DOSSIER: COMMON TASK: -2-

TITLE:

GMES SERVICE ELEMENT
PROMOTE

C6 Validation Report
LOCAL AIR QUALITY FORECAST SERVICE
Version 2

DOCUMENT STATUS SHEET

	FUNCTION	NAME	DATE	SIGNATURE
LEAD AUTHORS	editor	R. Delgado J. C. Lambert		
CONTRIBUTING AUTHORS	Service leader Service providers	Koen De Ridder Karen Van de Vel Hein Zelle Nuno Grosso		
REVIEWED BY	Reviewers			
APPROVED BY	Technical officer (ESA)			
ISSUED BY	Project manager			

DOCUMENT CHANGE RECORD

Issue	Date	Modified Items / Reason for Change
Version 1		
0.10	22.02.2007	Draft document created and sent to ACRI and CERC
0.20	20.03.2007	Document updated with input form service provider (ACRI)
0.30	09.05.2007	Document reformatted and updated (S5)
0.40	15.05.2007	Document edited and sent to all providers
0.50	04.06.2007	Input from RIU received and document edited
0.60	08.06.2007	Input from ACRI and DLR received and edited
0.70	11.06.2007	Integration and edition
0.75	11.06.2007	Document sent for partial review (Three sub-services: RIU, DLR, ACRI)
0.76	14.06.2007	Contribution FMI received and integrated in master document
0.77	15.06.2007	Contribution FMI received and integrated in master document
0.78	20.06.2007	Contribution from AUTH received and integrated in master document
0.79	20.06.2007	Contribution KNMI received and integrated in master document
0.80	21.06.2007	Contribution from VITO received and integrated in master document
1.00	26.06.2007	Document edition finished and properties updated
Version 2		
1.05	15.04.2008	Available Phase 2 validation plans integrated in template
1.10	04.06.2008	Template updated and distributed
1.2	26.06.2008	Document updated (no CERC contribution)
1.5	07.07.2008	Document reviewed, edited and ready for final review

LIST OF TABLES

LIST OF FIGURES

LIST OF ACRONYMS

AQI	Air Quality Index
AQMP	Regional Air Quality Service for Mecklenburg-Western Pomerania
AUTH	Aristotle University of Thessaloniki
AVN	Global Forecast Model System (also GFS)
CERC	Cambridge Environmental Research Consultants
CTM	Chemistry-Transport Model
DFD	German Remote Sensing Data Center
DIMS	Data Ingestion and Management System
DLR	German Aerospace Center
EMEP	Co-operative Programme for Monitoring and Evaluation of the Long-range Transmission of Air pollutants in Europe
ENVISAT	European Environmental Satellite
EURAD	European Air Pollution Dispersion Model System
FMI	Finnish Meteorological Institute
KNMI	Royal Netherland Meteorological Service
LUNG	Landesumweltamt für Umwelt, Naturschutz und Geologie
MWP	Mecklenburg-Western Pomerania
NCEP	National Center for Environmental Prediction
NOAA	National Oceanic and Atmospheric Administration
PM10	Particulate Matter within 10 um scale
RIU	Rhenish Institute for Environmental Research
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Cartography
VITO	Flemish Institute for Technological Research
WDC-RSAT	World Data Center for Remote Sensing of the Atmosphere
3d-var	Three-Dimensional Variational [Data Assimilation]

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

TABLE OF CONTENTS

1 LOCAL AND REGIONAL AIR QUALITY FORECAST

1.1 Service overview

This service is composed of a suite of local air pollution forecasting services provided by a collection of service providers in several European countries. During the lifetime of PROMOTE, the service is expected to reach approximately 25 million people, or about 5 % of the European population.

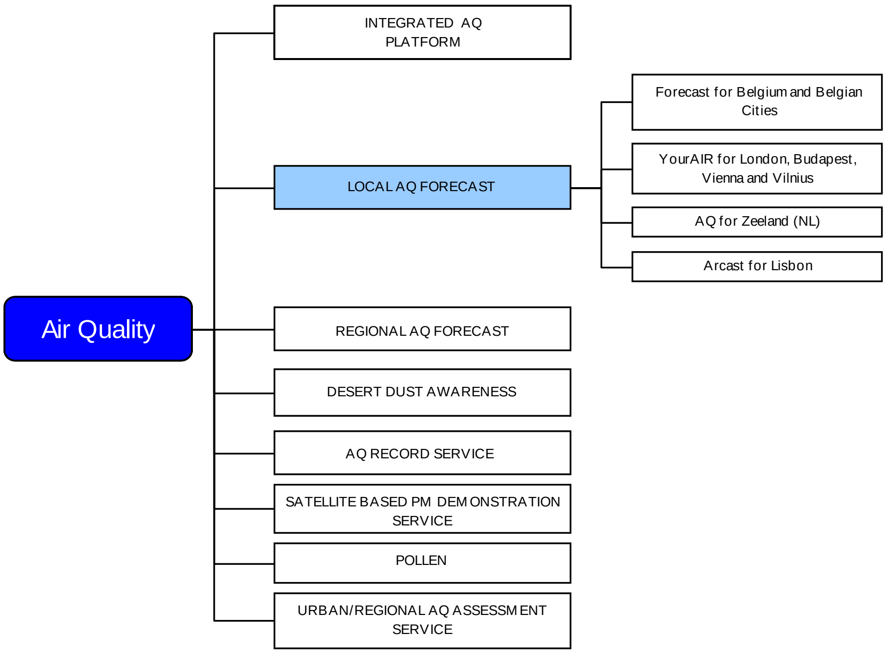

Figure 1.1-1 Position and structure of the Local Air Quality Forecast Service within PROMOTE 2 Air Quality.

This figure is rather low compared to population coverage in the regional- and continental-scale services. Yet, the products in the local air quality services contain much more spatial detail; hence provide a better estimate of human exposure to air pollution in urban agglomerations, which, after all, are home to 80 % of the Europeans. The comparatively low population coverage also means that this service has a significant growth potential.

The services use a number of different modelling approaches, with spatial resolutions ranging from tens of metres up to a few kilometres. Many of the services integrate outputs from other PROMOTE partners. In particular air composition forecasts from continental and hemispheric scale forecasts are used as boundary conditions for the forecasts at the highest resolution.

The services engage users at all levels, from the general public to regional and national environmental authorities.

The service comprises air quality forecasting systems for

- London, Liverpool, Budapest, Vienna, and Vilnius, provided by CERC;
- Belgium and Belgian cities, provided by VITO;
- the province of Zeeland (the Netherlands), provided by ARGOSS;
- Lisbon, provided by YDREAMS/IMAR.

1.2 AQ Forecast for Belgium and Belgian Cities

Description: Daily 48-hr forecasts of relevant pollutants (PM10, PM2.5, O3, NO2), for Belgium and 5 Belgian cities (Antwerp, Brussels, Gent, Liège , Charleroi)

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

Research partners: -

Service Provider(s): VITO

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

1.2.1 Product characterization

O_3	
Parameter	fields of ground-level O_3 concentrations
Typical range	0 – 360 µg m^{-3}
Determination of the typical range (Method, criteria)	European guidelines and concentration scales used at IRCEL (User), see URL01
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 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 URL02
NO_2	
Parameter	fields of ground-level NO_2 concentrations
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 URL01
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 URL02
PM_{10}	
Parameter	fields of ground-level PM_{10} concentrations
Typical range	0 to > 200 µg m^{-3}
Determination of the typical range (Method, criteria)	European guidelines and concentration scales used at IRCEL (User), see URL01
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 URL02

Table 1.2-1 Characterization of the products provided by the Air Quality Forecast for Belgium and Belgian Cities Sub-service

1.2.2 Validation plan and validation data

The main outcome of this service consists of 48-hour forecasts of hourly gridded ground-level concentration data of the pollutants O_3, NO_2, PM_{10}, and $PM_{2.5}$, at spatial resolution of 1 km (urban agglomerations of Antwerp, Ghent, Brussels, Liège, Charleroi), using the AURORA model. The final product consists of digital files (maps or data) containing daily mean and maximum values of these quantities. The validation focuses on both geophysical validation and operational functioning.

Geophysical validation is performed on-line by comparing simulated concentrations with observed values for the past two days, using data from the telemetric network of air quality observation stations (see Table below). The quality of the simulated values is assessed using error statistics including root mean square error and bias. As AURORA forecasts are significantly affected by lateral boundary conditions, which we take from the EURAD model, concentrations simulated by the latter are also assessed.

Apart from the concentrations themselves, also emissions are evaluated to some extent by comparing regional mean emission values generated with the 'emission mapper' (i.e., tool to spatially disaggregate national emission totals) with the emissions reported by the Flemish, Walloon, and Brussels regions. This is done per sector (e.g., industry, road traffic, agriculture etc...) and per pollutant.

Validation of **operational functioning** is done by generating failure statistics, including reporting on the cause, and statistics regarding the timely delivery of the forecasts.

It should be noted that both the geophysical and operational validation of the air quality forecasts is being done at two different levels:

- in near-real-time the forecasts of the preceding days are validated and made available through the website
- in this report also a validation of the past year is provided, to provide a broader overview

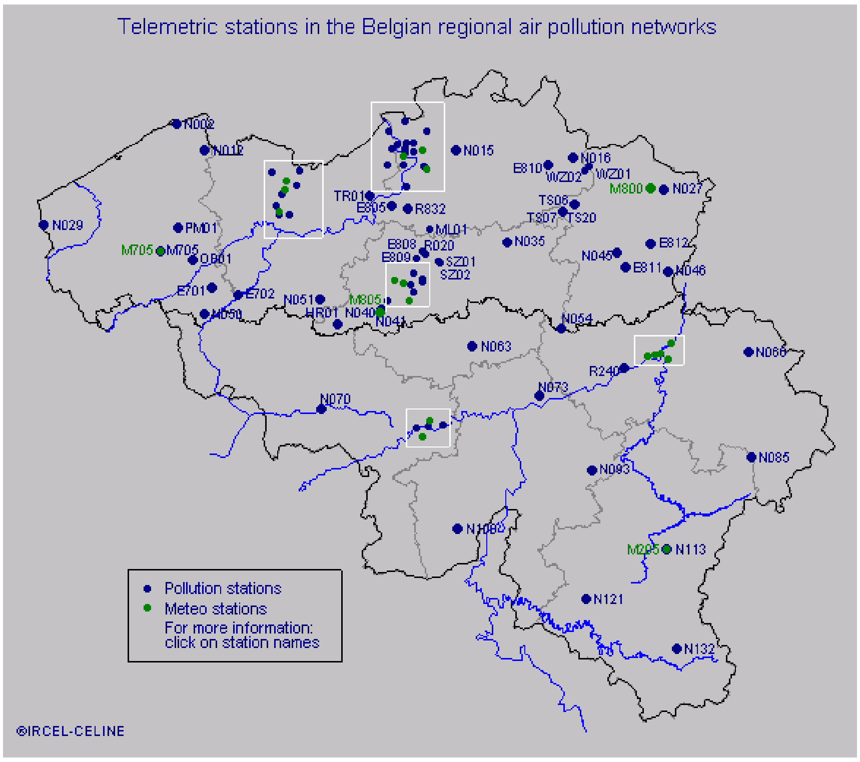

Figure 1.2-1. Location of IRCEL's pollutant measurement stations in Belgium

The validation focuses on comparing simulated pollutant concentrations with measured values. The latter are taken in near-real time from IRCEL's automatic measurement etwork. Positions of individual stations are shown in Figure 1.2-1.

VALIDATION DATA	
Ground based observations	
Ground-based observations	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 is shown in Figure 1.2-1– further details are available from URL01. 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.
***In-situ* observations**	
Instrument/station/trajectory	n.a.
Model outputs	
MODEL (name/version)	n.a.

Table 1.2-2 Data used for the products provided by the Air Quality Forecast for Belgium and Belgian Cities Sub-service

1.2.3 Validation of individual components

1.2.3.1 Geophysical validation

Two types of comparisons are performed: in the daily operational forecasting cycle, near-real time measured pollutant concentrations are retrieved from IRCEL, and their values are compared with simulated values, for several stations scattered over the territory, for the past two days, as shown in Figure 1.2-2 Moreover, annually, simulated and observed values are compared on a monthly (phase 1 – see Figure 1.2-3 and Figure 1.2-4) or, more recently, annual basis (phase 2).

