Final Report

PANDA 熊貓

PArtnership with ChiNa on space DAta

SEVENTH FRAMEWORK PROGRAMME

Executive Summary

The rapid economic development and intense urbanization in many areas of Asia has led to a severe degradation of air quality with acute human health problems, specifically in the vicinity of large metropolitan areas. By combining space observations, in situ surface measurements and surface emissions of chemical pollutants with complex mathematical models of atmospheric composition, detailed analyses and reliable predictions of regional air quality in Asia can be produced and should help environmental managers to take early appropriate actions to avoid the occurrence of acute air pollution episodes.

The objective of the PANDA project was to establish a team of European and Chinese scientists who jointly use space observations and in-situ data as well as advanced numerical models to monitor, analyze and forecast global and regional air quality. Through a close cooperation between 14 European and Chinese research institutions, the PANDA Project has worked towards the understanding of the processes responsible for the formation, dispersion and destruction of air pollutants, and to the improvement of air quality monitoring process from space and from the surface. In an effort to disseminate information and data to a broad community and to the public, the project has produced a so-called toolbox for easy access to information, and developed related educational activities.

The toolbox of the PANDA project is located at the joint MarcoPolo-Panda web portal hosted by the MarcoPolo partner KNMI. It gathers available measurements and observations, emission inventories and model data on atmospheric composition, as well as the system for the prediction of air quality for China.
They can be accessed from the main page http://www.marcopolo-panda.eu/ via the main menu item ‘Products’, and is available in English and Chinese.
The toolbox contains six sections: (1) Air quality Forecasts, (2) Model Results, (3) Model Evaluation, (4) Observations, (5) Emissions, and (6)Tutorials, presenting the main results of the Panda project and making them available to the scientific community and the public.

A system for the prediction of air quality in China has been established jointly with the MarcoPolo Project, providing daily forecasts of air pollution for 37 Chinese cities with a multi model ensemble over China, operationally since the beginning of 2016. To our knowledge, this is only the second time that an activity of such a scale is done (after the MACC series of project in Europe). The forecasts are showing a reasonable degree of skill –especially for the ensemble-based products (median or average of the multi-model ensemble). The scientific evaluation of the forecasting system has been started during the project and will be continued as longer time series of models/observations are building up with time. The evaluation is used for the improvement of the forecasting system and our understanding of atmospheric pollution.

Project Context and main objectives

The rapid economic development and intense urbanization in many areas of Asia has led to a severe degradation of air quality with acute human health problems, specifically in the vicinity of large metropolitan areas. By combining space observations, in situ surface measurements and surface emissions of chemical pollutants with complex mathematical models of atmospheric composition, detailed analyses and reliable predictions of regional air quality in Asia can be produced and should help environmental managers to take early appropriate actions to avoid the occurrence of acute air pollution episodes.

The objective of the PANDA project was to establish a team of European and Chinese scientists who jointly use space observations and in-situ data as well as advanced numerical models to monitor, analyze and forecast global and regional air quality. Through a close cooperation between 14 European and Chinese research institutions, the PANDA Project has worked towards the understanding of the processes responsible for the formation, dispersion and destruction of air pollutants, and to the improvement of air quality monitoring process from space and from the surface. In an effort to disseminate information and data to a broad community and to the public, the project has produced a so-called toolbox for easy access to information, and developed related educational activities.
A system for the prediction of air quality in China has been established jointly with the MarcoPolo Project, providing daily forecasts of air pollution for 37 Chinese cities with a multi model ensemble over China, operationally since the beginning of 2016.

The Panda project provides to users and stakeholders knowledge, methodologies and toolboxes that can serve as a basis for global and regional air quality analysis and forecasts. It provides science-based information that improves air quality management by regional and local authorities. A strong dissemination and education activity has been established to train users to use the key products and data generated by the project.

Specific goals of the project are listed in the following, being addressed by the different Workpackages of the Panda project. Each of them has been developed to support a clear partnership between Chinese and European scientists, who are members of prominent research institutions. To ensure this cooperation, each WP was co-led by a European and by a Chinese participant.

