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GMES SERVICE ELEMENT
PROMOTE 2

C6 Validation Report

Chapter 10
URBAN AND REGIONAL AIR QUALITY ASSESSMENT SERVICE

Version 3

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CONTRIBUTING AUTHORS	Service leader Service providers	Koen De Ridder Peter Viaene Hein Zelle Nuno Grosso	23/06/2009	
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LIST OF ACRONYMS

AirBase	European air quality databaseAdvanced regional prediction system
ARPS	Advanced regional prediction system
AURORA	Air quality modelling in urban regions using optimal resolution approach
AVHRR	Advanced very high resolution radiometer
CHIMERE	Chemistry-transport model
CITEAIR	Common information to European air
CORINAIR	Core Inventory of Air Emissions (EEA)
CORINE	European land cover mapping project
ECMWF	European centre for medium-range weather forcasting
EEA	European environment agency
E-MAP	Emission MAPping GIS tool
EMEP	European (air quality) monitoring and evaluation programme
EPER	European pollutant emission register
FNL	NCEP final analysis
GDAS	Global Data Assimilation System
IRCEL	Interregional Cell for the Environment (~ Belgian Environmental Agency)
KNMI	Royal Netherlands Meteorological Institute
LML	Dutch national measuring network (air quality)
MERIS	Medium-resolution imaging spectrometer
MODIS	Moderate resolution imaging spectroradiometer
NAEI	National Atmospheric Emission Inventory for UK
NASA	US national space agency
NCAR	National centre for atmospheric research
NCEP	National Centers for Environmental Prediction
NDVI	Normalised difference vegetation index
OMI	Ozone Monitoring Instrument (aboard AURA satellite)
PM	Particulate matter
RIVM	Dutch National institute for public health and environment
SCIAMACHY	Scanning imaging absorption spectrometer for atmospheric cartography
SPOT	Satellite pour l'observation de la Terre
SST	Sea surface temperature
TREMOVE	Transport and Emissions Simulation Model (EC)
USGS	United states geological survey
VGT	Vegetation instrument (onboard the SPOT platform)
WRF	Weather Research and Forecasting model

N/A	Not Available
n.a.	not applicable
n.s.	not specified

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10 URBAN AND REGIONAL AIR QUALITY ASSESSMENT

10.1 Service Summary

Description:

Whereas air quality forecasts are useful in the context of issuing warnings to the general public, the use of deterministic atmospheric models in hindcasting (assessment) mode is particularly relevant for policy makers.

While other Services within PROMOTE do create atmospheric data in hindcasting mode, the resolution of the models involved (tens of kilometres) is rather coarse, which is related to the fact that they employ domains covering the entire European continent or large portions of the continent. As a result, the strong concentration gradients that occur over urban areas are not captured in these models.

Considering the above, the goal of the present Service is to downscale (using nesting techniques) coarse-resolution atmospheric data generated in other Services to urban and regional domains, at a resolution of the order of one to ten kilometres. Note that, even though the focus is on urban-scale domains (typical extent a few tens of kilometres across), the scope of the "Urban/regional air quality assessment" Service is at the scale of Europe, in the sense that the Service will consider a representative sample of urban areas throughout Europe.

This Service contains the following subservices :

- Model-based urban air quality indicators for up to ten European cities (VITO);
- Scenario tool for regional air quality policy support (VITO);
- Zeeland air quality assessments (ARGOSS);
- Portuguese air quality records (YDREAMS/IMAR).

Service is/will be operational since/after: May 2007

Research partners: -

Provider(s): ARGOSS, VITO, YDREAMS/IMAR

Validation contact: Koen De Ridder, VITO, koen.deridder at vito.be

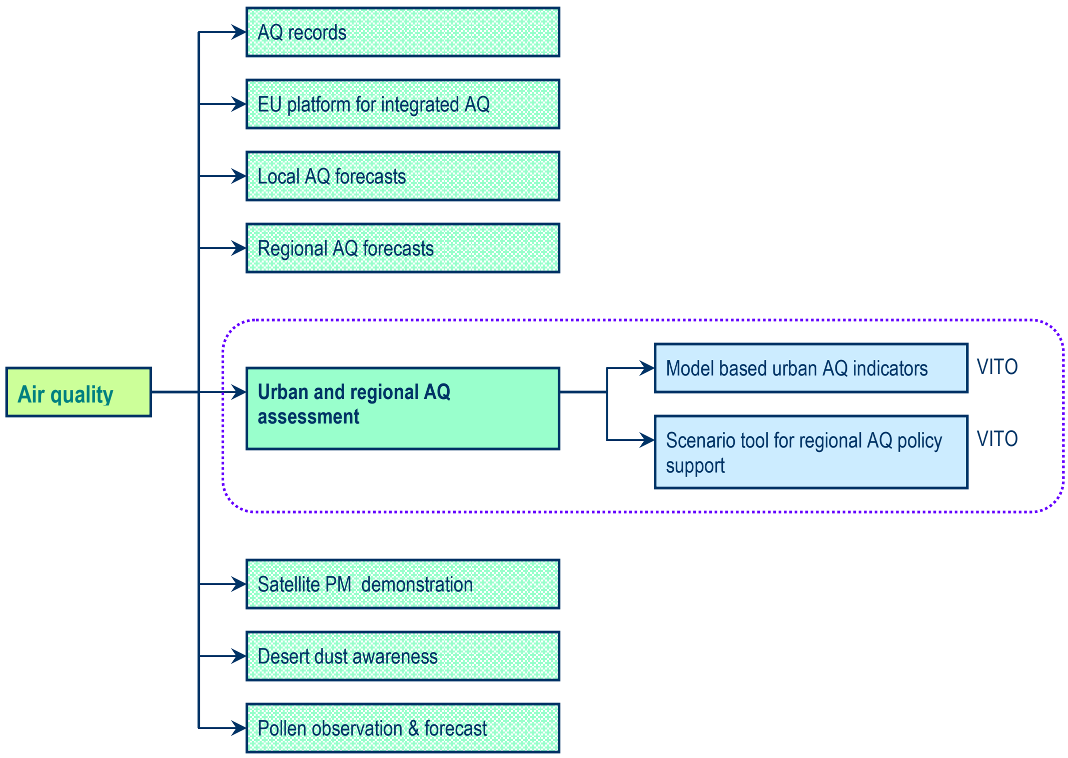


Figure 1.1-1 The *Urban and regional air quality assessment* service within the PROMOTE-2 *Air Quality* theme.

10.2 Product characterization

Model based urban air quality indicators	
SO_2 concentration fields	
Parameter	gridded ground-level SO_2 concentration values
Typical range	0 to > 250 µg m^{-3}
Determination of the typical range (Method, criteria)	European guidelines and concentration scales used at IRCEL (User), see http://www.irceline.be/~celinair/english/homeen_nojava.html
Maximum range	n.s.
Units	µg m^{-3}
Standards	Council Directive 96/62/EC of 27 September 1996 on ambient air quality assessment and management, Official Journal L 296 , 21/11/1996 P. 0055 – 0063 Council Directive 1999/30/EC relating to limit values for sulphur dioxide, nitrogen dioxide and oxides of nitrogen, particulate matter and lead in ambient air. [OJ L 163, 29.6.1999, p. 41] see http://ec.europa.eu/environment/air/existing_leg.htm
NO_2 concentration fields	
Parameter	gridded ground-level NO_2 concentration values
Typical range	0 to > 400 µg m^{-3}
Determination of the typical range (Method, criteria)	European guidelines and concentration scales used at IRCEL (User), see http://www.irceline.be/~celinair/english/homeen_nojava.html
Maximum range	n.s.
Units	µg m^{-3}
Standards	Council Directive 96/62/EC of 27 September 1996 on ambient air quality assessment and management, Official Journal L 296, 21/11/1996 P. 0055 – 0063 Council Directive 1999/30/EC relating to limit values for sulphur dioxide, nitrogen dioxide and oxides of nitrogen, particulate matter and lead in ambient air. [OJ L 163, 29.6.1999, p. 41] see http://ec.europa.eu/environment/air/existing_leg.htm
PM_{10} concentration fields	
Parameter	gridded ground-level PM_{10} concentration values
Typical range	0 to > 200 µg m^{-3}
Determination of	European guidelines and concentration scales used at IRCEL (User), see

the typical range (Method, criteria)	http://www.irceline.be/~celinair/english/homeen_nojava.html
Maximum range	n.s.
Units	µg m^{-3}
Standards	Council Directive 96/62/EC of 27 September 1996 on ambient air quality assessment and management, Official Journal L 296 , 21/11/1996 P. 0055 – 0063 Council Directive 1999/30/EC relating to limit values for sulphur dioxide, nitrogen dioxide and oxides of nitrogen, particulate matter and lead in ambient air. [OJ L 163, 29.6.1999, p. 41] see http://ec.europa.eu/environment/air/existing_leg.htm
CiteAir YACAQI city index	
Parameter	YACAQI (Year Average Common Air Quality Index) city index
Typical range	0-2
Determination of the typical range (Method, criteria)	Determined through the CiteAir Interreg IIIc project, more information available on http://citeair.rec.org/
Maximum range	3
Units	Dimensionless
Standards	Determined through the CiteAir Interreg IIIc project, more information available on http://citeair.rec.org/
CiteAir YACAQI traffic index	
Parameter	YACAQI (Year Average Common Air Quality Index) traffic index
Typical range	0-2
Determination of the typical range (Method, criteria)	Determined through the CiteAir Interreg IIIc project, more information available on http://citeair.rec.org/
Maximum range	3
Units	Dimensionless
Standards	Determined through the CiteAir Interreg IIIc project, more information available on http://citeair.rec.org/
Scenario tool for regional air quality policy support	
Concentration change patterns	
Parameter	fields of (changes of) ground-level concentrations of pollutants as requested by the User (typically O_3, PM_{10}, $PM_{2.5}$, NO_2, ...)
Typical range	concentrations: 0 to a few hundred µg m^{-3} (depending on the pollutant species) concentration changes: typically up to several ten percent
Determination of the typical range	European guidelines and concentration scales used at IRCEL (User), see http://www.irceline.be/~celinair/english/homeen_nojava.html

(Method, criteria)	experience from past scenario studies
Maximum range	n.s.
Units	µg m^{-3} (concentrations and their changes) and % (conc. changes)
Standards	Council Directive 96/62/EC of 27 September 1996 on ambient air quality assessment and management, Official Journal L 296 , 21/11/1996 P. 0055 – 0063 Council Directive 1999/30/EC relating to limit values for sulphur dioxide, nitrogen dioxide and oxides of nitrogen, particulate matter and lead in ambient air. [OJ L 163, 29.6.1999, p. 41] Directive 2002/3/EC of the European Parliament and of the Council relating to ozone in ambient air. [OJ L 67, 9.3.2002, p. 14] see http://ec.europa.eu/environment/air/existing_leg.htm
Zeeland air quality assessment	
Annual average, standard deviation and maximum concentration of several constituents	
Annual air quality concentration statistics	Annual concentration, standard deviation and maximum concentrations for the parameters PM10, PM2.5, NH3, CH4, CO, NO2, NO, O3, SO2
Typical range	Range differs for each constituent. Scales are set to allow the typical range as well as provide information on extremes. The following lists the typical range and the extreme value currently in use, in units of ug/m^3. NOTE: these values are yet to be discussed with the user, and will certainly be modified. PM10: 0-75, 200 PM2.5: 0-75, 200 NH3: 0-30, 50 CH4: 1150 - 1300,1500 CO: 0-750, 5000 NO2: 0-100, 500 NO: 0-100, 250 O3: 0-100, 400 SO2: 0-100, 400
Determination of the typical range (Method, criteria)	Estimated from annual averages and typical forecast data. TO BE EVALUATED with the user, WILL BE CHANGED. Criteria will be determined (amongst others) based on the concentration limits where the user should start warning people or issuing alerts.
Maximum range	See the above table with typical ranges. There is no maximum value: all data above the maximum is displayed in the same colour. Contours can be extended to higher maxima if requested so numerical information remains available. Currently the maxima for contours are as specified in the table above.

Units	ug/m^3
Standards	To be determined in phase 3 with the user. Standards as currently in use for reporting to the national government will be adhered to whenever possible.
Portuguese air quality records	
Daily air quality index	
Parameter	Daily Air Quality Index (global and for PM_{10}; NO_2; SO_2; CO;O_3) As defined by the user in: http://www.qualar.org/INDEX.PHP?page=1&subpage=7
Typical range	Global: 1-5 Very good to bad PM_{10}: 10 to 70 NO_2: 5 to 70 SO_2: 0 to 15 CO: 100 to 1000 O_3: 5 to 100
Determination of the typical range (Method, criteria)	The typical range is defined as approximately percentile 5 and percentile 95 of the parameter results for the year 2006 in all the monitoring stations
Maximum range	Global: Very good to bad or 1 to 5 PM_{10}: 0 to >120 NO_2: 0 to >400 SO_2: 0 to >500 CO: 0 to >10000 O_3: 0 to >240
Units	For global index is qualitative(very good to bad or 1 to 5) For the pollutants is $\mu g\ m^{-3}$
Standards	Council Directive 96/62/EC of 27 September 1996 on ambient air quality assessment and management, Official Journal L 296 , 21/11/1996 P. 0055 – 0063 Council Directive 1999/30/EC relating to limit values for sulphur dioxide, nitrogen dioxide and oxides of nitrogen, particulate matter and lead in ambient air. [OJ L

	163, 29.6.1999, p. 41] Council Directive 2000/69/CE relating benzene and carbon monoxide in ambient air [OJ L 313, 13.12.2000, p. 12] Council Directive 2002/3/EC relating to ozone in ambient air. [OJ L 67, 9.3.2002, p. 14] http://www.apambiente.pt/politicasambiente/Ar/QualidadeArAmbiente/Paginas/default.aspx
Monthy parameters for PM10	
Parameter	PM10 monthly average
Typical range	PM10 monthly average: 10 to 55
Determination of the typical range (Method, criteria)	The typical range is defined as approximately percentile 5 and percentile 95 of the parameter results for the year 2006 in all the monitoring stations
Maximum range	PM10 monthly average: <5 to >80
Units	µg m^{-3}
Standards	Council Directive 96/62/EC of 27 September 1996 on ambient air quality assessment and management, Official Journal L 296 , 21/11/1996 P. 0055 – 0063 Council Directive 1999/30/EC relating to limit values for sulphur dioxide, nitrogen dioxide and oxides of nitrogen, particulate matter and lead in ambient air. [OJ L 163, 29.6.1999, p. 41] http://www.apambiente.pt/politicasambiente/Ar/QualidadeArAmbiente/Paginas/default.aspx
Annual parameters for PM1	
Parameter	PM_{10} annual average and 36º maximum daily average
Typical range	PM_{10} annual average: <20 to >45 36º maximum daily average: <30 to >70
Determination of the typical range (Method, criteria)	The typical range is defined as approximately percentile 5 and percentile 95 of the parameter results for the year 2006 in all the monitoring stations

Maximum range	PM_{10} annual average: <10 to >60 36º maximum daily average: <20 to >90
Units	µg m^{-3}
Standards	Council Directive 96/62/EC of 27 September 1996 on ambient air quality assessment and management, Official Journal L 296 , 21/11/1996 P. 0055 – 0063 Council Directive 1999/30/EC relating to limit values for sulphur dioxide, nitrogen dioxide and oxides of nitrogen, particulate matter and lead in ambient air. [OJ L 163, 29.6.1999, p. 41] http://www.apambiente.pt/politicasambiente/Ar/QualidadeArAmbiente/Paginas/default.aspx

Table 10.2-1 Characterization of the products provided by the Urban Regional AQ assessment sub-service

10.3 Urban air quality indicators and scenario tools

10.3.1 Validation plan and validation data

The "urban indicators and scenario studies" sub-service produces air quality indices/indicators and scenario evaluations based on annual hourly pollutant concentrations simulated with the AURORA model. In phase 2 the following domains (and resolutions) are considered: Rotterdam (1 km), Prague (1 km), Flanders-Holland (3 km – for the scenario evaluation). Regarding the geophysical validation, the focus is on assessing the different components of the model: meteorology (only for a case study), emissions, transport-chemistry.