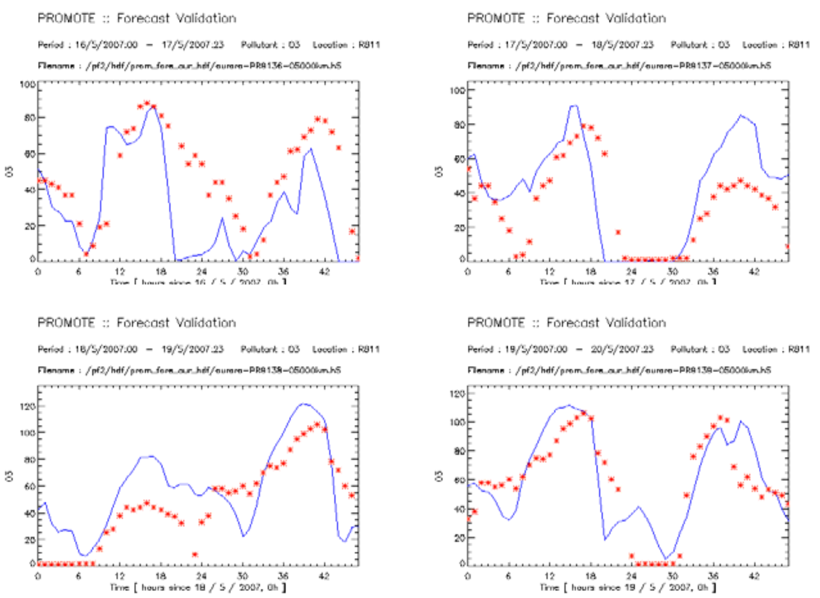

Figure 1.2-2. Daily validation plots for O_3, for a few days in April 2007.

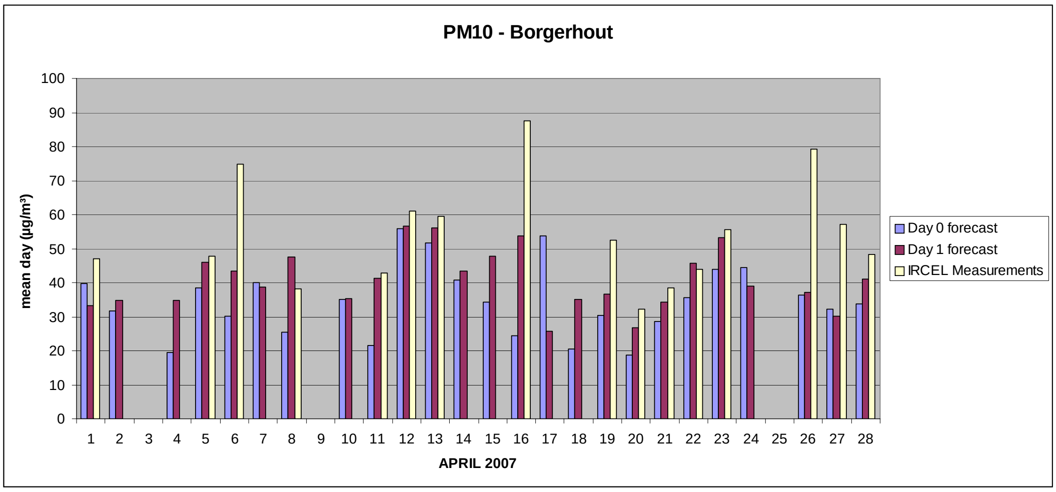

Figure 1.2-3. Validation of daily mean forecasted PM_{10} values, April 2007.

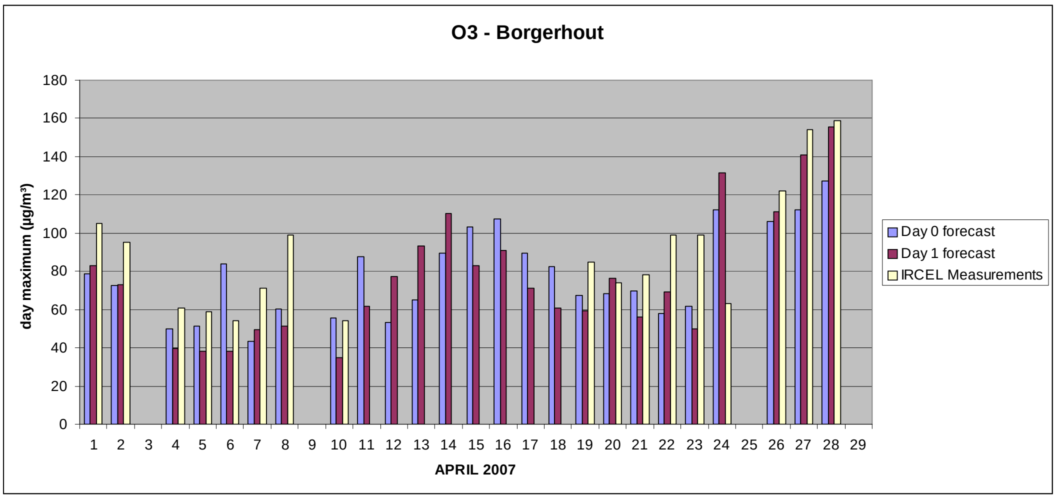

Figure 1.2-4. Validation of daily mean forecasted O_3 values, April 2007.

During the first phase the validation was not beyond the stage of producing graphs comparing simulated and observed pollutant concentrations. However, starting in phase 2, the goal was to generate a rigourous error analysis, including all measurement stations in Belgium for the production of relevant statistics (e.g., bias, error, proportion of simulation values within 50 % of the measured values, ...). This has now (in June 2008) been achieved, as demonstrated below.

Error statistics for the 5-km forecasts for Belgium were generated for each station in the domain, for the period 1 June 2007 – 31 May 2008. An example of the corresponding scatter plot and associated error statistics is provided in

Figure 1.2-5. The information that is provided as text on each validation plot is as follows:

- number of observations and number of model results;
- percentage of simulated values within ± 50 % of the observed value;

- Root Mean Square Error (RMSE);
- Mean Bias (MB);
- Mean Absolute Gross Error (MAGE)
- Normalised Mean Bias (NMB)
- Normalised Mean Absolute Error (NMAE)
- Correlation Coefficient (CORR).

The statistics are calculated based on daily values, using the daily maximum for O_3, and the daily mean for NO_2, PM_{10}, and $PM_{2.5}$.

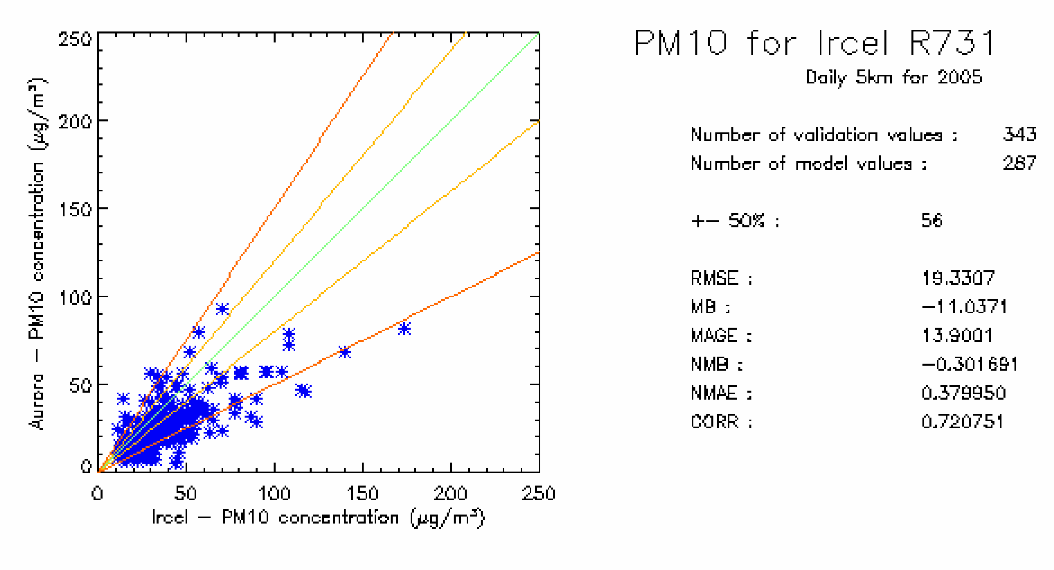

Figure 1.2-5. Example of an annual error statistics plot, showing the scatter between the observed (horizontal axis) and simulated (vertical axis) values for daily mean PM_{10} concentration at the position of station R731.

Moreover, error statistics per station are aggregated into one Table, thus providing a synoptic overview of model performance across all stations, at an annual basis. For the period 1 June 2007 – 31 May 2008, error statistics for all stations are shown in Figure 1.2-6. Each symbol in the diagrams corresponds to one station, and the plots give for each station the NMB, the NMAE, and the correlation coefficient. These plots reveal that, for O_3, there is a problem of a systematic positive bias. In response to this information, investigations are currently underway to improve the photochemistry in the model. Moreover, in phase 3, a scheme will be developed to remove bias from the forecasts, using observations from the days preceding the forecast, and spatially interpolating the bias error from the station's positions to the rest of the simulation domain.

For NO_2 the situation is better, as a large cluster of stations exhibits values of NMB centred on NMB ~ 0, and with a relative error (NMAE) between 20-40 %. nevertheless, a significant portion of the stations shows values veering off towards values as high as 0.8 for both the relative bias and error.

Surprisingly, PM_{10} is simulated rather well, exhibiting a small negative bias and a relative error around 40 % for many stations. For $PM_{2.5}$ (less points since this quantity is measured in a limited number of IRCEL stations only) the situation is comparable, apart from two stations that show larger error and bias.

For all pollutants, the correlation coefficients are generally fairly acceptable, mostly in the range 0.6-0.7, with a minority of values in the range 0.4-0.5.

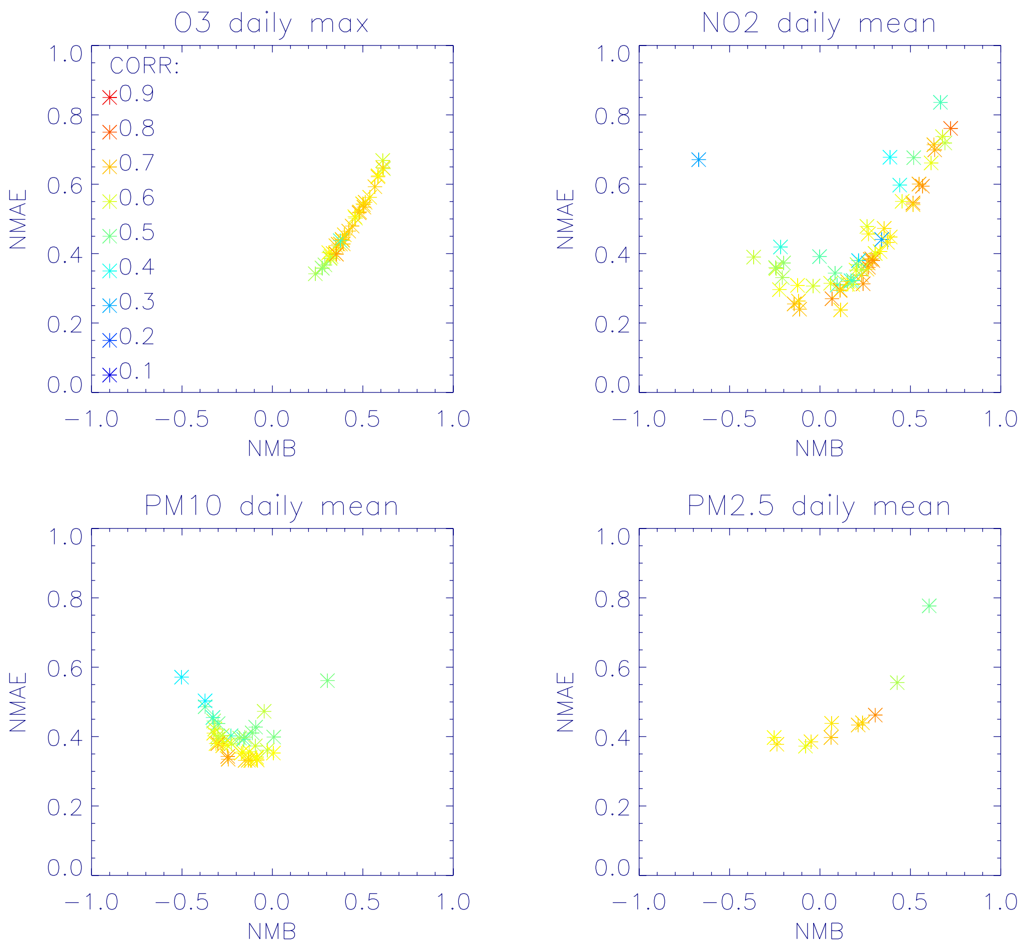

Figure 1.2-6. Error statistics for the 5-km forecasts for Belgium, for the period 1 June 2007 - 31 May 2008, for O_3, NO_2, PM_{10}, $PM_{2.5}$. In these graphs, each symbol corresponds to the position of a station, the horizontal and vertical co-ordinates corresponding to the Normalised Mean Bias (NMB) and Normalised Mean Absolute Error (NMAE), respectively. The correlation coefficients of the simulated concentrations vs. the observations is given by the color code, the legend of which is shown in the upper left diagram.

