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C6 Validation Report
URBAN AND REGIONAL AIR QUALITY ASSESSMENT SERVICE
Version 2

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1.5	03/07/2008	Document edited and ready for final review

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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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1 URBAN/REGIONAL AIR QUALITY ASSESSMENT

1.1 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

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1.2 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 the typical range	European guidelines and concentration scales used at IRCEL (User), see http://www.irceline.be/~celinair/english/homeen_nojava.html

(Method, criteria)	
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 (Method, criteria)	European guidelines and concentration scales used at IRCEL (User), see http://www.irceline.be/~celinair/english/homeen_nojava.html 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 1.2-1 Characterization of the products provided by the Urban Regional AQ assessment sub-service

1.3 Urban air quality indicators and scenario tools

1.3.1 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 1.3-1, 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 1.3-1. 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 1.3-1 Data used for the validation of the Urban Regional AQ assessment

1.3.2 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 1.3-2.

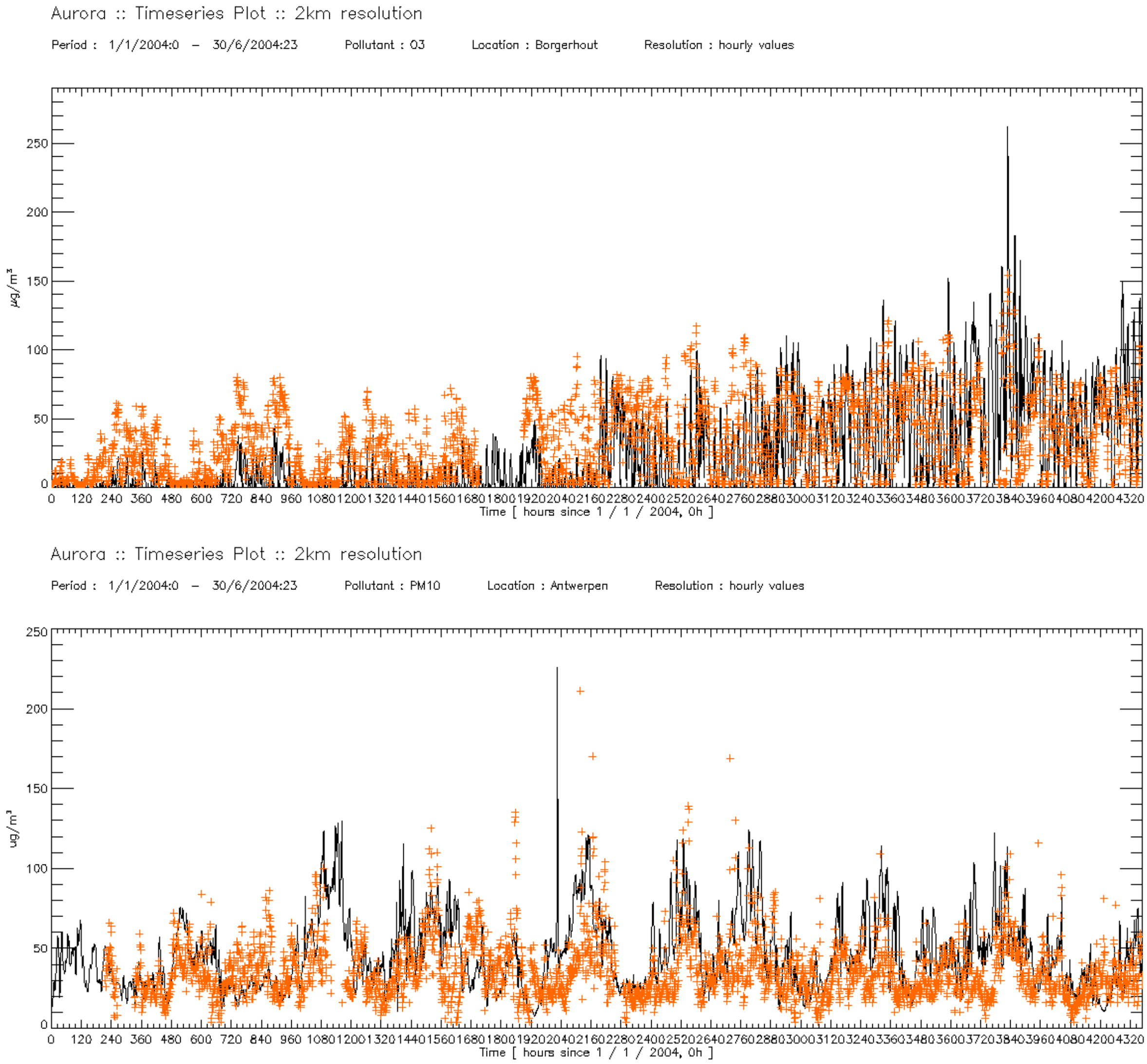


Figure 1.3-2. Comparison between simulated (line) and observed (symbols) concentrations of ozone (upper panel) and PM_{10} (lower panel) for the station "Borgerhout" (near Antwerp), January – June 2004.