1) To collect and provide historical (existing) and recent satellite datasets with improved retrieval algorithms for Asia and initiate a collaboration between European and Chinese Remote Sensing Groups in order to validate and intercompare the satellite data. (Workpackage 1)

2) To collect suitable sets of in situ air quality data from both publically available sources as well as from measurements made by Panda partners for comparison with the satellite data and for model evaluation and provide a harmonized air quality datasets to allow for comparison both with each other and the satellite data, and make the datasets available for the toolbox and model evaluation. (Workpackage 2)

3) To provide an improved emission dataset for China used for the air quality models to study and forecast air quality over China, a documentation about the emissions for China and a paper discussing the evaluation of surface emissions and their trends in China in order to improve our understanding about air quality forecasting and the forecasting system. (Workpackage 3)

4) To set-up global-to-regional model chains to study and forecast air quality over China, to use data assimilation processes for improving the air quality forecasts for China and to evaluate the model chains and the forecasting system in order to improve the predictions (Workpackage 4)

5) Development of the toolbox to facilitate the access to scientific results obtained in the project, interact with potential users of the toolbox, in particular in China to assess the needs for the toolbox, provide source allocation graphs for major cities in China

6) To disseminate results from the PANDA project through a bilingual website and the toolbox and through presentations at international conferences and meetings. In order to enhance knowledge transfer and cooperation among the Panda and MarcoPolo partners two summer schools have been organized (one in Europe, one in China). Through the production of a synthesis and integration report for Panda, summarizing the scientific output of the project, the results can be further disseminated. (Workpackage 6)

7) To deepen the cooperation with other projects, especially the EU MarcoPolo project, a separate Workpackage has been initiated (Workpackage 9). The cooperation has been strengthened by joint project meetings (Kickoff meeting, 1st and 2nd General assembly), joint summerschools, joint scientific workshops to address scientific questions.

Description of the main S & T results/foregrounds

In an effort to disseminate information and data to a broad community and to the public, the project has produced a so-called toolbox for easy access to information, and developed related educational activities. The toolbox of the PANDA project is located at the joint MarcoPolo-Panda web portal hosted by the MarcoPolo partner KNMI. It gathers available measurements and observations, emission inventories and model data on atmospheric compositionas well as the system for the prediction of air quality for China.

They can be accessed from the main page http://www.marcopolo-panda.eu/ via the main menu item 'Products'. An overview is provided in the same menu item, both in English and in Chinese. Direct links to the overview:
http://www.marcopolo-panda.eu/products/toolbox/ (English version)
http://www.marcopolo-panda.eu/products_cn/toolbox_cn/ (Chinese version).

The toolbox contains six sections: (1) Air quality Forecasts, (2) Model Results, (3) Model Evaluation, (4) Observations, (5) Emissions, and (6) Tutorials, presenting the main results of the Panda project and making them available to the scientific community and the public.

(1) Air quality Forecasts:

MarcoPolo and Panda are applying a number of air quality models to provide daily air quality forecasts for a selection of Chinese agglomerations and for the region of East Asia (37 cities). Currently, seven models, Chimere (run at KNMI), C-IFS (run at ECMWF), WRFchemSCUEM (run at SCUEM), SILAM (run at fmi), WRFchemMPI (run at MPI), EMEP (run at met.no) and LOTOS-EUROS (run at VITO) are providing daily forecasts every day at 0:00 UTC for the next 72hours (three days) for NO2, O3, PM10 and PM2.5 for a selection of ~35 cities (see Figure 2). Hourly data contain surface concentrations in µg/m3 for grid values which are bilinearly interpolated to city center coordinates. In-situ data is obtained from www.pm25.in. The average of the urban network is given (usually around 5-12 stations), together with the standard deviation and the number of contributing stations. Figure 1 shows an example of the forecast for Beijing from the 20^{th} October 2016.

In addition to the individual models, a simple multi-model ensemble was constructed by using simple statistical methods such as median and mean. The multi model approach provides more accurate forecasts and reduces the underlying uncertainties.
The database can be accessed by project partners through the internal webpage through an interface.

