**



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

## **Individual case study report: 14 Assessment of modelling uncertainties**

Deliverable:	D7.1 Part 14
Dissemination level:	PU
Editor:	Carlos Borrego
Version:	Final
Date:	March 2007
Contract:	503596

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## Table of Content

<b>SUMMARY (ABSTRACT)</b> .....	<b>5</b>
<b>1. EXECUTIVE SUMMARY</b> .....	<b>7</b>
<b>2. CASE STUDY DESCRIPTION</b> .....	<b>7</b>
2.1 Background.....	7
2.2 Aim and description.....	7
2.3 Relevance to recommendations in Air4EU.....	8
<b>3. METHODOLOGY</b> .....	<b>9</b>
<b>4. RESULTS</b> .....	<b>10</b>
4.1 Urban scale.....	11
4.1.1 Uncertainties according to the EU Directives.....	12
4.1.2 Uncertainties from statistical analysis.....	14
4.1.2 Uncertainty mapping.....	17
4.2 Hot spot scale.....	20
4.2.1 Uncertainties according to EU Directives.....	21
4.2.2 Statistical analysis.....	23
4.2.3 Uncertainty mapping.....	25
<b>5. CONCLUSION AND DISCUSSION</b> .....	<b>29</b>
5.1 Assessment of the case study.....	29
5.2 Improvements in assessment derived from case study.....	29
5.3 Recommendations resulting from the case study.....	29
5.4 Suitability for implementation in other cities.....	29
<b>REFERENCES</b> .....	<b>30</b>

## Summary (Abstract)

The uncertainty concept is one of the crucial points of Quality Assurance/Quality Control (QA/QC) procedures that should provide quantitative information about the modelling precision, identifying the uncertainty sources and their potential reduction. The present European legislation defines the Modelling Quality Objectives as an acceptability measure, to guarantee good model performance and reliable modelling results for decision makers. However, a practical application of these requirements and interpretation of the uncertainty analysis results based on the recommended methodology is ambiguous, and in some cases incomprehensible for non-expert users. The development of a consistent procedure for uncertainty evaluation is still a challenge for the scientific community.

The aim of this case study is to provide an example of the methodology described in the Air4EU-M2 cross cutting report regarding the estimation of air quality modelling uncertainty. An uncertainty analysis was performed to the modelling results of the Berlin case, concerning an urban and hot spot scales, for the main critical pollutants. According to the basic recommendations, defined in the Air4EU-M2 report, the estimation of total model uncertainty will be determined through comparison between model predictions and air quality observations, based on the Air Quality Framework Directive (FWD) settlements and on statistical parameters. The referred recommendations consider three levels of application adaptable to end-users needs, goals and ability. The first level is a simple qualitative analysis. The estimation of total model uncertainty based on statistical parameters and on FWD settlements is covered by the second level. In order to improve model performance, it is necessary to investigate the contribution of the different components of total model uncertainty. Therefore, the third level details the total model uncertainty, through the estimation of its different components. For a more complete evaluation, sensitivity analysis to model and input parameters should also be performed. This sequence of recommendations should be regarded in these three levels of complexity and could be applied by end-users according to their desire and need of detail (Borrego et al., 2005). For the Berlin case study the second level of recommendations will be applied. The alternative model error RPE (Relative Percentile Error) will be considered to estimate model uncertainty. The Berlin case study is composed by two different scale model approaches. First of all, simulations were performed with the RCG model over the urban area of Berlin, with 4x4 km<sup>2</sup> grid resolution. The Gaussian multi-source dispersion model IMMISnet was used for the local scale modelling simulations over Berlin. The modelling and monitoring data were provided by the Senat Berlin for the year 2002 and for PM<sub>10</sub> and NO<sub>2</sub> pollutants. The uncertainty estimation methodology described was applied separately for each numerical model scale application.

Results of the first step point to the fulfilment of the modelling acceptability criteria defined in the FWD, for all the analysed pollutants for the urban scale and partially for NO<sub>2</sub>, at the local scale. For the same scale and for PM<sub>10</sub> most of the RPE values determined are above the modelling quality objective of 50%. In the second step, the statistical analysis, comprising a set of parameters, gave information about the ability of the model to predict the tendency of observed values ( $r$ ), relative and absolute errors on the simulation (RMSE and NMSE), and type of errors (Bias). This analysis shows that the urban scale model is able to predict concentrations for the Berlin case with correlation factors higher than 0.7 for O<sub>3</sub> and for PM<sub>10</sub>. For the local scale, the averaged correlation factor is 0.48 and 0.51 for NO<sub>2</sub> and PM<sub>10</sub> pollutants, respectively, indicating that the model is not able to simulate correctly the physic processes involved in the dispersion of the referred pollutants. Besides that, the models average error shows no significant discrepancies between model values and observed data. At the urban scale the Bias shows no model tendency for some pollutants, suggesting that local phenomena could be responsible for model errors at each specific monitoring site, but exists a clear model overestimation for PM<sub>10</sub>. The uncertainty spatial mapping showed that all the analysed indicators are adequated to perform the spatial representation of the uncertainty. Considering that the basic level of recommendations is completed for this case study, it is recommended for future work to investigate the stochastic contribution to the total model uncertainty and to perform a sensitivity analysis or model intercomparison to evaluate the uncertainty related to each model modules.



# **Berlin case study report: Assessment of modelling uncertainties**

## **1. Executive Summary**

Air quality models need to be properly evaluated before their predictions can be used with confidence, because model results often influence decisions with consequences on health and economy. A systematic description of the methodologies for modelling uncertainty estimation was performed and discussed in the scope of the AIR4EU European project based on a bibliography review and addressed according to the end users needs. This methodology consists first on the estimation of model uncertainty and comparison with the data quality objectives defined by the EU legislation and, consecutively, a complementary analysis of the total model uncertainty based on a statistical analysis. The developed procedure was applied to the city case of Berlin, considering both urban and local scale modelling applications. The uncertainty analysis exercise shows an incomplete definition of the Quality Assurance/Quality Control procedures for air quality modelling by the present EU legislation. The statistical analysis performed suggests the use of specific group of indicators in order to complete the model uncertainty estimation.

## **2. Case study description**

### **2.1 Background**

There is no record of previous studies concerning uncertainty modelling estimation over the city of Berlin.

### **2.2 Aim and description**

The aim of this case study is to provide an example of the methodology described in the cross cutting report "M2: Uncertainties of models & monitoring" regarding the estimation of air quality modelling uncertainty. An uncertainty analysis was performed for the modelling results of Berlin City concerning the urban and hot spot scales for the main critical pollutants. Following the basic recommendations, the estimation of total model uncertainty, based on the Air Quality Framework Directive (FWD) settlements and on statistical parameters was applied.

The present European legislation defines the requirements of QA/QC procedures for air quality modelling, including the definition of Quality Objectives as an acceptability measure, in order to guarantee that they indicate a good model performance and reliable modelling results for decision makers. The interpretation and applicability of this legislation is discussed in the cross cutting report M2: Uncertainties of models & monitoring. An alternative relative error at the percentile correspondent to the allowed number of exceedances of the limit value, suggested in the above mentioned report, was tested and compared with the legislated uncertainty estimation measure, showing that it is more robust and also evaluates the model performance as required.

The statistical analysis suggested to evaluate model performance and to estimate uncertainties comprising a set of parameters, give information about the ability of the model to predict the tendency of observed values, errors on the simulation of average and peak observed concentrations, and type of errors (systematic or unsystematic). Despite the importance of all parameters, a subset of parameters defined previously in M2 report were used with the goal to reproduce the general

uncertainties estimation, comprising the correlation coefficient, the bias and the root and normalized mean square errors (Borrego *et al.*, 2005).

## 2.3 Relevance to recommendations in Air4EU

This study case constitutes an application example of the basic recommendations (see Table 1), regarding model uncertainty, defined in the scope of Air4EU project. In this sense, it could serve as a guideline and baseline document for other cities that use local or urban scale model applications. Nevertheless, considering that only the basic level of recommendations was performed for this case study it is recommended for future work:

- to investigate the stochastic contribution to the total model uncertainty in order to improve model performance
- to perform a sensitivity analysis and/or model intercomparison to evaluate the different model modules (Chemical mechanisms, physical parameterisations and numerical algorithms) and to determine the intrinsic model uncertainty
- to present assessment maps combined with a spatial representation of the uncertainty.

*Table 1: Guidelines/recommendations for model applications evaluation by end-users.*

Level of Complexity	Guidelines description
---------------------	------------------------

Qualitative analysis	Analysis of model results against measured values from the air quality network
Total model uncertainty	Quantitative analysis of model results using a set of statistical parameters defined in the cross cutting report M2: Uncertainties of models & monitoring, chapter 2.2;  Model performance evaluation according to the Air Quality Framework Directive Quality Objectives - Due to ambiguities in the FWD text it is suggested to apply an alternative model error measure as proposed and justified in the cross cutting report M2: Uncertainties of models & monitoring, chapter 2.3;
Total model uncertainty by components (variability, model uncertainty and input data)	Variability - for stochastic variations quantification spectrum analysis or exploration of cyclical patterns should be performed to measured air quality data. The purpose of the analysis is to decompose a complex time series with cyclical components into a few underlying sinusoidal functions of particular wavelengths and, in this way, separate different phenomena present in the time series. Fast Fourier Transformation technique can be used to accomplish this goal.  Model Uncertainty- Sensitivity analysis and/or model intercomparison to evaluate different model modules (Chemical mechanisms, physical parameterisations and numerical algorithms);  Input Data- Sensitivity analysis to input parameters (initial and boundary conditions, meteorological parameters, emissions, land use and topography).

### 3. Methodology

According to the second level of basic recommendations, the total model uncertainties will be determined through comparison between model predictions and air quality observations for the urban and hot spot scales, using an alternative model error measure to the Air Quality Framework Directive and a set of statistical parameters defined in the cross cutting report M2: Uncertainties of models & monitoring, chapter 2.2. The modelling and monitoring data for both scales were provided by the Senat Berlin for the year 2002 and for PM<sub>10</sub> and NO<sub>2</sub> pollutants.

The Framework Directive (FWD) and Daughter Directives establish requirements for air quality modelling, including the definition of the Modelling Quality Objectives, as a measure of modelling results acceptability.

The quality objectives defined for each quality indicator and for NO<sub>2</sub> and PM<sub>10</sub> pollutants are listed in Table 3.

*Table 3: Modelling Quality objectives established by EU Directives.*

Pollutant	Quality Indicator	Quality Objective	Directive
SO <sub>2</sub> , NO <sub>2</sub> , NO <sub>x</sub>	Hourly mean	50-60%	1999/30/EC

	Daily mean	50%
	Annual mean	30%
PM <sub>10</sub> , Pb	Annual mean	50%

The alternative model error RPE (Relative Percentile Error) will be considered to estimate model uncertainty, corresponding to the allowed number of exceedances of the limit value normalized by the observation:

$$RPE = \frac{|C_{o_p} - C_{p_p}|}{C_{o_p}}$$

Table 2 presents the main statistical parameters used as quality indicators in this case study.

Table 2: Quality indicators for air quality model performance evaluation.

Quality indicators	Formula	Observations	Range of acceptable values
Correlation coefficient	$r = \frac{\sum_{i=1}^N (C_{o_i} - \bar{C}_o)(C_{p_i} - \bar{C}_p)}{\sigma_o \sigma_p}$	C <sub>o</sub> and C <sub>p</sub> are the concentration observed and predicted,	1.0
Bias	$\text{Bias} = \frac{\sum_{i=1}^N (C_o - C_p)}{n}$	$\bar{C}_o$ and $\bar{C}_p$ are the averaged concentration observed and predicted, $\sigma_o$ and $\sigma_p$ are the standard deviations of observations and predictions	0.0
Root mean squared error	$RMSE = \sqrt{\sum_{i=1}^N (C_{o_i} - C_{p_i})^2}$	C <sub>oi</sub> and C <sub>pi</sub> are the observed and predicted concentration in monitoring station "i"; n the total number of monitoring stations.	0.0
Normalized mean square error	$NMSE = \frac{(C_o - C_p)^2}{C_o C_p}$		0.0

## 4. Results

The Berlin case study is composed by two different scale model approaches. First of all, simulations were performed with the REM-Calgrid (RCG) model over the urban area of Berlin, with 1x1 km<sup>2</sup> and 4x4 km<sup>2</sup> grid resolutions. For local scale numerical simulations, the Gaussian multi-source dispersion model IMMISnet was applied over Berlin (information regarding domain and resolution was not provided by the Senat Berlin).

The uncertainty estimation methodology described above was applied separately for each numerical model scale application and follows the basic recommendations agreed in the Cross-cutting Report Air4EU-M2: Uncertainties of models and monitoring.

## 4.1 Urban scale

The German HOVERT campaign aimed at increasing the observational data basis for chemically and size specified aerosols in a Central European region with strong anthropogenic influence, the Berlin Brandenburg area. Dedicated daily measurements in a network of traffic, urban, peri-urban and rural sites for an about one year period (from September 2001 to September 2002) provided valuable information to assess the urban contrast in concentrations, sources of different aerosol components and to perform a complete model evaluation. The HOVERT data base is enhanced by routine observations from the air quality networks existent within the Berlin urban area domain and from specific measurements at a traffic influenced site in Berlin, supported by the SENAT of Berlin.