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.**

1.3.2.1 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).

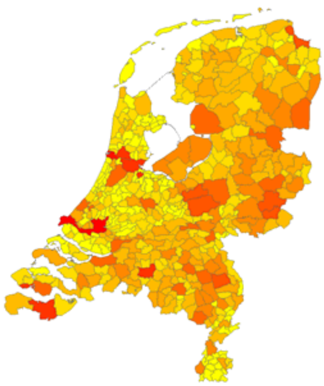
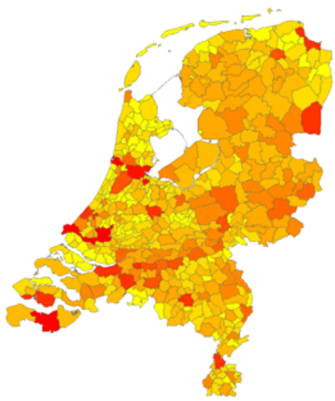
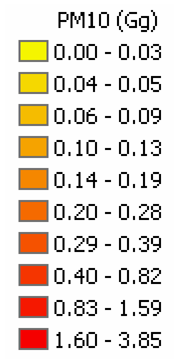
E-MAP emissions PM_{10}	National Emission Registration PM_{10}	
		

Figure 1.3-3. 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 1.3-3 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 1.3-4 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).

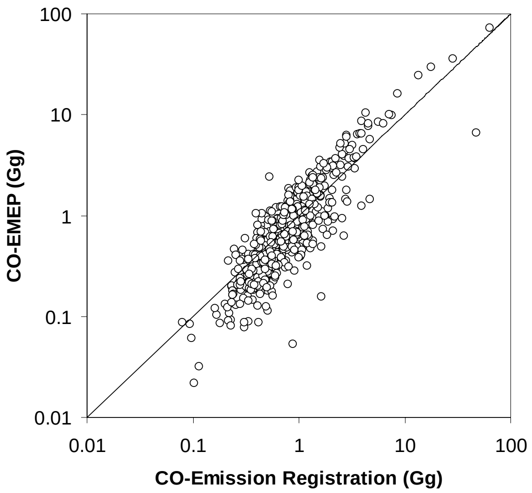


Figure 1.3-4. Dutch CO emissions for municipalities in the Netherlands (CO-Emission Registration) plotted against the disaggregated EMEP/CORINAIR CO emissions. The line represents the 1:1 relation.

1.3.2.2 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 1.3-5. shows an example of a scatterplot of modelled PM_{10} concentrations against measured values for the station of Bentinckplein, Rotterdam.

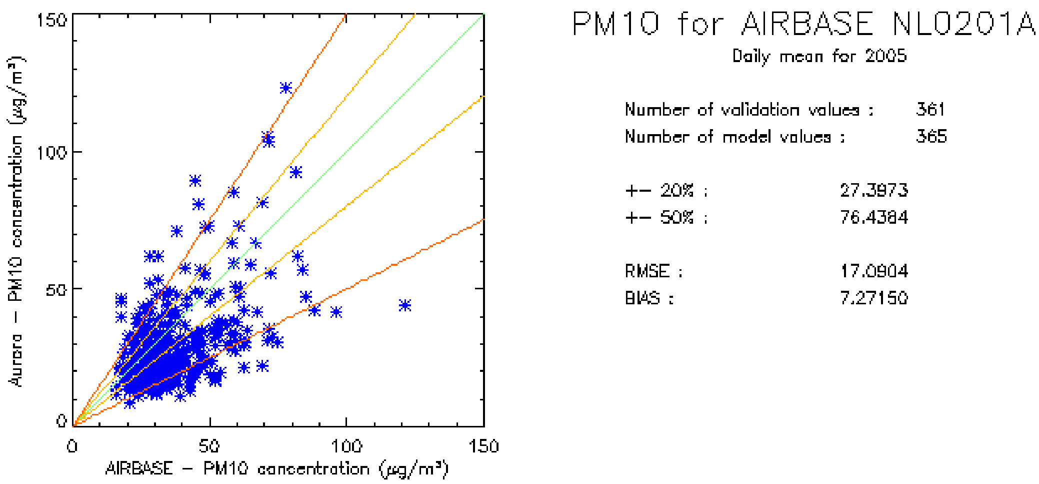


Figure 1.3-5. Scatterplot of AURORA PM_{10} daily mean concentrations as a function of measured values, for the station of Bencinckplein, Rotterdam.