The emissions of atmospheric pollutants and their precursors are subject to a high degree of uncertainty, especially at the spatial scales considered here (order 1 km). Therefore, the uncertainty on emissions into the air were also estimated.

A first estimate on this uncertainty is obtained by considering the difference between the officially reported emissions totals for the three regions establishing Belgium, against the

EMEP expert emissions for their sum. In principle these figures should of course be exactly the same. Table 1.2-1 does indeed show that the uncertainty on annual totals are fairly small, of the order of at most 4 to 5 %.

Table 3. Comparison of reported emissions for 2007, between the sum of the emissions reported by the three Belgian regions (Flanders, Brussels, Wallonia) and the EMEP expert emissions.

	SOx	NOx	VOS	NH3	PMcrs	PM2.5
sum regionally reported (tonnes)	157779	313181	227512	77910	31129	31516
EMEP expert emissions (tonnes)	157634	299935	230178	81637	31131	31515
difference (%)	0.092	4.230	-1.172	-4.784	-0.007	0.004

Yet, the uncertainty on annual total emissions for a large area are certainly much smaller than what one should expect as uncertainty for spatially disaggregated emission values. In order to assess this latter aspect, a detailed study was performed, in which different emission inventories were compared (Maes et al., 2008) From this it emerged that different emission inventories may give values differing by up to several tens of %, depending on the pollutant, the sector, and the spatial resolution.

1.2.3.2 Validation of operational aspects

Apart from the validation activities described above, an evaluation is also made of the reliability of the forecast, from the operational point of view. In other words, statistics and graphs are generated regarding the percentage of time in a given period that a forecast was effectively produced. Figure 1.2-7 shows the results for January-May 2007, clearly displaying the starting-up period during most of the winter 2007, and the increasing availability of the daily forecast.

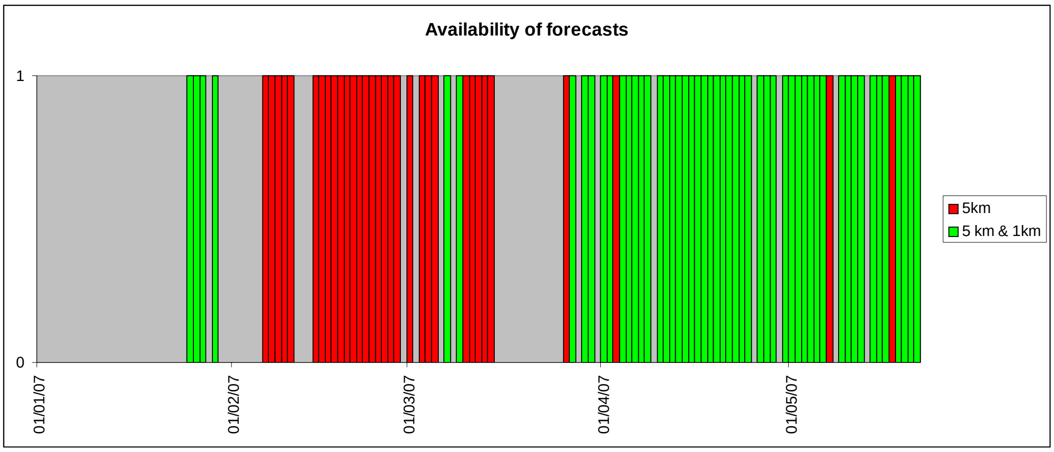

Figure 1.2-7. Availability of forecasts for the period January - May 2007, green colours indicating that the full forecast (5 & 1 km) was produced, red when only the 5-km forecast was generated, and grey when no forecast was made at all.

During the course of Phase 2, a more detailed analysis of service operationality was introduced. Forecast delivery rate is shown in Figure 1.2-8. Note that, owing to late delivery of hardware the Ghent and Charleroi domains have not been activated yet (hence these display a 0 % delivery rate).

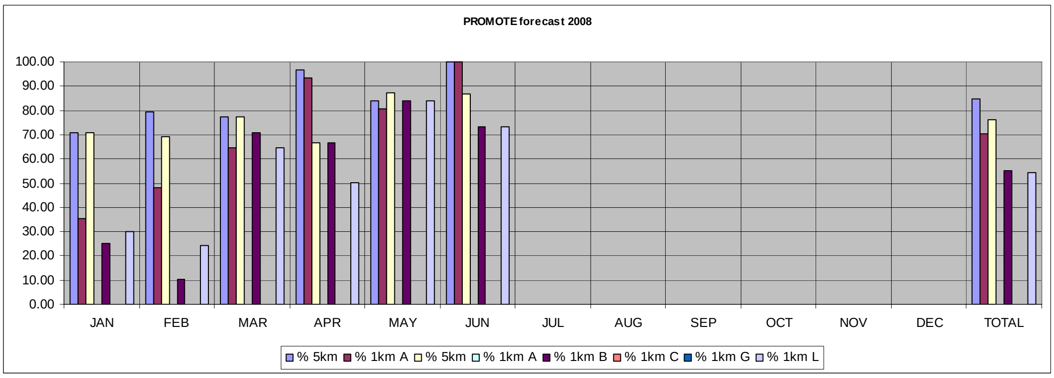

Figure 1.2-8. Forecast delivery rate for the Belgium (B) domain, and the city domains of Antwerp (A), Brussels (B), Ghent (G), Liège (L), and Charleroi (C).

Furthermore, statistics are now being generated to better document the cause of the failure of a forecast. An example is provided for the month of february 2008 (Figure 1.2-9, the legend is given in Table 1.2-4).

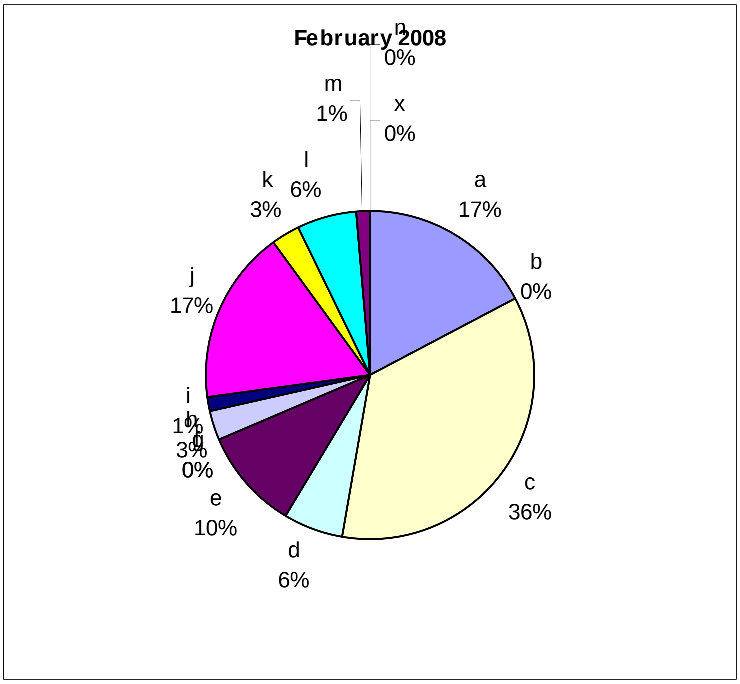

Figure 1.2-9. Forecast failure statistics for february 2008.

Table 1.2-4 Legend used for the failure cause statistics.

a	modifications in cfg files being tested
b	technical cause (e.g. installation new servers – system down)
c	EURAD data not fully available / or available too late
d	EURAD data unavailable
e	ARPS crash
f	sysadmin error
g	not yet implemented
h	NFS down
i	bug in code
j	inner run faster than outer run
k	aurora … max num of loops waiting for emissions
l	no binary
m	arps faster than lateral baundary conditions

n	disk full
x	unknown

VALIDATION OF INDIVIDUAL COMPONENTS	
Quality assessment and uncertainty estimators	
root mean square error (RMSE)	$\sqrt{\frac{1}{N}\sum_i (M_i - O_i)^2}$
mean bias (MB)	$\frac{1}{N}\sum_i (M_i - O_i)$
mean absolute gross error (MAGE)	$\frac{1}{N}\sum_i \lvert M_i - O_i \rvert$
normalised mean bias (NMB)	$\frac{\sum_i (M_i - O_i)}{\sum_i O_i}$
normalised mean absolute error (NMAE)	$\frac{\sum_i \lvert M_i - O_i \rvert}{\sum_i O_i}$
correlation coefficient (CORR)	$\sum_i (M_i - \overline{M})(O_i - \overline{O}) \Big/ \sqrt{\sum_i (M_i - \overline{M})^2 (O_i - \overline{O})^2}$
MODELS/ASSIMILATION	
MM5 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, though typical examples of mesoscale model variability can be inferred from Thunis *et al.* (2003).
EURAD	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.
	Accuracy is very case-dependent, example from the forecast of 21 June 2007: RMSE and bias for O_3 resp. 33.7 and 22.7 µg m^{-3}; for PM_{10} the

	values were 29.2 and -18.7 µg m^{-3} (see URL05).
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. A particular issue is that some emissions are very difficult to predict or to include in the modelling, e.g., the timing of forest fires or of manure spreading, both of which may give rise to unexpected high PM episodes.
	Overall validation of emission cadastres is extremely difficult because of a lack of suitable independent data. Comparison of modelled and measured emission factors for individual vehicles often show differences of the order of a factor 2 (Mensink *et al.*, 2000). However, for long time periods and large spatial scales, these differences are expected to be less. Also see Mensink (2000), Mensink *et al.* (2001), Van den Bossche *et al.* (2007), and Maes et al. (2008).
ARPS	Equations of atmospheric physics and dynamics. Whereas large-scale atmospheric features are dominated by the lateral boundary conditions (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.* (2007). In a study by De Ridder and Lefebre (2003), it was found that for the pollutant benzene, and using observations from an experimental campaign (URL03), the correspondence between measured and simulated values improved significantly when comparing model (grid-level) results with aggregated point measurements from different stations.