First, results are given of a recent study that was performed during a three-week period, with a simulation domain covering the Ruhr area in Germany. Calculated traffic emissions are compared to results from a local mission inventory. Simulated meteorological parameters and pollutant concentrations are compared with observations from local stations. Simulated land surface temperature is compared with AVHRR brightness temperature.

For the Rotterdam model domain, simulated pollutant concentrations are compared with local data, from the Interregional Cell for the Environment (IRCEL) and the DCMR Environmental Protection Agency Rijnmond (both are Users). For Prague, observed pollutant concentrations are taken from the AirBase database (EEA). The main statistics used here are bias and root mean square error. While the EU Directives set required accuracies at the level of 30-50 % (depending on the pollutant and the averaging period), we strive for accuracies of 20 % for gaseous pollutants and 30 % for particulate matter.

While for the Rotterdam modelling domain detailed shipping emission data were made available by the User DCMR–, no local emissions data are available for the city of Prague,. Therefore, for the latter we used the E-MAP GIS tool to perform a spatial disaggregation of CORINEAIR/EMEP emission inventories by using spatial surrogate data (Maes *et al.*, 2008). For applications over Europe the spatial variables include the CORINE land cover data, EPER database, TREMOVE data, EUROSTAT statistics together with ESRI data and maps. The resulting emission maps have been compared with local emission data for the region of London and for the Netherlands. This gives an estimate for the uncertainty associated with this top-down emission inventorisation method.

The main outcome of the "urban/regional air quality assessment service" consists of hourly fields of ground-level pollutant concentrations, for a number of species including O_3, NO_2, PM_{10}, $PM_{2.5}$ and SO_2. For the stations measuring the pollutants O_3, NO_2 and PM_{10} it is possible to derive the CiteAir city index and the CiteAir traffic index, hence allowing for direct validation of the calculated CiteAir indices. Validation of simulation results is done by comparing simulated concentration values with data from networks of pollutant measurement stations.

The validation procedure is based on the calculation of the root mean square error, bias, correlation coefficient of simulated air pollution statistics that are considered in the

European Air Quality Directives, e.g., for PM_{10} that would be daily and annual average values (see more details from http://www.irceline.be/~celinair/english/homeen_nojava.html).

The accuracy requirements for simulated pollutant concentrations, according the EU Air Quality Directives, and also used in our validation work, are shown in Figure 10.3-1, taken from Borrego et al. (2003). Note that the required accuracies depend on the averaging time, so that, e.g., the required accuracy on annual mean values is generally higher than on daily or hourly mean values.

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%	
CO	8-h mean	50%	2000/69/EC
Benzene	Annual mean	50%	
Ozone	8-h daily maximum	50%	2002/3/EC
	1-h average	50%	

Figure 10.3-1. Required accuracy for simulated pollutant concentrations according the EU Air Quality Directives (from Borrego et al., 2003).

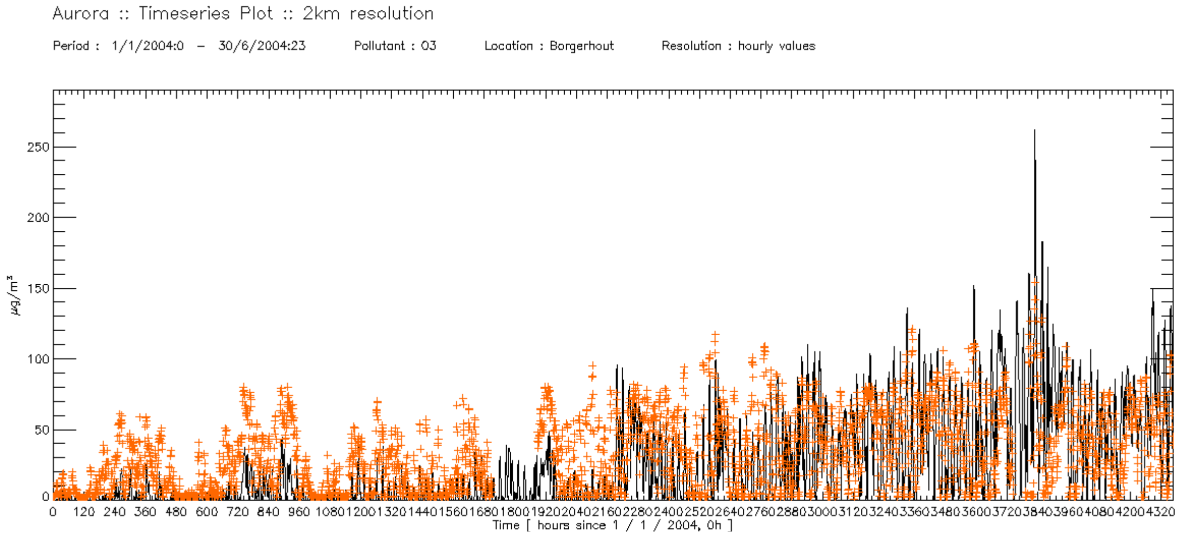
VALIDATION DATA	
Ground based observations	
near real-time observed concentrations from the telemetric stations in Belgium Phase: 1+2	Data availability and access: the data are made available by the Interregional Cell for the Environment (IRCEL) Spatial coverage and resolution: more than 80 stations scattered throughout Belgium (though not all stations measure all pollutants at all times) Temporal coverage and resolution: continuous measurements at hourly resolution Location(s) (coordinates): see http://www.irceline.be/~celinair/english/homeen_nojava.html Uncertainty quantification (e.g. Accuracy): depends on the pollutant, ranges from around 10-20 % for gaseous pollutants to 30 % and more for particulate matter
AirBase - the European Air quality dataBase Phase: 2	Data availability and access: freely available from the European Topic Centre on Air and Climate Change (EIONET) Spatial coverage and resolution: several tens of stations in the wider Prague area Temporal coverage and resolution: the year 2005, hourly time resolution Location(s) (coordinates): see

	http://www.fsm.it/padova/homepage.html Uncertainty quantification (e.g. Accuracy): see http://www.fsm.it/padova/homepage.html, click on "QA/QC aspects"
DCMR air quality concentration database Phase: 2	Data availability and access: made available through User DCMR Spatial coverage and resolution: 3 stations in the Rotterdam area Temporal coverage and resolution: the year 2005, hourly time resolution Location(s) (coordinates): see http://www.dcmr.nl/luchtkwaliteit/index.htm Uncertainty quantification (e.g. Accuracy): depends on the pollutant, ranges from around 10-20 % for gaseous pollutants to 30 % and more for particulate matter
ground-based air pollution concentration measurements	Data availability through the User, who generally is the local/national environmental agency (for Belgium the data come from the measurement network operated by IRCEL) Spatial coverage varies, for Belgium, most pollutants are measured by a network containing several tens of stations for the entire territory. Measurement stations constitute point measurements, i.e., they are representative of the immediate surroundings only. Temporal coverage for most stations/pollutants is of the order of several years, time resolution is mainly hourly. Location of the stations depends on the domain (country), for Belgium the position of the stations and further details are available from http://www.irceline.be/~celinair/english/homeen_nojava.html Accuracy: depends on the pollutant, ranges from around 10-20 % for gaseous pollutants to 30 % and more for particulate matter (these measurements are subject to some uncertainty, given the difficult sampling methods and the (at times somewhat subjective) applied correction factors

Table 10.3-1 Data used for the validation of the Urban Regional AQ assessment

10.3.2 Validation of individual components

Often it is very difficult or impossible to validate individual components or to get an idea of their error. Therefore, the validation generally focuses on assessing the final result, *i.e.*, comparing the pollutant concentrations simulated by the AURORA model with observed values. For the simulations carried out in PROMOTE to generate the "urban air quality indicators" for the Brussels-Antwerp-Ghent area, in phase 1 a validation was performed for ozone and PM_{10}, for the period January to June 2004, using measurements from the station Borgerhout (operated by IRCEL) in the vicinity of Antwerp. The results are shown in Figure 10.3-2.



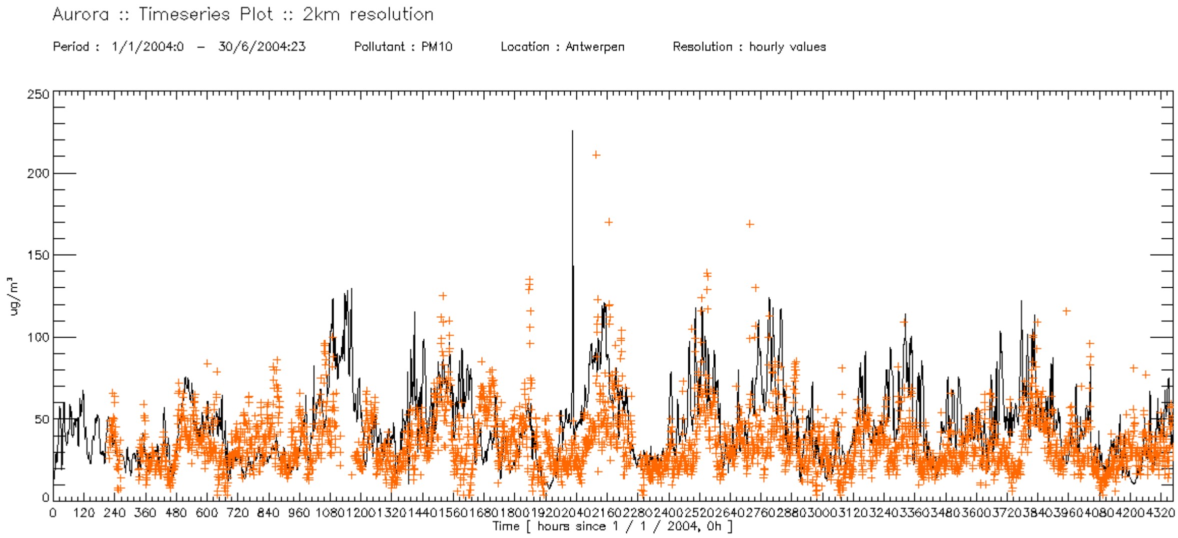


Figure 10.3-2. Comparison between simulated (line) and observed (symbols) concentrations of ozone (upper panel) and PM_{10} (lower panel) for the station "Borgerhout" (near Antwerp), January – June 2004.

While in phase 1 validation was fairly much limited to visual inspection of the simulated against the observed pollutant concentrations, phase 2 focuses more on error statistics, as shown in the remainder of this section. Below, a description will be given of the validation of the emissions, and the concentrations. Also the results of a comprehensive validation exercise, considering all the components of the air quality modelling system (emissions, meteorology, transport-chemistry) are described.**Error! Reference source not found.**

10.3.2.1 Emissions

The E-MAP top down methodology to generate emissions is validated by comparing the resulting emission maps with bottom up emission inventories. This has been performed for the city of London, by comparing E-MAP results with the NAEI data, which are available for he London area at a resolution of 1km. The explained variance at a spatial resolution of 5km (aggregation of 25 1-km² NAEI cells) was >70% for CO, NMVOC and NOx, >60% for PM10 and almost 50% for SO2. When going to a resolution of 1km (as also used in the current simulations over Rotterdam and Prague) the explained variance decreased for most pollutants (approx 30% for CO, approx. 50% for NMVOC, NOx and PM10).

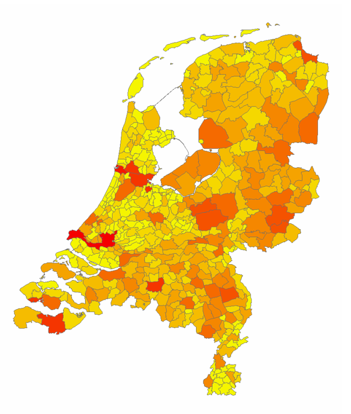
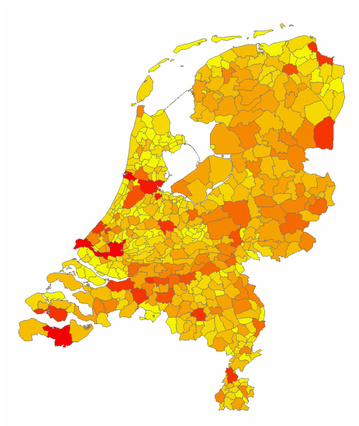
E-MAP emissions PM_{10}	National Emission Registration PM_{10}	
		PM10 (Gg) 0.00 - 0.03 0.04 - 0.05 0.06 - 0.09 0.10 - 0.13 0.14 - 0.19 0.20 - 0.28 0.29 - 0.39 0.40 - 0.82 0.83 - 1.59 1.60 - 3.85

Figure 10.3-3. Emission maps for PM_{10} showing disaggregated CORINAIR/EMEP emission totals for the Netherlands using spatial surrogates (left) and emissions taken from the National Dutch Emission Registration (right), for all the Dutch municipalities.

For the Netherlands we compared E-MAP with emission data that are available on the municipality level. Figure 10.3-3 shows PM_{10} emission maps at the municipal level for the Netherlands. The E-MAP derived emission data agree well with the National Dutch Emission Registration. Figure 10.3-4 shows a scatterplot of CO, with E-MAP plotted against data from the National Dutch Emission Registration. More details on the validation of the E-MAP methodology can be found in Maes *et al.* (2008).

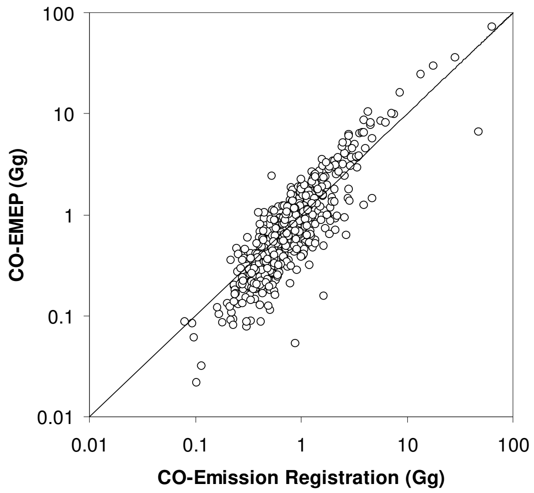


Figure 10.3-4. Dutch CO emissions for municipalities in the Netherlands (CO-Emission Registration) plotted against the disaggregated EMEP/CORINAIR CO emissions. The line represents the 1:1 relation.

10.3.2.2 Pollutant concentrations

The validation for the Rotterdam model domain was done by comparing simulation results with AirBase measurement data as well as with data provided by the User (further referred to as DCMR data). Figure 10.3-5. shows an example of a scatterplot of modelled PM_{10} concentrations against measured values for the station of Bentinckplein, Rotterdam.