In this case study, the HOVERT campaign data base was used for the uncertainty analysis of the RCG model. The RCG model, developed at Free University of Berlin with the support of the German Environmental Protection Agency (Umweltbundesamt) (Stern, 2003), is a Chemical-Transport-model of medium complexity designed for the regional and urban scale. In the past, RCG has been mainly used for the simulations of emission abatement scenarios (Stern, 2003) and for ozone forecast (Tilmes et al., 2002). Figure 4 shows the mesoscale domain (covering 11°-15°W degrees of longitude and 51°-53,5°N degrees of latitude) used for the Berlin urban area simulation, with 4x4 km<sup>2</sup> resolution.

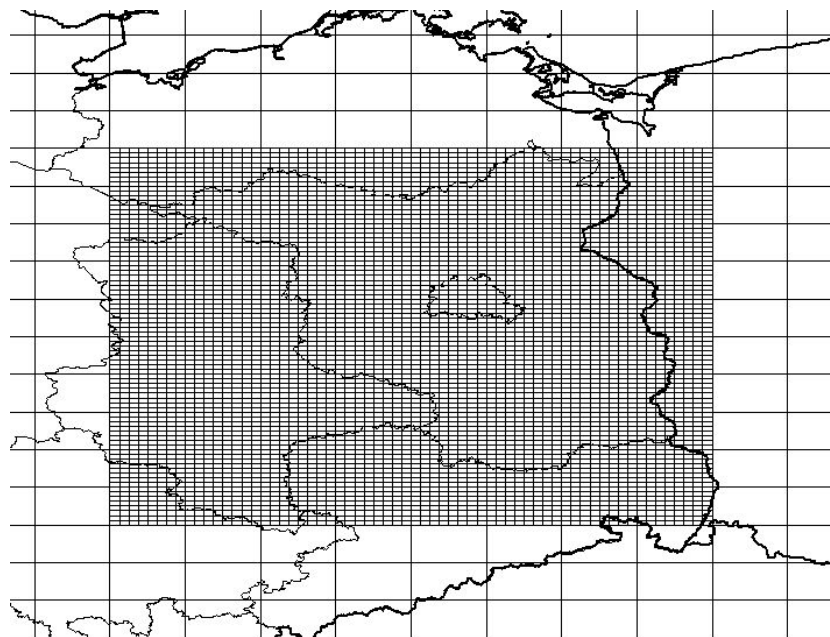


Figure 4: Domain of RCG model application for Berlin urban area (4x4 km<sup>2</sup> grid resolution). From 11° to 15°W degrees of longitude and from 51° to 53,5°N degrees of latitude.

Besides this grid resolution, the RCG model was also applied for a fine resolution (1x1km<sup>2</sup>) for a small domain, covering the urban city area of Berlin. A representation of this smaller domain is shown in Figure 5.

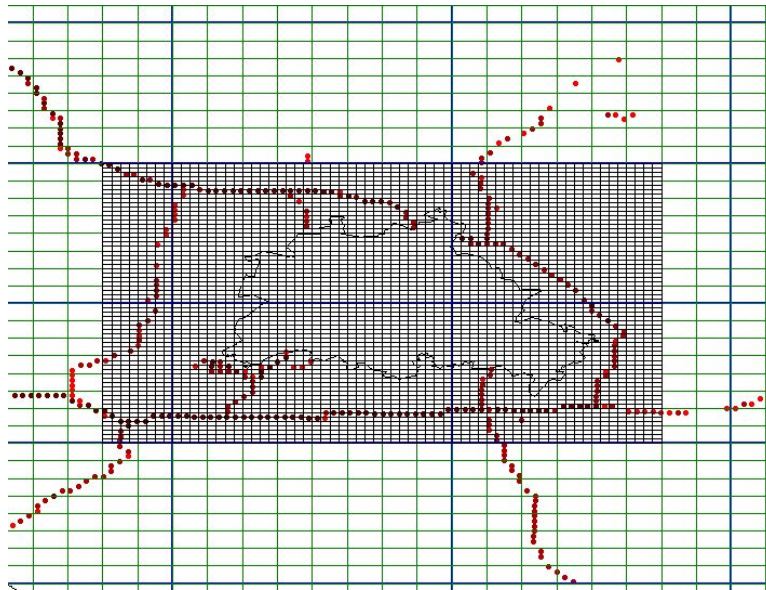


Figure 5: Domain of RCG model application for Berlin urban area (1x1 km<sup>2</sup> grid resolution).

#### 4.1.1 Uncertainties according to the EU Directives

Following the recommendations defined in the M2 report, the first level of model uncertainty estimation consists on the calculation of the Relative Percentil Error (RPE) parameter, according to the model data quality objectives defined by the EU legislation. An example of a shell script (called "MODEL\_UNCERTAINTY\_STEP1") is listed in Annexe A, which was developed in order to automate the calculation of RPE, for any pair of observed/modelled data. The input data required for applying this script is listed below:

- Model specifications (name, resolution)
- Period of simulation
- Pollutant analysed
- List of monitoring stations
- Input/output directories and files specification
- hourly, octo and annual obs/model data files

In Figure 6 and 7 are plotted the RPE values concerning O<sub>3</sub> and PM<sub>10</sub>, respectively. In the case of ozone, RPE is estimated for the percentile 99.7, corresponding to the 26<sup>th</sup> maximum daily 8-hour mean within one calendar year (2001 year), and according to the target value defined for human health protection. For PM<sub>10</sub>, RPE is based on the annual average concentration, according to the annual limit value for human health protection.

In both figures are indicated the data-quality objectives defined by the FWD for modelling uncertainty: 50% for O<sub>3</sub> 8-hours data and annual averages for PM<sub>10</sub>.

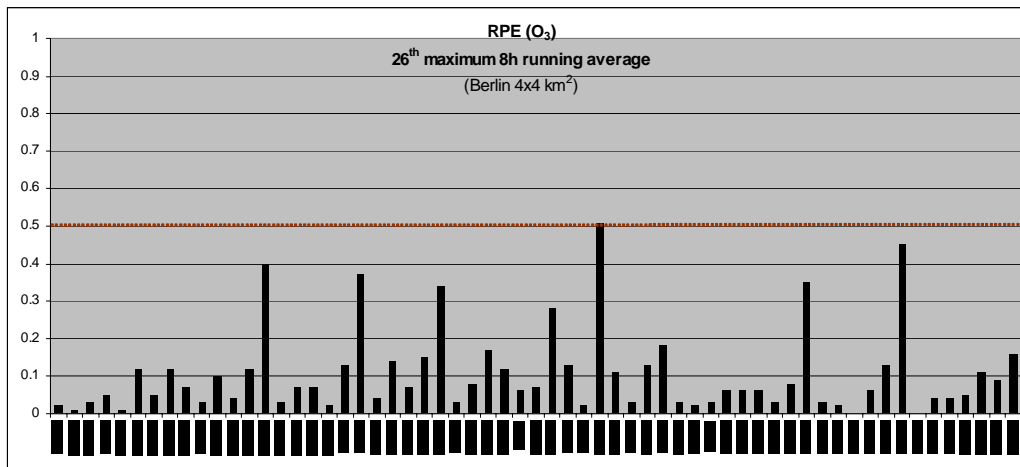


Figure 6: RPE estimated for each O<sub>3</sub> monitoring station, for the 4x4km<sup>2</sup> Berlin case study simulation.

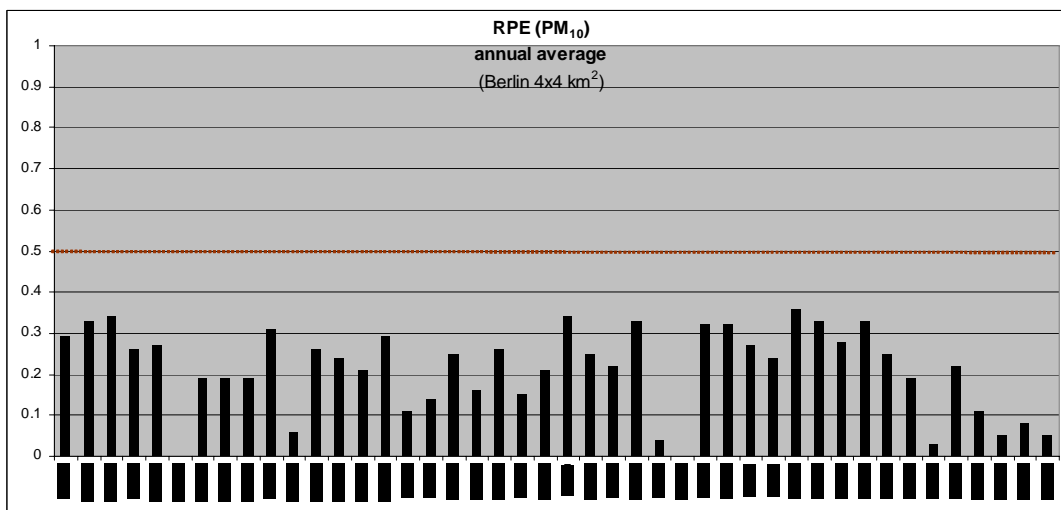


Figure 7: RPE estimated for each PM<sub>10</sub> monitoring station, for 4x4km<sup>2</sup> Berlin case study simulation.

Results show that, for both pollutants, the RPE values are below 50%, fulfilling the data quality objectives for allowed uncertainty of model assessment. There is only an exception regarding a specific monitoring site for ozone that presents a RPE close to 0.5, which can be justified by the traffic type and urban influence of the station (not representative of the model grid resolution). In summary, according to the FWD, the RCG model is able to simulate appropriately and with an acceptable level of uncertainty the Berlin case study at urban scale (4x4 km<sup>2</sup> grid resolution).

RPE was also estimated for the fine scale simulation (1x1 km<sup>2</sup>) and the comparison of the results is presented in Figure 8, for O<sub>3</sub> and PM<sub>10</sub>. This analysis points out that there is no direct relation between finer resolution and model results improvement, namely in what concerns ozone results. In fact, for some O<sub>3</sub> monitoring sites RPE is higher for the finer resolution (1x1km<sup>2</sup>) simulation. This suggests that when the model grid resolution is higher, the model uncertainties may be also superior.

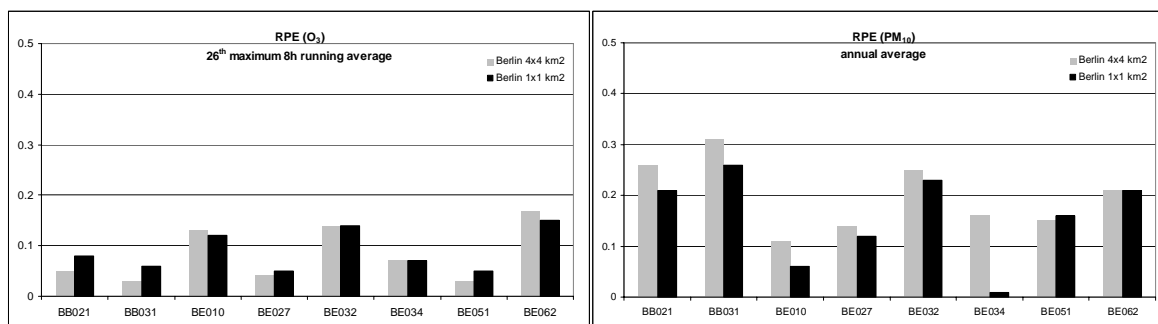


Figure 8: Comparison between RPE estimated for the different grid resolution simulations (4x4km<sup>2</sup> and 1x1km<sup>2</sup>), for O<sub>3</sub> and PM<sub>10</sub>.

#### 4.1.2 Uncertainties from statistical analysis

According to the first level of basic recommendations, a statistical analysis should be performed using a set of parameters that give some additional information to the model uncertainty analysis: namely, the correlation coefficient ( $r$ ), the root mean square error (RMSE), the normalised mean square error (NMSE) and the systematic error (BIAS). A shell script (MODEL\_UNCERTAINTY\_STEP2) was also developed for automates the calculation of these statistical parameters. The input data required for applying this script is listed below:

- Model specifications (name, resolution)
- Period of simulation
- Pollutant analysed
- List of monitoring stations
- Input/output directories and files specification
- Hour, octo, daily and annual obs/model data

In Figure 9 and 10 are plotted the referred group of statistical parameters concerning O<sub>3</sub> and PM<sub>10</sub>, respectively. The analysis, for each parameter, is follows:

- **Correlation coefficient ( $r$ ):** is significantly higher for ozone (>0.75) and less for PM<sub>10</sub> (>0.6), suggesting that the model is able to simulate the physics and chemistry processes involved in the O<sub>3</sub> formation and (but with a less good performance) the aerosols chemistry
- **RMSE:** presents an average of 15-25  $\mu\text{g}\cdot\text{m}^{-3}$  for O<sub>3</sub> and 10-20  $\mu\text{g}\cdot\text{m}^{-3}$  for PM<sub>10</sub>, showing that besides the lower correlation, the magnitude of the errors between observed and modelled values are lower for PM<sub>10</sub> than for O<sub>3</sub>.
- **NMSE:** presents an average of 0.2-0.25 for O<sub>3</sub> and 0.4-0.85 for PM<sub>10</sub>, indicating that besides the absolute error is higher for O<sub>3</sub>, the normalized error is lower for this pollutant. This could be due to the level of PM<sub>10</sub> values that are usually lower than O<sub>3</sub> concentrations.
- **Bias:** presents an average range between -10 and +5  $\mu\text{g}\cdot\text{m}^{-3}$  for O<sub>3</sub> and is always positive (<10  $\mu\text{g}\cdot\text{m}^{-3}$ ) for PM<sub>10</sub>, suggesting that there is an overestimation of the PM emissions, but not existent regarding ozone precursors (that could inclusive be underestimated).