Table 1.3-2 and Table 1.3-3 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 1.3-2 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 1.3-3 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 1.3-6. Table 1.3-4 summarizes the correlation coefficients and RMSE values. It shows that the spatial pattern of AURORA captures well the relative differences between the measurement stations.

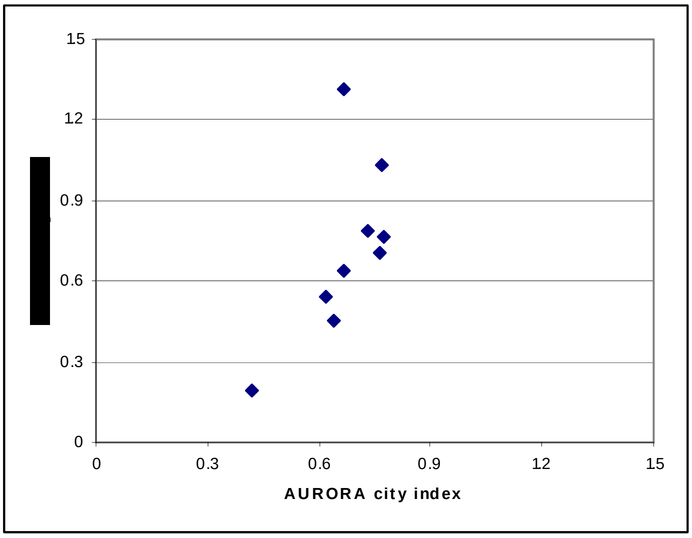


Figure 1.3-6. Scatterplot of the Airbase city index as a function of the AURORA-derived city index (on the location of the Airbase stations).

Table 1.3-4. 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 1.3-7 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.

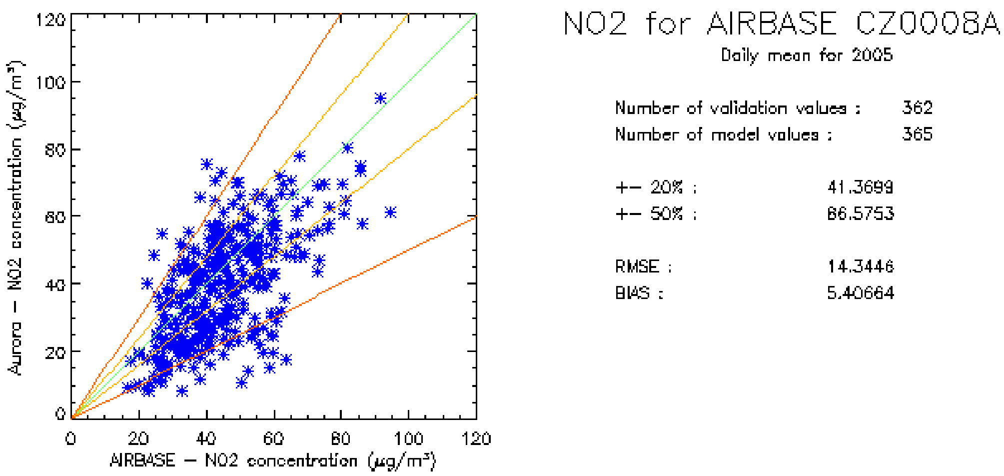


Figure 1.3-7. Scatterplot of AURORA NO2 daily mean concentrations as a function of measured NO2 daily mean concentrations, for the Airbase station CZ0008A.

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 1.3-5 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.

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

Table 1.3-5 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 1.3-6. 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 1.3-7. 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 1.3-7. 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 1.3-8 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 1.3-8. 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 1.3-9. 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 1.3-9 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.

1.3.2.3 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 1.3-8 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 1.3-8 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 1.3-8 were set to that value.