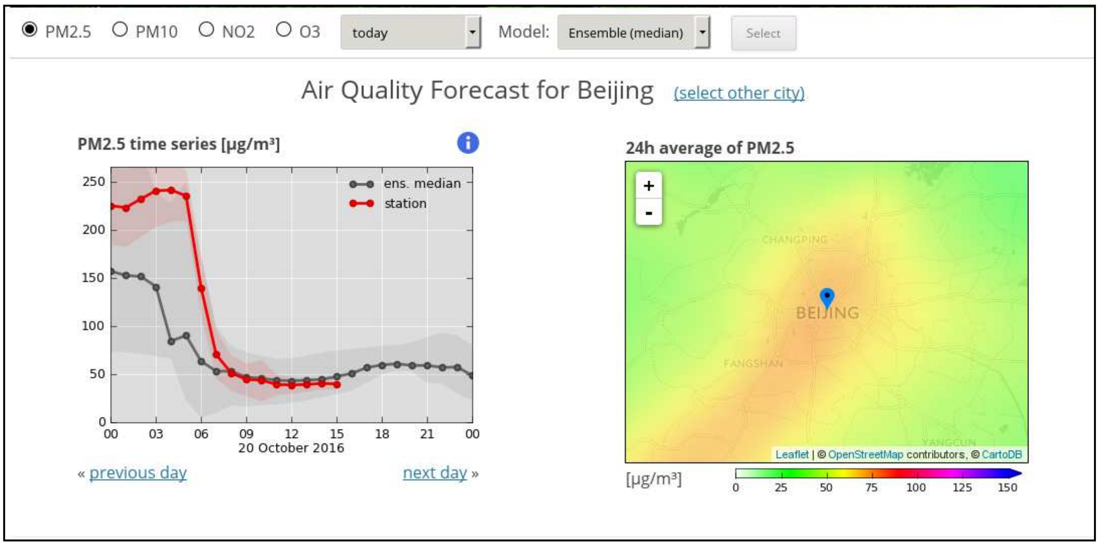


Figure 1: Air quality forecast for Beijing of 20th October 2016.

The next table indicates when the models have joined the forecasting system, the period for which observations have been acquired and the period for which the model/observation comparisons have been made.

Models	CHIMERE v2013 (KNMI)	24 May 2015 - ...
	C-IFS (ECMWF)	4 September 2015 - ...
	WRF-Chem (SCUEM)	9 November 2015 - ...
	SILAM (FMI)	20 January 2016 - ...
	WRF-Chem (MPI)	1 March 2016 - ...
	EMEP (Met.no)	6 April 2016 - ...
	LOTOS-EUROS (TNO)	12 May 2016 - ...
	Ensemble (median/mean)	25 April 2016 - ...
Cities	北京 Beijing, 上海 Shanghai, 广州 Guangzhou, 深圳 Shenzhen, 杭州 Hangzhou, 天津 Tianjin, 成都 Chengdu, 南京 Nanjing, 西安 Xi'an, 武汉 Wuhan, 沈阳 Shenyang	14 April 2015 - ...
	东莞 Dongguan, 重庆 Chongqing, 哈尔滨 Harbin, 苏州 Suzhou, 青岛 Qingdao, 济南 Jinan, 郑州 Zhengzhou, 大连 Dalian, 昆明 Kunming, 无锡 Wuxi, 厦门 Xiamen, 长春 Changchun, 宁波 Ningbo, 南宁 Nanning, 太原 Taiyuan, 合肥 Hefei, 常州 Changzhou, 唐山 Tangshan, 长沙 Changsha, 徐州 Xuzhou, 温州 Wenzhou, 贵阳 Guiyang, 乌鲁木齐 Ürümqi, 淄博 Zibo, 福州 Fuzhou, 石家庄 Shijiazhuang	17 January 2016 - ...
Species	(in-situ) PM2.5, PM10, NO2, O3, SO2, CO	14 April 2015 - ...
	(model) PM2.5, PM10, NO2, O3	14 April 2015 - ...
	(model) NO, SO2	9 March 2016 - ...
	(model) CO	25 March 2016 - ... (not all models)