It should be notice that there are some exceptions to these average ranges, all explained by the monitoring station traffic type or strong urban influence. In Annexe is listed the type and coordinates of each monitoring station.

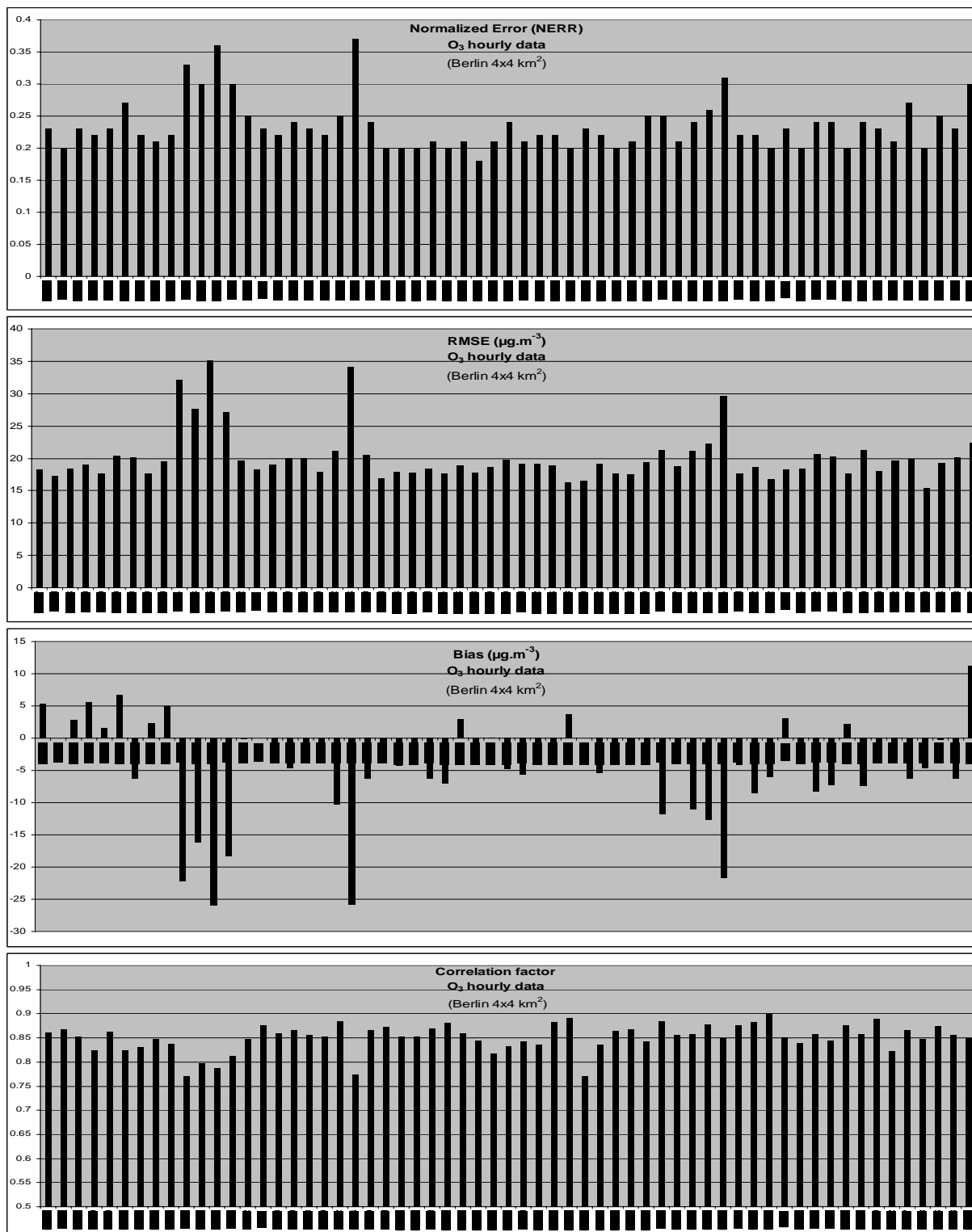


Figure 9: Statistical parameters obtained for the  $4 \times 4 \text{ km}^2$  Berlin simulation for each  $O_3$  monitoring station.

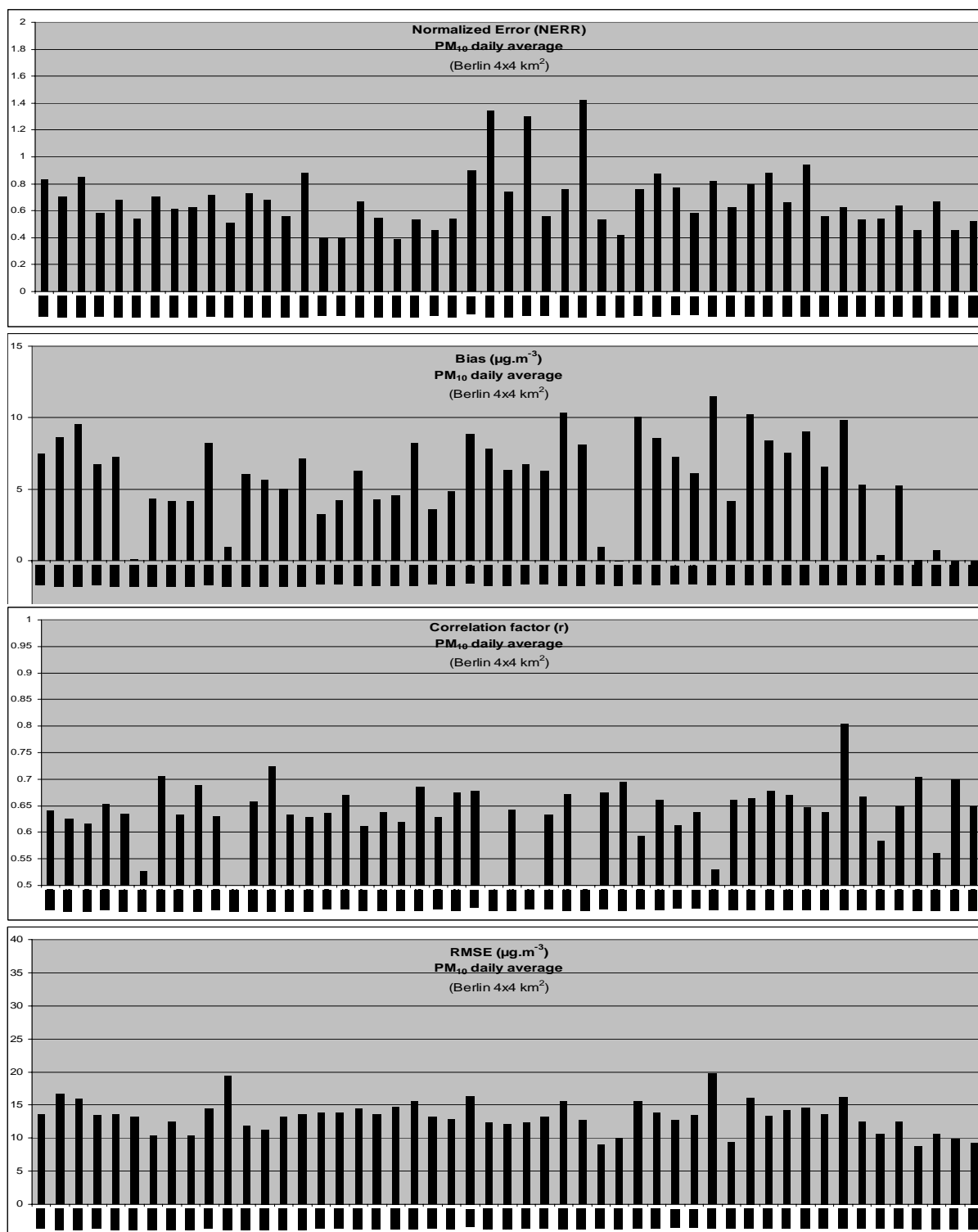


Figure 10: Statistical parameters obtained for the 4x4km<sup>2</sup> Berlin simulation for each PM<sub>10</sub> monitoring station.

In Table 4 and 5 is presented the comparison between the statistical parameters estimated for the large (4x4km<sup>2</sup>) and finer (1x1km<sup>2</sup>) grid resolution simulations, for O<sub>3</sub> and PM<sub>10</sub>, respectively.

Relatively to ozone, once more there is no evident tendency for results improvement (and reduction of model uncertainties) when using fine-scale resolution. But, regarding PM<sub>10</sub>, the errors (absolute, normalized and systematic) are lower for the 1x1km<sup>2</sup> simulation for the major part of the monitoring sites. However, the correlation factor does not reflect the same behaviour, being higher for the large-scale resolution application (4x4km<sup>2</sup>).

*Table 4: Comparison between the statistical parameters obtained for the urban scale (4x4km<sup>2</sup>) and finer scale resolution (1x1km<sup>2</sup>) simulations, for O<sub>3</sub>.*

		1x1km <sup>2</sup>	4x4km <sup>2</sup>	1x1km <sup>2</sup>	4x4km <sup>2</sup>	1x1km <sup>2</sup>	4x4km <sup>2</sup>	1x1km <sup>2</sup>	4x4km <sup>2</sup>
<b>TYPE</b>	<b>STATION</b>	<b>RMSE</b>	<b>RMSE</b>	<b>BIAS</b>	<b>BIAS</b>	<b>NERR</b>	<b>NERR</b>	<b>CORR</b>	<b>CORR</b>
Urban	BB021	18.97	18.44	-7.70	-6.34	0.21	0.21	0.87	0.87
Urban	BB031	19.60	19.18	-8.11	-5.72	0.20	0.21	0.84	0.85
Urban	BE010	21.73	21.34	-11.97	-11.81	0.25	0.25	0.88	0.88
Urban	BE027	19.11	18.82	-0.79	-1.28	0.20	0.21	0.86	0.86
Urban	BE032	20.98	21.27	-10.91	-10.95	0.23	0.24	0.86	0.86
Urban	BE034	22.33	22.27	-12.24	-12.64	0.24	0.26	0.88	0.87
Urban	BE051	18.53	17.63	-5.60	-4.10	0.21	0.22	0.88	0.87
Urban	BE062	17.58	16.89	-6.68	-5.99	0.20	0.20	0.90	0.89

*Table 5: Comparison between the statistical parameters obtained for the urban scale (4x4km<sup>2</sup>) and finer scale resolution (1x1km<sup>2</sup>) simulations, for PM<sub>10</sub>.*

		1x1km <sup>2</sup>	4x4km <sup>2</sup>	1x1km <sup>2</sup>	4x4km <sup>2</sup>	1x1km <sup>2</sup>	4x4km <sup>2</sup>	1x1km <sup>2</sup>	4x4km <sup>2</sup>
<b>TYPE</b>	<b>STATION</b>	<b>RMSE</b>	<b>RMSE</b>	<b>BIAS</b>	<b>BIAS</b>	<b>NERR</b>	<b>NERR</b>	<b>CORR</b>	<b>CORR</b>
Urban	BB021	12.82	13.47	5.46	6.71	0.49	0.58	0.66	0.65
Urban	BB031	14.20	14.40	7.03	8.19	0.61	0.72	0.60	0.63
Urban	BE010	13.96	13.91	1.77	3.23	0.36	0.40	0.62	0.64
Urban	BE015	13.75	13.89	3.45	4.20	0.38	0.40	0.66	0.67
Urban	BE027	14.24	14.41	5.75	6.26	0.58	0.67	0.63	0.61
Urban	BE032	13.24	13.53	3.40	4.24	0.52	0.55	0.63	0.64
Urban	BE034	15.07	14.69	-0.17	4.55	0.31	0.39	0.57	0.62
Urban	BE051	13.34	13.23	3.80	3.59	0.45	0.45	0.63	0.63
Urban	BE062	13.41	12.88	5.35	4.85	0.57	0.54	0.65	0.67

#### **4.1.2 Uncertainty mapping**

According to the basic recommendations, the spatial mapping of model uncertainty is first represented based on point assessment and on the RPE parameter, for both pollutants (Figure 11). This type of spatial representation indicates already the distribution of the model uncertainty and where are located the most critical areas in terms of model deviation to the observed values.

The domain represented concerns the 4x4km<sup>2</sup> model simulation.