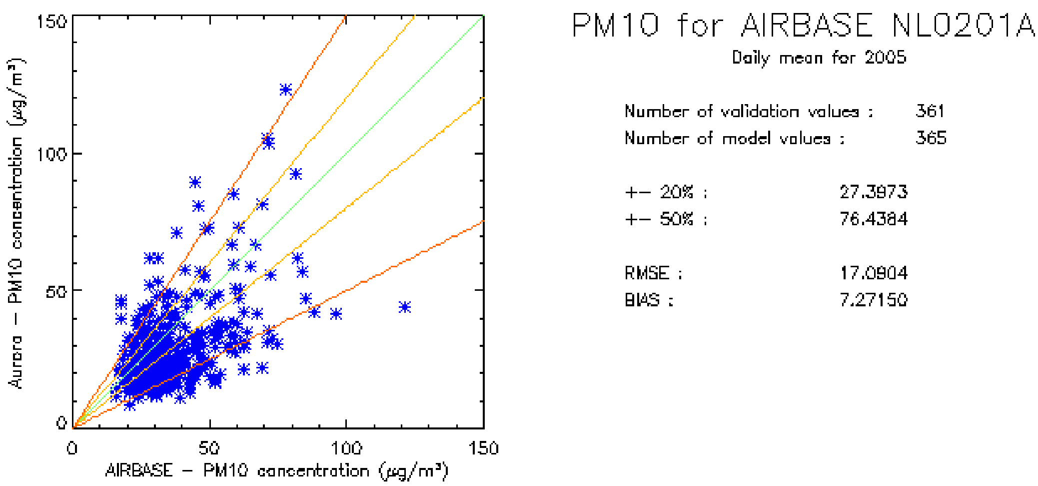


Figure 10.3-5. Scatterplot of AURORA PM_{10} daily mean concentrations as a function of measured values, for the station of Bencinckplein, Rotterdam.

Table 10.3-2 and Table 10.3-3 give an overview of the validation of the AURORA results against Airbase and DCMR data, respectively. The concentration values shown in the second and third columns are annual means of the parameters shown in the last column (daily maximum of 8-h average concentration for O_3, while for NO_2, SO_2, PM_{10} and $PM_{2.5}$ daily mean values). Also the statistical parameters (bias, RMSE and correlation coefficient) are calculated on the basis of these daily parameters. The values shown are an average over all measurement data available for the pollutant under consideration.

Table 10.3-2 Overview of the AURORA validation for the Rotterdam area with Airbase data. The figures are averages over the stations.

	AURORA	Airbase	bias	RMSE	correlation coefficient	based on
O3	48.790	51.949	3.576	29.002	0.588	8-h dayly max
NO2	38.808	36.871	1.937	19.339	0.415	daily mean
PM10	28.874	31.244	-2.370	15.070	0.456	daily mean
SO2	22.174	7.079	15.095	17.550	0.350	daily mean
city index	0.672	0.715	-	-	-	annual mean
traffic index	0.809	0.902	-	-	-	annual mean

Table 10.3-3 Overview of the AURORA validation for the Rotterdam area with DCMR data.

	AURORA	DCMR	bias	RMSE	correlation coefficient	based on
O3	47.227	56.802	9.274	28.092	0.647	8-h dayly max
NO2	40.684	38.136	2.548	18.377	0.403	daily mean
PM10	29.775	25.995	3.780	14.582	0.475	daily mean
PM25	24.458	15.301	9.157	14.706	0.515	daily mean
SO2	23.788	13.201	10.587	15.936	0.270	daily mean
city index	0.764	0.553				annual mean
traffic index	0.899	0.689				annual mean

We would like to draw the attention to the fact that the SO_2 concentrations measured by the DCMR network are much higher than the ones measured by the Airbase network because of different locations.

In order to assess the correctness of the spatial pattern of the AURORA results, we calculated the correlation between the individual measurement stations (on an annual basis). A scatterplot of the Cite Air city index derived from AURORA versus the Airbase measurement data is shown in Figure 10.3-6. Table 10.3-4 summarizes the correlation coefficients and RMSE values. It shows that the spatial pattern of AURORA captures well the relative differences between the measurement stations.

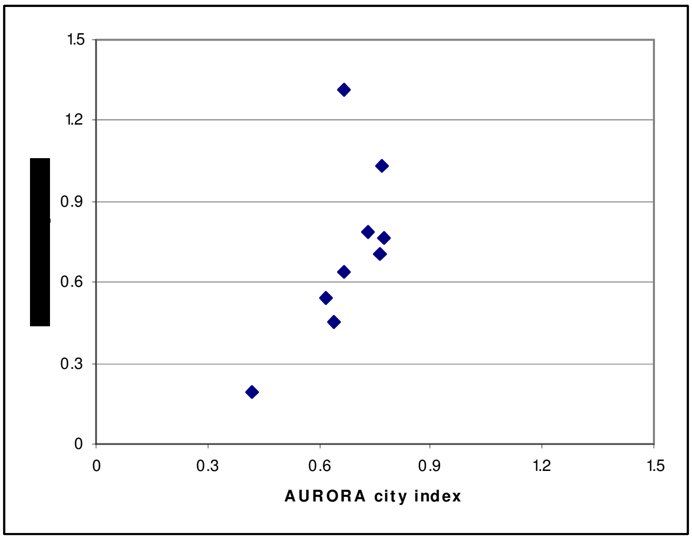


Figure 10.3-6. Scatterplot of the Airbase city index as a function of the AURORA-derived city index (on the location of the Airbase stations).

Table 10.3-4. Overview of the spatially-based validation for the Rotterdam area with Airbase and DCMR data. In contrast to previous tables, the RMSE is not calculated based on time series but based on annual mean concentartions from the total sample of stations in the domain.

AURORA vs Airbase	correlation coefficient	RMSE
O3	0.862	4.711
NO2	0.686	8.346
PM10	0.767	5.578
SO2	0.903	15.319
city index	0.647	0.254
traffic index	0.785	0.347

AURORA vs DCMR	correlation coefficient	RMSE
O3	0.858	9.583
NO2	0.641	2.978
PM10	0.245	3.890
PM25	1.000	9.166
SO2	0.641	2.978
city index	0.743	0.123
traffic index	0.788	0.122

The validation of the AURORA results for the city of Prague was done on the basis of Airbase data. Figure 10.3-7 shows an example of a scatterplot of modelled NO2 concentrations as a function of measured NO_2 concentrations for the Airbase station CZ0008A in central Prague.

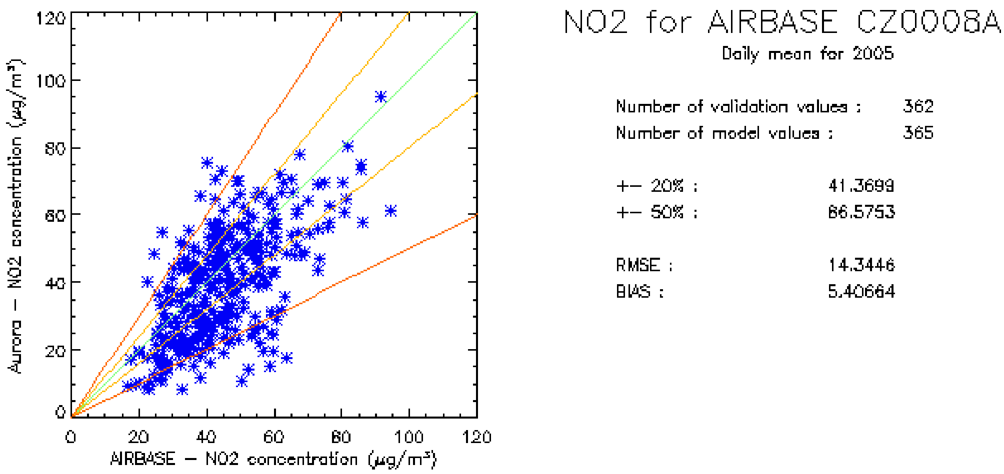


Figure 10.3-7. Scatterplot of AURORA NO2 daily mean concentrations as a function of measured NO2 daily mean concentrations, for the Airbase station CZ0008A.

An overview of the relative errors, compared to the required accuracy, is provided in **Error! Reference source not found.**.For SO2 there clearly is a problem, which we believe is related to the emissions data. Indeed, the emissions for this pollutant are known to vary widely between emissions inventories. It should also be noted that between different observational datasets, as e.g. DCMR's and that from AirBase, significant differences arise.

Table 10.3-5 Synoptic table showing required versus actual relative accuracy for the Rotterdam and Prague 1-km domains, for the different pollutants. For Rotterdam different data sets (DCMR & AirBase) were used.

		required	actual accuracy in %		
constituent	averaging	accuracy	Rotterdam		Prague
	time	in %	DCMR	AirBase	Airbase
SO2	daily	50	120.5	246.5	203.1
	annual	30	80.2	212.7	160.9
NO2	daily	50	48.3	52.3	46.6
	annual	30	6.6	5.1	0.3
PM	annual	50	14.6	7.7	4.1
O3	8h daymax	50	16.4	49.5	49.9

Table 10.3-5 gives an overview of the validation of the AURORA results against Airbase data. The concentration values shown in the second and third columns are annual means of the parameters shown in the last column (daily maximum of 8h average concentration for O_3, while for NO_2, SO_2, PM_{10} and $PM_{2.5}$ daily mean values). Also the statistical parameters (bias, RMSE and correlation coefficient) are calculated on the basis of these daily parameters. The values shown are an average over all measurement data available for the pollutant under consideration.

Table 10.3-6. Overview of the AURORA validation for the Prague area with Airbase data.

	AURORA	Airbase	bias	RMSE	correlation coefficient	based on
O3	66.104	65.308	7.510	32.630	0.687	8-h daymax
NO2	35.772	35.839	-0.067	16.652	0.607	daily mean
PM10	35.569	34.152	1.417	31.804	0.552	daily mean
PM25	20.371	25.309	-4.938	22.781	0.509	daily mean
SO2	16.779	6.439	10.340	13.028	0.549	daily mean
city index	1.279	1.051	-	-	-	annual mean
traffic index	1.366	1.267	-	-	-	annual mean

An overview of the relative errors, compared to the required accuracy, is provided in Table 10.3-7. For SO_2 there clearly is a problem, which we believe is related to the emissions data. Indeed, the emissions for this pollutant are known to vary widely between emission inventories. It should also be noted that between different observational data sets, as e.g. DCMR's and that from AirBase, significant differences arise.

Table 10.3-7. Synoptic table showing required versus actual relative accuracy for the Rotterdam and Prague 1-km domains, for the different pollutants. For Rotterdam different data sets (DCMR & AirBase) were used.

constituent	averaging time	required accuracy in %	actual accuracy in %		
			Rotterdam		Prague
			DCMR	AirBase	Airbase
SO2	daily	50	120.5	246.5	203.1
	annual	30	80.2	212.7	160.9
NO2	daily	50	48.3	52.3	46.6
	annual	30	6.6	5.1	0.3
PM	annual	50	14.6	7.7	4.1
O3	8h daymax	50	16.4	49.5	49.9

The validation of the results from the simulation domain covering the south of Netherlands and northern Belgium (also referred to as the Flanders/South-Holland domain), used in the development of the scenario tool for regional air quality policy support, at a resolution of 3 km was done by means of of Airbase data.

Table 10.3-8 gives an overview of the validation of the AURORA results against Airbase data. The concentration values shown in the second and third columns are annual means of the parameters shown in the last column (daily maximum of 8h average concentration for O_3, while for NO_2, SO_2, PM_{10} and $PM_{2.5}$ daily mean values). Also the statistical parameters (bias, RMSE and correlation coefficient) are calculated on the basis of these daily parameters. The values shown are an average over all measurement data available for the pollutant under consideration.

Table 10.3-8. Overview of the AURORA validation for the Flanders/South-Holland area with Airbase data.

	AURORA	Airbase	bias	RMSE	correlation coefficient	based on
O3	55.012	60.758	9.859	42.048	0.122	8-h daymax
NO2	43.064	28.953	14.111	21.271	0.351	daily mean
PM10	32.226	32.121	0.105	19.330	0.352	daily mean
SO2	20.183	3.861	16.322	18.695	0.212	daily mean

Table 10.3-9. Required versus actual relative accuracy for the Flanders/South-Holland domain.

constituent	averaging time	required accuracy in %	actual accuracy in %
SO2	daily	50	479.5
	annual	30	417.9
NO2	daily	50	73.4
	annual	30	48.6
PM	annual	50	0.3
O3	8h daymax	50	68.9

Table 10.3-9 gives the required versus the actual accuracy. The latter is poorer than that obtained for the 1-km domains above, which suggests that the in-situ data from the individual stations used here may not be appropriate for comparison with 3-km scale grid cells. In other words, the station data ("point data") may not be representative for 3-km scale pollution features.

10.3.2.3 Prague re-run with alternative emissions

In 2009 the 1-km Prague simulation was carried out again, though using different emissions. The reason for doing so is that the simulated concentrations of the previous year were found to yield (too) high values over the urban areas. As the emissions were not specified from a detailed emissions inventory, but instead were produced by means of the 'emission mapper' (e-MAP) tool described above, another key for the distribution of urban emissions was implemented, e.g. attributing relatively less traffic emissions in the urban core and assigning some of these emissions to rural areas.

Table 10. AirBase stations used for the validation of the Prague simulation, and their characteristics. The stations with green background are 'background' stations (see text for explanation).

	station / pollutant ID	
1	2005_NO2_CZ0008A.h5	traffic urban commercial
2	2005_NO2_CZ0009A.h5	background suburban residential
3	2005_NO2_CZ0010A.h5	background urban residential/natural
4	2005_NO2_CZ0011A.h5	traffic urban residential/commercial
6	2005_NO2_CZ0013A.h5	traffic urban residential
7	2005_NO2_CZ0014A.h5	traffic urban residential
8	2005_NO2_CZ0015A.h5	background suburban residential
11	2005_NO2_CZ0020A.h5	background suburban residential
14	2005_NO2_CZ0041A.h5	background rural natural
15	2005_NO2_CZ0065A.h5	traffic urban residential/commercial
16	2005_NO2_CZ0066A.h5	traffic urban residential/commercial
17	2005_NO2_CZ0068A.h5	traffic urban residential/commercial
18	2005_NO2_CZ0081A.h5	background urban residential
19	2005_NO2_CZ0082A.h5	traffic urban commercial
20	2005_NO2_CZ0083A.h5	traffic urban residential/commercial
21	2005_NO2_CZ0089A.h5	background urban residential
22	2005_NO2_CZ0090A.h5	background urban residential
23	2005_NO2_CZ0107A.h5	industrial urban commercial/industrial
24	2005_NO2_CZ0108A.h5	background suburban residential

The validation was done by means of observed hourly pollutant concentrations from the AirBase network, for the area of Prague and surroundings. Table 10 lists the stations used, as well as their characteristics. The green background on some stations means that the concerned stations are representative of background conditions. These are in fact the only stations that should be used for comparing simulated values at a spatial resolution of 1 km. The other stations are mainly 'traffic' stations, i.e., located near busy streets, and not representative for 1-km grid cells. We have retained these stations, though, as they provide insight into the effect of the model's spatial resolution, and provide a case for adding a high-resolution component to the modelling.

Table 11. Validation statistics for O3. Every row corresponds to another station. The third and fourth columns give the annual mean values observed and simulated, respectively. The fifth column gives the fractional bias, and the sixth column the fractional mean absolute deviation. The rightmost column gives the correlation between measured and simulated values. All statistics were established based on daily mean values.

O3						
	station / pollutant ID	obs MEAN	mod MEAN	fractional BIAS %	fractional MAD %	CORR
1	2005_O3_CZ0008A.h5	32.6	50.0	53.5	77.0	0.65

2	2005_O3_CZ0009A.h5	48.8	49.4	1.2	43.0	0.63
8	2005_O3_CZ0015A.h5	45.7	50.5	10.6	46.0	0.66
11	2005_O3_CZ0020A.h5	52.3	50.7	-3.2	42.0	0.61
14	2005_O3_CZ0041A.h5	65.0	52.9	-18.7	35.0	0.65
15	2005_O3_CZ0065A.h5	32.8	50.6	54.5	80.8	0.57
18	2005_O3_CZ0081A.h5	49.5	50.3	1.6	40.6	0.67
20	2005_O3_CZ0083A.h5	33.7	49.4	46.5	77.2	0.55
21	2005_O3_CZ0089A.h5	53.8	51.3	-4.8	36.0	0.71
24	2005_O3_CZ0108A.h5	52.4	50.1	-4.6	40.1	0.65

Table 12. Validation statistics for NO2, see table for O3 above for explanations.