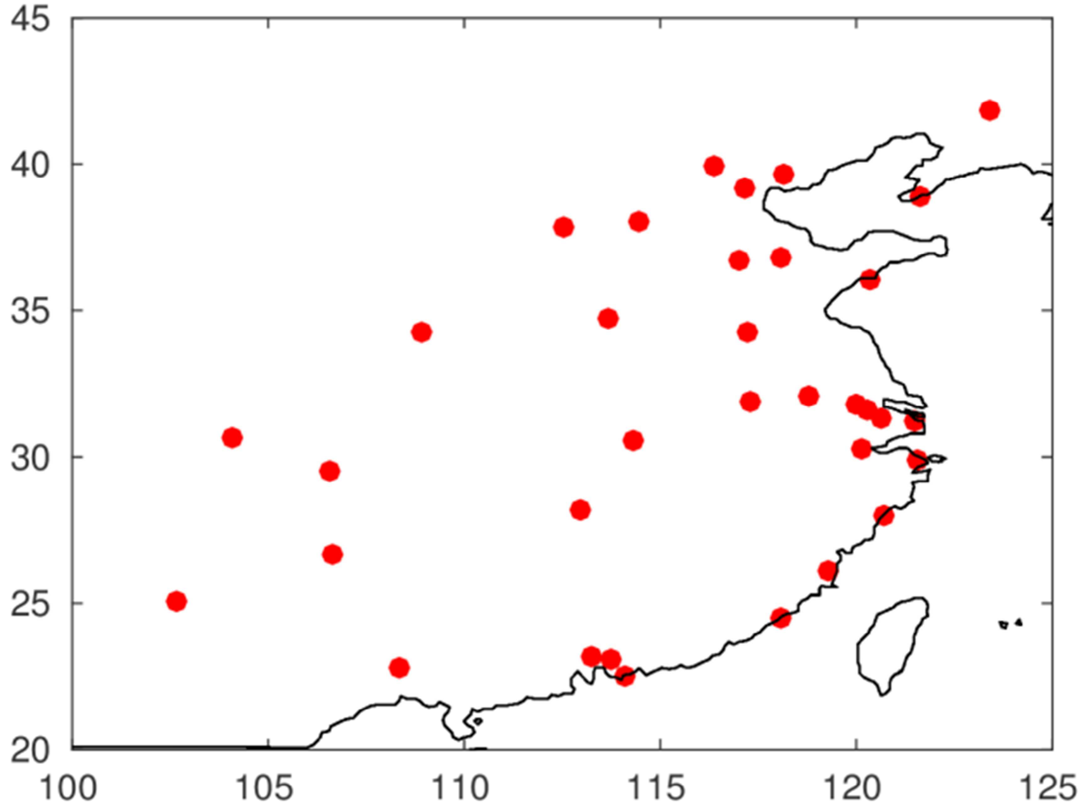


Figure 2: Map of the cities/urban clusters (population over 3 million (2010 census)) with available data (observational and model ensembles)

Results are still in the process of being analysed (together with some MarcoPolo project partners), looking at the various models and at their ensemble properties. For the evaluation of the forecasting ensemble, statistical values have been calculated for each model for the species NO2, O3, PM10 and PM2.5 which are shown on the public website. The statistical values used for the evaluation are the mean BIAS, RMSE, correlation coefficients and the refined index of agreement (Willmott et al., 1981).

The statistical values have been calculated for the whole time period (1.April to 15.October 2016) and for each month separately to evaluate the performance for different seasons, and separately for each city to see if some models have regional issues in the performance. Apart from the statistical values, the mean diurnal variations of O3 and NO2 for different cities have been plotted for a better understanding of the model performance. For the evaluation of issues related to the planetary boundary layer (PBL) representation, the correlation of predicted values versus observed values of O3 and NO2, nighttime and daytime data has been plotted in different colors. Some models have problems in the representation of the PBL during nighttime.

As an example of the evaluation exercise, we show on Figure 3 the BIAS, RMSE and the correlation coefficient of the ensemble mean of all models for the ozone and PM2.5.

More details about the evaluation of the forecasts so far have been prepared by Partner MPI-M and can be found in the deliverable D4.7.