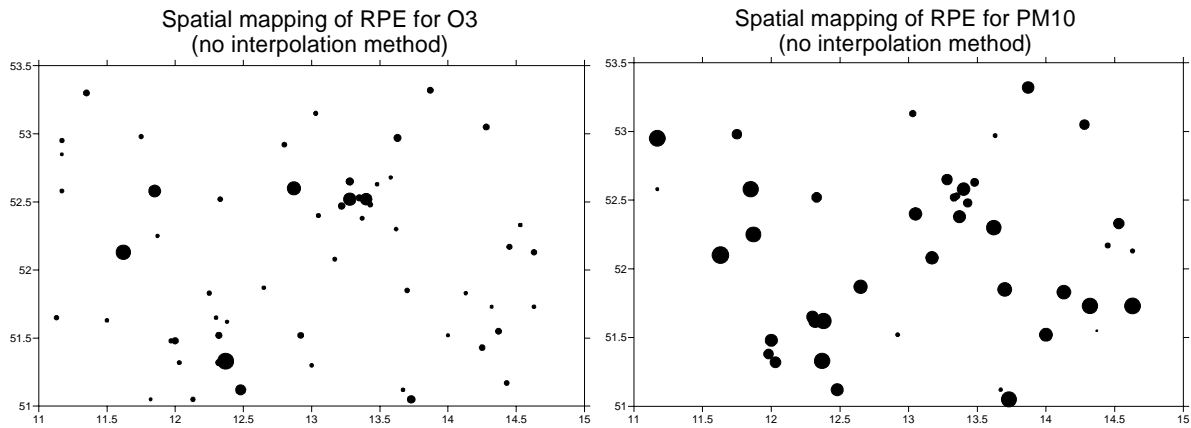
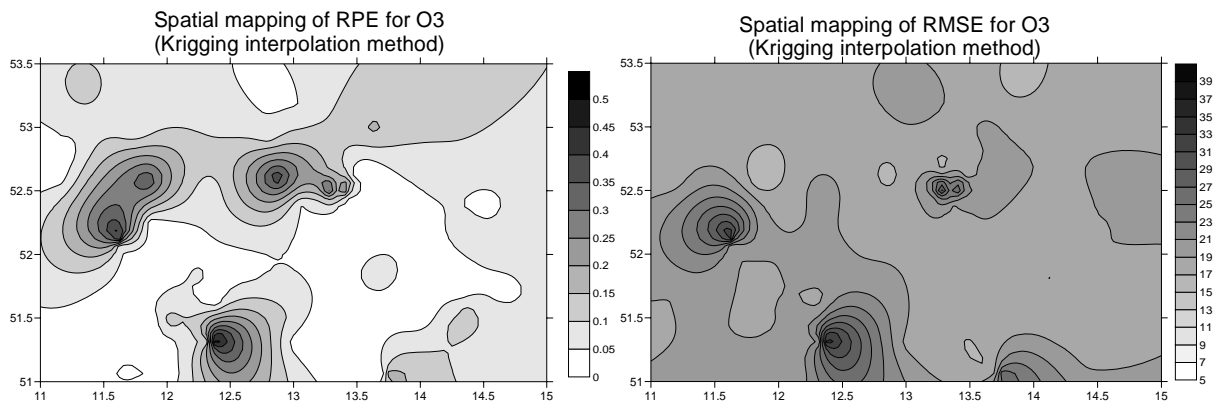


Figure 11: Spatial mapping (without interpolation) of the RPE parameter for  $O_3$  and  $PM_{10}$ .

However, since there is a considerable high density monitoring network, it is suitable to spatially interpolate the error data. In Figures 12 and 13 are presented the spatial interpolation (using Kriging method) of the several analysed parameters, for  $O_3$  and  $PM_{10}$ , respectively. For both cases, it is possible to verify that each error parameter can be used as a (relative or absolute) indicator of the model uncertainty. In fact, the spatial distribution is similar for all the variables presented, reflecting the same pattern when identifying the areas with higher uncertainty levels. The ideal should be to combine the different maps to produce a final one for model uncertainty spatial representation.



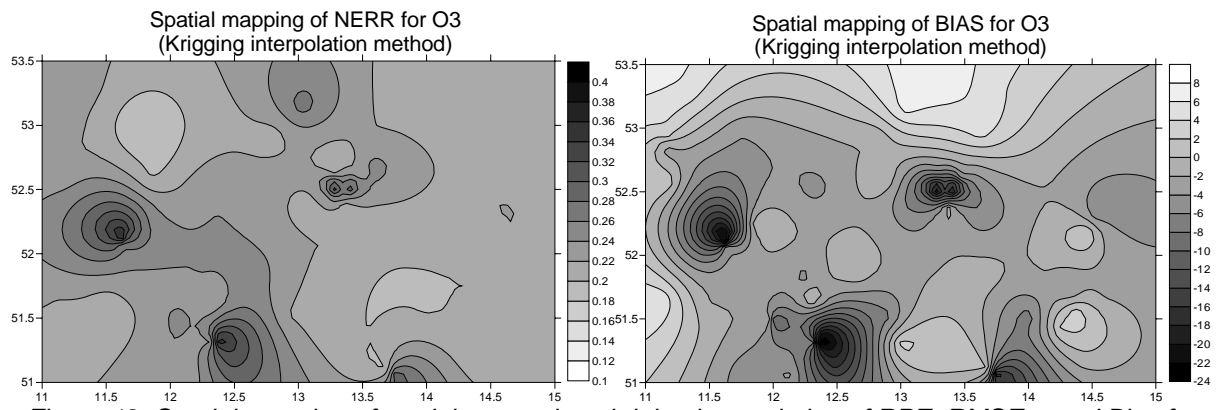


Figure 12: Spatial mapping of model uncertainty: kriging interpolation of RPE, RMSE, r and Bias for O<sub>3</sub>.

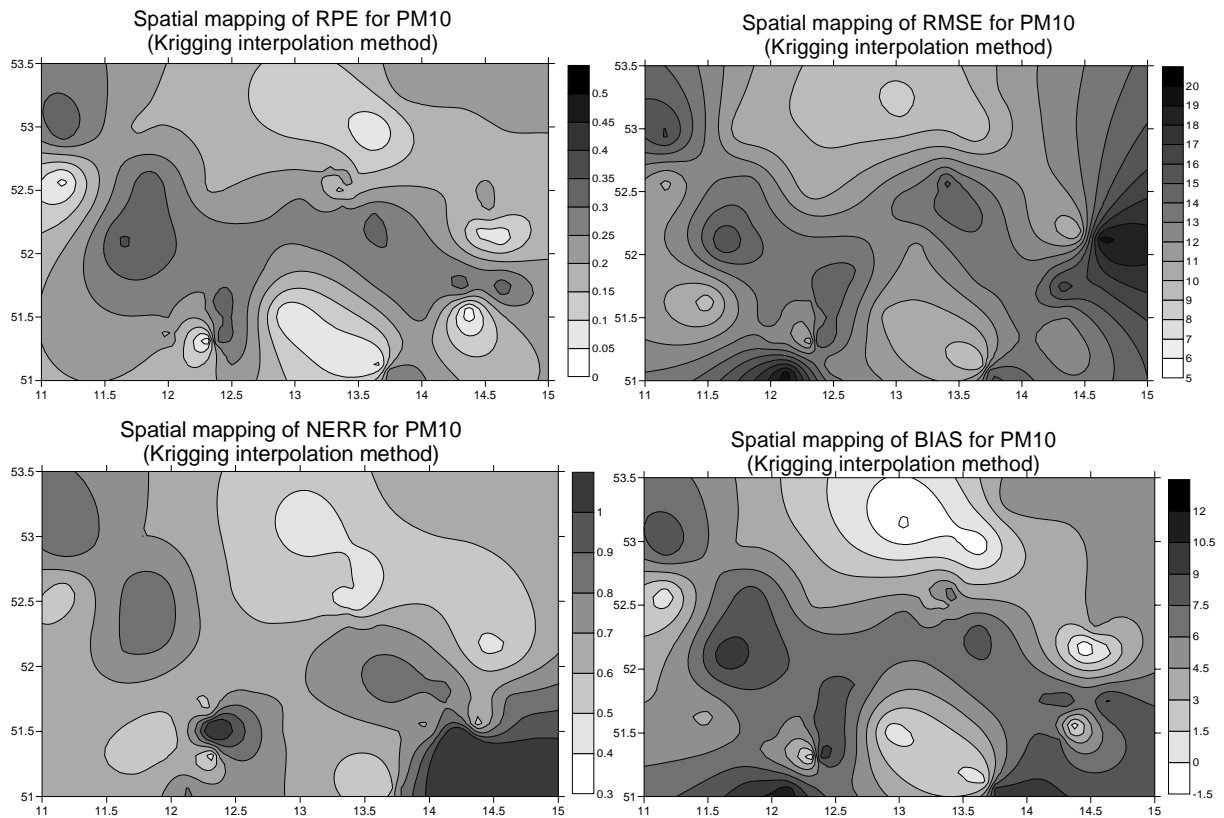


Figure 13: Spatial mapping of model uncertainty: kriging interpolation of RPE, RMSE, r and Bias for PM<sub>10</sub>.

## 4.2 Hot spot scale

The Gaussian multi-source dispersion model IMMIS<sup>net</sup> was used for the local scale modelling simulations over Berlin (information regarding domain and resolution was not provided by the Senat Berlin). Hourly concentration data were simulated for the year 2002, for PM<sub>10</sub> and NO<sub>2</sub> pollutants, by the Senat Berlin. For the same period and for the same time resolution, measured concentrations of the above mentioned pollutants were also provided from the 121 air quality measuring points located over the study domain (Figure 14). These air quality measuring devices were located at different heights ( $z=2\text{m}$ ;  $z=3.5\text{m}$ ;  $z=6\text{m}$ ;  $z=10\text{m}$ ;  $z=14\text{m}$ ;  $z=18\text{m}$ ;  $z=20\text{m}$ ), for 20 points located over a straight line ( $y=0$ ) that crosses the domain, creating the XZ plane shown in Figure 15.

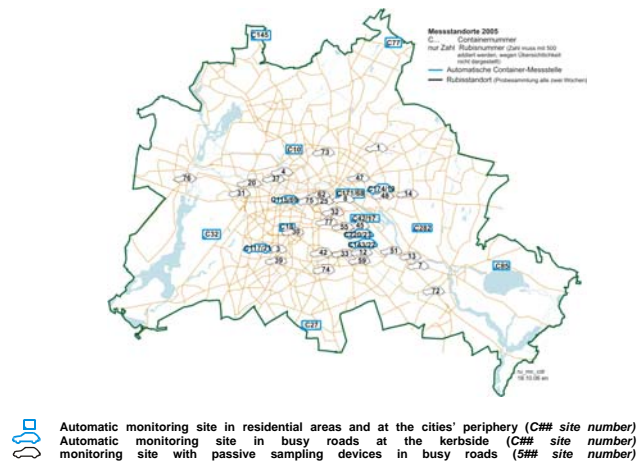


Figure 14: Berlin air quality network.

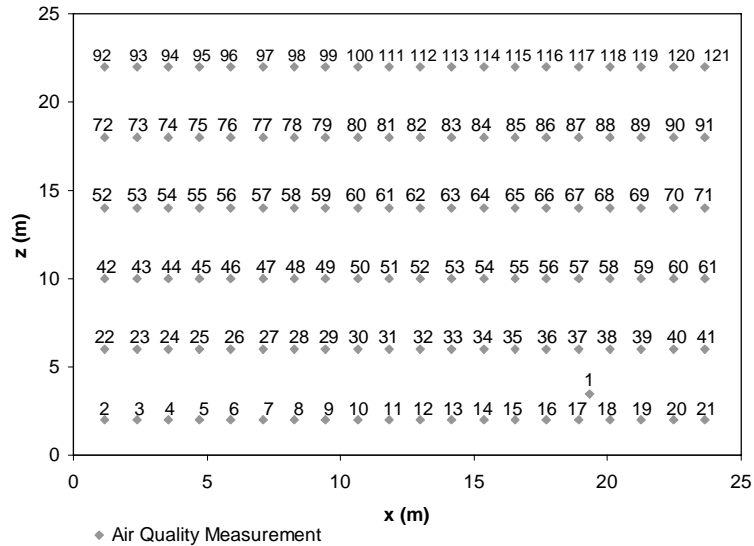


Figure 15: Location of the air quality measuring devices over the study domain for  $\text{NO}_2$  and  $\text{PM}_{10}$  pollutants (XZ plane).

#### 4.2.1 Uncertainties according to EU Directives

According to the second level of basic recommendations defined in the Air4EU-M2 report, the model uncertainty estimation will be determined through the calculation of the Relative Percentile Error (RPE) parameter for any pair of observed/modelled data of the 121 points previously indicated in Figure 15.

Figures 16 and 17 present the RPE values for  $\text{NO}_2$  and  $\text{PM}_{10}$ , respectively. In the case of  $\text{NO}_2$ , RPE is estimated for percentile 99.79, corresponding to the 18<sup>th</sup> maximum hourly mean within one calendar year (2002 year), and according to the target value defined for the protection of human health. For  $\text{PM}_{10}$ , RPE is based on the annual average concentration, according to the annual limit value for human health protection.

In both figures are indicated the data-quality objectives defined by the FWD for modelling uncertainty: 50-60% for  $\text{NO}_2$  hourly mean and 50% for  $\text{PM}_{10}$  annual averages.