Table 1.2-5 Validation of the individual components of the Air Quality Forecast for Belgium and Belgian Cities Sub-service

1.2.4 Validation against specifications and against user requirements

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

VALIDATION AGAINST SERVICE SPECIFICATIONS			
o The cities of Ghent and Charleroi, scheduled for phase 2, are not yet covered in the forecasts, owing to delays in the delivery of hardware. However, the domains for these cities have been fully configured, and as the required hardware has arrived in June 2008, it is expected that forecasts for Ghent and Charleroi will start in the Summer of 2008. o Timeliness is still problematic (results become available after 09:00 most of the time, while 09:00 is targeted). o Simulated ozone exhibits a strong positive bias (see Figure 1.2-6). An assessment of the phtochemistry scheme has revealed problems with the numerics of the chemistry calculations. This is currently being remedied by implementing another scheme (which has already shown a lower bias) in the AURORA model. After further testing this new scheme will be implemented in the operational AURORA version (Fall 2008).			
VALIDATION AGAINST USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Product	Air pollution alert and detailed forecasting for O3, NO2, PM10, CO and SO2		
Accuracy	nx10%	n.s.	O3: 30-70 % NO2: 25-80 % PM10: 30-60 % PM2.5: 40-80 %
Accuracy minimum	n.s.	EU's Daughter Directives ambient [Please indicate here and Air Quality framework (92/62/EC) *30%*	50 % on daily maxima (O3) and mean (NO2, PM10, PM2.5) values
Accuracy target	n.s.	*5%*	10-20 % for gases and 30-40 % for particles
Spatial coverage	Belgium with zoom on Antwerp, Brussels, Ghent,	Belgium: Antwerp	Antwerp, Brussels,

	Liege and Charleroi	*Antwerp, Ghent, Brussels; Charleroi, Liege*	Liège Belgium
Horizontal resolution	5x5 Km2 (Belgium) 1x1 Km2 (Cities) 20-50 m (Antwerp)	5X5 Km^2 to 1x1 Km^2 P2: Daily forecast for Belgium & Antwerp P2: Daily forecast for Belgium & Antwerp, Brussels, Charleroi, Ghent and Liège. P3: Street level resolution for one city	1 km (Antwerp, Brussels, Liège) 5 km (Belgium)
Vertical resolution	n.s.	n.s.	20 m near the surface
Grid/Projection	Cartesian grid in Lambert projection	*UTM; EURAD; Georeferenced*	Cartesian grid in Lambert projection
Temporal coverage	48 h	48 h - *72 h*	48 h
Temporal resolution	n.s.	1 h	1 h
User Interfaces			
PROMOTE Web	n.s.	Complete, operational and up-to-date	operational
ftp	n.s.	automated	n.a.
On demand	n.s.	n.s.	available daily
Data formats and data delivery			
Data availability	From 12 March 2007 on	09:00 a.m. local time	daily, delivery time varies between 09:00 and 14:00 – timeliness is still an issue
Data access	Online	Online, ftp	online
Delivery Mode	NRT	NRT	NRT
Delivery frequency	24 h	24 h	24 h

Data Format	HDF, PNG	*e.g.* HDF, geoTIFF, TXT, JPG, PNG, GIF *SMS, Bulletins and warning systems, ASCII*	PNG
Historical archive	Data have been archived since April 2007	*Daily archiving of full 3D Datasets*	daily archive 3D data sets
Visualization	To be defined with User	*Maps, Images*	maps with ground-level concentrations
REMARKS			
None			

Table 1.2-6 Validation against specifications and against user requirements for the Air Quality Forecast for Belgium and Belgian Cities Sub-service

1.2.5 Quality assessment and control procedures

Service Quality				
Service delivery start date: Phase 1 (though new elements added in phase 2)				
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**	**N checks/Delivery period °** **entire Phase 2**
Quality checks	To be defined with user	*yes*	daily graphs model vs. observation for preceding 2 days	checked daily
Product confidence data	n.s.	*95%*	N/A	N/A
Error bar definition and representation	N/A	*EURAD; 2 std*	N/A	N/A

Representation of missing data	In case of process failure the missing data are indicated with '-999' in the output data, no further data processing takes place.	*-99.99 or similar value < 0; Interpolated; as EURAD; colour in maps*	N/A	a forecast is either complete (no missing data) or else completely missing (in which case no results are shown)
Documentation of process failure	Every month a summary is made of the percentage of process failures and the cause of failure. Some failures cannot be circumvented (e.g. no delivery of EURAD boundary conditions). Some issues giving rise to process failure in the course of Phase 1 are being met now.	*n.s.*	archived	daily

Version control mechanisms and representation	P2: 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.	*Product version number and last date of modification to be available in background*	P1: N/A	update whenever a new version is to be implemented (variable frequency)

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

°Between 1st March and 30th of May.

Table 1.2-7 Quality assessment and control procedures for the final products of the Air Quality Forecast for Belgium and Belgian Cities Sub-service

1.2.6 References

1.2.6.1 Electronic references and online data access paths

URL01 http://www.irceline.be/~celinair/english/homeen_java.html (click on 'Air Quality' – 'Stations' – 'Location')

URL02 http://ec.europa.eu/environment/air/existing_leg.htm

URL03 http://www.fsm.it/padova/homepage.html

URL04 http://www.vito.be/bugs/deliverables.htm

URL05 http://www.eurad.uni-koeln.de/index_e.html (select 'Analysis' - 'Germany')

1.2.6.2 Bibliographic references

De Ridder, K., 2000: Remote sensing of parameters that regulate energy and water transfer at the land-atmosphere interface. *Physics and Chemistry of the Earth,* **25**, 159-165.

De Ridder, K., and F. Lefebre, 2003. Benefits of urban green space – regional air quality simulations. Deliverable 13, EVK4-CT-2000-00041 (BUGS), available from URL04.

De Ridder, K., F Lefebre, S Adriaensen, U Arnold, W Beckroege, C Bronner, O Damsgaard, I Dostal, J Dufek, J Hirsch, L IntPanis, Z Kotek, T Ramadier, A Thierry, S Vermoote, A Wania, C Weber, 2008. Simulating the impact of urban sprawl on air quality and population exposure in the German Ruhr area. Part I: reproducing the base state. *Atmospheric Environment*, in press.

Maes, J., J. Vliegen, K. Van de Vel, S Janssen, F Deutsch, K De Ridder, C Mensink, 2008. Spatial surrogates for the disaggregation of CORINAIR emission inventories. *Atmospheric Environment*, submitted.

Mensink, C., 2000. Validation of urban emission inventories. *Environmental Monitoring and Assessment,* **65**, 31-39.

Mensink, C., I. De Vlieger, and J. Nys, 2000. An urban transport emission model for the Antwerp area. *Atmospheric Environment*, **34**, 4595-4602.

Mensink, C., Janssen L. and Bomans B., 2001. An assessment of urban VOC emissions and concentrations by comparing model results and measurements, *Int. J. Environment and Pollution*, Vol. **16**, Nos 1-6, pp. 345-356.

Thunis, P., S. Galmarini, A. Martilli, A. Clappier, S. Andronopoulos, J. Bartzis, M Vlachogianni, K. De Ridder, N. Moussiopoulos, P. Sahm, R. Almbauer, P. Sturm, D. Oettl, S. Dierer, H. Schluenzen, 2003. Mesocom: an inter-comparison exercise of mesoscale flow models applied to an ideal case simulation. *Atmospheric Environment*, **37**, 363-382.

Van den Bossche, G., V. Vandenberghe, O. Thas, P. Vanrollegem, 2007. Validatie van het VLOPS model 1.2. Eindrapport, Universiteit Gent, 31 January 2007.

1.3 Zeeland air quality forecast

Service description

This service delivers daily air quality forecasts for the Province of Zeeland, the Netherlands. The forecasts provide concentration information for 9 chemical constituents. Forecast results are presented as concentration charts, currently every 3 hours and hourly upon request. The forecasts are computed twice per day, for a period of 48 hours into the future.

Service is/will be operational since/after:

April 2007, with archived data available starting in December 2007.

Research partners: -

Provider(s): ARGOSS

Validation contact: Hein Zelle <zelle@argoss.nl>

1.3.1 Product characterization table

The products of this subservice are concentration charts, once chart per chemical constituent, every 3 hours. The products are made accessible through a website which allows the user to select the forecast time. Charts for each constituent are then shown in table form, an enlarged chart is shown when a constituent is selected.

The constituents (PM10, PM2.5, NO2, NO, O3, CO, CH4, NH3, SO2) Are not listed separately in the table below. When there is constituent-specific information available, this is mentioned in the table.

Concentration charts for species PM10, PM2.5, NO2, NO, O3, CO, CH4, NH3, SO2	
Parameter	PM10, PM2.5, NO2, NO, O3, CO, CH4, NH3, SO2
Typical range	Ranges 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 to conform to standards in use by the user. 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 literature 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.

Table 1.3-1 Characterization of the products provided by the Zeeland air quality forecast subservice

1.3.2 Validation plan and validation data

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 (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 provided as daily averages. *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)/orbits:* Swath width = 2600 (OMI), viewing zenith angle at end of the swath = 57 degree *Accuracy:* NO2 column : typical 30-40 % (OMI and SCIAMACHY)

Table 1.3-2 Data used for the validation for the Zeeland air quality forecast subservice

1.3.3 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 a fixed period of forecasts).

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 (See the Zeeland air quality analysis subservice in the Urban air quality analysis service). This information can be made available upon request.

The numbers made available in table 1.3-4 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. This report will be made accessible as part of both the analysis service and the forecast service for Zeeland.

VALIDATION OF INDIVIDUAL COMPONENTS	
Quality assessment	
Comparison of 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.
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.
MODELS/ALGORITHM/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 analysis has been performed for forecast lead times of 0-48 hours. The numbers reported here are based on a 6 hour forecast lead time.
	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
CHIMERE	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. The validation is based on hindcast (*not forecast*) data, as the available data period with the latest model version is too short, and there is no matching observation data available. In phase 3 the validation will be expanded using forecast model data compared with newly available observation data for April-June 2008.
	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 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
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.
Consistency	
WRF vs KNMI SYNOP	**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)
CHIMERE vs RIVM LML observations	**O3:** RMSE = 20.9 µg/m3, MAE = 15.8 µg/m3, MB = -6.0 µg/m3 **PM10:** RMSE = 19.9 µg/m3, MAE = 12.9 µg/m3, MB = 7.5 µg/m3 **NH3:** RMSE = 3.6 µg/m3, MAE = 2.3 µg/m3, MB = -0.5 µg/m3 **NO:** RMSE = 18.1 µg/m3, MAE = 7.4 µg/m3, MB = 2.9 µg/m3 **NO2:** RMSE = 17.4 µg/m3,

	MAE = 12.8 µg/m3, MB = -5.0 µg/m3 **SO2:** RMSE = 11.1 µg/m3, MAE = 7.8 µg/m3, MB = -5.2 µg/m3

Table -1.3-3 Validation of the individual components of the Zeeland air quality forecast subservice

1.3.4 Validation against specifications and against user requirements

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

VALIDATION AGAINST SERVICE SPECIFICATIONS			
No limitations/delays for compliance between theoretical and actual service specifications reported			
VALIDATION AGAINST USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Product	Forecast concentration charts for Ozone (O3), nitrogen dioxide (NO2), nitrogen monoxide (NO), sulphur dioxide (SO2), carbon monoxide (CO), methane (CH4), ammonia (NH3), fine dust (PM10, PM2.5)		
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.	See results in table 1.3-3 under "Consistency"
Accuracy minimum	n.s.	*30%*	N/A
Accuracy target	n.s.	*5%*	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
Horizontal resolution	1x1 Km^2	1x1 Km^2	As specified in S5
Vertical resolution	n.s.	n.s.	Only surface data are part of the product, 10 model layers are

			available.
Grid/Projection	Lambert	*UTM; Georeferenced*	The Netherlands: Lambert projection (conical) with 4 km resolution. Zeeland: Lambert projection (conical) with 1 km resolution
Temporal coverage	48 hours from forecast start	0 h – *72 h*	As specified.
Temporal resolution	24 h	1 h	Currently 3 hourly, hourly charts can be provided upon request.
Outputs	Instantaneous Concentration charts	*1h, 8h, 24h running average and maxima*	Hourly averages and 8/24h running average and maxima will be made available in phase 3.
User Interfaces			
PROMOTE Web	n.s.	Complete, operational and up-to-date. Public access during evaluation phase with user approval. *Freely accessible.*	Complete, operational. The forecast results can be accessed upon request (password protected). The full validation report will be made available, expected 06 2008.
ftp	n.s.	n.s.	N/A
On demand	Yes	n.s.	Yes
Helpdesk par e-mail	Yes	Yes	Yes
Data formats and data delivery			
Data availabilty	Approximately 8-9 hours after forecast start time. Once per day. When sufficient computation power is available (based on circumstances) the forecast can be provided twice per day.	Data remains available for 48 h after forecast provided	Data has been delivered twice per day for the period April 2008 – present. Available time as specified.

Data access	Online/Offline	Online/Offline	Online, archive kept offline
Delivery Mode	NRT	NRT	NRT
Delivery frequency	24 h	24 h	12 h, provided sufficient computer power is available.
Data Format	Charts in PNG format	Html, reports, maps, charts in ESRI- or MRSid-	Charts in PNG format
Historical archive	Selected model output data and all forecast charts are archived for the period January 2008 – May 2008. A rolling archive of 5 months will be kept afterwards.	Analysis for a 5 years period AQ forecast for at least 48 hours (previous)	Selected model outputs and all forecast charts have been archived from January 2008 – present.
Visualization	charts are produced using the open-source software package “Ferret”. Charts are presented using a regular lat/lon projection, with interpolated color-levels and a colorbar linking colors and data values. Charts are delivered to the user on a website.	Charts	As specified in S5. In phase 3 visualization in the User’s GIS system will be provided.
REMARKS			
None			

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

Table -1.3-4 Validation against specifications and against user requirements for the Zeeland air quality forecast subservice

1.3.5 Quality assessment and control procedures: Service quality

Service delivery start date: n.s.