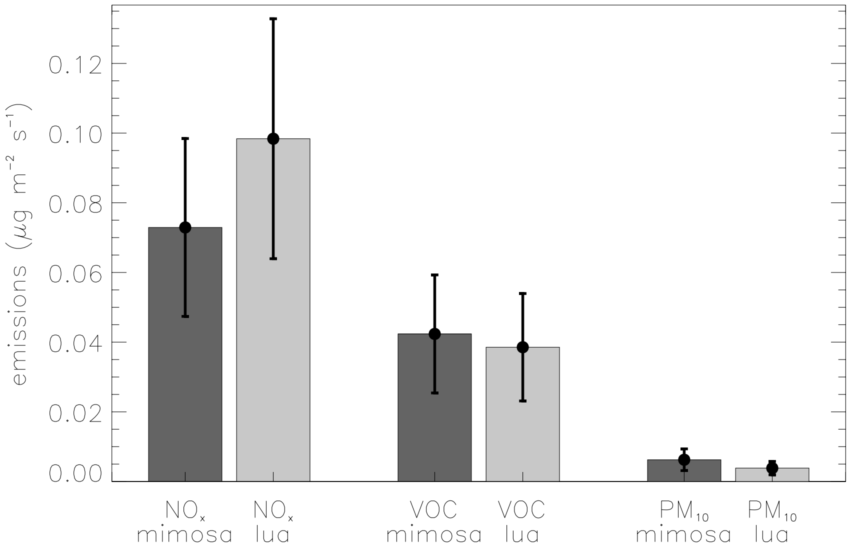


Figure 1.3-8. Comparison of vehicle exhaust emissions computed using the MIMOSA model with the emission inventory provided by LUA.

ARPS **meteorology** simulation results were validated by comparing model output with observed meteorological parameters. Figure 1.3-9 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 1.3-9 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.

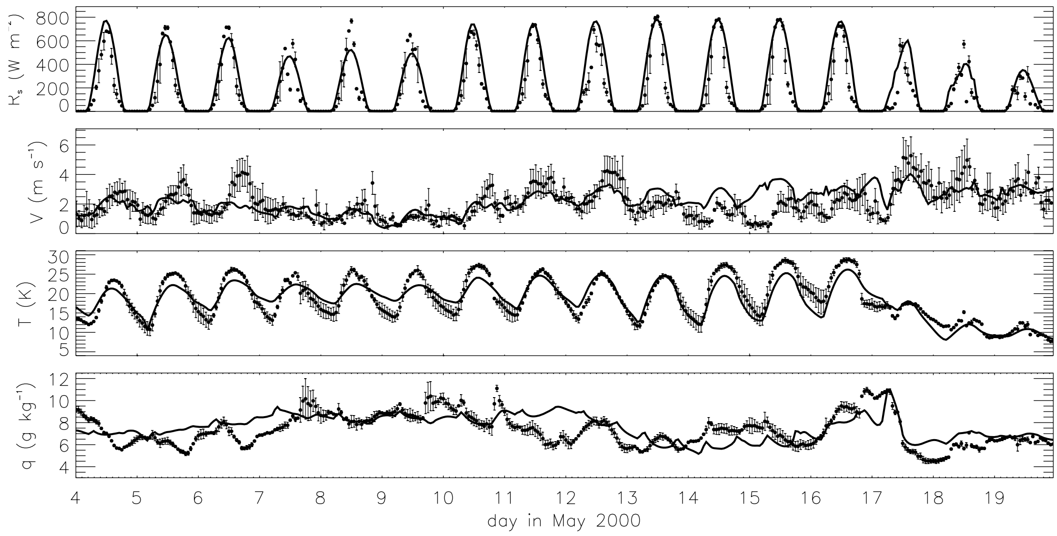


Figure 1.3-9. Simulated (solid line) versus observed (symbols) meteorological parameters. From top to bottom: down-welling shortwave radiation, 10-m wind speed, and 2-m temperature and specific humidity. Observations were taken from the Essen-Altenessen en Essen-Hirschlandplatz stations, separated by 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 1.3-10, 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 1.3-9).