RPE (NO<sub>2</sub>) Hourly mean

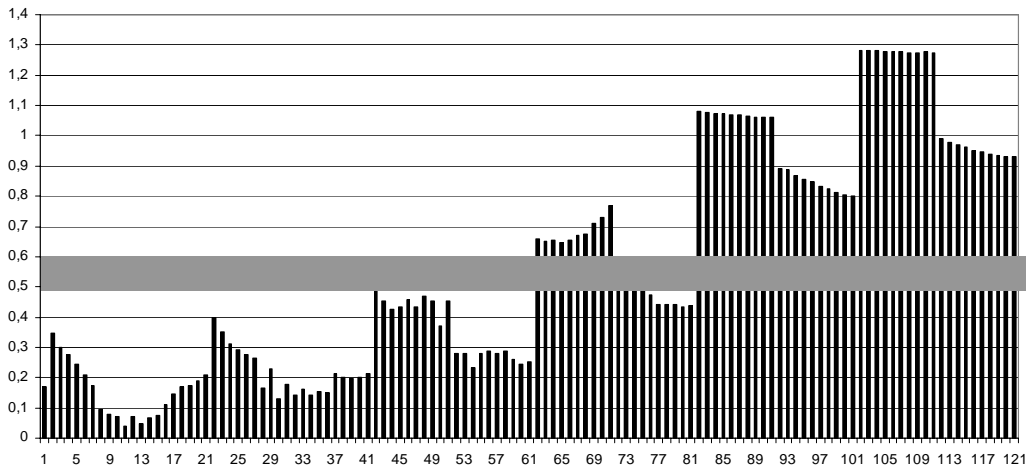


Figure 16: RPE hourly mean for NO<sub>2</sub> pollutant estimated for each air quality measuring point.

In Figure 16 is possible to notice that the RPE values are increasing with height, concluding that the Modelling Quality objectives of the FWD for NO<sub>2</sub> pollutant are over passed for heights above 15 m (RPE>50-60%). This suggests that the applied model has the capability to predict well the transport of NO<sub>2</sub> near the ground, but not at heights above 10-20 meters. The high discrepancy between observed and modelled values over the 15 m can justify RPE values higher than 1.0.

RPE (PM<sub>10</sub>) Annual mean

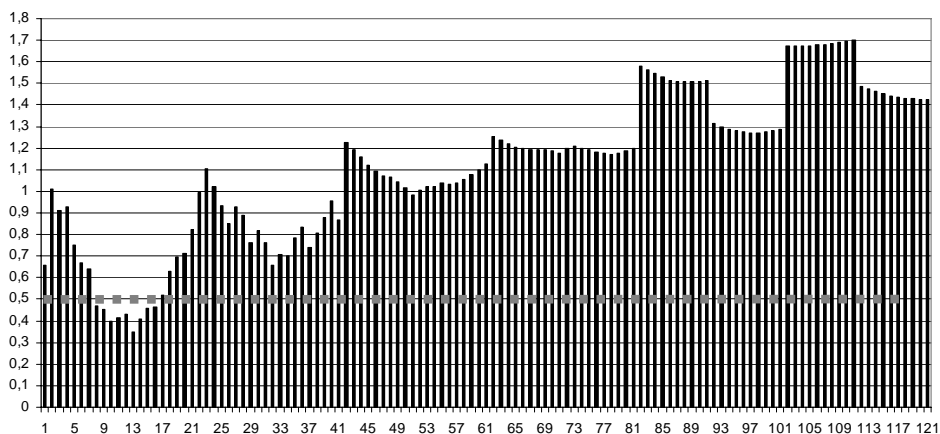


Figure 17: RPE annual mean for PM<sub>10</sub> pollutant estimated for each air quality measuring point.

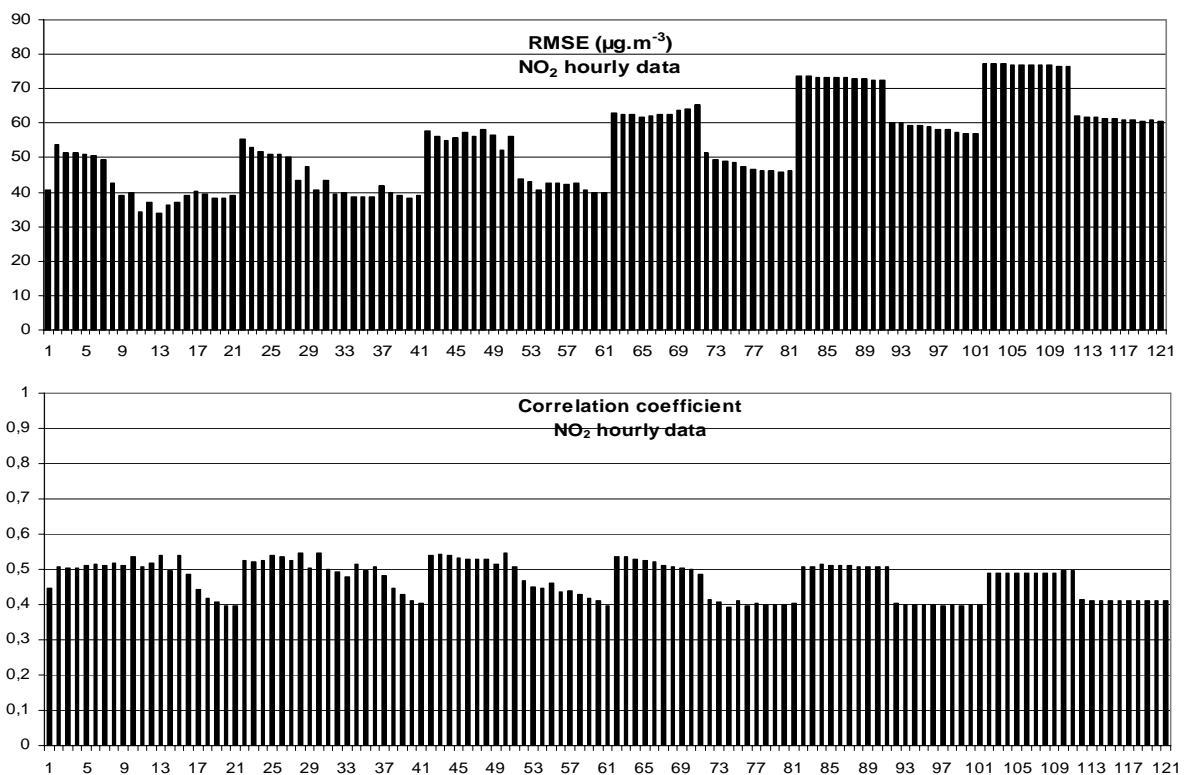
For PM<sub>10</sub> most of the RPE values determined are above the modelling quality objective of 50%. These results allow to conclude that the model has a deficient performance concerning PM<sub>10</sub> transport and diffusion processes. Moreover, this indicates that these modeling results should not be considered for air quality modeling assessment. Again, it is possible to observe lower RPE values near the ground that will increase with height.

## 4.2.2 Statistical analysis

According to the second level of basic recommendations, a statistical analysis should also be performed using the set of parameters previously indicated in sub-chapter 3, which can provide additional information to the model uncertainty analysis: namely, the correlation coefficient ( $r$ ), the root mean square error (RMSE), the normalised mean square error (NMSE) and the systematic error (BIAS).

In Figure 18 and 19 are plotted the referred group of statistical parameters concerning  $\text{NO}_2$  and  $\text{PM}_{10}$ , respectively. The analysis, for each parameter, is the following:

- **Correlation coefficient ( $r$ ):** presents minimum values of approximately 0.40 for both  $\text{NO}_2$  and  $\text{PM}_{10}$  pollutants and maximum values of 0.55 and 0.61, respectively, suggesting that the model present deficiencies/limitations to simulate correctly the physic processes involved in the dispersion of the above mentioned pollutants.
- **RMSE:** presents an average of  $50 \mu\text{g}\cdot\text{m}^{-3}$  for  $\text{NO}_2$  and  $10 \mu\text{g}\cdot\text{m}^{-3}$  for  $\text{PM}_{10}$ , showing that the magnitude of the errors between observed and modelled values are lower for  $\text{PM}_{10}$  than for  $\text{NO}_2$ .
- **NMSE:** presents an average of 0.24 for  $\text{NO}_2$  and 0.79 for  $\text{PM}_{10}$ , indicating that besides the absolute error is higher for  $\text{NO}_2$ , the normalized error is lower for this pollutant.
- **Bias:** presents averages of  $-40 \mu\text{g}\cdot\text{m}^{-3}$  and  $-9.6 \mu\text{g}\cdot\text{m}^{-3}$  for  $\text{NO}_2$  and  $\text{PM}_{10}$ , respectively, with values always negative for both pollutants, indicating an overestimation of modelled concentrations that should be related and a consequence of an emissions overestimation.



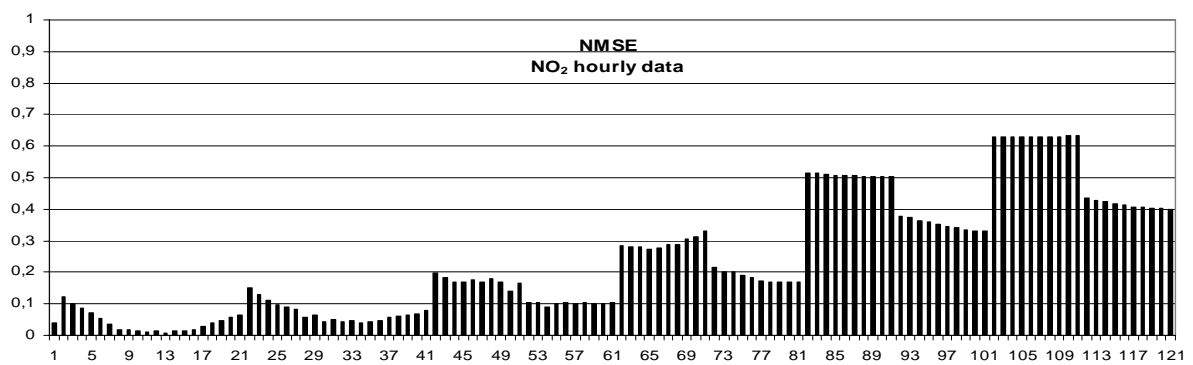
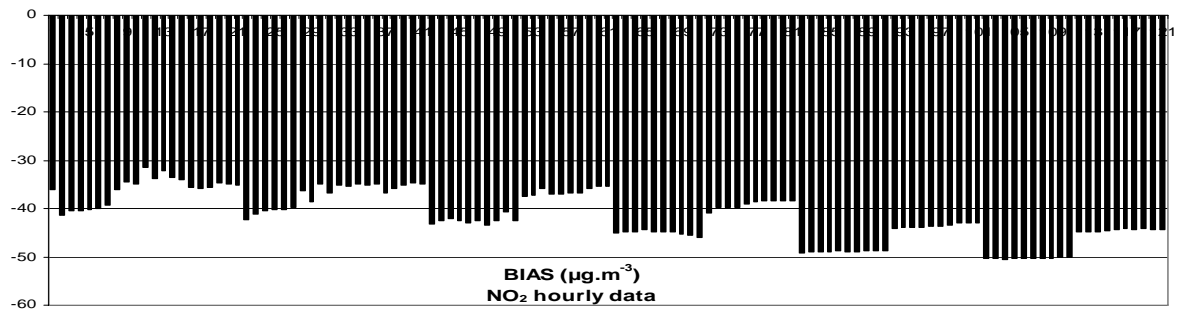
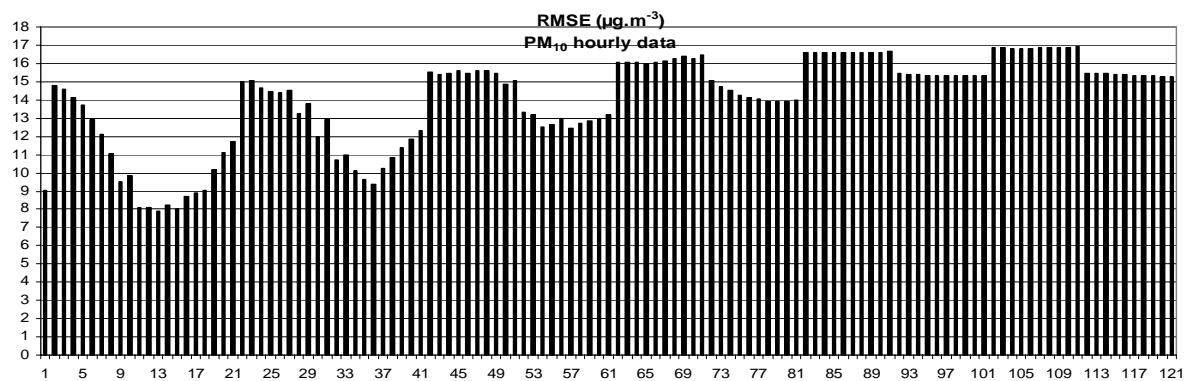
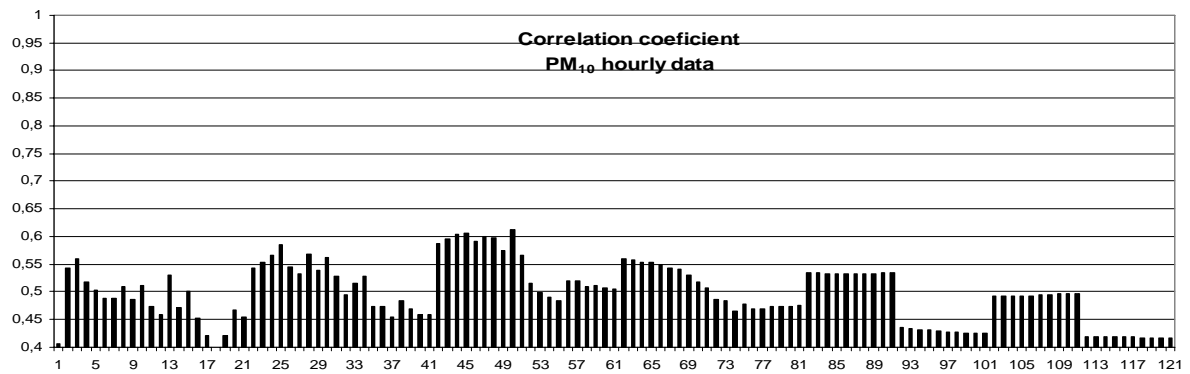


Figure 18: Statistical parameters for the local scale simulation for NO<sub>2</sub> pollutant.