NO2						
	station / pollutant ID	obs MEAN	mod MEAN	fractiona l BIAS %	fractiona l MAD %	CORR
1	2005_NO2_CZ0008A.h5	44.7	25.1	-43.8	45.9	0.54
2	2005_NO2_CZ0009A.h5	27.6	25.6	-7.2	32.7	0.64
3	2005_NO2_CZ0010A.h5	33.8	26.6	-21.3	33.3	0.62
4	2005_NO2_CZ0011A.h5	38.2	26.4	-30.9	38.5	0.56
6	2005_NO2_CZ0013A.h5	38.5	26.3	-31.6	38.7	0.60
7	2005_NO2_CZ0014A.h5	41.1	26.2	-36.4	40.2	0.56
8	2005_NO2_CZ0015A.h5	29.8	24.4	-18.3	38.0	0.58
11	2005_NO2_CZ0020A.h5	25.7	23.3	-9.6	37.6	0.53
14	2005_NO2_CZ0041A.h5	12.5	20.1	60.7	71.5	0.73
15	2005_NO2_CZ0065A.h5	46.5	24.8	-46.7	50.3	0.30
16	2005_NO2_CZ0066A.h5	75.6	25.5	-66.3	66.4	0.48
17	2005_NO2_CZ0068A.h5	37.0	24.8	-33.0	39.7	0.59
18	2005_NO2_CZ0081A.h5	28.9	24.5	-15.3	33.7	0.64
19	2005_NO2_CZ0082A.h5	48.0	28.4	-40.8	43.6	0.56
20	2005_NO2_CZ0083A.h5	42.3	27.1	-35.8	41.2	0.43
21	2005_NO2_CZ0089A.h5	22.6	22.6	0.0	33.1	0.73
22	2005_NO2_CZ0090A.h5	24.0	23.3	-2.9	30.8	0.73
23	2005_NO2_CZ0107A.h5	38.1	25.5	-33.1	52.3	0.12
24	2005_NO2_CZ0108A.h5	24.5	24.4	-0.3	36.5	0.65

Table 13. Validation statistics for PM10, see table for O3 above for explanations.

PM10						
	station / pollutant ID	obs MEAN	mod MEAN	fractiona l BIAS %	fractiona l MAD %	CORR
1	2005_PM10_CZ0008A.h5	34.6	21.5	-37.9	47.5	0.44
2	2005_PM10_CZ0009A.h5	34.1	22.2	-35.0	45.5	0.58
3	2005_PM10_CZ0010A.h5	33.3	22.0	-33.9	46.9	0.45
4	2005_PM10_CZ0011A.h5	35.0	21.2	-39.3	48.7	0.50

6	2005_PM10_CZ0013A.h5	28.0	21.7	-22.4	40.0	0.54
7	2005_PM10_CZ0014A.h5	28.2	22.6	-19.7	35.4	0.62
8	2005_PM10_CZ0015A.h5	36.2	19.0	-47.6	51.7	0.46
11	2005_PM10_CZ0020A.h5	30.9	20.4	-34.0	47.3	0.44
15	2005_PM10_CZ0065A.h5	32.3	21.4	-33.8	44.6	0.46
17	2005_PM10_CZ0068A.h5	43.3	20.6	-52.4	56.4	0.59
18	2005_PM10_CZ0081A.h5	25.6	20.3	-20.7	43.4	0.48
19	2005_PM10_CZ0082A.h5	38.1	22.1	-42.0	49.2	0.51
20	2005_PM10_CZ0083A.h5	37.9	21.9	-42.1	49.3	0.46
21	2005_PM10_CZ0089A.h5	33.5	20.4	-39.0	47.6	0.50
22	2005_PM10_CZ0090A.h5	52.1	20.5	-60.7	61.8	0.59
23	2005_PM10_CZ0107A.h5	30.8	20.8	-32.6	52.7	0.30
24	2005_PM10_CZ0108A.h5	23.7	18.7	-21.0	39.9	0.52

Table 14. Validation statistics for PM2.5, see the table for O3 above for explanations.

PM2.5						
	station / pollutant ID	obs MEAN	mod MEAN	fractional BIAS %	fractional MAD %	CORR
4	2005_PM25_CZ0011A.h5	23.0	18.4	-20.2	39.4	0.60
11	2005_PM25_CZ0020A.h5	24.5	17.6	-28.1	43.0	0.54
17	2005_PM25_CZ0068A.h5	31.8	18.4	-42.3	49.2	0.65
19	2005_PM25_CZ0082A.h5	21.6	18.1	-16.2	47.1	0.10
20	2005_PM25_CZ0083A.h5	24.7	18.2	-26.3	37.1	0.61
21	2005_PM25_CZ0089A.h5	26.3	17.6	-33.1	41.8	0.57

From the tables above the following conclusions can be drawn:

- For O3, the model exhibits a very low bias, at least for the background stations, generally of the order of 5-10%, except for the rural backgroudn station CZ0041A where the model has a negative bias of almost 20 %. In the traffic stations, the model exhibits a strong positive bias, which is not surprising as the resolution of 1 km does not allow to account for local titration of O3 bij NO from car emissions. The fractional mean absolute deviation (MAD) for O3 is of the order of 35-45% for all background stations. For these stations, the correlations are of the order of 60-70%.
- Simulated NO2 generally also exhibits low biases for the background stations, except for the rural one, the same for which O3 also was not simulated well. This might possibly point to an overestimation of NOx emissions in rural areas, leading to too high NO2 and too low O3 concentrations. Fractional MAD is of the order of 30-40%, except (again) for the rural station. Correlation coefficients are in the range 55-75%.
- PM10 exhibits a persistent negative bias for all stations, underestimating annual mean concentrations by several tens of percent. This is not uncommon in air pollution simulations, and is often attributed to missing emissions of primary PM10 (natural sources such as wind-blown dust, and re-suspension).

The fractional MAD is of the order 40-50%. Correlation coefficients are in the range 45-60%.

- The bias of simulated PM2.5 is quite a bit lower, confirming the hypothesis of the missing prilary PM10 in the emisison inventory. The fractional MAD is around 40%, and correlation coefficients are around 55%.

A final conclusion from this exercise is that performance could be improved by

1. improving the emissions estimates: even though the approach where emissions were estimated using the e-MAP tool does show some skill, the model does not catch the urban-rural gradients well;
2. adding a high-resolution component to the modelling, e.g. a gaussian line source model coupled to the 1-km grid model;
3. improving the emissions of primary PM10 (natural sources, resuspension).

10.3.2.4 Results from a comprehensive validation study

In a recent European research project, VITO carried out a validation of several components of the air quality modelling system. This was done for a three-week period in May 2000, for a domain covering the major cities in the German Ruhr area. The validation addressed the components constituting the whole modelling chain, including emissions, meteorology, and the pollutant concentrations themselves.

In this exercise, traffic-related **emissions** were calculated using the MIMOSA model (Lewyckyj *et al.*, 2004). Based on the COPERT III-methodology, MIMOSA calculates geographically and temporally distributed traffic emissions using traffic information including fluxes of vehicles and their speeds. Vehicle exhaust emissions simulated by MIMOSA using traffic modelling and traffic data as input were found to compare favourably to the official emission inventory figures from LUA-NRW (Environmental Agency of North-Rhine Westphalia, Germany), see Figure 10.3-8 Compared with data from the latter, NO_x emissions from MIMOSA for the entire KVR domain were lower by 26 %, VOC emissions were higher by 10 %, and PM_{10} emissions were higher by 62 %. In Figure 10.3-8 the emissions per pollutant are compared. The error bars on NO_x and VOC emissions are 35 and 40 % respectively, in accordance with uncertainty estimates given by Kühlwein and Friedrich (2000) for urban emission inventories. For PM_{10} no such uncertainty figures were available. However, Parra et al. (2006) found differences in traffic-related PM_{10} emission estimates between inventories of 54 %, and Lindley et al. (1999), also comparing different inventories, found a figure of 50 %. Therefore, it would appear that using a figure of 50 % to characterise the uncertainty on PM_{10} emissions is fair, hence the error bars on this pollutant in Figure 10.3-8 were set to that value.

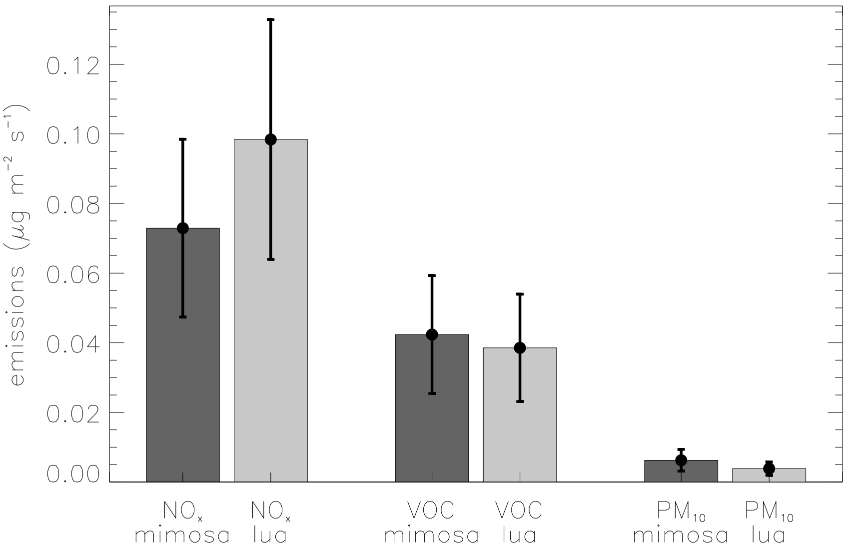


Figure 10.3-8. Comparison of vehicle exhaust emissions computed using the MIMOSA model with the emission inventory provided by LUA.

ARPS **meteorology** simulation results were validated by comparing model output with observed meteorological parameters. Figure 10.3-9 shows validation results for down-welling solar radiation, 10-m wind speed, and 2-m air temperature and humidity. As the first model level above the ground is located at 12.5 m, simulated temperature, humidity and wind speed were extrapolated to the 2-m and 10-m levels of the observations using Monin-Obukhov similarity profiles, accounting for stability effects. In the comparison, use was made of observations from two meteorological stations, Essen-Altenessen (51.49 °N, 7.01 °E) and Essen-Hirschlandplatz (51.46 °N, 7.01 °E) separated by a distance of around 3 kilometres only. The range of values from both stations at each hour is plotted in Figure 10.3-9 by vertical bars. While these do not correspond to instrumental error, they give an idea of the representativity error of the measured values compared to model output, i.e., their difference indicates the capacity of point (station) measurements to provide spatial average values at the scale of a model grid cell.

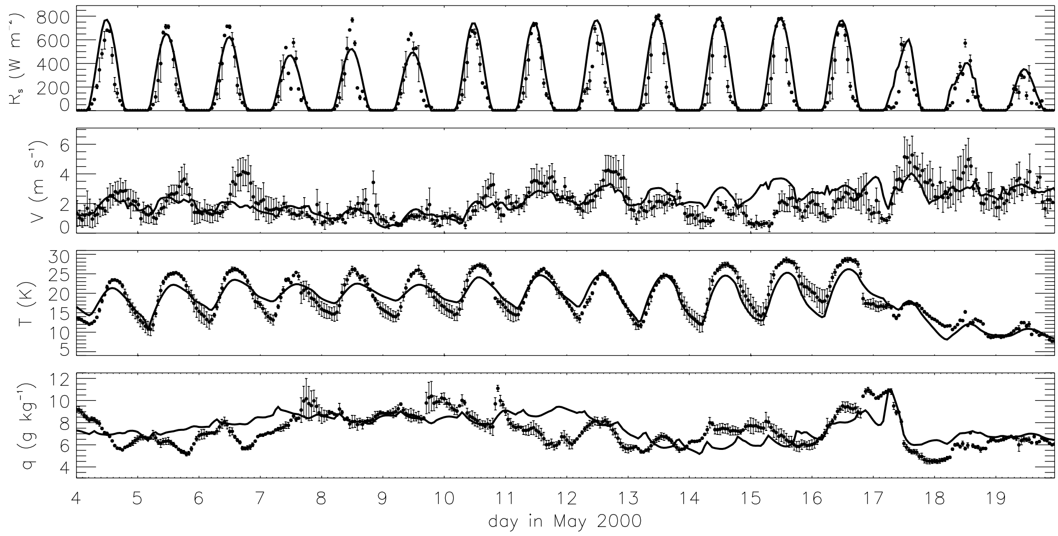


Figure 10.3-9. Simulated (solid line) versus observed (symbols) meteorological parameters. From top to bottom: down-welling shortwave radiation, 10-m wind speed, and 2-m temperature and specific humidity. Observations were taken from the Essen-Altenessen en Essen-Hirschlandplatz stations, separated by approximately 3 km. The differences between the observations from the two stations are shown as vertical bars, their mean value is shown as a solid circle.

Error statistics for the simulated meteorological variables are provided in Table 10.3-15, including values for the mean absolute gross error (*E*), bias (*B*), and correlation coefficient (*r*). The mean absolute gross error of simulated radiation is in the range 60-80 W m^{-2}, that of wind speed is less than 1 m s^{-1}, and values for temperature and specific humidity are around 2 K and 1 g kg^{-1}, respectively. Note that, in particular, the abrupt transition on the 17th of May – caused by a frontal passage – is well captured (Figure 10.3-9).

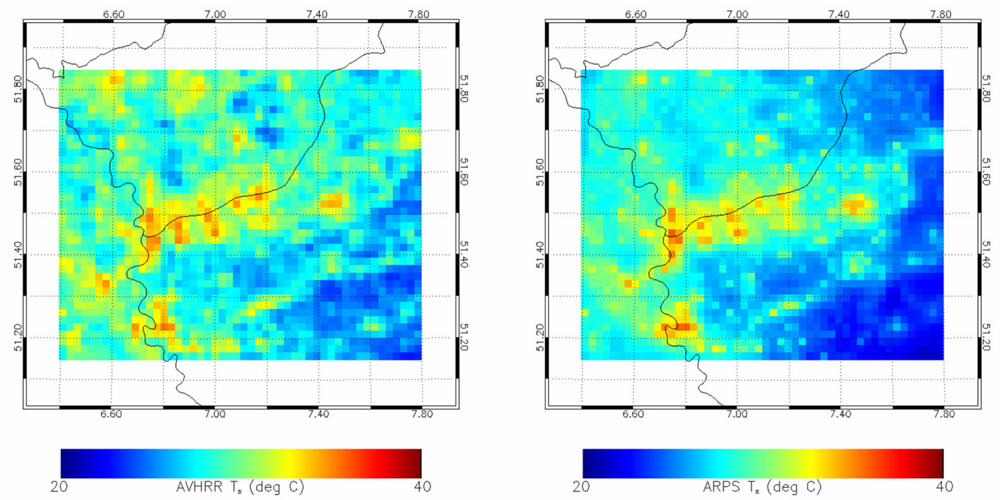


Figure 10.3-10. Simulated (right panel) and observed (left panel) surface temperature, for 14:40 GMT on 13 May 2000. The observed values were constructed from AVHRR instrument channels 4 and 5 (thermal infrared) onboard the NOAA-14 polar orbiting satellite platform.