SPECIFICATION	S5	REQUIRED*	ACTUAL	N checks/Delivery period °
Quality checks	n.s.	Yes	Yes, input data (meteo) and output data (chemistry concentration charts) are regularly inspected visually.	Approximately twice per week.
Product confidence data	n.s.	*95%*	N/A	n.a.
Error bar definition and representation	RMS error of concentration (model compared to observations)	*EURAD; 2 std*	As specified in S5	n.a.
Representation of missing data	Missing data is typically caused by a process failure, and is tracked in the same log document which is made available to the user on a regular basis.	*-99.99 or similar value < 0; Interpolated; as EURAD; color in maps*	Missing data is either specified as “white” in charts, or as “no image available” when the forecast result is not completed yet.	n.a.
Documentation of process failure	Process failures can include technical problems (storage full, network failure) or problems in boundary condition delivery (weather forcing data, chemistry boundary conditions). Such	n.s.	As specified in S5, tracked in a log. An automatic warning system is in place which notifies the operator of failures to	3 process failures have occurred between January 2008 – present.

	failures are tracked in a log document by the service provider. This document is made available on a regular basis to the user.		enable quick recovery in case of process errors.	
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.	*Product version number and last date of modification to be available in background*	Latest product version: 1.0.2, 20-May-2008 Versions before this date contained model instabilities with results that were often unreliable.	3 versions: 1.0 (01-April-2008), 1.01 (8-April-2008) and 1.02 (20-May-2008)

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

Table -1.3-5 Quality assessment and control procedures during the Zeeland air quality forecast subservice provision

1.3.6 References

1.3.6.1 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

1.3.6.2 Bibliographic references

-

1.4 YourAir Local pollution forecast for London (airTEXT service), Budapest, Vienna and Vilnius

Description: YourAir provides ultra-high (circa 7.5m) resolution air quality forecasts using a combination of local data on traffic patterns, weather forecasts and PROMOTE's European regional forecasts of atmospheric composition. In addition the system allows air quality alerts to be broadcast by email and SMS text messaging (AirTEXT).

Service is/will be operational since/after:

Research partners:

Service Provider(s): CERC

Validation Contact:

1.4.1 Product characterization table

O3	
Parameter	Daily maximum of the hourly mean gridded O_3 over the domain, expressed as an air quality index (AQI – see later).
Typical range	20-300ug/m^3
Determination of the typical range (Method, criteria)	Statistical analysis of historic data by UK Department of the Environment Photo-oxidants Review Group (1997).
Units	ug/m^3
Standards	
NO2	
Parameter	Daily maximum of the hourly mean gridded NO_2 over the domain, expressed as an air quality index (AQI)
Typical range	20-500ug/m^3
Determination of the typical range (Method, criteria)	Statistical analysis of historic data by UK Department of the Environment Air Quality Expert Group (2004).
Units	ug/m^3
Standards	
PM10	

Parameter	Daily mean of the gridded PM_{10} over the domain, expressed as an air quality index (AQI).
Typical range	5-100ug/m^3
Determination of the typical range (Method, criteria)	Statistical analysis of historic data by UK Department of the Environment Air Quality Expert Group (2005).
Maximum range	5-100ug/m^3
Units	ug/m^3
Standards	Gravimetric measurement provide the standard.
CO	
Parameter	Daily maximum 8 hour mean
Typical range	0-3mg/m^3
Determination of the typical range (Method, criteria)	Historic data
Maximum range	
Units	mg/m^3
Standards	
Total Health Index	
Parameter	
Typical range	
Determination of the typical range (Method, criteria)	
Maximum range	
Units	
Standards	

Table 1.4-1 Characterization of the products provided by YourAIR for AirTEXT

1.4.2 General validation plan and validation data (Phase 1 plan)

Phase 1: Preliminary validation estimate is carried out by completing resimulations of the system for the period 5/5/05 – 31/3/07 using forecast meteorology and chemical boundary conditions for the periods concerned, and measurements at the observation stations within the model domain for the parameters A_1 and E_1 (see below).

Phases 2 & 3: Validation continues by automatic calculation of validation statistics based on yesterdays data. These are reviewed monthly. System extended to 2 day forecasts if parameters A_2 & E_2 both above 65%.

PARAMETERS USED TO DETERMINE THE ACCURACY OF THE COMPLETE YOURAIR SYSTEM	
For each receptor within the forecast domain:	
A_1	Proportion of alerts issued correctly for tomorrow = total number of correct alerts issued / total number of alerts issued
E_1	Proportion of episodes correctly forecast for tomorrow = total number of episodes forecast / total number of episodes observed
A_2	Proportion of alerts issued correctly for the day after tomorrow = total number of correct alerts issued / total number of alerts issued
E_2	Proportion of episodes correctly forecast for the day after tomorrow = total number of episodes forecast / total number of episodes observed

An **episode** is defined as observations at a measurement station breaching any of the thresholds from the **Air Quality Index Banding** (see reference [3] for details):

Units of ug/m³	***MODERATE threshold >=***	***HIGH threshold >=***	***VERY HIGH threshold >=***	***Averaging time***
Ozone	100	180	360	1 hour
Nitrogen Dioxide	287	573	764	1 hour
PM_{10}	50	75	100	24 hours

A correct forecast is defined as the forecast predicting values within the bands observed during the period of the forecast and the system broadcasting the alert.

VALIDATION DATA	
Ground based observations	
Ground-based observations London: AURN/LAQN Budapest: in-situ network	Data availability and access: London – online, Budpest – by arrangement. Spatial coverage and resolution: London: 33 measurement site in four classes for London. Temporal coverage and resolution: point measurements, hourly since 1998. Location(s) (coordinates): see e-reference [1] Accuracy: unknown, but based on UK/EU reference standards.
Model outputs	
ADMS-Urban 2.2	Data availability and access: online Spatial coverage and resolution: Parameters specified in Table 1.8-1. Temporal coverage and resolution: Hourly data for the period 1.4.05-31.3.07 Location(s) (coordinates)/computational domain: Locations of LAQN stations. Accuracy: Under investigation

Table 1.4-2 Data used for the validation of YourAIR for London AirTEXT

1.4.2.1 YourAir-airTEXT Service for London and Slough

YourAir-airTEXT was officially launched across Greater London and Slough, an area of 2500km^2, on 28 March 2007. It produces daily forecasts of daily PM_{10}, maximum hourly average ozone and NO_2 for T0 - T+36. Predictions are presented as a pollution index (UK COMEAP Pollution Index) on a scale from 1 to 10 for each pollutant and a Total Pollution Index that is the maximum of the 3 pollutant indices. The forecasts are presented as very high resolution colour contour plots (circa 7.5m resolution) in GoogleMaps.

An alert is issued in a Borough if the Total Pollution Index is MODERATE (>3) or HIGH (>6) over an area exceeding 10% of the Borough. The issuing of alerts was assessed in Phase 1 by comparing the alerts issued with measured air pollution concentrations at Automated Urban & Rural Network (AURN) sites in Greater London with respect to the following parameters:

i) Proportion of alerts issued correctly for tomorrow = total number of correct alerts issued / total number of alerts issued

ii) Proportion of episodes correctly forecast for tomorrow = total number of episodes forecast / total number of episodes observed

In Phase 2 data from the LAQN monitoring sites will be used in addition to that from the AURN sites. Using the combined AURN and LAQN data the following additional measures will be assessed:

a) Percentage of daily forecasts that were accurate (defined as the predicted concentration of a pollutant at the receptor point being ± 1 UK air quality index (1-10) of the index in which the receptor measurement falls).

b) Number of alerts that were issued for the incorrect air quality banding as a percentage of the total number of alerts.

c) Percentage of daily forecasts that were accurate (defined as the predicted concentration of a pollutant at the receptor point being within the same UK air quality index as that measured at the receptor).

d) Percentage of daily forecasts that were inaccurate (defined as the predicted concentration of a pollutant at the receptor point being more than ± 1 UK air quality index compared with the index measurement at the receptor).

e) Percentage of daily forecasts that were inaccurate (defined as the predicted concentration of a pollutant at the receptor point being outside the UK air quality index measured at the receptor).

f) A comparison of the absolute pollutants concentrations predicted and measured at receptor locations.

1.4.2.2 YourAir-Viennair Service for Vienna

The Service in Vienna is expected to be installed and to start its 6-month intensive validation period in operation by the end of June 2008. Before the 6-month validation period the emissions inventory and model set-up will be validated for the last full year for which meteorological and ambient monitoring data are available.

Historical validation for emissions inventory & model set up
The emissions inventory will be supplied by City of Vienna and collated in the EMIT model (Emissions Inventory Toolkit). Attention will be paid to characterising the diurnal, monthly and seasonal variation in emissions and the variation with known special events e.g. public holidays, European Championship. From EMIT the emissions data will be exported to the ADMS-Urban dispersion model. For the historical validation the model inputs will be: the emissions inventory, ambient monitoring data from a rural site and meteorological data recorded by the Austrian Meteorological Service. The model output will be hourly concentrations of the pollutants of interest (to be finalised) at ambient monitoring locations in the City.

The predicted hourly concentrations will be compared with ambient monitoring data at each monitoring location and a statistical analysis carried out:

<u>Set of measures (1)</u>

- Mean
- Standard deviation
- Bias
- Normal mean squared error
- Correlation

- Fraction of modelled within a factor of 2 of observed

The model predictions will then be further compared with the ambient observations on the basis on which the predictions are to made and alerts issued. These are to be finalised but might include:

Set of measures (2)

- Comparison of the daily maximum hourly average concentration for NO_2 and ozone
- Comparison of the daily average concentration of PM_{10}
- Comparison of pollution indices
- Comparison against the alert threshold

Intensive validation in operation

During the intensive validation phase the model inputs for ambient rural background and meteorological data will be forecast values. Near real time ambient monitoring will be available as an additional model input.

There will be a weekly analysis of the predictions against Set of measures (1) and a monthly analysis against Set of measures (2).

1.4.2.3 YourAir Service for Vilnius

The Service in Vilnius is likely to start its 3-month intensive validation period in operation 6 weeks after the SLA is signed (expected to start in operation at the beginning of June 2008). The methodology for historical validation of the emissions inventory and model set up and the validation during the intensive validation period will be similar to the methodology used for Vienna.

VALIDATION DATA	
Ground based observations	
Name LONDON AURN Phase: 1+2	Data availability and access: On-line www.airquality.co.uk Spatial coverage and resolution: 33 measurements sites in four classes. Temporal coverage and resolution: Point measurements, 15-minute averages since 1998. Location(s) (coordinates): See UK automatic monitoring network archive: www.airquality.co.uk Uncertainty quantification (e.g. Accuracy): Unknown but based on UK/EU reference standards.
Name LONDON LAQN Phase: 2	Data availability and access: On-line http://www.londonair.org.uk/ Spatial coverage and resolution: Temporal coverage and resolution: Hourly averages. Location(s) (coordinates): See http://www.londonair.org.uk/

	Uncertainty quantification (e.g. Accuracy): The monitoring sites are operated by individual local authority boroughs within London, different boroughs have different operational policies. Information on each site is available from http://www.londonair.org.uk/
Name Vienna MA 22 air quality monitors Phase: 2	Data availability and access:On application Spatial coverage and resolution: 17 monitoring stations in Vienna Temporal coverage and resolution: Hourly averages. Location(s) (coordinates): See http://www.wien.gv.at/umweltschutz/luft/messnetz.html Uncertainty quantification (e.g. Accuracy):Unknown but based on EU reference standards.
Name Lithuanian monitoring network Phase: 2	Data availability and access:Online http://gamta.lt Spatial coverage and resolution: 13 monitoring stations Temporal coverage and resolution: Hourly averages Location(s) (coordinates): See http://gamta.lt Uncertainty quantification (e.g. Accuracy):Unknown

Table 1.4-3 Data used for the validation of all the products of this service/sub-service

1.4.3 Validation of individual components

Validation of individual components will only take place for the forecasts data (both meterological and chemical) used as boundary conditions and inputs to the ADMS-Urban model. We will use the validation data provided by the suppliers of these components for this purpose, a significant preparation of which already lies within the purview of the PROMOTE validation scheme.