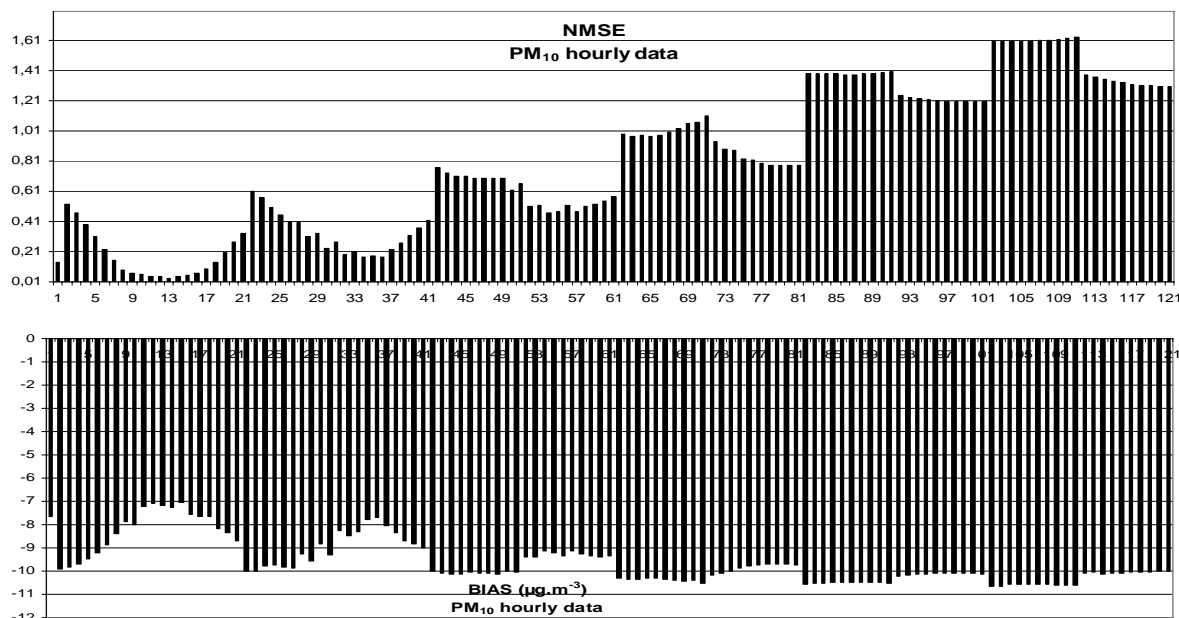


Figure 19: Statistical parameters for the local scale simulation for  $PM_{10}$  pollutant.

### 4.2.3 Uncertainty mapping

The spatial mapping of model uncertainty (RPE parameter) can be first represented based on point assessment at monitoring sites. Figure 20 presents the spatial mapping (without interpolation) of the RPE parameter for  $NO_2$  and  $PM_{10}$  for an XZ plane. This type of spatial representation can already indicate the distribution of the model uncertainty and where are located the most critical areas in terms of model deviation compared with the observed values.

Such point like assessments can be spatially interpolated to create maps from the given values through a direct spatial interpolation method of the model errors, such as, kriging or some other interpolation method. For the application of the interpolation method is necessary to guarantee a good spatial coverage of the study domain by the air quality network.

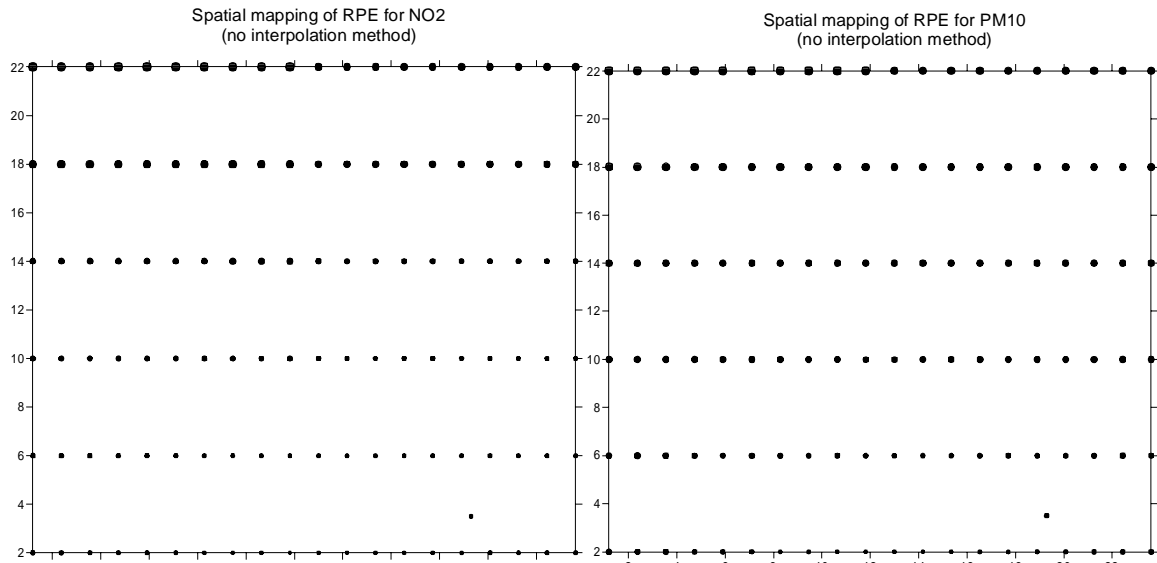


Figure 20: Spatial mapping (without interpolation) of the RPE parameter for  $\text{NO}_2$  and  $\text{PM}_{10}$  (XZ plane).

Again for both pollutants the point representation of RPE parameter shows lower uncertainty values near the ground that will increase with height (Figure 20). The sizes of the dots represented in the map are proportional to the values of RPE.

In Figures 21 and 22 are presented the spatial interpolation (using Kriging method) of the several analysed parameters, for  $\text{NO}_2$  and  $\text{PM}_{10}$ , respectively. For both cases, it is possible to verify that each error parameter can be used as a (relative or absolute) indicator of the model uncertainty. In fact, the spatial distribution is similar for all the variables presented, reflecting the same pattern when identifying the areas with higher uncertainty levels. The ideal should be to combine the different maps to produce a final one for model uncertainty spatial representation.

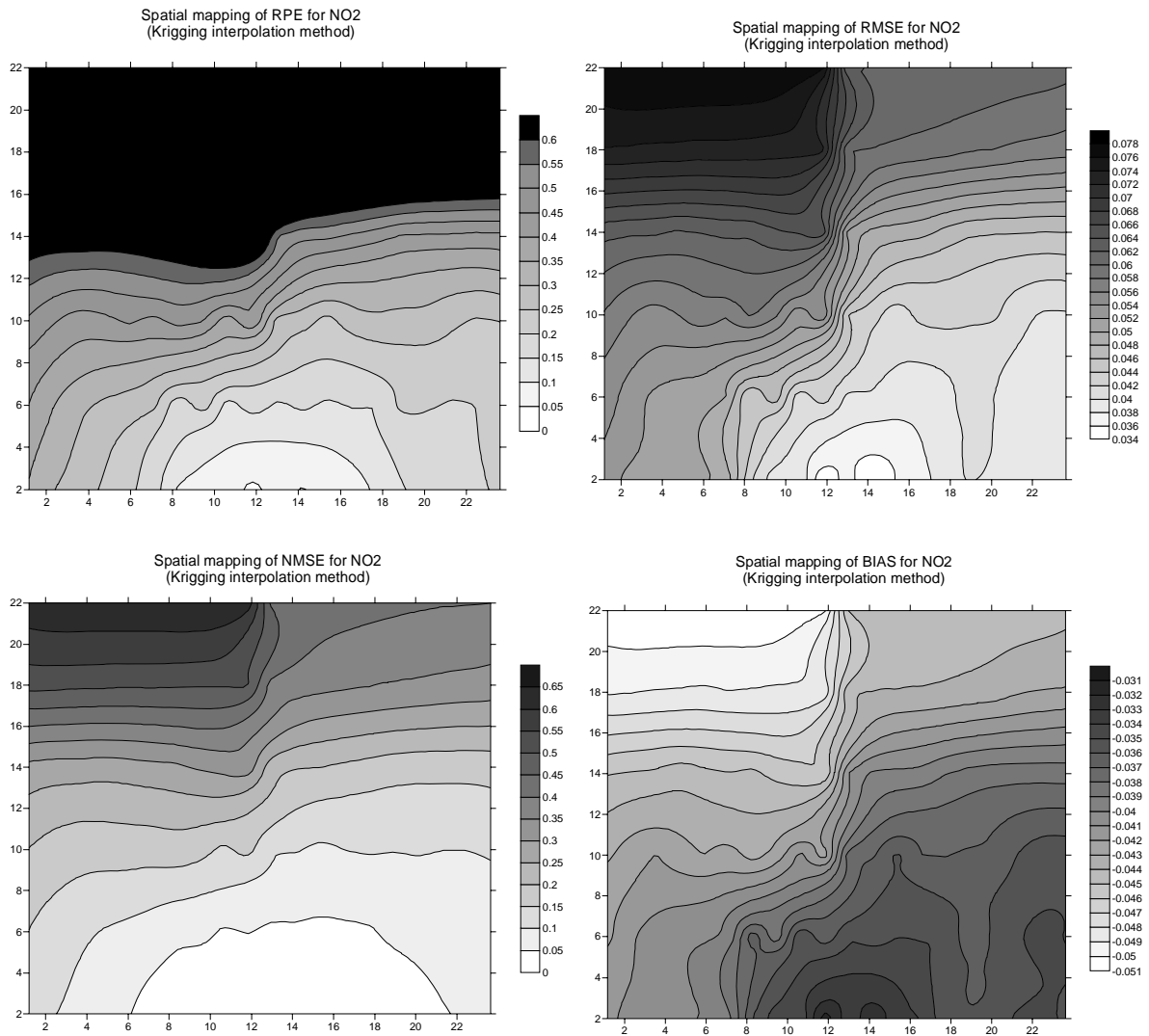


Figure 21: Spatial mapping of model uncertainty: Kriging interpolation of RPE, RMSE, r and Bias for NO<sub>2</sub> (XZ plane).