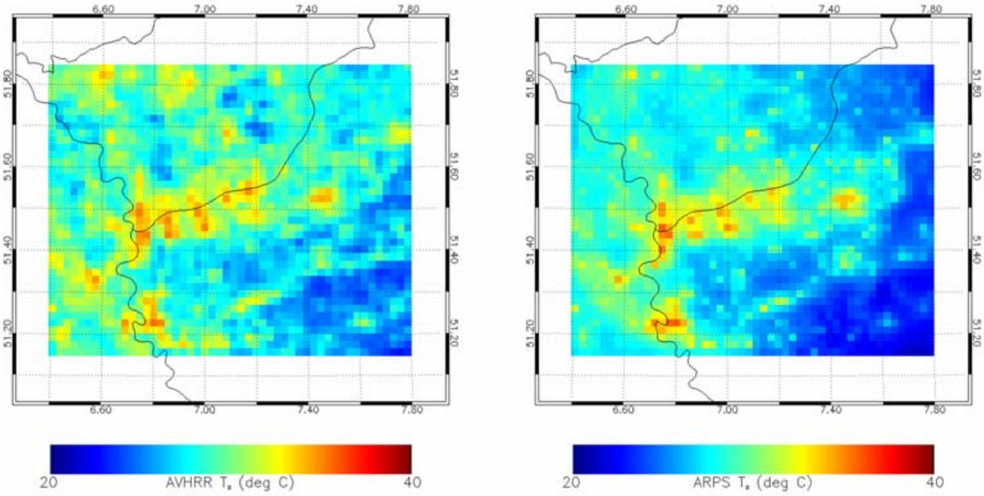


Figure 1.3-10. Simulated (right panel) and observed (left panel) surface temperature, for 14:40 GMT on 13 May 2000. The observed values were constructed from AVHRR instrument channels 4 and 5 (thermal infrared) onboard the NOAA-14 polar orbiting satellite platform.

In another validation exercise (

Figure 1.3-10), 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 1.3-10. 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 1.3-11 and Table 1.3-11), 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.

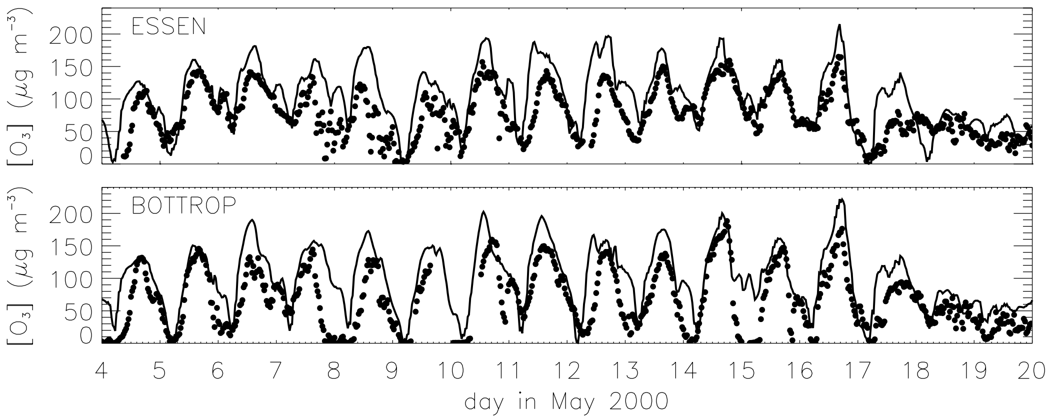


Figure 1.3-11. Simulated (solid line) as compared to observed (symbols) ground-level O_3 concentrations for the stations Essen (upper panel) and Bottrop (lower panel).

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 1.3-11. 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 (µg m^{-3})	32.8	26.7	0.74	36.9	33.9	0.81
$[O_3]$ daymax (µg 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 µg m^{-3}, for the rural background stations it was 14.8 µg m^{-3}, the average urban-rural difference being 9.5 µg m^{-3}. With a standard deviation on the measured time series of urban-rural particulate matter concentration differences of 1.5 µg m^{-3}, this difference was found to be relatively stable. The mean difference of 9.5 µg m^{-3} is to be compared with simulated PM_{10} concentrations (not shown here), with values of the order of 10 µg 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	o comparison with accuracy requirements as in Figure 1.3-1

	o 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} (NO2), 6 µg m^{-3} (O3), 12 µg m^{-3} (PM10), 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 1.3-12 Validation of the individual components for the Urban Local AQ Assessment Sub-service

1.3.3 Validation against specifications and against user requirements

1.3.3.1 Model based urban air quality indicators

* Requirements written in *Italics* are only recommended and not compulsory for Phase 2

VALIDATION AGAINST SERVICE SPECIFICATIONS			
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.			
VALIDATION AGAINST USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Product	Average human exposure to atmospheric pollution, for SO_2, NO_2, O_3, PM_{10}		
Accuracy	~nx10%	Standards in Daughter Directives of the EU	daily mean SO2: 120-246 %

		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 %	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 %
Accuracy minimum	n.s.	Standards in Daughter Directives of the EU ambient and Air Quality framework directive (96/62/EC)	id.
Accuracy target	n.s.	n.s.	~ 10-20 % (gases) ~ 30 % (particles)
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* are only recommended and not compulsory for Phase 2

Table 1.3-13 Validation against specifications and against user requirements for the Urban and Regional AQ Assessment Sub-service

1.3.3.2 Scenario tool for regional air quality policy support

VALIDATION AGAINST SERVICE SPECIFICATIONS
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.