VALIDATION OF INDIVIDUAL COMPONENTS	
Uncertainty estimators	
Mean	N/A
Standard deviation	N/A
Fractional bias	N/A
Fractional within factor of 2	N/A
Normal mean square error	N/A

Correlation	N/A
MODELS/ASSIMILATION	
MeteoGroup Meteorology	Validation performed by MeteoGroup
ADMS-Urban (2.2)	N/A
EURAD & PREVAIR synthesized data	N/A
Consistency	
ADMS Urban vs AURN	N/A
Alert issued vs. alert recorded (London)	N/A
Prediction vs. UK AQI Bands	N/A

Table 1.4-4 Validation of the individual components of YourAIR London

1.4.4 Validation against specifications and against user requirements of YourAir for London airTEXT service

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

VALIDATION AGAINST SERVICE SPECIFICATIONS			
No limitations/delays for compliance between theoretical and actual service specifications reported			
VALIDATION AGAINST USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Product	Air pollution alert and detailed forecasting system for ozone, nitrogen dioxide, pm10, co, Total Health Index		
Accuracy	P1: 70-95% for AQ Index; Alerts estimated 80% Accurate in 2005 P2: Varies from point to point 70-95% for AQI. Alerts estimated 75% Accurate in 2007	Daily forecast with 99.7% reliability **Good" level** A_1 >= 75%, E_1 >= 75%.	P1: From Ref [12] (Run 3) A_1 = 68%, E_1 = 64% as initial estimates at one station.
Accuracy minimum	n.s.	*30%*	P1: **Minimum acceptable level** A_1>=65%, E_2>=65%.
Accuracy target	n.s.	*5%*	P1: Awaiting from user
Spatial coverage	London (70x50km^2)	Greater London	P1: Greater London (70x50km^2)
Horizontal resolution	Irregular 50-10 m resolution varying with source density	Down to 6x6 m	P1: 7.5m grid
Vertical resolution	n.a.	n.a.	n.a.
Grid/Projection	Mercator	n.s.	P1: Irregular mesh of resolution 5m-30m following street geometry, interpolated to a regular grid.

Temporal coverage	24 h	48 h - *72 h*	P1: 36 h forecast excluding CO (Agreed with users)
Temporal resolution	12 hours	24 hours	P1: 24 hours
User Interfaces			
Public WWW	www.airtext.info	www.airtext.info operational	www.airtext.info operational
PROMOTE Web	n.s.	Operational, complete and up-to-date	http://www.gse-promote.org/ services/ aq_YourAir/ YourAir.html
ftp	n.a.	n.a.	ftp.airtext.info
Voicemail	n.a.	no	P1: Available for episode alerts
e-mail alerts	Available for episode alerts	Available for episode alerts	P1: Available for episode alerts
SMS	Available for episode alerts	183/year daily forecasts including up to 60 alerts for a max of 500 recipients per borough *365/year daily forecasts including alerts*	P1: Available for episode alerts
Data formats and data delivery			
Data availability	Since March 28th 2007	+	
Data access	Online	Online	P1: Operational
Delivery Mode	NRT	NRT	NRT
Delivery frequency	12 h forecast /alerts on event	Daily (7 a.m.-7 p.m.)/on event	P1: Daily (7 a.m.-7 p.m., timing agreed with user)/on event

Data Format	Online Contour maps as png integrated with Google Maps map serverMaps, SMS, e-mails, voicemail	Maps, SMS, e-mail	P1: Maps, gridded data if requested, SMS, voicemail, e-mail
Historical archive	Available on-line from March 28, 2007	n.s.	P1: From 28.3.2007, online.
Visualization	GoogleMaps adapted for use by colour blind individuals or screen readers. Currently there is an option to read the forecasts as text. Development is almost complete of a text-only option for the whole web site following guidelines on font and colour for users with a visual impairment.	*Maps*	P1: Online maps provided using zooming interface.
REMARKS			
No remarks			

Table 1.4-5 Validation against specifications and against user requirements for YourAIR London

1.4.5 Quality assessment and control procedures

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

Service Quality				
Service delivery start date: n.s.				
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**	**N checks/Delivery period °**
Quality checks	Manually against hourly measurements	*yes*	Accuracy currently determined manually, automatic to be introduced in Phase 2. Change management process requires request-review-test cycle before documentation.	n;s.
Product confidence data	n.s.	*95%*	N/A	N/A
Error bar definition and representation	N/A	*EURAD; 2 std*	N/A	N/A
Representation of missing data	Emails to operators are automatically generated if the EO data or met data are not available on time.	*-99.99 or similar value < 0; Interpolated; as EURAD; colour in maps*	-999; where data missing in maps, this is indicated by the colour WHITE.	n.s.

Documentation of process failure	For the calculation process emails to operators are automatically generated giving a description of the point at which the system has failed.	*n.s.*	When a failure occurs a preliminary investigation takes places within 1 working day and the details of this are logged for further investigation later. These are then given six monthly reviews as part of the system update process.	n.s.
Version control mechanisms and representation	The ADMS-Urban code and Forecasting System code are version controlled using MKS (Mortice Kern Systems) software. Changes to the software are controlled by a QA system of Change Requests and Technical Reports..	*Product version number and last date of modification to be available in background*	MKS	n.s.

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

°Between 1st March and 30th of May.

Table 1.4-6 Quality assessment and control procedures

1.4.6 References

1.4.6.1 Electronic references and online data access paths

Archive of forecast maps www.airtext.info
UK automatic monitoring network archive: www.airquality.co.uk
London Air Quality Network: www.londonair.org.uk

Vienna MA 22 air quality monitoring network
www.wien.gv.at/umweltschutz/luft/messnetz.html
Lithuanian monitoring netVilnius http://gamta.lt

1.4.6.2 Bibliographic references

References regarding validation of ADMS-Urban model

1) I.J. Kilbane-Dawe, S. Potter (2007), First Results from Croydon airTEXT, Proceedings of the ESA Montreux symposium, April 2007.
2) CERC (October 2003), Modelling Air Quality for London using ADMS-Urban, TOPIC REPORT Prepared for DEFRA, National Assembly for Wales, The Scottish Executive, and the Department of the Environment, Northern Ireland http://www.airquality.co.uk/archive/reports/cat12/final_doc.pdf
3) CERC (January 2003), Validation and Sensitivity Study of ADMS-Urban for London, TOPIC REPORT Prepared for DEFRA, National Assembly for Wales, The Scottish Executive, and the Department of the Environment, Northern Ireland www.airquality.co.uk/archive/reports/cat09/Validation&Sensitivity(22JAN03)10_TR-0191-h.pdf
4) CERC (2001) ADMS-Urban Technical Specification. Cambridge Environmental Research Consultants Ltd., 3 Kings Parade, Cambridge, CB2 1SJ
5) CERC (2001a) Validation of ADMS-Urban and ADMS-Roads Against M4 and M25 Motorway Data, Cambridge Environmental Research Consultants Ltd.
6) CERC (2001b) Validation of ADMS-Roads Using the Caltrans Highway 99 Data Set, Cambridge Environmental Research Consultants Ltd.
7) CERC (2001c) Comparison of ADMS-Roads, CALINE4 and UK DMRB model, Cambridge Environmental Research Consultants Ltd.
8) Carruthers, D. J., Dixon, P., McHugh, C. A., Nixon, S. G. and Oates, W. (2001) Determination of Compliance with UK and Air Quality Objectives From High Resolution Pollutant Concentration Maps Calculated Using ADMS-Urban. Proc of the 6th Workshop on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, in Intl. J. of Environment and Pollution, 16, Nos. 1-6
9) Carruthers, D. J., Edmunds, H. A., Lester, A. E., McHugh, C. A. and Singles, R. J. (1998) Use and Validation of ADMS-Urban in Contrasting Urban and Industrial Locations. Intl. J. Environment and Pollution, 14, 364-374
10) McHugh, C. A., Carruthers, D. J. and Edmunds, H. A. (1997) ADMS-Urban: an Air Quality Management System for Traffic, Domestic and Industrial Pollution. Int. J. Environment and Pollution 8, 437-440.

1.5 Aircast Air Quality Data for Lisbon

1.5.1 Sub-Service Summary

The Aircast Service is aimed at the integration of statistical models, geostatistical and multi-regression methods and remote sensing algorithms in an operational web based service platform that delivers optimized forecast and monitoring daily maps of observations and forecasts of PM and other atmospheric pollutants. The Urban Air Quality Forecast Sub-service will provide Level 1 point and zone average 1-day forecast of O3 and PM10 for the Lisbon Metropolitan Area. Level 2 will include, for the same geographic region, PM10 forecast spatialized patterns based on the Level 1 product and multiregression spatial modelling. This next day forecast was created and implemented by DCEA/FCT/UNL for Lisbon Metropolitan Area and will be available for the whole country during this year. It is based on statistical models applying the 'Classification and regression trees - CART' method to construct the multiple regression models called PrevQualar. For each station, a model was developed based on empirical relationships between each pollutant concentration and meteorological variables (using historical datasets from ground air quality and meteorological stations). In an operational basis this modelling system uses the pollutant data from the day before and the predictions given by ECMWF for the key meteorological parameters (maximum, minimum and average temperature, mean relative humidity, dew point average temperature, number of sun hours pressure difference between stations, atmospheric vertical profile (only for Lisbon), geopotencial height and temperature at 1000,925,850,700,500 hPa) defined in the model to generate the forecast for the next day for each ground monitoring station. These point daily concentrations forecast will then be spatialized using a spatial modelling method that combines geostatistics 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 to generate air pollutants spatial patterns.

Service is/will be operational since/after:

Phase 2 Level 1 Product – September 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

Service is/will be operational since/after:

Research partners: -

Provider(s): Validation contact:

1.5.2 Product characterization

Portuguese air quality recordsforecast	
Daily hourly maximum or global index, O3 hourly maximum, NO2 Hourly maximum, etc.	
[Daily air quality index – next day forecast]	
Parameter [give name]Parameter [give name]	Daily Air Quality Index (global and for PM_{10}; O_3) As defined by the user in: http://www.prevqualar.org/indices.do [Name of the parameter or physical quantity, measured property or parameter chosen to represent the product named above.]
Typical rangeTypical range	Global: 1-5 Very good to bad PM_{10}: 10 to 70 O_3: 5 to 100
Determination of the typical range (Method, criteria)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 O_3: 0 to >240
Units Units	For global index is qualitative(very good to bad or 1 to 5) For the pollutants is $\mu g\ m^{-3}$
StandardsStandards	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

Table 1.5-1 Characterization of the products provided by the Local Forecast AQ service for Lisbon

1.5.3 Validation plan and validation data

The Aircast service is composed of four levels of products aimed at the integration of statistical models, geostatistical and multi-regression methods and remote sensing algorithms in an operational web based service platform that delivers optimized forecast and monitoring daily maps of observations and forecasts of PM and other atmospheric pollutants.

The validation plan described bellow refers to the products included in Level 1 scheduled to be delivered by the end of Phase 2 of PROMOTE. This document is divided into forecast and monitoring products since each present a different quality control/quality assurance or validation methodology and includes information on input data quality, product accuracy and reporting.

All the information in this document will be presented in a report to be delivered annually to the user (Portuguese Environmental Agency) and will be available in the project website. 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.

Level 1

Monitoring

Monitoring Level 1 products include 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).

The calculated parameters are directly based on ground observations so no validation plan is required. Nevertheless some Quality Assurance/Quality control (QA/QC) procedures are defined to assure the usefulness and consistency of the calculated parameters. Such procedures are applied in the several steps towards the calculation of the defined parameters:

1) Raw pollutant concentration data collection

All data (raw data and statistics) transmitted to the Commission are considered to have undergone the validation and quality assurance/quality control procedures implemented by the Member States according to their own methods and procedures and so to be valid.

Within those procedures the following is included according to European Legislation

- Approval of the measuring devices (methods, equipment, networks, laboratories),
- Ensuring accuracy of measurement by measuring devices and checking the maintenance of such accuracy by those devices, in particular by internal quality controls carried out in accordance, inter alia, with the requirements of European quality assurance standards.

For Portugal all this information is already overseen and compiled by the Portuguese Environmental Agency and the Commission of Coordination and Regional Development and its validation is therefore outside the scope of Aircast.

2) Data aggregation and Calculation of statistical parameters

The aggregation of raw data and the calculation of statistical parameters must comply with quality criteria established on air quality Directives. All those criteria are described bellow and will be compiled in annual reports to Environmental Portuguese Agency and in tables to be included in the Aircast web portal and updated whenever new data is available. Although data for all years is available through the web portal, the current year data is not yet validated (validation is made annually by regional authorities until March of the next year).