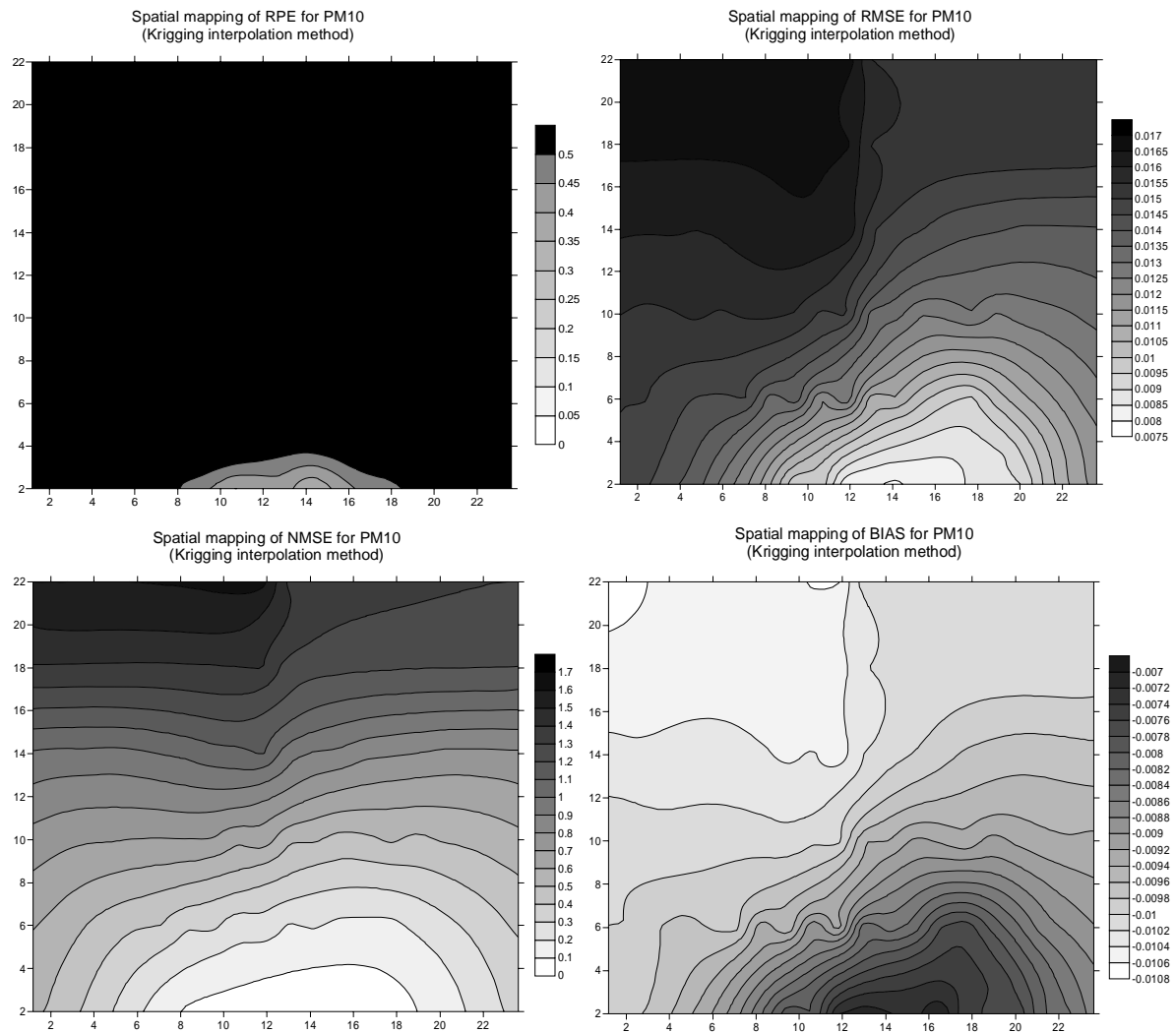


Figure 22: Spatial mapping of model uncertainty: Kriging interpolation of RPE, RMSE,  $r$  and Bias for  $PM_{10}$  (XZ plane).

## **5. Conclusion and discussion**

### **5.1 Assessment of the case study**

The Berlin case study is especially interesting due to the important city size and to the different available scale model applications (local and urban scale), supported by extensive monitoring field campaigns. At the local scale, a Gaussian model was used to simulate NO<sub>2</sub> and PM<sub>10</sub> air concentrations, revealing uncertainty values considerable high that are not in agreement with the defined modelling quality objectives of the tested pollutants and indicating that this model could not be suitable for air quality assessment. On the other hand, at the urban scale, the applied RGC chemistry-transport model was able to simulate O<sub>3</sub> and PM<sub>10</sub> with a satisfactory uncertainty level, according to the quality objectives defined by the EU Directive and to the statistical parameters calculated.

### **5.2 Improvements in assessment derived from case study**

Regarding the local scale model, the low levels of uncertainty determined for NO<sub>2</sub> and PM<sub>10</sub> near the ground and their increase with height can be associated to the necessity of considering recirculation phenomena typical of urban areas. In this way, it is recommendable to test other type of local scale model. Relatively to the urban scale, the uncertainty analysis performed in this study suggests that the RCG applied model can be used and adopted as modelling tool to perform air quality assessment with an adequate spatial detail, verification of the fulfilment of the limit targets and threshold values imposed by the EC directives, and also assessment of appropriate emission reduction strategies.

### **5.3 Recommendations resulting from the case study**

Considering that the basic level of recommendations is now completed for this case study it is recommended:

- to investigate the stochastic contribution to the total model uncertainty in order to improve model performance
- to perform a sensitivity analysis and/or model intercomparison to evaluate the different model modules (Chemical mechanisms, physical parameterisations and numerical algorithms) and to determine the intrinsic model uncertainty
- to present assessment maps combined with a spatial representation of the uncertainty.

### **5.4 Suitability for implementation in other cities**

Cities that perform air quality assessment using numerical models (urban and/or local scale models) and reasonable air quality measurements over the study area can easily implement the basic recommendations of the AIR4EU project concerning total model uncertainty estimation. Moreover, the presentation of uncertainty maps combined with assessment maps is directly dependent on the application of the defined methodology.

## References

1. Borrego, C.; Monteiro, A.; Ferreira, J.; Miranda, A.I.; Costa, A.M.; Sousa, M. Modelling uncertainty estimation procedures for air quality assessment. In 3rd International Symposium on Air Quality Management at Urban, Regional and Global Scales (AQM), 26-30 September 2005; Istanbul, Turkey - Proceedings of the 3rd International Symposium on Air Quality Management at Urban, Regional and Global Scales. Eds. S. Topçu, M.F. Yardim, A. Bayram, T. Elbir and C. Kahya, Vol. I, pp. 210-219.
2. Stern, J.; Flemming, R. Formulation of criteria to be used for the determination of the accuracy of model calculations according to the requirements of the EU Directives for air quality – Examples using the chemical transport model REM-CALGRID, Freie Universität Berlin, Institut für Meteorologie; 2004.
3. Beekmann M., Kerschbaumer A., Reimer E., Stern R. (2004). PM Measurement campaign HoVerT: Model Evaluation with chemically specified observations for a one year period. *Atmos. Chem. Phys. Discuss.*, 6, 7285–7321, 2006.
4. Stern, R.: Entwicklung und Anwendung des chemischen Transportmodells REM/CALGRID, Berichte zum UBA Forschungsvorhaben 298 41 252, Freie Universität Berlin, Institut für Meteorologie, 2003.
5. Tilmes, S., Brandt, J., Flatøy, F., Bergström, R., Flemming, J., Langner, J., Christensen, J. H., Frohn, L. M., Hov, Ø., Jacobsen, I., Reimer, E., Stern, R., and Zimmermann, J.: Comparison of five eulerian air pollution systems for the summer 1999 using the German ozone 30 monitoring data, *J. Atmos. Chem.*, 42, 91–121, 2002.

## Appendix A

Example of a shell script to automate the calculation of RPE for any pair of observed/modelled data

```
#!/bin/sh
```

```
#####INFORMATION#####
```

```

#THIS SCRIPT READS THE MODEL OUTPUTS AND PREPARE A FILE WITH #
#MODELED/OBSERVED DATA FOR FUTURE UNCERTAINTY ANALYSIS. #
#THIS SCRIPT SHOULD BE RUNNED BEFORE MODEL_UNCERT_STEP1 AND #
#MODEL_UNCERT_STEP2 #
# #
#*****ADAPTED FOR BERLIN CASE***** #
# #
#SOFTWARE REQUIRED: gawk, pgf90 or ifort90 compiler #
#ONLY TESTED ON LINUX MACHINE!!!!!!!!!!!!!!!!!!!! #
# #
#AUTHORS: Alexandra Monteiro #
# Ana Cristina Carvalho #
# #
#INSTITUTION: UNIVERSITY OF AVEIRO #
# 3810-193 AVEIRO #
# PORTUGAL #
# #
#PLEASE CONTACT FOR FURTHER INFORMATION: #
# alexandra@dao.ua.pt #
# #
#DATE: JUNE 2006 #
#####
#####INPUT INFORMATION REQUIRED #####

#####Model name
model=REM_BERLIN_1x1

#####Pollutant to be analysed
pol=PM10

#####Period simulation
year=2002

#####Pollutant-station file
#####please see example of file "PM10-STATIONS"
stat_file=/home/LONG-TERM/validation/AIR4EU/PM10-STATIONS-BERLIN-1x1

#####Directory where you want to save the output files
odir=/home/LONG-TERM/validation/AIR4EU/BERLIN_DATA/1x1

#####Programs/scripts needed to run this script:
#dave.awk; peak.awk; anual.awk (gawk scripts)
#aerostat.f; o3octo_average.f (fortran programs)

#####OUTPUT FILES CREATED#####
#1. hourly files for each station: (model)_(station)_(pol)_(year).dat
#2. diurnal average for each station: (model)_(station)_(pol)_(year)_DAVE.dat
#3. anual average for each station: (model)_(station)_(pol)_(year)_ANUAL.dat
#4. octo-average for each station: (model)_(station)_(pol)_(year)_OCTO.dat

#####
# END USER MODIFICATION #
#####
#Compilation of Fortran programs
#-----
f77 o3octo_average.f -o o3octo_average.e

#Extracting obs/mod data for the BERLIN case
#-----

```

```

#ni=2
#nf=8762
#for f in `gawk '{print $2}' ${stat_file}` ; do
# echo Processing $f
# nend=`gawk 'END {print FNR}' ${model}_${pol}_${year}.dat`
# gawk '{if(NR<='${nf}'&&NR>='${ni}') {printf "%8.1f%8.1f\n", $2, $3}}'
${odir}/${model}_${pol}_${year}_1x1.dat > .tmp
# paste idate2002 .tmp > ${odir}/${model}_${f}_${pol}_${year}_1x1.dat

# nf=$(( $nf+8762 ))
# ni=$(( $ni+8762 ))
#done

# Calculation of daily/peak averages
#-----
echo Calculating the daily/peak averages for ${pol}
cd ${odir}
for f in `gawk '{print $2}' ${stat_file}` ; do
  case $pol in
    PM10) gawk -f ../../dave.awk ${model}_${f}_${pol}_${year}.dat >
${model}_${f}_${pol}_${year}_DAVE.dat ;;
    O3) gawk -f ../../peak.awk ${model}_${f}_${pol}_${year}.dat >
${model}_${f}_${pol}_${year}_PEAK.dat ;;
  esac
done

# Calculation of anual/octo averages
#-----
cd ../../
echo Calculating the anual/octo averages for ${pol}
for f in `gawk '{print $2}' ${stat_file}` ; do
  ntotal=`gawk 'END {print FNR}' ${odir}/${model}_${f}_${pol}_${year}.dat`

  if [[ ${pol} = "PM10" ]]
  then
    gawk -f anual.awk ${odir}/${model}_${f}_${pol}_${year}.dat >
${odir}/${model}_${f}_${pol}_${year}_ANUAL.dat
# else
# echo "***ATTENTION: THERE IS NO ENOUGH DATA TO CALCULATE PM10 ANNUAL
AVERAGE!****"
# exit 0
# fi

  else
    rm ${odir}/${model}_${f}_${pol}_${year}_OCTO.dat
    echo ${ntotal} "'${odir}/${model}_${f}_${pol}_${year}.dat'" |
./o3octo_average.e
    cat O3_OCTAV >> ${odir}/${model}_${f}_${pol}_${year}_OCTO.dat
    fi
done

#!/bin/sh

#####INFORMATION#####
#THIS SCRIPT CALCULATES THE RPE DEFINED BY THE EU LEGISLATION AS A #
#DATA QUALITY OBJECTIVE FOR MODEL UNCERTAINTY ACEPTANCE. #
#THIS SCRIPT SHOULD BE RUNNED AFTER SCRIPT MODEL_UNCERTAINTY_STEP1. #
# #
#SOFTWARE REQUIRED: gawk, pgf90 or ifort90 compiler #
#ONLY TESTED ON LINUX MACHINE!!!!!!!!!!!!!!!!!!!!!! #

```

```

#                                                                 #
#AUTHORS:      Alexandra Monteiro                                #
#              Ana Cristina Carvalho                            #
#                                                                 #
#INSTITUTION:  UNIVERSITY OF AVEIRO                             #
#              3810-193 AVEIRO                                  #
#              PORTUGAL                                         #
#                                                                 #
#PLEASE CONTACT FOR FURTHER INFORMATION:                       #
#              alexandra@dao.ua.pt                              #
#                                                                 #
#DATE:         JUNE 2006                                        #
#####

#####INPUT DATA/FILES REQUIRED#####

#####Model name
model=REM_BERLIN_1x1

#####Pollutant analysed
pol=PM10

#####Pollutant-station file
stat_file=/home/LONG-TERM/validation/AIR4EU/PM10-STATIONS-BERLIN-1x1

#####Directory of input files
odir=/home/LONG-TERM/validation/AIR4EU/BERLIN_DATA/1x1

#####Period of simulation
year=2002
ddeb=20020101                #day of beginning   (yyyymmdd)
dend=20021231                #day of termination (yyyymmdd)

#####other input files needed
#####output files from MODEL_UNCERT_FILE:
#(model)_(station)_PM10_(year)_ANUAL.dat      #in the case of PM10 pollutant
#(model)_(station)_O3_(year)_OCTO.dat        #in the case of O3 pollutant

#####OUTPUT FILES CREATED#####
#RPE_(model)_(pol)_(year)_1x1

#####
#                                                                 #
#  END USER MODIFICATION                                       #
#                                                                 #
#####

# Calculating RPE (Relative Percentile Error)...
#-----
rm ${odir}/RPE_${model}_${pol}_${year}_1x1
echo "Calculating RPE for" ${pol}
cd ${odir}
echo "STATION" "AVO" "AVM" "RPE" | gawk '{printf "%8s%8s%8s%8s\n", $1, $2, $3, $4}' >
.rpe
echo "LONG" "LAT" "TYPE" | gawk '{printf "%10s%10s%10s\n", $1, $2, $3}' > .sta
gawk '{printf "%10s%10s%10s\n", $5, $6, $4}' ${stat_file} >> .sta
for f in `gawk '{print $2}' ${stat_file}` ; do

    if [[ ${pol} = "PM10" ]]