VALIDATION AGAINST USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Product	Concentration change patterns following user-defined emission scenario		
Accuracy	~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 %
Accuracy minimum	n.s.	Standards in Daughter Directives of the EU ambient and Air Quality framework directive (96/62/EC)	id.
Accuracy 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* are only recommended and not compulsory for Phase 2

Table 1.3-14 Validation against specifications and against user requirements for scenario tool for Regional Air Quality Policy support sub-service.

1.3.4 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* are 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 1.3-15 Quality assessment and control procedures for the for the Urban and Regional AQ Assessment Sub-service

1.3.5 References

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1.4 Local air quality analysis for the province of Zeeland

1.4.1 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 <zelle@argoss.nl>

1.4.2 Validation Plan and validation data

This validation plan applies to the air quality analysis reports based on a 5-year hindcast database of air quality information for the province of Zeeland, the Netherlands.

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, 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 will be 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, 2003-2007. 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. Due to data availability problems the satellite data validation will be limited to short case studies, we strive to complete at least the summer 2003 heat wave case, and a longer period if possible.

Validation of the services against specifications and user requirements will 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 the period January-May 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 1.4-1 Data used for the validation of all the products of this service/sub-service

1.4.2.1 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) will be made available in a validation report which will become a chapter in the air quality analysis report for PROMOTE phase 3. This information can be made available upon request.

The numbers made available in table 1.4-2 give a rather crude presentation of the overall quality of the air quality data from the CHIMERE model. Taking the variable PM10 as an example, although the overall timeseries match fairly well (visually), the error statistics are made severely worse because of a single peak where the model strongly overestimates the concentration. Similar problems occur for NO concentration peaks. O3 generally shows good to very good agreement between model and observations, but the model overestimates the low episodes during the nighttime. The daily cycle of NO2 is estimated well by the model, but it overestimates the low concentration episodes especially during the weekends. The variables NH3 and SO2 are currently not trusted yet. NH3 sometimes shows an opposed daily cycle, suggesting a problem with the emission data over time. SO2 is strongly overestimated by the model, combined with unexpected spatial emission distributions this leads us to believe the emission data are faulty.

The final air quality analysis report will contain a more 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.

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. $\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum (X_i - O_i)^2}$ 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. The stations can also be taken together to show the overall regional error statistics.
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	For phase 2 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. In phase 3 these boundary conditions will be replaced by output from a European-scale model within PROMOTE.
	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 July 2003-2006, to be expanded to 2003-2007 before the end of PROMOTE phase 2).

	The 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 all stations in the Netherlands, these results are not included here but are available upon request. The results presented here are only for stations in the province of Zeeland. 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 CO: No observations available from LML / RIVM CH4: No observations available from LML / RIVM
Consistency	
	N/A

Table 1.4-2 Data used for the validation of all the products of this service/sub-service

1.4.2.2 Validation of specifications and user requirements

VALIDATION AGAINST SPECIFICATIONS and USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Accuracy	Not available until completion of phase 2 validation. 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) **O3:** RMSE = 20.9 μg/m^3, MAE = 15.8 μg/m^3, MB = -6.0 μg/m^3 **PM10:** RMSE = 19.9 μg/m^3, MAE = 12.9 μg/m^3, MB = 7.5 μg/m^3 **NH3:** RMSE = 3.6 μg/m^3, MAE = 2.3 μg/m^3, MB = -0.5 μg/m^3 **NO:** RMSE = 18.1 μg/m^3, MAE = 7.4 μg/m^3, MB = 2.9 μg/m^3 **NO2:** RMSE = 17.4 μg/m^3, MAE = 12.8 μg/m^3, MB = -5.0 μg/m^3 **SO2:** RMSE = 11.1 μg/m^3, MAE = 7.8 μg/m^3, MB = -5.2 μg/m^3
Accuracy minimum	n.s.	n.s.	N/A
Accuracy 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 July 2003 – September 2006, expansion to full 2003-2007 is running and expected complete July 2007.
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. The final analysis and validation report must still be added, expected 06-2008.
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 expected 07/2008
Data accessibility	All results of the analysis service are available offline. Delivery by WWW or on request. Other data / statistics that are not included in the analysis reports are available offline on request. Validation reports are made available online.	online	As specified, validation will be made available online when final version is completed (expected 07/2008)
Delivery Mode	Offline	Offline	Offline
Delivery frequency	Initial delivery spans the period 2003 – 2007, to be expanded annually	N/A	As specified, once per year

	starting in phase 3 and continuing afterwards.		
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.
REMARKS			
Trial report delivered May 2008 Final report delivery July 1, 2008 Reports will be delivered annually, one for each phase.			