In another validation exercise (

Figure 10.3-10), simulated surface temperature values were compared with measurements from the AVHRR instrument onboard the NOAA-14 polar orbiting satellite platform, for 13 May 2000 at approximately 14:40 GMT. Surface temperature was extracted from AVHRR channels 4 (10.3-11.3 µm) and 5 (11.5-12.5 µm), applying a correction for atmospheric and surface emissivity effects using the split-window technique by Ulivieri *et al.* (1994) together with NDVI-dependent spectral emissivity values. There is a very good agreement (absolute gross error of 1.21 K, bias of -0.78 K, correlation coefficient of 0.86) between the spatial patterns of simulated and observed values. When using another split-window method to correct the AVHRR imagery, the one by Kerr et al. (1992), the agreement was even better, with an absolute gross error of 1.15 K, a bias of -0.26 K, and again a correlation coefficient of 0.86. Comparing AVHRR observations processed with either the Ulivieri or the Kerr algorithm, the absolute gross difference amounted to 0.85 K, showing that the error on the simulated values is close to the uncertainty related to the satellite image processing. In any case, both the observations and the simulation clearly show the urbanized portions of the domain exhibiting high temperatures contrasting with the lower rural temperature values.

Table 10.3-15. Mean absolute gross error (*E*), bias (*B*), and correlation (*r*) between simulated an observed meteorological variables, and between the two sets of observations. The variables are downward solar radiation (R_s), 10-m wind speed (*V*), and 2-m temperature (*T*) and specific humidity (*q*). ARPS refers to the model result and Essen-Altenesen /Hirschlandplatz refer to the measurement stations.

	ARPS vs Essen-Altenessen			ARPS vs Essen-Hirschlandplatz			Essen-Altenessen vs -Hirschlandplatz		
	E	*B*	*r*	*E*	*B*	*r*	*E*	*B*	*r*
R_s (W m^{-2})	81	67	0.89	60	41	0.93	42	-25	0.94
V (m s^{-1})	0.83	0.71	0.54	0.90	-0.44	0.50	1.17	1.15	0.87
T (K)	2.2	0.58	0.89	2.1	-1.32	0.91	1.9	-1.91	0.96
q (g kg^{-1})	1.1	0.31	0.54	0.99	0.06	0.57	0.61	-0.25	0.89

Air quality simulated with AURORA was validated by comparing simulated ozone concentrations with hourly values obtained from two stations in the study area operated by LUA-NRW at Bottrop and Essen. Simulated ozone values compare fairly well with observations (Figure 10.3-11 and Table 10.3-16), the simulated concentrations having a positive bias and a mean absolute gross error of approximately 30-35 µg m^{-3}. This is relatively high, but comparable to results obtained in other model evaluation exercises (e.g., Monteiro *et al*., 2005; Mircea *et al*., 2008). With respect to the daily maxima, the mean absolute gross error is of comparable magnitude, but in a relative sense the error is smaller, in the range 21-27 %, and exhibiting correlation coefficients of approximately 0.9. It should be noted that the positive bias exhibited by the model is consistent with the negative bias of the NO_x emissions mentioned above, as low NO_x emissions induce less titration, hence higher ozone concentration values. In particular the difference of night time concentrations between the two locations, which is due to the titration effect (reduction of ozone by traffic-related NO emissions) caused by the more intense traffic at Bottrop, is well captured by the model, meaning that the spatial distribution of traffic densities as well as the chemical processes accounted for in the model perform correctly.

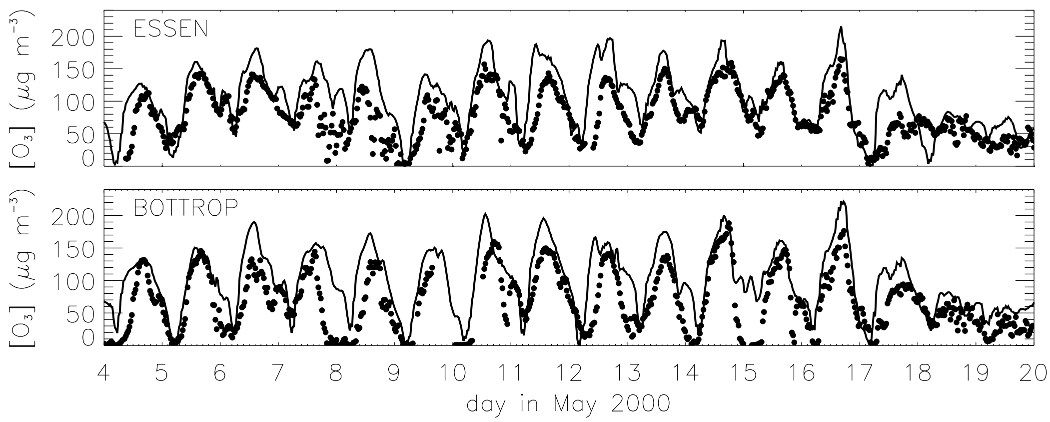


Figure 10.3-11. Simulated (solid line) as compared to observed (symbols) ground-level O_3 concentrations for the stations Essen (upper panel) and Bottrop (lower panel).

A validation for particulate matter (PM_{10}) was more difficult to achieve, given the absence of PM_{10} measurements in the area for the period studied. Even if such data had been available, a comparison with measured concentration values would not have been straightforward given that no lateral boundary values for particulate matter were available in these simulations. However, since the focus here was mainly on the urban-rural contrast, it was verified whether the model is capable of reproducing typical urban-rural PM_{10} concentration differences. This was done for April-September 2004, for which suitable measurements were available from the AirBase (http://air-climate.eionet.europa.eu/databases/airbase/) database of the European Environment Agency. The stations used were those of Mülheim, Krefeld, and Dortmund, for the 'urban-background' observations; and those of Westerwald, Rothaargebirge, and Soest, representing nearby 'rural-background' conditions.

Table 10.3-16. Mean absolute gross error (E), bias (B), and correlation (r) between values simulated with AURORA and observations, for hourly concentration values as well as daily maxima using data from the Essen and Bottrop stations.

	AURORA vs Essen			AURORA vs Bottrop		
	E	*B*	*r*	*E*	*B*	*r*
$[O_3]$ hourly ($\mu g\ m^{-3}$)	32.8	26.7	0.74	36.9	33.9	0.81
$[O_3]$ daymax ($\mu g\ m^{-3}$)	34.2	34.2	0.91	27.5	27.2	0.90

Time series of representative urban and rural PM_{10} concentrations were obtained by averaging over the three stations in the respective groups. As the purpose is to compare typical urban-rural differences over a time period of 20 days (i.e., the duration of the simulation), the time series were smoothed by applying a 20-day sliding averaging operator. In the resulting time series, the station- and time-average concentration for the urban background stations was 24.3 $\mu g\ m^{-3}$, for the rural background stations it was 14.8 $\mu g\ m^{-3}$, the average urban-rural difference being 9.5 $\mu g\ m^{-3}$. With a standard deviation on the measured time series of urban-rural particulate matter concentration differences of 1.5 $\mu g\ m^{-3}$, this difference was found to be relatively stable. The mean difference of 9.5 $\mu g\ m^{-3}$ is to be compared with simulated PM_{10} concentrations (not shown here), with values of the order of 10 $\mu g\ m^{-3}$ for the portions of the domain characterized by urban land cover types. Hence, it is fair to conclude that the model is fairly well capable of capturing the typical observed differences between urban and rural concentrations of particulate matter.

VALIDATION OF INDIVIDUAL COMPONENTS	
Uncertainty estimators (M_i and O_i are simulated and observed values, $\overline{M}$ and $\overline{O}$ their means)	
Mean absolute error	$\frac{1}{N}\sum_i \lvert M_i - O_i \rvert$
Root mean square error	$\sqrt{\frac{1}{N}\sum_i (M_i - O_i)^2}$
Bias	$\frac{1}{N}\sum_i (M_i - O_i)$
Normalized bias	$\frac{\sum_i (M_i - O_i)}{\sum_i O_i}$

Correlation coefficient	$\sum_i (M_i - \overline{M})(O_i - \overline{O}) \Big/ \sqrt{\sum_i (M_i - \overline{M})^2 (O_i - \overline{O})^2}$
Quality assessment	
Quality checks	○ comparison with accuracy requirements as in Figure 10.3-1 ○ percentage of simulated values that are within ± 20 % and ± 50 % of the observed values
MODELS /ALGORITHMS/ASSIMILATION	
MODIS SST	Used to specify sea surface temperature as a lower boundary condition, the accuracy of this data (order 1 K) is sufficient for its use in atmospheric modelling, i.e. the sensitivity of the atmospheric model to SST within the error range is relatively low
	Comparison with AVHRR data (Brown *et al.*, 1999)
SPOT-VEGETATION NDVI	Used as lower boundary condition, accuracy is of the order of 0.1-0.2 for the NDVI.
	Comparison with AVHRR, MODIS, ETM (Morisette *et al.* 2004)
FNL-ECMWF Meteorology	Used as lateral boundary conditions for the meteorology, our final results (i.e., the simulated urban/regional pollutant concentrations) are very sensitive to the correct specification of these.
	N/A
BelEUROS	Used as lateral boundary conditions for the chemistry, our final results (i.e., the simulated urban/regional pollutant concentrations) are quite sensitive to the correct specification of these.
	RMSE of simulated versus observed annual mean concentrations, using several measurement stations in Belgium, is of the order of 8 µg m^{-3} (NO_2), 6 µg m^{-3} (O_3), 12 µg m^{-3} (PM_{10}), see Deutsch *et al.* (2007a), also see Deutsch *et al.* (2007b).
EMISSIONS	Emission cadastres are generated using a bottom-up approach, the final outcome produced by the AURORA model is very sensitive to the correct specification of the spatial distribution of emissions.
	As mentioned above the E-MAP derived emission inventory has been compared with local emission data for the London area (1km and 5km resolution grids) and the Netherlands (municipality level). Details can be found in Maes *et al.*, (2008)
ARPS	Equations of atmospheric physics and dynamics. Whereas large-scale

	atmospheric features are dominated by the lateral boundary conditoons (from FNL, see above), ARPS regional simulations generate finer spatial detail, mainly as a consequence of more detailed terrain data sets (e.g., NDVI from SPOT-VEGETATION, CORINE Land cover, high-resolution digital elevation model, etc...).
	RMSE of surface fluxes (De Ridder, 2000) and meteorological quantities (Thunis *et al.*, 2003). The latter reference contains results of an intercomparison study for mesoscale meteorological models, the differences between the participating models providing an indication of typical model uncertainty.
AURORA	Equations of transport (advection-diffusion) and chemistry of the atmosphere.
	Simulated versus observed pollutant concentrations are available from De Ridder *et al.* (2008). In a study by De Ridder and Lefebre (2003), it was found that for the pollutant benzene, and using observations from an experimental campaign (http://www.fsm.it/padova/homepage.html), the correspondence between measured and simulated values improved significantly when comparing model (grid-level) results with aggregated point measurements from different stations.
AirBase ground-based data retrieval	Measured concentrations represent the area immediately surrounding the instrument doing the measurements. This is somewhat problematic of course when comparing with results that represent concentrations over grid volumes (see also remark in the lines above).
	No independent data available, assumed to be 'truth', but in general the accuracy of pollutant measurements is of the order of 10-20 % for gaseous pollutants and 30 % for particles (Van de Bossche *et al.*, 2007). More general information about QA/QC aspects of AirBase data is given in Larssen *et al.* (1999)

Table 10.3-17 Validation of the individual components for the Urban Local AQ Assessment Sub-service

10.3.3 Validation against specifications and against user requirements

10.3.3.1 Model based urban air quality indicators

* Requirements written in *Italics* were not compulsory for Phase 2

VALIDATION AGAINST SERVICE SPECIFICATIONS & USER REQUIREMENTS
Accuracy is most strikingly not compliant for SO_2, which is probably related to poor knowledge of the emissions of this pollutant. In phase 3 it will be investigated whether progress is possible for SO_2. However, confrontation of measurements from different networks (DCMR vs AirBase) also show large discrepancies, perhaps owing to the very local character of this pollutant, thus making a

comparison to simulated (grid-level) values difficult.			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Product	Average human exposure to atmospheric pollution, for SO_2, NO_2, O_3, PM_{10}		
Accuracy			
Uncertainty	~nx10%	Standards in Daughter Directives of the EU ambient and Air Quality framework directive (96/62/EC) hourly/daily mean SO2, NO2: 50-60 % annual mean SO2, NO2: 30 % annual mean PM: 50 % 8-hr mean O3: 50 %	daily mean SO2: 120-246 % annual mean SO2: 80-213 % daily mean NO2: 47-52 % annual mean NO2: 0.3-7 % annual mean PM10: 4-15 % 8-hr daymax O3: 16-50 %
Uncertainty minimum	n.s.	Standards in Daughter Directives of the EU ambient and Air Quality framework directive (96/62/EC)	id.
Uncertainty target	n.s.	n.s.	~ 10-20 % (gases) ~ 30 % (particles)
Spatiotemporal characteristics			
Spatial coverage	10 cities throughout Europe	Belgium, North France, South Holland, Ruhr Area	Phase 1 : domain including Brussels-Antwerp-Gent Phase 2 : Rotterdam, Prague
Horizontal resolution	1 Km	10x10 Km, *1x1 Km*	Phase 1 : 2 km Phase 2 : 70x70km²,

			1km resolution
Vertical resolution	n.s.	n.s.	0-20 m (near ground)
Grid/Projection	Cartesian on Lambert projection	Gridded for cadastre info	Cartesian / Lambert projection
Temporal coverage	12 months	Phase 1: 2 Pollution episodes (winter vs summer) Phase 2: 12 months	12 months
Temporal resolution	1 h	1 h	1 h
User Interfaces			
PROMOTE Web	n.s.	*Operational, complete and up to date*	to be updated after approval User
ftp	n.s.	n.s.	available
On demand	n.s.	n.s.	Phase 1 : handed over to User May 2007 Phase 2 : handed over to User June 2008
Data formats and data delivery			
Data availability	The availability will be synchronised with the availability of the AirBase data, i.e., every time the EEA releases another year of AirBase ground-level concentration data, the Service can calculate the urban air quality indicators within a few months.	Few months after agreement on scenario	Phase 1 : year 2004 completed Phase 2 : year 2005 completed
Data access	n.s.	*online*	ftp
Delivery Mode	Offline/Not NRT	Agreed with user	figures / ftp
Delivery frequency	n.s.	N x months (agreed with user)	once per domain

Data Format	HDF or any other gridded, TIFF or any other graphic, ASCII for indicators	HDF, geoTIFF, TXT, JPG, PNG, GIF	JPG
Historical archive	N/A	n.s.	N/A
REMARKS			
None			

* Requirements written in *Italics* were not compulsory for Phase 2

Table 10.3-18 Validation against specifications and against user requirements for the Urban and Regional AQ Assessment Sub-service

10.3.3.2 Scenario tool for regional air quality policy support

VALIDATION AGAINST SERVICE SPECIFICATIONS & USER REQUIREMENTS			
Accuracy is most strikingly not compliant for SO_2, which is probably related to poor knowledge of the emissions of this pollutant. In phase 3 it will be investigated whether progress is possible for SO_2. However, confrontation of measurements from different networks (DCMR vs AirBase) also show large discrepancies, perhaps owing to the very local character of this pollutant, thus making a comparison to simulated (grid-level) values difficult. For other pollutants, investigations are required with respect to the representativity of the in-situ data when compared to 3-km model grid output.			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Product	Concentration change patterns following user-defined emission scenario		
Uncertainty	~nx10%	Standards in Daughter Directives of the EU ambient and Air Quality framework directive (96/62/EC) hourly/daily mean SO2, NO2: 50-60 % annual mean SO2, NO2: 30 % annual mean PM: 50 % 8-hr mean O3: 50 %	daily mean SO2: 120-480 % annual mean SO2: 418 % daily mean NO2: 73 % annual mean NO2: 49 % annual mean PM10: 0.3 % 8-hr daymax O3: 16-69 %
Uncertainty minimum	n.s.	Standards in Daughter Directives of the EU ambient and Air Quality framework directive (96/62/EC)	id.
Uncertainty target	n.s.	n.s.	10-20 % on gases and 30 % on particulate matter
Spatial coverage	10 cities throughout Europe	Belgium, North France, South Holland, Ruhr Area	Flanders/South-Holland domain
Horizontal resolution	10 Km	10x10 Km	Phase 1 : 15 km

			Phase 2 : 3km
Vertical resolution	n.s.	n.s.	0-50 m (ground-level)
Grid/Projection	Lat-long in shifted pole coordinates	Gridded for emissions cadastre	Lat-long in shifted pole coordinates
Temporal coverage	12 months	2 Pollution episodes (winter vs summer) *12 months*	12 months
Temporal resolution	1 h	1 h	1 h
User Interfaces			
PROMOTE Web	n.s.	*Operational, complete and up to date*	to be updated once User has 'cleared' the product
ftp	n.s.	n.s.	yes
On demand	n.s.	n.s.	yes
Data formats and data delivery			
Data availability	n.s.	Few months after agreement on scenario	few months after specification scenario
Data access	n.s.	*online*	online once User agrees
Delivery Mode	Offline/Not NRT	Agreed with user	agreed with user
Delivery frequency	n.s.	Agreed with user	once for each scenario
Data Format	HDF or any other gridded, TIFF or any other graphic, ASCII for indicators	*e.g.* HDF, geoTIFF, TXT, JPG, PNG, GIF	JPG
Historical archive	N/A	n.s.	-
Visualization	N/A	To be agreed	-
None			

* Requirements written in *Italics* were not compulsory for Phase 2

Table 10.3-19 Validation against specifications and against user requirements for scenario tool for Regional Air Quality Policy support sub-service.