Criteria for data capture

Data capture is the proportion (%) of a regarded period, to which valid values can be assigned. The extreme values of data capture are 0 % (no valid data) and 100 % (no missing value either not measured or not valid). It is calculated as ratio of the valid values measured during a certain period and the maximum of values that might have been measured during that period.

The minimum data capture required for continuous measurements of particulate matter is 90%.

The requirements for minimum data capture do not include losses of data due to the regular calibration or the normal maintenance of the instrumentation. A rough estimation could be applied: calibration cycle of one hour per day plus normal maintenance of the instrumentation assumed to take 10 days per year. Thus a device caused data loss of up to 6,9 % is possible.

Therefore it is accepted an 85 % minimum data capture, related to the whole year, including losses due to calibration and maintenance.

Criteria for the aggregation of data

These criteria are applicable for the calculation of one-hour and 24-hour values from data with a smaller averaging time.

To get the values for these recommended averaging times, it might be necessary to aggregate data (as presented in Example 1). In that case, the criteria on data capture described in Annex IV of Decision 2001/752/EC have to be fulfilled.

- Calculation of one-hour values: for one-hour values the minimum data capture is 75 %.
- Calculation of 24-hour values: this calculation is based on one-hour values, either sampled or calculated. For the calculation of 24-hour values at least 13 one-hour values (54,2 %) are necessary (minimum data capture), with a maximum of six successive one-hour missing values (maximum data capture gap).

Criteria for the calculation of statistical parameters

For those Member States who transfer statistics the following statistics are required: arithmetic mean, median, percentiles 98, and maximum, calculated from raw data corresponding to the recommended averaging times. It is suggested to perform data treatment on data which are considered as valid according to the QA/QC procedures followed in the Member State.

Criteria on data availability required for computing the statistics are expressed in Annex IV of the Decision. Annex IV of 2001/752/EC defines different criteria for, on the one hand, mean and median and, on the other hand, for (higher) percentiles and maximum. In addition to these criteria, a ratio between data capture in winter and data capture in summer is defined. Statistical parameters are calculated for the period of one year (their calculation is described in Annex I of 2001/752/EC).

The criteria established for the calculation of statistical parameters are as follows:

Calculation of mean and median:

since the percentile 50 is – like the mean – statistically more stable, the minimum data capture is – differing from the higher percentiles – only 50 %.

Calculation of (higher) percentiles and maximum:

the calculation of parameters with a lower statistical stability requires a higher data capture. The minimum data capture is defined as 75 %.

Minimum data capture requirement in relation to the seasons:

to avoid the calculation of statistical parameters on the basis of data with an uneven distribution of missing values, the following criterion has to be fulfilled in any case.

The possible “error” is larger for pollutants with a significant yearly variation.

This criterion ensures that none of the two main seasons (winter and summer) is overestimated. For that reason the ratio has to be checked winter by summer and summer by winter.

The ratio between the number of valid data for the two seasons of the year considered cannot be greater than 2, the two seasons being winter (from January to March inclusive and from October to December inclusive) and summer (from April to September inclusive).

Criteria for the calculation of the Portuguese Air Quality Index

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 (PM_{10}) - daily average.

The provisory index, calculated for the current day, is referred to the data measured from 00h00 to 15h00 of that day, and is available from 18h00. The definitive Index is available from 14h00 of the next day.

The calculation of the Air Quality Index for a specific zone/agglomeration must accomplish the following rules:

- There must be at least one monitor for NO2, O3 and PM10. The existence of SO2 and CO monitors is not mandatory although, if they are measured, they are used for the index calculation.
- Data capture in one monitor must be at least 75%, for one day, for each pollutant, to be considered in the daily index, as shown in Table 1.

Table 1. Criteria for data capture in order to calculate the Portuguese Air Quality Index

Pollutant	Provisory Index (00h00 to 14h59)	Definitive Index (00h00 to 23h59)	Averaging time
	minimum data capture (hours)	minimum data capture (hours)	
NO2	11	18	hourly average concentration
SO2	11	18	hourly average concentration
O3	11	18	hourly average concentration
CO	11	18	8-hourly average concentration
PM10	11	13, with no more then 6 consecutive hours without measurements	hourly average concentration

Forecast

Forecast Level 1 products include point and zone average for 1-day forecast of O3 and PM10 for the national scale (Lisbon since 2005, Porto since 2006, all the remaining sites since 2008). This next day forecast was created and implemented by DCEA/FCT/UNL for Lisbon and Porto Metropolitan Areas and will be available for the whole country during this year. It is based on statistical models applying the 'Classification and regression trees - CART' method to construct the multiple regression models called PrevQualar. For each station, a model was developed based on empirical relationships between each pollutant concentration and meteorological variables (using historical datasets from ground air quality and meteorological stations). In an operational basis this modelling system uses the pollutant data from the day before and the predictions given by ECMWF for the key meteorological parameters (maximum, minimum and average temperature, mean relative humidity, dew point average temperature, number of sun hours pressure difference between stations, atmospheric vertical profile (only for Lisbon), geopotencial height and temperature at 1000,925,850,700,500 hPa) defined in the model to generate the forecast for the next day.

Forecast validation gives information about the quality of both forecasted air pollutants concentrations and forecasted air quality index classes. It allows the technicians to assess models performance in different situations and to improve future forecasts. For the 1-day forecast made available daily trough the Aircast web portal all the validation procedures described bellow will be presented online and compiled in an annual report to the Portuguese Environmental Agency. The validation procedures ensuring the quality of the historical dataset of air quality measurements are already described in the previous section.

The validation process of the forecasted concentrations is applied for a whole year data set of PM10 and O3 hourly concentrations using the measured values by the Portuguese Air Quality Network ground stations as independent data. Validation parameters, such as normalized mean error, absolute mean error, bias, are calculated for each air quality monitoring station. For the air quality index the validation parameters include contingency tables, accuracy, probability of detection of high pollution episodes, and false alarm rate associated with those episodes.

- Normalized mean error (%): error associated with the total number of one-day forecast performed;
- Absolute mean error: indicates the mean error associated with each forecast. Given by the sum of differences between forecasted and observed values, in module;
- Bias: Indicates, in average, if the index forecasts are being under or overestimated. Its value is given by the difference between modelled and observed values. Negative values indicate index underestimation and positives indicate overestimation;
- Contigency table: table in which each level of the forecasted index is compared with the observations
- Percentage of correct forecasts: ratio of total number of correct forecasts to total number of days for which a forecast was made;
- Detection probability: model capability to predict the index level corresponding to observed high pollution values. Example: a detection probability of level 2 of PM10=66% indicates that two thirds of the level 2 PM10 forecasts (Poor Air Quality Index – above 50 μg/m^3) were correct. It is calculated by the ratio between the days in which the forecast was right for a given index and the total number of days where such index was observed;
- Percentage of False Alarms: indicates the number of wrong forecasts for any given index level. It is given by the ratio of the number of days for which that index level was not foreseen and the total number of days for which that index level was foreseen.

VALIDATION DATA	
Ground based observations	
Name SOURCE/NETWORK Air Quality Network Ground Stations Portuguese Environmental Agency /National Air Quality	*Data availability and access (include access details if data is freely available):* Data compiled by regional authorities and freely available trough the web portal www.qualar.org *Spatial coverage and resolution*: Coverage - entire Portuguese Territory with especial emphasis for largest agglomerations and industrial complexes

Network Phase 2	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)

Name	X (meters)	Y (meters)
Circular Sul	549540.27	4599985.75
Horto	545581.99	4601838.33
Lamas de Olo	601359.31	4580651.37
Senhora do Minho	517875.61	4619797.33
Sto Tirso	543923.90	4577189.17
Guimaraes-Centro	559040.63	4589584.57
Calendario	538958.43	4582600.53
Paredes-Centro	555501.31	4562058.01
Centro de Lacticinios	552262.39	4569362.25
Vila do Conde	522147.22	4577152.14
Vermoim	531198.95	4564740.35
Espinho	530136.31	4539563.08
Vila Nova da Telh	529383.16	4566588.52
Perafita	524251.95	4564601.00
Baguim	537901.30	4559855.06
Leca do Balio	531075.17	4563321.64
Custoias	529634.94	4562096.71
Boavista	529726.82	4556393.75
Senhora da Hora	530041.28	4559542.72
Matosinhos	526884.53	4559436.25
Antas	534443.11	4557093.54
Ermesinde	537749.88	4563007.42
Águas Santas	535837.39	4562023.67
Aveiro	529760.12	4498550.28
Ilhavo	527753.42	4493400.30
Fundão (Salgueiro)	644665.29	4454692.99
Fornelo do Monte	575827.23	4499512.60
Ervedeira (Leiria	509146.80	4419393.57
Av. Fernão Magalhães	548000.53	4451833.22
Instituto Geofísica	550024.09	4451063.48
Avanca	535326.87	4517156.12
Teixugueira	535968.11	4512022.67
Liberdade	487222.21	4285715.26
Restelo	481776.49	4284158.35
Beato	490126.89	4287191.13
Entrecampos	486966.85	4288822.41
Reboleira	479929.66	4289503.32
Alfragide	481967.66	4287821.45
Casal Ribeiro	487571.42	4287046.96
Loures	485679.07	4297813.06
Mercado	463307.25	4283650.52

	Marques	471883.70	4283262.00
	Chelas	490269.12	4289373.49
	Benfica	482274.77	4289164.73
	Olivais	490619.12	4291148.02
	Mem-Martins	469862.54	4292975.09
	Paio Pires	492933.26	4274562.39
	Lavradio	495772.49	4280003.85
	escavadeira	494346.16	4279049.77
	Laranjeiro	486273.92	4279460.14
	Alto Seixalinho	494512.39	4277539.01
	Fernando Pó	526932.28	4276380.46
	Arcos	509297.10	4264627.35
	Quebedo	509902.78	4264104.29
	Camarinha	511136.85	4264784.66
	Chamusca	545882.64	4356209.93
	Terena	639510.50	4275462.34
	Santiago do Cacém	526552.13	4208077.07
	Monte Velho	517663.83	4214371.55
	Monte Chãos	514228.46	4200742.02
	Sonega	524285.04	4191550.36
	Malpique	566550.86	4105168.56
	Município	567880.31	4105402.64
	Cerro	616967.07	4130206.96
	Afonso II	594357.87	4097946.61
	Joaq. Magalhães	595376.71	4096948.16
	Pontal	541205.71	4109070.48
	David Neto	540524.97	4110161.86
	Uncertainty quantification (e.g. Accuracy): N/A		

Table 1.5-2 Data used for the validation of all the products of this service/sub-service

1.5.4 Validation of individual components

Preliminary results of the validation for the next day forecast of Ozone and PM10 for the PrevQualAr statistical model for the Northern Lisbon Metropolitan Area are presented in the table and figures and bellow:

Table 1. Preliminary results of the PrevQualAr validation for the year 2007 and the Northern Lisbon Metropolitan Area

	Daily PM10 Mean (2007 data - 285 days)	Daily Average of the Ozone Hourly Maximum (2007 data - 294 days)
Absolute mean error	9 µg/m3	13.49µg/m3
Bias	5.2 µg/m3	-4.69 µg/m3
R^2	0.6	0.8