*Requirements written in *Italics* are 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 1.4-3 Validation of specifications and user requirements for this service

1.4.3 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.	Approximately 5 quality checks over the period March – June 2008.
Product confidence data	n.s.	*95%*	N/A	N/A
Error bar definition and representation	RMS error of concentration (model compared to observations)	2σ	As specified in s5	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 There were no process failures in the database / report generation process up to this point in time.	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: 1.0, 1-may 2008. The full database was generated with this version, and the report based on these results solely.	2 changes, V0.9 (April 7 2008) V1.0 (May 1 2008)

*Requirements written in *Italics* are 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

1.4.4 References

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1.4.4.1 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

1.4.4.2 Bibliographic references

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1.5 Portuguese air quality records service

1.5.1 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. The key feature presented by this service is the possibility to spatialize observed or modelled PM 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 is a spinoff of the current services available in QualAr, the current air quality monitoring information web service offered by APA, where the products are still only point or zone average based. Products integrated in this service level include 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.

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

1.5.2 Validation plan and validation data

Products scheduled to be delivered on Phase 2 of PROMOTE include Level 1 point and zone average for ground based daily information (concentration and air quality indexes) on PM10, O3, NO2, SO2 and CO for the national scale (historical data since 1995 to end year of project - 2009). This product level is directly calculated from measured ground observations so no validation plan is required. Nevertheless some Quality Assurance/Quality control (QA/QC) procedures to assure the usefulness and consistency of the calculated parameters are defined in section 1.5.5.

VALIDATION DATA	
Ground based observations	
Name SOURCE/NETWORK Phase: 2	Data availability and access (include access details if data is freely available): Spatial coverage and resolution: Temporal coverage and resolution: Location(s) (coordinates): Uncertainty quantification (e.g. Accuracy):
Name SOURCE/NETWORK Phase: 2	Data availability and access (include access details if data is freely available): Spatial coverage and resolution: Temporal coverage and resolution: Location(s) (coordinates): Uncertainty quantification (e.g. Accuracy):
In-situ observations	

Name SOURCE/NETWORK Phase: 2	Data availability and access (include access details if data is freely available): Spatial coverage and resolution: Temporal coverage and resolution: Location(s) (coordinates): Uncertainty quantification (e.g. Accuracy):
Name SOURCE/NETWORK Phase: 2	Data availability and access (include access details if data is freely available): Spatial coverage and resolution: Temporal coverage and resolution: Location(s) (coordinates): Uncertainty quantification (e.g. Accuracy):
EO Data	
Name SOURCE/NETWORK Phase: 2	Data availability and access (include access details if data is freely available): Spatial coverage and resolution: Temporal coverage and resolution: Location(s) (coordinates): Uncertainty quantification (e.g. Accuracy):
Name SOURCE/NETWORK Phase: 2	Data availability and access (include access details if data is freely available): Spatial coverage and resolution: Temporal coverage and resolution: Location(s) (coordinates): Uncertainty quantification (e.g. Accuracy):

Table 1.5-1 Data used for the validation of all the products of this service/sub-service

1.5.3 Validation of individual components

Most of the individual components present in table 1.5.3

VALIDATION OF INDIVIDUAL COMPONENTS FOR STRATOSPHERIC GASES	
Uncertainty estimators	
N/A	N/A
Quality assessment	
QA ground based data/removal of outliers/verification consistency	Phase 2 Raw pollutant data outlier removal is done by Portuguese air quality regional authorities and is therefore outside the scope of Aircast.
Error statistics	RMSE – root mean square error NRMSE – normalised mean square error
Models/algorithms/assimilation	

Air Quality parameter and index calculation module	Air quality is measured by monitors that record the concentrations of pollutants at several air quality monitoring stations across the country. The Portuguese Air Quality Index (IQAr) value results from the arithmetic average calculated for each pollutant in all the stations of the area. Those values are compared with concentration categories which have a correspondence with a colour scale. A specific colour is assigned to each IQAr concentration category. The pollutant that individually has the higher concentration is the responsible for the colour of the Air Quality Index. The index for one day is determined by the worst pollutant concentration measured in one or more monitoring stations (the average of the maximum values is considered in the second case) in that day. The Environmental Portuguese Agency provides IQAr in a daily basis, based on the concentrations measured at air quality monitoring stations managed by regional authorities. The pollutants and type of values aggregation used in the index are the following: – Sulphur dioxide (SO2) – daily maximum hour average; – Nitrogen dioxide (NO2) - daily maximum hour average; – Ozone (O3) - daily maximum 8-hours average; – Carbon monoxide (CO) - daily maximum 8- hours average; – Particulate matter (PM10) - daily average.
	N/A
Spatial model adjustment module	Phase 3 The quality of the product is expected to decrease with the decrease of time average. Annual and monthly products will have more quality than daily products. The daily product quality is very variable and dependent on meteorological conditions (boundary layer height, wind speed and direction, etc) RMSE for the annual parameters in the Lisbon area will probably be less than 50% and for the national scale is not yet available
MODIS Pre-processing reflectance, cloud and masking	Phase 3 MODIS AOT retrieval is based on the Level 1B 250 m calibrated radiance product. Pre-processing of this product includes subseting 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)
	N/A