10.3.4 Quality assessment and control procedures: service quality

Service delivery start date: n.s.				
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**	**N checks/Delivery period °**
Quality checks	No/only validation	yes	only validation (RMSE, bias, correlation coefficient)	beginning June 2008
Product confidence data	n.s.	*95%*	N.A.	N.A
Error bar definition and representation	n.s.	*2σ*	N.A.	N.A.
Representation of missing data	Missing date replaced by -999	*-99.99 or similar <0 or interpolation; color (black or white, in maps)*	In case of process failure the missing data are indicated with '-999' in the output data, no further data processing takes place.	done automatically
Documentation of process failure	Process failure is indicatd by missing data indicators	n.s.	The process failure controlling is performed manually	daily

Version control mechanisms and representation	All code is integrated in a Subversion Server. This allows development in different trees so the operational part won't be affected by the further development. This provide us with a "History" of the project. All SVN repositories are backed-up every day in different physical locations to prevent loss.	*References to Quality Control procedures and product version number and last date of modification to be available in background*	All code is integrated in a Subversion server. This allows development in different trees so the operational part won't be affected by the further development. Also this could provide us with a 'history' of the project. All SVN repositories are backup-ed every day in different physical locations to prevent data loss.	N.A.

*Requirements written in *Italics* were not compulsory for Phase 2

°Between 1st March and 30th of Mayor delivery date (you can send this information separately if this document is delivered at an earlier date.

Table 10.3-20 Quality assessment and control procedures for the for the Urban and Regional AQ Assessment Sub-service

10.3.5 References

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10.4 Local air quality analysis for the province of Zeeland

10.4.1 Sub-Service Summary

Service description

This service consists of the production and delivery of air quality analysis reports for the Province of Zeeland, the Netherlands. The reports are based on a multi-year database of air quality information, computed with a chain of numerical models and several input databases. The reports contain high resolution charts with several statistics for each year, for several chemical constituents. Information on the quality of the data is included in the reports.

Service is/will be operational since/after: July 2008

Research partners: -

Provider(s): Validation contact: Hein Zelle <hein.zelle@bmtargoss.com>

10.4.2 Validation Plan and validation data

This validation plan applies to the air quality analysis reports based on a multi-year hindcast database of air quality information for the province of Zeeland, the Netherlands.

BMT ARGOSS has set up a modelling system to deliver air quality information for Zeeland at high resolution (1 km), both in forecast mode up to 48 hours ahead, as well as in hindcast mode for a 5 year period (to be expanded in phase 3 and after). Forecast products are typically delivered as charts valid for one time, while hindcast-based products include charts and tables with several statistic indicators.

For the validation of these products, BMT ARGOSS makes use of three main datasets: ground-based air quality observations from the Dutch national sensor network (obtained from RIVM via internet), ground-based weather observations (SYNOP) from the Dutch national measuring network (obtained through KNMI) and data from the OMI instrument on the AURA satellite (obtained through KNMI and directly from NASA). Whenever possible, applicable data (for the period and geographical region involved) is obtained and used for the validation. For ground-based observations, relevant model data is collected at the location and time of the observations. These data are then compared and presented as standard statistical measures (mean error, mean absolute error, standard deviation / root mean square error). Validation of weather data was performed on forecast data for a period of 5 months (Jan-May 2008). Validation of hindcast air quality data will be performed for the complete hindcast period, 2006 – 2008 as of June 2009. The weather data is not validated for the full hindcast period due to restricted availability of weather observation data.

As for satellite-based observations, the validation results can not be easily represented in terms of such measures, as there are significant physical differences between the satellite observation (total/tropospheric columns with reduced sensitivity at lower altitudes) and the output of the model (partial atmospheric column with uniform sensitivity at most altitudes). Satellite data will therefore mainly be used for side-by-side comparison of concentration charts and presentation of spatial difference charts. This comparison is performed for selected cases in 2006, 2007 and 2008.

Validation of the services against specifications and user requirements is be performed based on the properties specified in the service specification and the service level agreement with the Province of Zeeland. When applicable, extra user requirements by the Province or changes to specifications requested by the Province will be indicated.

VALIDATION DATA	
Ground based observations	
Name: Dutch national measuring network LML (Air Quality, RIVM) Phase 2	*Data availability and access (include access details if data is freely available):* freely available on the internet from RIVM, with an effective delay of 3-6 months. http:www.lml.rivm.nl/data_val/index.html *Spatial coverage and resolution*: 49 stations distributed over the Netherlands *Temporal coverage and resolution*: hourly, 2000 – 2007. PM10 information is only provided as daily average values. *Location(s) (coordinates)*: See specification at http://www.lml.rivm.nl/data/tabel/actueel.html, charts under the link “kaart van dit uur” show most stations. *Uncertainty quantification (e.g. Accuracy):* N/A
Name: Dutch national measuring network (Meteo, SYNOP, obtained from KNMI) Phase 2	*Data availability and access (include access details if data is freely available):* Obtained from KNMI in the framework of the PROMOTE project, data available via ftp. *Spatial coverage and resolution*: 62 stations distributed over the Netherlands *Temporal coverage and resolution*: 10 minute intervals, 2007-07-01 / present *Location(s) (coordinates)*: See specification at http://www.knmi.nl/kodac/over_kodac/catalogus/nl-obs-surf-stationslijst-06.08.2007.htm, a chart is available at http://www.knmi.nl/klimatologie/images_algemeen/stations.jpg *Uncertainty quantification (e.g. Accuracy):* N/A
EO Data	
Name: NO2 and O3 measurements from OMI instrument on AURA satellite Phase 2	*Data availability and access (include access details if data is freely available):* Freely available from the internet, http://www.knmi.nl/omi. Gridded OMI NO2 information has been obtained from KNMI for selected periods in 2006, 2007 and 2008. *Spatial coverage and resolution*: Global, resolution 13×24 km at nadir *Temporal coverage and resolution*: Daily observations, limited by clouds *Location(s) (coordinates)*: n.a. *Uncertainty quantification (e.g. Accuracy):* N/A

Table 1.4-21 Data used for the validation of all the products of this service/sub-service

10.4.2.1 Validation of individual components

The WRF model (meteorological data) is validated separately from the CHIMERE (chemistry) model. For both models, the model data is compared to ground station data. The error values (difference between model and observation) are computed, and several statistical uncertainty estimators are computed from these error values. The table below indicates which uncertainty estimators are used. It indicates average values for the estimators (based on a set of relevant stations for the whole database period).

More detailed error information (station-based analysis, analysis per year, etcetera) is made available in the validation report, which is part of the analysis report as delivered for this service. The report provides detailed error information (station-based analysis, analysis per year, etcetera).

The numbers made available in the tables below give a rather crude presentation of the overall quality of the air quality data from the CHIMERE model. We refer to the detailed validation information in the analysis report for a better impression of the overall model accuracy. Compared to phase 2 significant improvements in accuracy have been achieved, leading to much better average concentrations, peak concentrations and daily cycles. High peaks in specific episodes as witnessed in phase 2 no longer occur, with the exceptions of a short period in july/august 2006 which has been corrected.

The air quality analysis report contains a detailed analysis of the quality of each analysed variable, with an indication of the reliability based on observed error statistics, spatial patterns and time behaviour. This report is accessible as part of both the analysis service and the forecast service for Zeeland.

VALIDATION OF INDIVIDUAL COMPONENTS	
Uncertainty estimators	
Mean Absolute Error (MAE)	The Mean Absolute Error is computed by taking the time-average of the absolute error over a given period. The relevant equation is $$\mathrm{MAE} = \frac{1}{N}\sum \lvert X_i - O_i \rvert$$ With N the number of observations / model data points, Xi the model value and Oi the corresponding observation value.
Mean bias (MB)	$\mathrm{MB} = \frac{1}{N}(\sum X_i - \sum O_i)$
Concentration RMS Error (RMSE)	The Root Mean Square Error is a frequently used measure for the deviation between model values and observed values. It is defined as

	the square root of the mean square error. $$\text{RMSE} = \sqrt{\frac{1}{N}\sum (X_i - O_i)^2}$$ The RMSE weighs larger errors heavier than small errors, which means large RMSE values may point to strong deviations during peak values.
Quality assessment	
Comparison model output with ground-based observations	Model output is co-located with observation data, both in space and in time. This results in a time series of concentrations for each species and each observation station. For each of these stations, the statistics MAE, MB and RMSE can be computed following the above definitions. Apart from the colocated validation, a validation is also performed on a weekly basis, e.g. by "grouping together" all data for monday, tuesday, etc. This results in a clear comparison of the weekly and daily concentration cycles on a station-by-station basis, including a 10% and 90% uncertainty interval.
Models/algorithms/assimilation	
WRF Regional Atmosphere Model	The output of the WRF model (temperature, humidity, winds and other parameters) are used as initial input and boundary conditions for the CHIMERE atmosphere model. The model takes global final analysis data from the NCEP GDAS system, and produces a high resolution weather hindcast based on these data. Using a high resolution model combined with high resolution ground datasets (USGS) results in fine weather detail above strongly varying terrain such as the province of Zeeland. The validation results below are based on a comparison between KNMI ground station observations (SYNOP) and the WRF model. All ground stations in the Netherlands were used for this validation, for the period March – April 2008.
	The validated parameters for the WRF model are 10 m wind speed and 2 m temperature. Other parameters that have been validated but are not included here are precipitation, wind direction and relative humidity. The procedure used is as described above – data is collocated in time and space matching model data and observation data. Statistics indicators are then computed as defined above. 10 m wind speed: MAE, MB, RMSE 2 m temperature: MAE, MB, RMSE

AQ Boundary conditions	The CHIMERE model makes use of boundary conditions from the INCA and GOCART climatological databases, included with the model. For certain species (e.g. PM10) the model is sensitive to the quality of these boundary conditions. Due to time constraints large-scale boundary conditions from a PROMOTE project partner have not been incorporated in the system for phase 3.
	No validation parameters available.
CHIMERE – air quality hindcast	The CHIMERE model is run using WRF model output as weather input data. EMEP emission data are used as input emissions, and GOCART / INCA provide chemical boundary conditions. The validation results below are based on a comparison between RIVM ground-based observations (LML) and the CHIMERE model output. Only the observation stations in Zeeland were used for this comparison, for the full database period (currently 2006, 2007 and 2008, to be expanded with 2005, 2004 if computation time allows before the end of PROMOTE phase 3).
	The validation method is analogous to the validation of the weather data described above: model data and observations are collocated, then the statistical indicators are computed. The validation can also be performed for 3 stations in the Province of Zeeland, as well as 1 or 2 stations elsewhere in the Netherlands for selected cases. Parameters that are validated: O3: MAE, MB, RMSE NH3: MAE, MB, RMSE NO: MAE, MB, RMSE NO2: MAE, MB, RMSE SO2: MAE, MB, RMSE PM10: MAE, MB, RMSE Parameters that are not validated: PM2.5: No observations available from LML / RIVM
Consistency	
	N/A

Table 1.4-22 Data used for the validation of all the products of this service/sub-service

10.4.2.2 Validation against specifications and user requirements

VALIDATION AGAINST SPECS and USER REQS			
SPECIFICATION	**S5**	**REQUIRED** *	**ACTUAL**
Uncertainty	Limited by the quality of emission data, meteorological input fields and chemistry boundary conditions.	n.s.	**10 m wind speed**: RMSE = 1.6 m/s, MAE = 1.2 m/s, MB = 0.2 m/s **2 m temperature**: RMSE = 1.5 C, MAE = 1.2 C, MB = -0.4 C (strongly depending on forecast lead time, -0.05 C average) **NOTE: RMSE values were not available at the time of writing (15/06/2009) but will be presented in august 2009.** **O3:** MAE = 13 µg/m3, MB = 16 µg/m3 **PM10:** MAE = 6.5 µg/m3, MB = -9.5 µg/m3 **NH3:** MAE = 1.4 µg/m3, MB = -0.2 µg/m3 **NO:** MAE = 6.4 – 8.9 µg/m3, MB = 0.7 – 6.5 µg/m3 **NO2:** MAE = 6.4 – 8.9 µg/m3, MB = 0.7 – 6.7 µg/m3 **SO2:** MAE = 2.0 – 2.4 µg/m3, MB = 0.34 – 2.3 µg/m3
Uncertainty minimum	n.s.	n.s.	Varying per species and station, typically within 25%

Uncertainty target	n.s.	n.s.	N/A
Spatial coverage	Province of Zeeland (51.2°N – 51.8°N, 3.2°E – 4.4°E)	Province of Zeeland	As specified in S5
Temporal coverage	Initial delivery spans the period 2003 – 2007, to be expanded annually starting in phase 3 and continuing afterwards.	5 years	Currently 2006, 2007 and 2008. This will be expanded with 2005, 2004 if computation time allows before August 2009.
Spatial resolution	Approximately 1 x 1 km^2	1 x 1 km^2	As specified.
Temporal resolution		1 h	Air quality data: available every hour. Meteo data: available every 10 minutes, may be reduced to hourly if needed.
Grid/Projection	Regular lat / lon at approximately 1 km resolution	n.s.	The Netherlands: Lambert projection (conical) with 4 km resolution. Zeeland: as specified, regular lat/lon at approximately 1 km resolution.
User Interfaces			
PROMOTE Web Site	n.s.	Complete, operational and up to date	Complete, operational.
ftp	n.s.	n.s.	n/a
On demand	yes	n.s.	Yes, upon request.
Data formats and data delivery			
Data availability	Initial delivery expected in May 2008, updated annually afterward.	online	As specified. Final delivery phase 3 expected 08/2009
Data accessibility	All results of the analysis service are available offline. Delivery by WWW or on request.	online	As specified, validation will be made available online when final version is completed (expected 08/2009)

	Other data / statistics that are not included in the analysis reports are available offline on request. Validation reports are made available online.		
Delivery Mode	Offline	Offline	Offline
Delivery frequency	Initial delivery spans the period 2003 – 2007, to be expanded annually starting in phase 3 and continuing afterwards.	N/A	As specified, once per year
Data Format	PDF reports with concentration / statistics charts in PNG format, tables with statistics and explanatory text. Charts will also be made available separately, see “visualization standards”.	Html, reports, charts in ESRI- or MRSid format	As specified.
Historical archive	Selected model output is archived for the 5 year hindcast database. The archive is not delivered to the user directly, but is accessible on request and new products / statistics can be generated afterwards.	5 years	As specified.
Visualization	n.s.	charts	Charts in PNG format are included in a report in PDF format. In phase 3 the charts will also be made available directly in the user’s GIS system, this is currently an ongoing trial, depending on available time on user side.