```

```

then

  if [ -f ${model}_${f}_${pol}_${year}_ANUAL.dat ]
  then
    avo=`gawk '{print $2}' ${model}_${f}_${pol}_${year}_ANUAL.dat`
    avm=`gawk '{print $3}' ${model}_${f}_${pol}_${year}_ANUAL.dat`
    rpe=`gawk '{if($2<0||$3<0) {print -999} else {n=n+1;x=x+(sqrt(($2-
$3)^2)/$2)}}END{print x/(n+1e-5)}' ${model}_${f}_${pol}_${year}_ANUAL.dat`
    else
      echo "*****ATTENTION: IT IS NOT POSSIBLE TO CALCULATE RPE FOR PM10 BECAUSE
THERE IS NO ENOUGH DATA!*****"
      exit 0
    fi

    else
      avo=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24'"
{n=n+1;x=x+$2}END{print x/(n+1e-5)}' ${model}_${f}_${pol}_${year}_OCTO.dat`
      avm=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24'"
{n=n+1;x=x+$3}END{print x/(n+1e-5)}' ${model}_${f}_${pol}_${year}_OCTO.dat`
      rpe=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24'"
{n=n+1;x=x+(sqrt(($2-$3)^2)/$2)}END{print x/(n+1e-5)}'
${model}_${f}_${pol}_${year}_OCTO.dat`

    fi

#printing RPE parameter
#-----
echo $f $avo $avm $rpe | gawk '{printf "%8s%8.2f%8.2f%8.2f\n", $1, $2, $3, $4}' >>
.rpe
paste .sta .rpe > ${odir}/RPE_${model}_${pol}_${year}_1x1
done

```

```

#!/bin/sh

#####INFORMATION#####
#THIS SCRIPT CALCULATES THE STATISTICAL PARAMETERS FOR UNCERTAINTY #
#ANALYSIS.THIS SCRIPT SHOULD BE RUNNED AFTER THE SCRIPT MODEL_UNCERT_FILE.#
#SOFTWARE REQUIRED: gawk, pgf90 or ifort90 compiler #
#ONLY TESTED ON LINUX MACHINE!!!!!!!!!!!!!!!!!!!!!! #
# #
#AUTHORS: Alexandra Monteiro #
# Ana Cristina Carvalho #
# #
#INSTITUTION: UNIVERSITY OF AVEIRO #
# 3810-193 AVEIRO #
# PORTUGAL #
# #
#PLEASE CONTACT FOR FURTHER INFORMATION: #
# alexandra@dao.ua.pt #
# #
#DATE: JUNE 2006 #
#####

#####INPUT DATA/FILES REQUIRED#####

#####Pollutant-station file
stat_file=/home/LONG-TERM/validation/AIR4EU/PM10-STATIONS-BERLIN-1x1

#####Model name
model=REM_BERLIN_1x1

#####Pollutant analysed
pol=PM10

#####Directory of input/output files
odir=/home/LONG-TERM/validation/AIR4EU/BERLIN_DATA/1x1

#####Period of simulation
year=2002
ddeb=20020100 #day of beginning (yyyymmdd)
dend=20021231 #day of termination (yyyymmdd)

#####other input files
#####output files from MODEL_UNCERT_FILE:
#(model)_(station)_(pollutant)_(year)_DAVE.dat #in case of PM10
#(model)_(station)_(pollutant)_(year)_PEAK.dat #in case of O3

#####OUTPUT FILES CREATED#####
#STAT_(model)_(pol)_(year)

#####
# END USER MODIFICATION #
#####

# Calculating statistical parameters...
#-----
rm ${odir}/STATS_${model}_${pol}_${year}
cd ${odir}
echo "Calculating statistical parameters for" ${pol}
echo "STATION" "AVO" "AVM" "RMSE" "NERR" "BIAS" "COR" | gawk '{printf
"%8s%8s%8s%8s%8s%8s%8s\n", $1, $2, $3, $4, $5, $6, $7}' > .par
echo "LONG" "LAT" "TYPE" | gawk '{printf "%10s%10s%8s\n", $1, $2, $3}' > .sta

```

```

gawk '{printf "%10s%10s%8s\n", $5, $6, $4}' ${stat_file} >> .sta

for f in `gawk '{print $2}' ${stat_file}` ; do
  if [[ ${pol} = "PM10" ]] then
    avo=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"'
{n=n+1;x=x+$2}END{print x/(n+1e-5)}' ${model}_${f}_${pol}_${year}_DAVE.dat`
    avm=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"'
{n=n+1;x=x+$3}END{print x/(n+1e-5)}' ${model}_${f}_${pol}_${year}_DAVE.dat`
    rms=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"' {n=n+1;x=x+($2-
$3)^2}END{print sqrt(x/(n+1e-5))}' ${model}_${f}_${pol}_${year}_DAVE.dat`
    nerr=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"'
{n=n+1;x=x+sqrt((($2-$3)^2)/$3}END{print x/(n+1e-5)}'
${model}_${f}_${pol}_${year}_DAVE.dat`
    bias=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"'
{n=n+1;x=x+$2;y=y+$3}END{print (x-y)/(n+1e-5)}'
${model}_${f}_${pol}_${year}_DAVE.dat`
    stdo=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"' {n=n+1;x=x+($2-
$avo)^2}END{print sqrt(x/(n+1e-5))}' ${model}_${f}_${pol}_${year}_DAVE.dat`
    stdm=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"' {n=n+1;x=x+($3-
$avm)^2}END{print sqrt(x/(n+1e-5))}' ${model}_${f}_${pol}_${year}_DAVE.dat`
    std=$stdm/$stdo
    cor=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"'
{n=n+1;x=x+$2;y=y+$3;xy=xy+$2*$3;xx=xx+$2^2;yy=yy+$3^2} END {n=n+1e-5;print (xy/n-
x*y/(n*n))/sqrt(1e-5+(xx/n-x*x/(n*n))*(yy/n-y*y/(n*n)))}'
${model}_${f}_${pol}_${year}_DAVE.dat`
  else
    avo=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"'
{n=n+1;x=x+$2}END{print x/(n+1e-5)}' ${model}_${f}_${pol}_${year}_PEAK.dat`
    avm=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"'
{n=n+1;x=x+$3}END{print x/(n+1e-5)}' ${model}_${f}_${pol}_${year}_PEAK.dat`
    rms=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"' {n=n+1;x=x+($2-
$3)^2}END{print sqrt(x/(n+1e-5))}' ${model}_${f}_${pol}_${year}_PEAK.dat`
    nerr=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"'
{n=n+1;x=x+sqrt((($2-$3)^2)/$3}END{print x/(n+1e-5)}'
${model}_${f}_${pol}_${year}_PEAK.dat`
    bias=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"'
{n=n+1;x=x+$2;y=y+$3}END{print (x-y)/(n+1e-5)}'
${model}_${f}_${pol}_${year}_PEAK.dat`
    stdo=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"' {n=n+1;x=x+($2-
$avo)^2}END{print sqrt(x/(n+1e-5))}' ${model}_${f}_${pol}_${year}_PEAK.dat`
    stdm=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"' {n=n+1;x=x+($3-
$avm)^2}END{print sqrt(x/(n+1e-5))}' ${model}_${f}_${pol}_${year}_PEAK.dat`
    std=$stdm/$stdo
    cor=`gawk '$2>0&&$3>0&&$1>="'${ddeb}00'"&&$1<="'${dend}24"'
{n=n+1;x=x+$2;y=y+$3;xy=xy+$2*$3;xx=xx+$2^2;yy=yy+$3^2} END {print (xy/n-
x*y/(n*n))/sqrt((xx/n-x*x/(n*n))*(yy/n-y*y/(n*n)))}'
${model}_${f}_${pol}_${year}_PEAK.dat`
  fi
done

#printing statistical parameters
#-----
echo $f $avo $avm $rms $nerr $bias $cor | gawk '{printf
"%8s%8.2f%8.2f%8.2f%8.2f%8.2f%8.3f\n", $1, $2, $3, $4, $5, $6, $7}' >> .par
paste .sta .par > ${odir}/STATS_${model}_${pol}_${year}
done

```

## Appendix B

List of monitoring stations included in the regional (4x4 km<sup>2</sup>) Berlin case domain

Table A1. List of monitoring stations included in the regional (4x4 km<sup>2</sup>) Berlin case domain

<b>O<sub>3</sub></b>	<b>PM<sub>10</sub></b>
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LONG	LAT	STATION	TYPE	LONG	LAT	STATION	TYPE
11.35	53.3	MV017	Rural	13.67	51.12	SN051	Rural
13.67	51.12	SN051	Rural	11.17	52.58	ST089	Rural
13	51.3	SN076	Rural	13.03	53.13	UB030	Rural
11.13	51.65	ST070	Rural	12.92	51.52	UB033	Rural
11.17	52.58	ST089	Rural	14.45	52.17	UB039	Rural
13.03	53.15	UB030	Rural	13.63	52.97	UB040	Rural
12.92	51.52	UB033	Rural	12.48	51.12	SN006	Suburban
14.45	52.17	UB039	Rural	12.37	51.33	SN025	Suburban
13.63	52.97	UB040	Rural	13.73	51.05	SN061	Suburban
13.28	52.52	BE014	Suburban	11.87	52.25	ST002	Suburban
12.48	51.12	SN006	Suburban	12.3	51.65	ST015	Suburban
12.37	51.33	SN025	Suburban	12.38	51.62	ST068	Suburban
13.73	51.05	SN061	Suburban	12	51.48	ST072	Suburban
11.87	52.25	ST002	Suburban	12.03	51.32	ST090	Suburban
12.3	51.65	ST015	Suburban	14.13	51.83	BB001	Urban
12.13	51.05	ST028	Suburban	14.32	51.73	BB006	Urban
12.25	51.83	ST030	Suburban	14.63	51.73	BB009	Urban
12.38	51.62	ST068	Suburban	13.05	52.4	BB021	Urban
11.17	52.85	ST069	Suburban	14	51.52	BB024	Urban
12	51.48	ST072	Suburban	14.37	51.55	BB026	Urban
11.62	52.13	ST076	Suburban	11.75	52.98	BB028	Urban
12.03	51.32	ST090	Suburban	14.28	53.05	BB029	Urban
13.28	52.65	BE037	Traffic	12.33	52.52	BB030	Urban
14.13	51.83	BB001	Urban	13.62	52.3	BB031	Urban
14.32	51.73	BB006	Urban	14.63	52.13	BB032	Urban
14.63	51.73	BB009	Urban	13.17	52.08	BB036	Urban
13.05	52.4	BB021	Urban	13.87	53.32	BB038	Urban
14	51.52	BB024	Urban	14.53	52.33	BB042	Urban
14.37	51.55	BB026	Urban	13.7	51.85	BB043	Urban
11.75	52.98	BB028	Urban	13.35	52.53	BE010	Urban
14.28	53.05	BB029	Urban	13.33	52.52	BE015	Urban
12.33	52.52	BB030	Urban	13.37	52.38	BE027	Urban
13.62	52.3	BB031	Urban	13.43	52.48	BE034	Urban
14.63	52.13	BB032	Urban	13.4	52.58	BE045	Urban
13.17	52.08	BB036	Urban	13.48	52.63	BE051	Urban
13.87	53.32	BB038	Urban	13.28	52.65	BE062	Urban
12.87	52.6	BB040	Urban	11.17	52.95	NI060	Urban
14.53	52.33	BB042	Urban	13.72	51.05	SN014	Urban
13.7	51.85	BB043	Urban	12.32	51.32	SN059	Urban
12.8	52.92	BB048	Urban	12.32	51.62	ST014	Urban
13.58	52.68	BB050	Urban	11.63	52.1	ST057	Urban
13.35	52.53	BE010	Urban	11.85	52.58	ST063	Urban
13.37	52.38	BE027	Urban	12.65	51.87	ST066	Urban
13.22	52.47	BE032	Urban	11.98	51.38	ST080	Urban
13.43	52.48	BE034	Urban				
13.4	52.52	BE044	Urban				
13.48	52.63	BE051	Urban				
13.22	52.47	BE052	Urban				
13.28	52.65	BE062	Urban				
11.17	52.95	NI060	Urban				
14.43	51.17	SN004	Urban				
12.32	51.52	SN012	Urban				
13.72	51.05	SN014	Urban				
14.25	51.43	SN050	Urban				
12.32	51.32	SN059	Urban				
11.97	51.48	ST050	Urban				
11.5	51.63	ST052	Urban				
11.63	52.1	ST057	Urban				
11.85	52.58	ST063	Urban				
12.65	51.87	ST066	Urban				
11.82	51.05	ST078	Urban				