MODIS AOT Retrieval	Phase 3 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 AERONET stations
Linear AOT/PM10 Assessment	Phase 3 product Linear model quality very variable and dependent on meteorological conditions (boundary layer height, wind speed and direction, etc)
	RMSE not yet available

Table 1.5-2 Summary of the validation of individual components this service/sub-service

1.5.4 Validation of specifications and user requirements

1.5.4.1 AIRCAST L1: Point and Zone average ground based air quality data

VALIDATION AGAINST SPECIFICATIONS and USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Accuracy	N/A	n.s.	N/A
Accuracy minimum	n.s.	n.s.	N/A
Accuracy target	n.s.	n.s.	N/A
Spatial coverage	Monitoring: Portugal Forecast: Lisbon	Portugal, Lisbon	Monitoring: Portugal
Temporal coverage	1995-2009	1995-2009	1995-2009
Spatial resolution	Point monitoring and zone monitoring	Point monitoring and zone monitoring	Point monitoring and zone monitoring
Temporal resolution	1h, 24h, 30 days	1h, 24h, 30 days	24h, 30 days and 12 months (the last two only for PM10)
Grid/Projection	various	n.s.	various

User Interfaces			
PROMOTE Web Site	n.s.	Complete, operational and up to date	Operational and will be up to date during the second week of June
ftp	n.s.	n.s.	FTP not available. Products available for download trough website
On demand			
Data formats and data delivery			
Data availability	Operational implementation by May 2008	Phase 2	Operational implementation by second week of June 2008
Data accessibility	Offline	Online	NRT
Delivery Mode	n.s.	Download	Download trough website
Delivery frequency	n.s.	Daily, month 6	Daily
Data Format	Shapefile	Ascii, gif	XLS file
Historical archive	Hourly AQ data from ground stations. Timeseries 1995-2009	1995-2009	Hourly AQ data from ground stations. Timeseries 1995-2009
Visualization	Thourhg Web Mapping Services	Thourhg Web Mapping Services	Webiste 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 1.5-3 Validation of specifications and user requirements.

1.5.5 Quality assessment and control procedures: service quality

Quality assessment and control procedures are applied in the several steps towards the calculation of the defined Level 1 products.

The raw pollutant concentration data used to calculate the air quality indexes 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).

Data aggregation and calculation of statistical parameters must comply with quality criteria established on air quality Directives (namely Annex IV of Decision 2001/752/EC) regarding miminum data capture and maximum data capture gap for data aggregation (hourly, daily and seasonal values). The criteria for the calculation of the Portuguese Air Quality Index (IQAr) were defined by the Environmental Portuguese Agency and include a list of mandatory pollutants to be included in the index and also a minimum data capture for each pollutant.

Criteria check for all of these stages is performed each day automatically during the different parameters calculation steps implemented in the air quality parameter and index calculation module.

The quality checks will be done periodically and all the information in this document will be presented in a 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	monitoring	yes	yes	Automatic quality checks included in air quality indices calculation Monthly non-automatic quality checks. Annual Service report to user
Product confidence data	n.s.	*95%*	n.s.	N/A
Error bar definition and representation	N/A	*2σ*	*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	*-99.99 or similar <0 or interpolation; color (black or white, in maps)*	n.s.	Station/Zone missing data will be represented in the daily air quality maps (by a "no data available" warning) and the downloadable xls files (value not yet defined)
Documentation of process failure	Process failure report sent to the user within one week	n.s.	n.s.	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	*References to Quality Control procedures and product version number and last date of modification to be available in background*	n.s.	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* are 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 1.5-4 Quality assessment and control procedures this service/sub-service

1.5.6 References

1.5.6.1 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)

1.5.6.2 Bibliographic references

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Ferreira, F., Nogueira, L., Meireles, P., Mesquita, S., Almeida, C., Tente, H. Torres, P. Integrating INTEGRATING DIFFUSIVE SAMPLING AND MONITORING STATIONS TO EVALUATE AIR QUALITY IN URBAN AREAS, in UAQ4 Conference, 25-28 March 2003, Charles University Prague, Czech Republic.

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