REMARKS
Trial report delivered June 2009 Final report delivery August 2009. Reports are delivered annually, one for each phase. Reports may be split up by year to reduce report volume.

* Requirements written in italics were not compulsory for Phase 2.

Table 1.4-3 Validation of specifications and user requirements for this service

10.4.3 Quality assessment and control procedures: service quality

Service delivery start date: July 1, 2008

The service web site has been operational since April 2008, however the complete analysis report is only completed per July 1, 2008.

SPECIFICATION	S5	REQUIRED*	ACTUAL	N checks/Delivery period °
Quality checks	n.s.	yes	Yes, input data has been validated, trial charts have been visually inspected and checked by provider and user. Several checks on unit conversion process and validation computation have been performed. Final results are intensively validated before publication.	Several quality checks performed over the period February – June 2009

Product confidence data	n.s.	*95%*	10% and 90% confidence intervals made available as part of validation report	N/A
Error bar definition and representation	RMS error of concentration (model compared to observations)	*2σ*	See above, 10% and 90% intervals	N/A
Representation of missing data	Missing data is unlikely to occur in an off-line service, unless there is a lack of input data (boundary conditions). Missing data will be tracked in the failure log document which is made available to the user on a regular basis.	*-99.99 or similar <0 or interpolation; color (black or white, in maps)*	There is no missing data in the product, due to the hindcast nature of the database.	N/A

Documentation of process failure	Process failures can include technical problems during the database computation (storage full, network failure) or problems in boundary condition delivery (weather forcing data, chemistry boundary conditions). Such failures are tracked in a log document by the service provider. This document is made available on a regular basis to the user.	n.s.	As specified in S5 The initial similation for 2007 contained faulty emission data, and has therefore been re-done. Up-to-date results will be available in August 2009.	0 process failures Checked weekly during database production (approximately 10 checks) and once before final delivery.

Version control mechanisms and representation	A modelling system version is defined and tracked in a version control document. Relevant changes to the system are tracked in this document, together with an updated system version number. The reason for the change is documented with expected advantages and other possible side effects. The user is informed by email when changes are performed that may have a noticeable impact on the product. The change log is made available to the user on a regular basis.	*References to Quality Control procedures and product version number and last date of modification to be available in background*	Latest product version: 2.2, May 2009. 2006 data was generated with version 2.1 (not including point sources). 2007 and 2008 data is generated with version 2.2 (including point sources). All subsequent years will use this latest version.3 changes in phase 3, current version 2.2 (may 2009)

*Requirements written in *Italics* were not compulsory for Phase 2

°Between 1st March and 30th of Mayor delivery date (you can send this information separately if this document is delivered at an earlier date.

Table 1.4-4 Quality assessment and control procedures for this service/sub-service

10.4.4 References

10.4.4.1 Electronic references and online data access paths

CHIMERE model information: http://euler.lmd.polytechnique.fr/chimere/

WRF model information: http://wrf-model.org/index.php

Access to product summary page: http://promote.argoss.nl/promote/

Access to sample analysis report and final report with validation information will be made available through this same page.

Access to EMEP emission data information: http://www.emep.int/, http://webdab.emep.int/

Information about RIVM LML air quality observations: http://www.lml.rivm.nl/data/smog/index.html

Information about KNMI SYNOP observations: http://www.knmi.nl/kodac/over_kodac/catalogus/nl-obs-surf-10m-ext.htm

10.4.4.2 Bibliographic references

- Zelle, H. and Hartog, W.: Satellite-Enabled Air Quality Service (SERQ), Final Report, Techn. Rep., BMT ARGOSS, 2008.

10.5 Portuguese air quality records service

10.5.1 Sub-Service Summary

Aircast is an air quality service integrated in PROMOTE that aims to answer PM10 monitoring needs by integrating ground data (from national network and monitoring campaigns), remote sensing data, emission inventories and territorial characteristics using geostatistical and multi-regression methods, in an operational web based service platform to deliver optimized forecast daily maps and monitoring daily, monthly and annual maps of PM for Portugal. When operational it will be introduced in the current range of services made available by the Portuguese Environment Agency (Agência Portuguesa do Ambiente - APA), the main organisation responsible for the air quality management in Portugal.

In the current services available in QualAr, the current air quality monitoring information web service offered by APA, the products are still only point or zone average based. In Aircast. The key feature presented by this service is the possibility to spatialize observed or modelled concentrations where current products offered by APA only offer point or zone averaged values. These spatialized patterns will enable the estimative of population exposure to PM10 levels.

To achieve this objective the Aircast Air Quality Records Sub-service is separated in three levels of products.

Level 1 includes daily air quality indexes on PM10, O3, NO2, SO2 and CO and a global index, and monthly and annual parameters for PM10 for each station and zone average at national scale. This level also uses interpolation method Inverse Distance Weighted IDW to produce a national background surface in a 1km grid for daily air quality indexes on PM10, O3, NO2, and monthly and annual parameters for PM10.

Level 2 uses geostatistics and multi-regression models to relate air quality data series with data on territorial characteristics (altimetry, climatic, land use, population, location of pollution sources and building density), and emissions inventory to provide spatial patterns of the PM concentrations distribution. The application of this methodology will generate daily (daily average), monthly (monthly average) and annual (annual average and 36º daily maximum) PM10 gridded maps at national (1x1 km) and urban scale (100x100 m) for the Lisbon Metropolitan Area. This Level 2 product is optimized by introducing as air quality ground data the satellite based PM data into the built up of the multi-regression models.

Level 3 is a satellite based PM product for urban/regional areas based on linear regression models determined by the correlation of Aerosol Optical Thickness (AOT), an aerosol parameter retrieved from satellite images, PM10 ground stations measurements and auxiliary meteorological information on boundary layer height and relative humidity. Those linear models will be used to create daily PM10 3x3 km gridded maps for the Lisbon Metropolitan Area. These maps will improve the assessment of the spatial structure of PM pollution and interactions on dispersion patterns at several scales the by increasing substantially the spatial coverage of current air quality monitoring data.

Service is/will be operational since/after:

Phase 2 Level 1 Product – June 2008

Phase 3 Level 2 Product – June 2009

Phase 3 Level 3 Product – June 2009

Research partners:

IMAR / YDREAMS

Provider(s): Validation contact:

Nuno Grosso ncsg@fct.unl.pt

10.5.2 Validation plan and validation data

Products scheduled to be delivered on Phase 3 of PROMOTE are validated using ground based data from the Portuguese Air Quality Stations Network. For the national or Lisbon metropolitan area background products only background stations are used. For the Lisbon metropolitan area high resolution products all stations located in the area are used. Since the Level 1 **- IDW Interpolation** and Level 2-**Geostatistical and multi-regression** products are based on interpolation methods their validation is based on cross-validation procedures. The cross-validation consists on modelling the data without one point at a time and comparing the model result for this point to the measured data. This procedure is repeated for all the points and the measured and predicted values are compared.

For Level 3 -**Satellite based product** the validation of the PM_{10} AOT based estimation is performed using all the stations located in the Lisbon metropolitan area. The AOT values were previously validated using 2005 AERONET photometer data from five sites (discriminated in the table bellow).

VALIDATION DATA	
Ground based observations	
Name Portuguese Environmental Agency	*Data availability and access (include access details if data is freely available):* Data compiled by regional authorities and freely available trough the web

<table>
<tr><td>/National Air Quality Stations Network

Phase: 3</td><td>portal www.qualar.org

Spatial coverage and resolution:

Coverage - entire Portuguese Territory with especial emphasis for largest agglomerations and industrial complexes

Resolution - n.a

Temporal coverage and resolution:

Hourly Air quality measurements of PM_{10}, O_3, NO_2, SO_2 and CO starting in 1995 until now

Location(s) (coordinates):

68 Air quality Stations covering the entire Portuguese territory (coordinates in UTM)

<table>
<tr><th>Name</th><th>X (meters)</th><th>Y (meters)</th></tr>
<tr><td>Circular Sul</td><td>549540.27</td><td>4599985.75</td></tr>
<tr><td>Horto</td><td>545581.99</td><td>4601838.33</td></tr>
<tr><td>Lamas de Olo</td><td>601359.31</td><td>4580651.37</td></tr>
<tr><td>Senhora do Minho</td><td>517875.61</td><td>4619797.33</td></tr>
<tr><td>Sto Tirso</td><td>543923.90</td><td>4577189.17</td></tr>
<tr><td>Guimaraes-Centro</td><td>559040.63</td><td>4589584.57</td></tr>
<tr><td>Calendario</td><td>538958.43</td><td>4582600.53</td></tr>
<tr><td>Paredes-Centro</td><td>555501.31</td><td>4562058.01</td></tr>
<tr><td>Centro de Lacticinios</td><td>552262.39</td><td>4569362.25</td></tr>
<tr><td>Vila do Conde</td><td>522147.22</td><td>4577152.14</td></tr>
<tr><td>Vermoim</td><td>531198.95</td><td>4564740.35</td></tr>
<tr><td>Espinho</td><td>530136.31</td><td>4539563.08</td></tr>
<tr><td>Vila Nova da Telha</td><td>529383.16</td><td>4566588.52</td></tr>
<tr><td>Perafita</td><td>524251.95</td><td>4564601.00</td></tr>
<tr><td>Baguim</td><td>537901.30</td><td>4559855.06</td></tr>
<tr><td>Leca do Balio</td><td>531075.17</td><td>4563321.64</td></tr>
<tr><td>Custoias</td><td>529634.94</td><td>4562096.71</td></tr>
<tr><td>Boavista</td><td>529726.82</td><td>4556393.75</td></tr>
<tr><td>Senhora da Hora</td><td>530041.28</td><td>4559542.72</td></tr>
<tr><td>Matosinhos</td><td>526884.53</td><td>4559436.25</td></tr>
<tr><td>Antas</td><td>534443.11</td><td>4557093.54</td></tr>
<tr><td>Ermesinde</td><td>537749.88</td><td>4563007.42</td></tr>
<tr><td>Águas Santas</td><td>535837.39</td><td>4562023.67</td></tr>
<tr><td>Aveiro</td><td>529760.12</td><td>4498550.28</td></tr>
<tr><td>Ilhavo</td><td>527753.42</td><td>4493400.30</td></tr>
<tr><td>Fundão (Salgueiro)</td><td>644665.29</td><td>4454692.99</td></tr>
<tr><td>Fornelo do Monte</td><td>575827.23</td><td>4499512.60</td></tr>
<tr><td>Ervedeira (Leiria</td><td>509146.80</td><td>4419393.57</td></tr>
<tr><td>Av. Fernão Magalhães</td><td>548000.53</td><td>4451833.22</td></tr>
<tr><td>Instituto Geofísica</td><td>550024.09</td><td>4451063.48</td></tr>
<tr><td>Avanca</td><td>535326.87</td><td>4517156.12</td></tr>
<tr><td>Teixugueira</td><td>535968.11</td><td>4512022.67</td></tr>
<tr><td>Liberdade</td><td>487222.21</td><td>4285715.26</td></tr>
<tr><td>Restelo</td><td>481776.49</td><td>4284158.35</td></tr>
<tr><td>Beato</td><td>490126.89</td><td>4287191.13</td></tr>
</table>
</td></tr>
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<table>
<tr><td></td><td>
<table>
<tr><td>Entrecampos</td><td>486966.85</td><td>4288822.41</td></tr>
<tr><td>Reboleira</td><td>479929.66</td><td>4289503.32</td></tr>
<tr><td>Alfragide</td><td>481967.66</td><td>4287821.45</td></tr>
<tr><td>Casal Ribeiro</td><td>487571.42</td><td>4287046.96</td></tr>
<tr><td>Loures</td><td>485679.07</td><td>4297813.06</td></tr>
<tr><td>Mercado</td><td>463307.25</td><td>4283650.52</td></tr>
<tr><td>Marques</td><td>471883.70</td><td>4283262.00</td></tr>
<tr><td>Chelas</td><td>490269.12</td><td>4289373.49</td></tr>
<tr><td>Benfica</td><td>482274.77</td><td>4289164.73</td></tr>
<tr><td>Olivais</td><td>490619.12</td><td>4291148.02</td></tr>
<tr><td>Mem-Martins</td><td>469862.54</td><td>4292975.09</td></tr>
<tr><td>Paio Pires</td><td>492933.26</td><td>4274562.39</td></tr>
<tr><td>Lavradio</td><td>495772.49</td><td>4280003.85</td></tr>
<tr><td>escavadeira</td><td>494346.16</td><td>4279049.77</td></tr>
<tr><td>Laranjeiro</td><td>486273.92</td><td>4279460.14</td></tr>
<tr><td>Alto Seixalinho</td><td>494512.39</td><td>4277539.01</td></tr>
<tr><td>Fernando Pó</td><td>526932.28</td><td>4276380.46</td></tr>
<tr><td>Arcos</td><td>509297.10</td><td>4264627.35</td></tr>
<tr><td>Quebedo</td><td>509902.78</td><td>4264104.29</td></tr>
<tr><td>Camarinha</td><td>511136.85</td><td>4264784.66</td></tr>
<tr><td>Chamusca</td><td>545882.64</td><td>4356209.93</td></tr>
<tr><td>Terena</td><td>639510.50</td><td>4275462.34</td></tr>
<tr><td>Santiago do Cacém</td><td>526552.13</td><td>4208077.07</td></tr>
<tr><td>Monte Velho</td><td>517663.83</td><td>4214371.55</td></tr>
<tr><td>Monte Chãos</td><td>514228.46</td><td>4200742.02</td></tr>
<tr><td>Sonega</td><td>524285.04</td><td>4191550.36</td></tr>
<tr><td>Malpique</td><td>566550.86</td><td>4105168.56</td></tr>
<tr><td>Município</td><td>567880.31</td><td>4105402.64</td></tr>
<tr><td>Cerro</td><td>616967.07</td><td>4130206.96</td></tr>
<tr><td>Afonso II</td><td>594357.87</td><td>4097946.61</td></tr>
<tr><td>Joaq. Magalhães</td><td>595376.71</td><td>4096948.16</td></tr>
<tr><td>Pontal</td><td>541205.71</td><td>4109070.48</td></tr>
<tr><td>David Neto</td><td>540524.97</td><td>4110161.86</td></tr>
</table>

Uncertainty quantification (e.g. Accuracy): N/A
</td></tr>
<tr><td>Name

AERONET photometer network

Phase: 3</td><td>
Data availability and access (include access details if data is freely available):

Data freely available trough the web portal http://aeronet.gsfc.nasa.gov/. Level 2.0 (cloud-screened and quality-assured)

Spatial coverage and resolution:

Worlwide (more information available trough the web portal named above)

Resolution - n.a

Temporal coverage and resolution:

Temporal coverage and resolution varies with station but only 2005 measurements were used (the measurements chosen for the validation process were the nearest to the time of passage of the satellite to a maximum time interval of 30 minutes)
</td></tr>
</table>

Location(s) (coordinates):

5 Aeronet site (coordinates in decimal degrees)

Name	Longitude (decimal degrees)	Latitude (decimal degrees)
Cabo da Roca	-9.50	38.78
Barcelona	2.17	41.39
Lille	3.14	50.61
Modena	10.94	44.63
Paris	2.33	48.87

Uncertainty quantification (e.g. Accuracy):

0.01 - 0.02 overall uncertainty in AOD (wavelength dependent) due to calibration uncertainty for the field instruments

Table 10.5-1 Data used for the validation of all the products of this service/sub-service

10.5.3 Validation of individual components

The error values from cross-validation and validation data are obtained from the difference between modelled values and measured values and several error statistics are calculated. These calculations are preformed, and made available on-line, for every day and for every product.