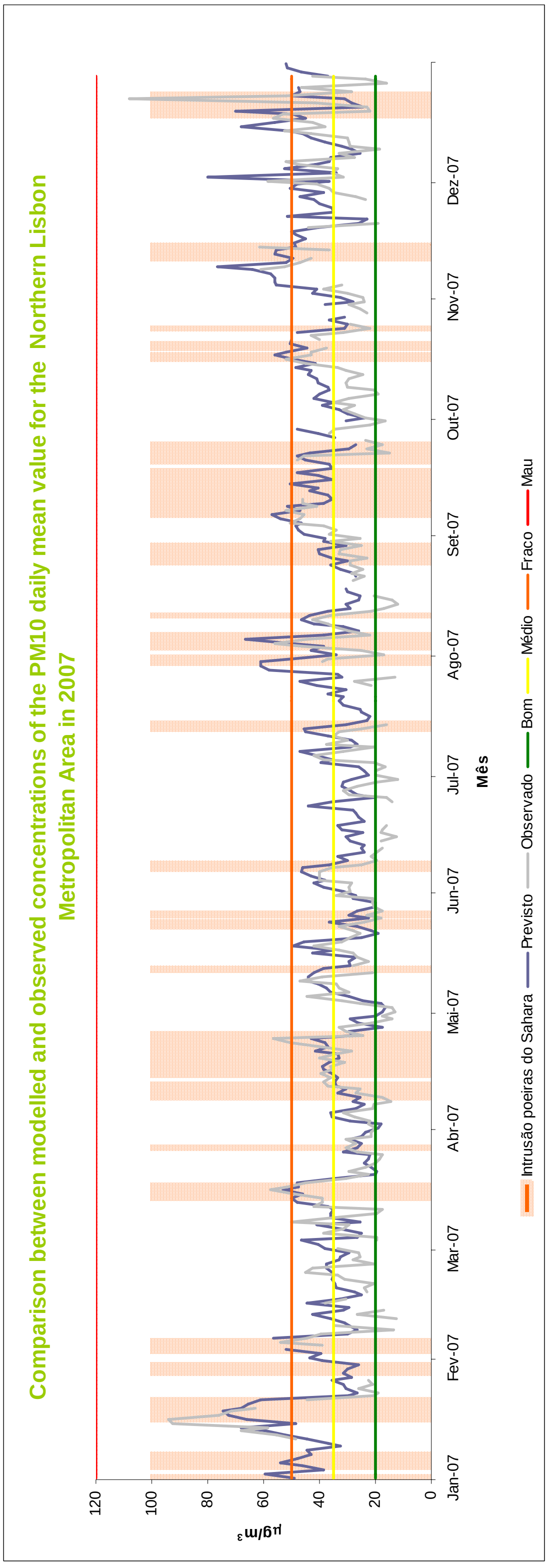

Figure 1. Comparison between modelled and observed concentrations of the PM10 daily mean value for the Northern Lisbon Metropolitan Area in 2007

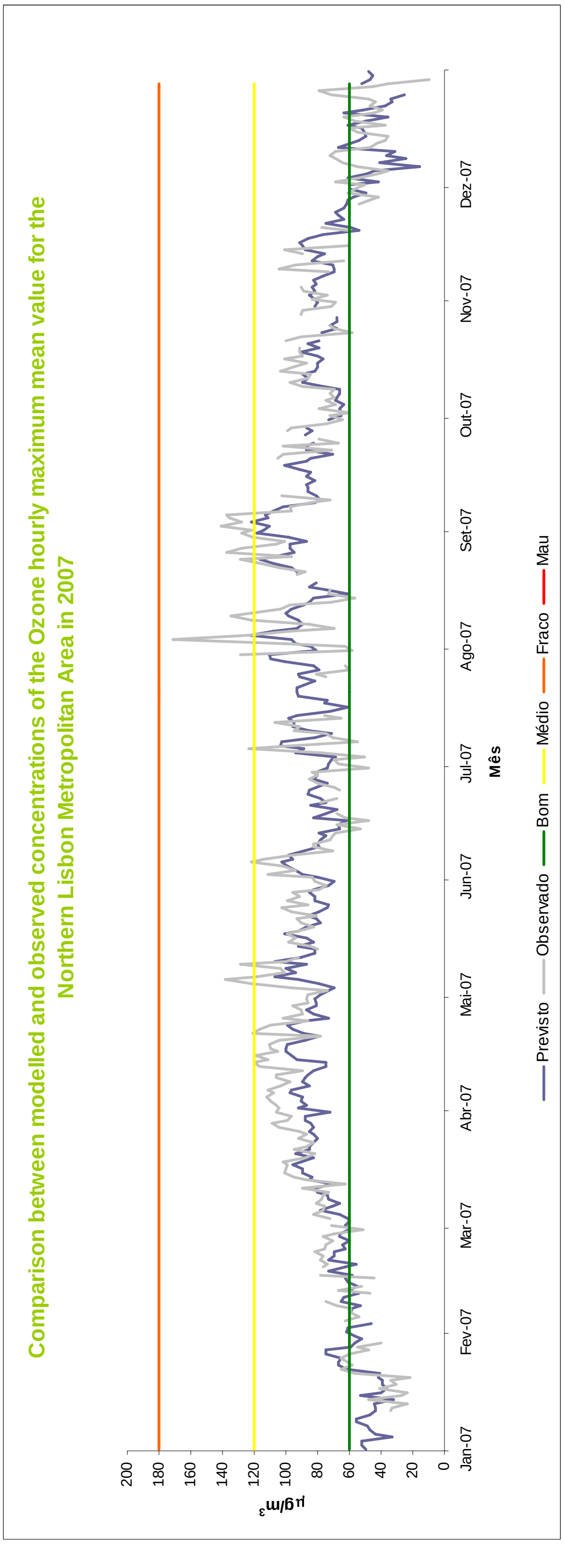

Figure 2. Comparison between modelled and observed concentrations of the Ozone hourly maximum mean value for the Northern Lisbon Metropolitan Area in 2007

VALIDATION OF INDIVIDUAL COMPONENTS FOR STRATOSPHERIC GASES	
Uncertainty estimators	
Bias	Indicates, in average, if the index forecasts are being under or overestimated. Its value is given by the difference between modelled and observed values. Negative values indicate index underestimation and positives indicate overestimation
Quality assessment	
QA ground based data/removal of outliers/verification consistency	N/A
Error statistics	Normalized mean error (%): error associated with the total number of one-day forecast performed; Absolute mean error: indicates the mean error associated with each forecast. Given by the sum of differences between forecasted and observed values, in module.
Contigency table	Table in which each level of the forecasted index is compared with the observations
Percentage of correct forecasts	Ratio of total number of correct forecasts to total number of days for which a forecast was made
Detection probability	Model capability to predict the index level corresponding to observed high pollution values. Example: a detection probability of level 2 of PM10=66% indicates that two thirds of the level 2 PM10 forecasts (Poor Air Quality Index – above 50 $\mu g/m^3$) were correct. It is calculated by the ratio between the days in which the forecast was right for a given index and the total number of days where such index was observed;
Percentage of False Alarms	indicates the number of wrong forecasts for any given index level. It is given by the ratio of the number of days for which that index level was not foreseen and the total number of days for which that index level was foreseen.
Models/algorithms/assimilation	
PrevQualAr - Next day Spatial model adjustment moduleforecast statitistical model for PM10 and ozone	Based on statistical models applying the 'Classification and regression trees - CART' method to construct the multiple regression models called PrevQualar. For each station, a model was developed based on empirical relationships between each pollutant concentration and meteorological variables (using historical datasets from ground air quality and meteorological stations). In an operational basis this

	modelling system uses the pollutant data from the day before and the predictions given by ECMWF for the key meteorological parameters (maximum, minimum and average temperature, mean relative humidity, dew point average temperature, number of sun hours pressure difference between stations, atmospheric vertical profile (only for Lisbon), geopotencial height and temperature at 1000,925,850,700,500 hPa) defined in the model to generate the forecast for the next day.
	RMSE for the annual parameters in the Lisbon area will probably be less than 50% and for the national scale is not yet available[Validation Parameter=Result; Procedure/method – ref data (ref)]
Consistency	
Forecast against ground data PM10 from National Air Quality Network	Level 1 product preliminary validation results [Constraints/Information content]presented in Table 1 for PM10 Daily Average and Daily Average of Ozone Hourly Maximum for the Northern Lisbon Metropolitan Area considering 2007 data
	[Validation Parameter=Result; Procedure/method – ref data (ref)]see Table 1 above

Table 1.5-3 Summary of the validation of individual components this service/sub-service

1.5.5 Validation of specifications and user requirements

1.5.5.1 AIRCAST L1: Point and zone Average PM10 and O3 next day forecast for the Lisbon Metropolitan AreaPoint and Zone average ground based air quality data

VALIDATION AGAINST SERVICE SPECIFICATIONS			
No limitations/delays for compliance between theoretical and actual service specifications reported			
VALIDATION AGAINST USER REQUIREMENTS			
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**
Accuracy	N/A	n.s.	Percentage of correct forecasts of the Air Quality Index – 60%
Accuracy minimum	n.s.	n.s	n.s.
Accuracy target	n.s.	n.s	n.s.

Spatial coverage	Monitoring: Portugal Forecast: Lisbon	Portugal/lisbon	Forecast: Lisbon Metropolitan Area
Temporal coverage	1995-2009	1995-2009	2005-2008
Spatial resolution	Point monitoring and zone monitoring	n.s.	Point (ground stations) and zone forecast
Temporal resolution	1h, 24h, 30 days	1h, 24h, 30 days	next day forecast
Grid/Projection	various	n.s.	various
User Interfaces			
PROMOTE Web Site	n.s.	Complete, operational and up to date	Operational in September 2008
ftp	n.s.	n.s.	N/A
On demand		n.s.	N/A
Data formats and data delivery			
Data availability	Operational implementation by May September 2008	Forecast delivery in month 6	Operational implementation by September 2008
Data accessibility	Offline	n.s.	NRT
Delivery Mode	n.s.	online	Trough the website
Delivery frequency	n.s.	24 h	Daily
Data Format	Shapefile	ASCII, gif	XLS File (shapefile data format to be implemented)
Historical archive	Hourly AQ data from ground stations. Timeseries 1995-2009	Hourly AQ data from ground stations. Timeseries 1995-2009	Daily Air Quality Index. Time series 2005-2008
Visualization	Through Web Mapping Services	Website	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 1.5-4 Validation of specifications and user requirements.

1.5.6 Quality assessment and control procedures: service quality

Service delivery start date: 16 June 2008				
SPECIFICATION	**S5**	**REQUIRED***	**ACTUAL**	**N checks/Delivery period**
Quality checks	monitoring	yes	yes	Automatic quality checks included in next day forecast calculation module Monthly non-automatic quality checks. Annual Service report to user
Product confidence data	n.s.	*95%*	95%	N/A
Error bar definition and representation	N/A	*2σ*	*2σ*	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)*	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)	N/A
Documentation of process failure	Process failure report sent to the user within one week	n.s.	Process failure report sent to the user within one week	N/A

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*	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	N/A

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

Table 1.5-5 Quality assessment and control procedures this service/sub-service

1.5.7 References

1.5.7.1 Electronic references and online data access paths

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

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

1.5.7.2 Bibliographic references

Briggs, D.J., Collins, S., Elliott, P., Fischer, P., Kingham, S., Lebret, E., Pryl, K., (...), Van Der Veen, A. (1997). Mapping urban air pollution using GIS: A regression-based approach. International Journal of Geographical Information Science, 11 (7), pp. 699-718.

Briggs, D.J., De Hoogh, C., Gulliver, J., Wills, J., Elliott, P., Kingham, S., Smallbone, K. (2000). A regression-based method for mapping traffic-related air pollution: application and testing in four contrasting urban environments. Science of the Total Environment 253 (1-3), pp. 151-167

EPA. Guidelines for Developing an Air Quality (Ozone and PM2.5) Forecasting Program, U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, North Carolina, EPA-456/R-03-002. 2003.

Ferreira F., Neto, P., J., Torres, Tente H.: Ozone Levels in Portugal: the Lisbon Region Assessment. In Proceedings of Air & Waste Management's 97th Annual Conference Exhibition. Indianapolis, Indiana, June 22-25, 2004.

Ferreira, F.m Torres, P, Neto, J & Tente, H.: Statistical Air Quality Prediction for Lisbon. In Valência_5th Urban Air Quality Conference, 2005.

Marques F., Cassmassi, J., Ferreira, F. E Mesquita, S. : Air quality forecast for Lisbon, Portugal: from data analysis to outreach. U.S. EPA's 2006 National Air Quality Conferences. February 5-8, 2006, em San Antonio, Texas, USA.

Neto, J., Torres, P. e Ferreira F. e Boavida, F.: Lisbon air quality forecast using statistical methods. In: Proceedings of the Third International Symposium on Air Quality Management at Urban, Regional and Global Scales, pp. 591-597 , 26-30 September, Istanbul, Turkey, 2005.

Thompson, M.L ; Reynolds, J; Cox, L.H., Guttorp, P: Sampson,P.D.: "A review of statistical methods for meteorological adjustment of tropospheric ozone" . Atmospheric Environment,35,617-630. 2001

Wang, W., Weizhen, L., Wang, X., Leung, A. : "Prediction of maximum daily ozone level using combined neural network and statistical characteristics". Environment International 29, pp. 555–562.. 2003