According to the Annex I relating data quality objectives, from the Directive 2008/50 CE of the European Parliament and Council of 21 May 2008, on ambient air quality and cleaner air for Europe, “the uncertainty for modelling is defined as the maximum deviation of the measured and calculated concentration levels for 90 % of individual monitoring points, over the period considered, by the limit value (or target value in the case of ozone), without taking into account the timing of the events. The uncertainty for modelling shall be interpreted as being applicable in the region of the appropriate limit value (or target value in the case of ozone). The fixed measurements that have to be selected for comparison with modelling results shall be representative of the scale covered by the model.”

The following table resumes modelling uncertainty data quality objectives for ambient air quality assessment for the pollutants PM_{10}, NO_2, and O_3.

Modelling uncertainty			
	NO_2	PM_{10}	O_3
Hourly	50%		50%
Eight-hour averages			50%
Daily average		Not yet defined	
Annual Average	30%	50%	

For all the aircast produts the uncertainty objective will be 50%. All maps produced with higher uncertainties will be considered invalid and will not be made available on the website.

Most of the individual components present in table 1.5.3

VALIDATION OF INDIVIDUAL COMPONENTS FOR STRATOSPHERIC GASES	
Uncertainty estimators Calculated from cross-validation results for level 1 and 2 and from simple validation results for level 3	
Error average	$\frac{1}{N}\sum_i M_i - O_i$ With N the number of observations and modeled values, Mi the model value and Oi the corresponding observation value. This notation is valid for all other calculated parameters specified bellow.
Absolute error average	$\frac{1}{N}\sum_i \lvert M_i - O_i \rvert$

Root mean square error (RMSE)	$\sqrt{\frac{1}{N}\sum_i (M_i - O_i)^2}$
Normalized Absolute error average	$\frac{\frac{1}{N}\sum_i \lvert M_i - O_i \rvert}{\sum_i O_i}$
Normalized RMSE	$\frac{\sqrt{\frac{1}{N}\sum_i (M_i - O_i)^2}}{\sum_i O_i}$
Quality assessment	
Comparison between the produced maps and the stations real value	In the comparison of the products results with the monitoring stations results only the relevant types of stations for each product are considered. The produced maps must have less then 50% of overall uncertainty. Product quality verification is done online and only the maps that comply with those thresholds are visualized on the website. A Failure rate is calculated for each year and each product. The stations real values are shown overlaid with the produced maps. Also error maps resulting from validation and cross-validation with point error in the stations location are presented.
Models/algorithms/assimilation	
IDW interpolation algorithm	The IDW interpolation algorithm is only applied to national scale and using background stations. The small number of stations in the interior and specially south of the country is limitative to use this method. The production of IDW interpolation PM_{10} annual maps only considers stations with measurement efficiency over 85%. So for these products the number of available stations can be even smaller.
	All the error statistics presented above are calculated from IDW interpolation cross-validation results. The preferred error statistic to evaluate the products is the NRMSE.
Geostatistical and Multiregression models	Several patterns representative of different meteorological conditions are produced by spatial modelling using a combination of geostatistical and multi-regression methods. The influence of nearby influence factors (such as population density, topography, land use, type of road, traffic volumes or emissions), is incorporated in these models at several distances by using GIS techniques, such as spatial buffering and data

	extraction for the monitoring locations. Since we need to have a number of representative patterns (one for campaign or average of campaigns) to adjust to the daily, monthly and annual data, the small number of developed measuring campaigns, with different meteorological conditions, is a limitation of the method.
	All the error statistics presented above are calculated geostatistical/multiregression patterns cross-validation results.
Linear regression assimilation	The daily, yearly and annual PM10 parameters are assimilated by the best fitted pattern using linear regression. Atypical days, for instance with concentrations in background stations higher than in traffic stations or concentrations in rural stations higher than in urban stations, can have negative slopes. These days are considered invalid. The small efficiency of some of the stations in the national network influences negatively the adjustments of patterns specially to daily parameters. As for IDW interpolation the production of regression PM_{10} annual maps only consider stations with measurement efficiency over 85%. Since outlier's stations can be detected in the level 2 data assimilation using linear regression (>2SD). The excluded stations are not shown in the concentration and error maps.
	All the error statistics presented above are calculated linear regression cross-validation results.
Contrast reduction based MODIS AOT Algorithm	MODIS AOT retrieval is based on the Level 1B 250 m calibrated radiance product. Pre-processing of this product includes subsetting to area of interest (Lisbon Metropolitan Area), reflectance values calculation and cloud masking using the cloud mask product (MOD35_L2) (only non cloudy pixels are considered). AOT will only be retrieved if at least 50% of the 250 m resolution good quality pixels (according to flags) inside a 3x3 km window are present.
	RMSE ~ 0.07 Validation done against 2005 AERONET data from five stations (name and location coordinates in table 1.5.1)
	N/A

Linear AOT/PM10 Regression Model	Linear regression model calibrated and validated using 2005 ground measurements stations daily PM_{10} data. Only days with a relative humidity lower than 60% are considered for PM_{10} satellite based estimation Online product quality verification excludes Level 3 map products with an overall NRMSE greater than 50%
	Expected RMSE ~ 20 µg/m3

Table 10.5-2 Summary of the validation of individual components this service/sub-service

10.5.4 Validation of specifications and user requirements

10.5.4.1 Level 1 – Point, zone average and IDW Interpolation (1 km grid for national background concentrations)

VALIDATION AGAINST SPECIFICATIONS and USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Uncertainty	<50%	<50%	The cross-validation of the national background interpolation maps (2008) have the following ranges of NRMSE and failure rates: PM10 daily average NRMSE: 39% Failure rate: 15% PM10 monthly average NRMSE: 29% Failure rate: 0% PM10 annual average NRMSE: 31% Failure rate: just 2008 PM10 36º daily maximum NRMSE: 32% Failure rate: just 2008 NO2 daily hourly maximum

			NRMSE: 63% Failure rate: 94% O3 daily hourly maximum NRMSE: 20% Failure rate: 0%
Uncertainty minimum	n.s.	n.s.	N/A
Uncertainty target	<50%	<50%	<50%
Spatial coverage	Portugal	Portugal	Portugal
Temporal coverage	Point and zone average 1995-2009 IDW 2002-2009	Point and zone average 1995-2009 IDW 2002-2009	Point and zone average 1995-2009 IDW 2002-2009
Spatial resolution	National: 1 km	National: 1 km	National: 1 km
Temporal resolution	24h, 30 days, 12 months (the last two only for PM10)	24h, 30 days, 12 months (the last two only for PM10)	24h, 30 days and 12 months (the last two only for PM10)
Grid/Projection	Latitude-longitude grid, various projections possible	Latitude-longitude grid, various projections possible	Latitude-longitude grid, various projections possible
User Interfaces			
PROMOTE Web Site	n.s.	Complete, operational and up to date	Complete, operational and up to date
ftp	n.s.	n.s.	FTP not available. Products available for download trough website
On demand	n.s.	n.s.	n.s.
Data formats and data delivery			
Data availability	Operational	Operational	Operational
Data accessibility	Online NRT	Online NRT	Online NRT
Delivery Mode	n.s.	Download	Download trough website
Delivery frequency	n.s.	Daily	Daily

Data Format	png	png	png
Historical archive	2002-2009	2002-2009	2002-2009
Visualization	Through Web Mapping Services	Through Web Mapping Services	Website using Web Mapping Services
REMARKS			
The compliance with user specifications will be evaluated in periodic meetings with the Portuguese Environmental Agency and before delivery of each level of product by organising a workshop in which representatives of the user can also test the capabilities of the developed web interface			

Table 10.5-3 Level 1 - Validation of specifications and user requirements.

10.5.4.2 Level 2 – Geostatistical and multi-regression based PM_{10} maps

VALIDATION AGAINST SPECIFICATIONS and USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Uncertainty	<50%	<50%	The cross-validation of the adjustment using linear regression of the actual patterns for PM10 have NRMSE: **For the Lisbon metropolitan scale (100m)** PM10 daily average NRMSE: 29% Failure rate: 4% PM10 monthly average NRMSE: 29% Failure rate: 0% PM10 annual average NRMSE: 25% Failure rate: just 2008 PM10 36º daily maximum NRMSE: 23% Failure rate: just 2008 **For the national scale (1km)** PM10 daily average NRMSE: 31% Failure rate: 2% PM10 monthly average NRMSE: 23% Failure rate: 0% PM10 annual average NRMSE: 22% Failure rate: just 2008 PM10 36º daily

			maximum NRMSE: 22% Failure rate: just 2008
Uncertainty minimum	n.s.	n.s.	N/A
Uncertainty target	<50%	<50%	<50%
Spatial coverage	Portugal	Portugal	Portugal
Temporal coverage	2002-2009	2002-2009	2002-2009
Spatial resolution	National:1 km Lisbon metropolitan area: 100 m	National:1 km Lisbon metropolitan area: 100 m	National:1 km Lisbon metropolitan area: 100 m
Temporal resolution	24h, 30 days, 12 months (the last two only for PM10)	24h, 30 days, 12 months (the last two only for PM10)	24h, 30 days and 12 months (the last two only for PM10)
Grid/Projection	Latitude-longitude grid, various projections possible	Latitude-longitude grid, various projections possible	Latitude-longitude grid, various projections possible
User Interfaces			
PROMOTE Web Site	n.s.	Complete, operational and up to date	Complete, operational and up to date
ftp	n.s.	n.s.	FTP not available. Products available for download trough website
On demand			
Data formats and data delivery			
Data availability	Complete, operational and up to date	Complete, operational and up to date	Complete, operational and up to date
Data accessibility	Online NRT	Online NRT	Online NRT
Delivery Mode	n.s.	Download	Download trough website
Delivery frequency	Daily	Daily	Daily

Data Format	png	png	png
Historical archive	2002-2009	2002-2009	2002-2009
Visualization	Through Web Mapping Services	Through Web Mapping Services	Website using Web Mapping Services
REMARKS			
The compliance with user specifications will be evaluated in periodic meetings with the Portuguese Environmental Agency and before delivery of each level of product by organising a workshop in which representatives of the user can also test the capabilities of the developed web interface			

Table 10.5-4 Level 2 - Validation of specifications and user requirements.

10.5.4.3 Level 3 – Satellite based PM10 product for the Lisbon Metropolitan Area

VALIDATION AGAINST SPECIFICATIONS and USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Uncertainty	<50%	<50%	TBD
Uncertainty minimum	<50%	<50%	TBD
Uncertainty target	<50%	<50%	TBD
Spatial coverage	Monitoring: Lisbon	Monitoring: Lisbon	Monitoring: Lisbon
Temporal coverage	2008-2009	2008-2009	2008-2009
Spatial resolution	3x3 km grid	3x3 km grid	3x3 km grid
Temporal resolution	daily	daily	Daily
Grid/Projection	Latitude-longitude grid, various projections possible	Latitude-longitude grid, various projections possible	Latitude-longitude grid, various projections possible
User Interfaces			
PROMOTE Web Site	n.s.	Complete, operational and up to date	Almost operational and will be up to date mid July (one month delay)
ftp	n.s.	n.s.	FTP not available. Products available for download trough website (PNG version)
On demand			
Data formats and data delivery			
Data availability	Operational implementation by June 2009	Operational implementation by June 2009	Operational implementation by July 2009 (one month delay)
Data accessibility	Online	Online	Online not yet

			implemented
Delivery Mode	Download	Download	Not yet implemented
Delivery frequency	Daily	Daily	Not yet implemented
Data Format	GIF	PNG	PNG
Historical archive	Daily maps from 2008-2009	Daily maps from 2008-2009	Not yet processed
Visualization	Through Web Mapping Services	Through Web Mapping Services	Website using Web Mapping Services
REMARKS			
The compliance with user specifications will be evaluated in periodic meetings with the Portuguese Environmental Agency and before delivery of each level of product by organising a workshop in which representatives of the user can also test the capabilities of the developed web interface			

Table 10.5-5 Level 3 - Validation of specifications and user requirements.

10.5.5 Quality assessment and control procedures: service quality

Quality assessment and control procedures are applied in the several steps towards the generation of the defined products for all levels (Level 1, Level 2, and Level 3).

The raw pollutant concentration data used to calculate the air quality data of Level 1 and Level 2 products undergoes validation and quality assurance/quality control procedures implemented by the Portuguese Environmental Agency and the regional authorities (those procedures are therefore outside the scope of Aircast). The incorporation of this validation results into the Aircast products are guaranteed by the frequency of data reprocessing:

- Hourly reprocessing of current and previous day products starting at 15h;
- Daily reprocessing of d-2 to d-5 products once a day;
- Weekly reprocessing of current and previous year products.

The quality assessment of the mapping products produced within Aircast results from their comparison with the monitoring stations measurements. For each product only the relevant types of stations are considered.

To compare modelled and observed values, several error statistics are calculated including error average, root mean square error (RMSE) and normalised root mean square error (NRMSE). Product quality verification is done online and only the maps that comply with the 50% or lower NRMSE threshold are visualized on the website. A Failure rate is calculated for each year and each product. Also error maps resulting from validation and cross-validation with point error in the stations location are presented.

The annual quality checks will be done and all the information in this document will be presented in an annual report to be delivered to the user (Portuguese Environmental Agency) and will be available in the project website.

Service delivery start date: 16 June 2009				
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**	**N checks/Delivery period °**

Quality checks	Quality checks of all the products are done online upon processing and reprocessing Annual Service report to user including all error and failure rate statistics per product	Quality checks of the all product results done upon processing and reprocessing using error statistics Annual Service report to user including all error and failure rate statistics per product	Quality checks of the all product results done upon processing and reprocessing using error statistics Annual Service report to user including all error and failure rate statistics per product	Hourly reprocessing of current and previous day products starting at 15h; Daily reprocessing of d-2 to d-5 products once a day; Weekly reprocessing of current and previous year products
Product confidence data	n.s.	*95%*	*95%*	N/A
Error bar definition and representation	n.s	n.s	n.s	N/A
Representation of missing data	Missing data warnings will be posted in the Web Portal and a report staring the reasons sent to the user within one week	*Missing data corresponds to value -1 and is identified in the map by the color grey* *Invalid map products (NRMSE>50%) are identified by the color blue*	*Missing data corresponds to value -1 and is identified in the map by the color grey* *Invalid map (NRMSE>50%) products are identified by the color blue*	Verification of missing or invalid data for all levels of products is done online each time the product is processed or reprocessed. The frequency of checks is therefore dependent on the processing and reprocessing frequency.
Documentation of process failure	Process failure report sent to the user within one week	Process failure report sent to the user within one week	Process failure report sent to the user within one week	Process failure report sent to the user within one week

Version control mechanisms and representation	Whenever a new version is available reprocessing and archiving of the new collection will made on the previous version and a set of improvement indicators will be sent to the user within a month	Whenever a new version is available reprocessing and archiving of the new collection will made on the previous version and a set of improvement indicators will be sent to the user within a month	Whenever a new version is available reprocessing and archiving of the new collection will made on the previous version and a set of improvement indicators will be sent to the user within a month.	Whenever a new version is available reprocessing and archiving of the new collection will made on the previous version and a set of improvement indicators will be sent to the user within a month

*Requirements written in *Italics* were not compulsory for Phase 2

°Between 1st March and 30th of Mayor delivery date (you can send this information separately if this document is delivered at an earlier date.

Table 10.5-6 Quality assessment and control procedures this service/sub-service

10.5.6 References

10.5.6.1 Electronic references and online data access paths

http://www.qualar.org/ (original service version)

http://development.ydreams.com:81/Aircast (new service version - temporary link)

10.5.6.2 Bibliographic references

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