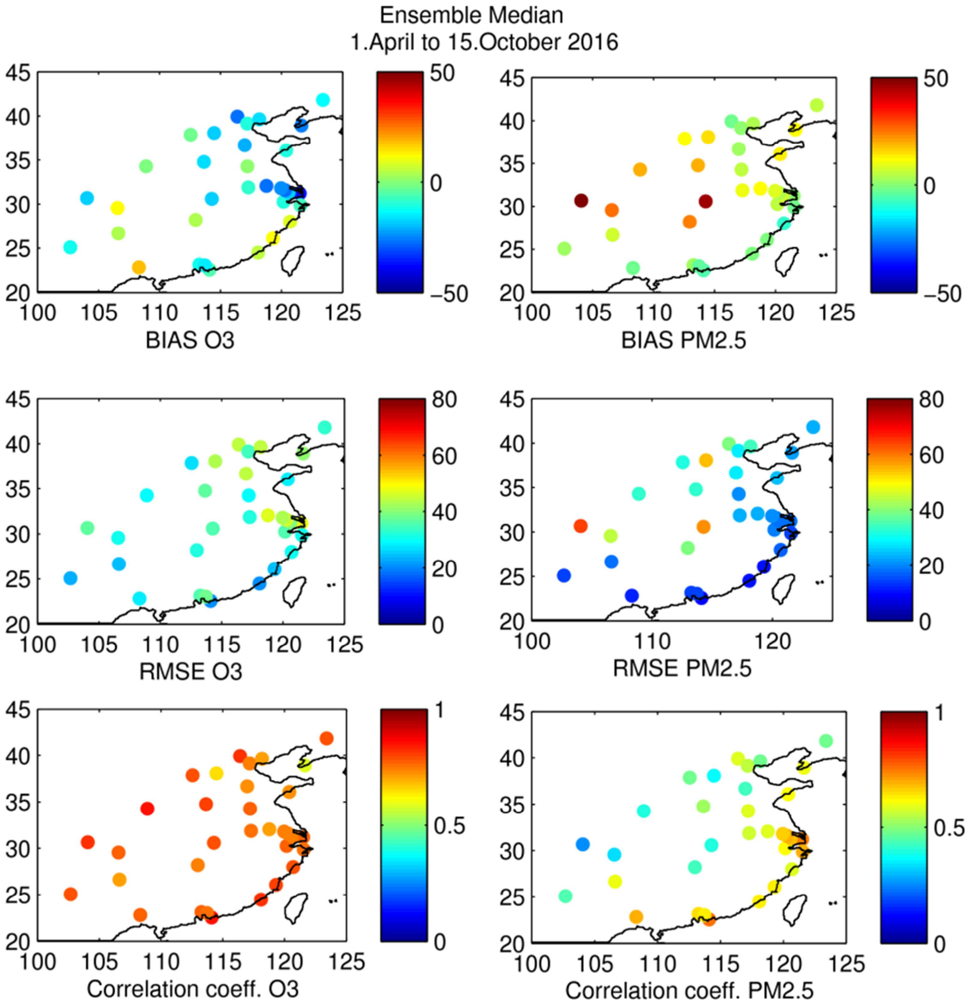
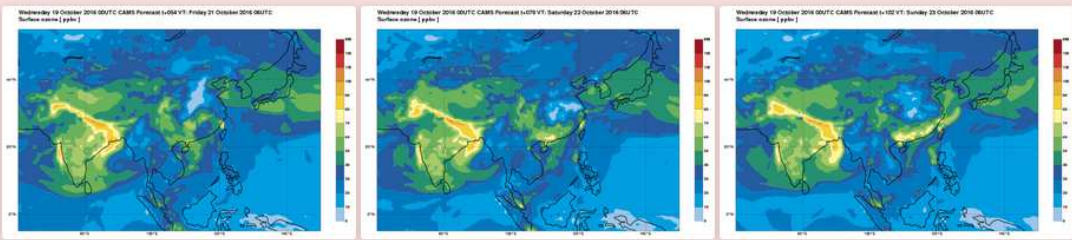


Figure 3: Ensemble median skill scores (bias, RMSE, correlation) for ozone (left) and PM2.5 (right) for the period April 1st to October 15th 2016.

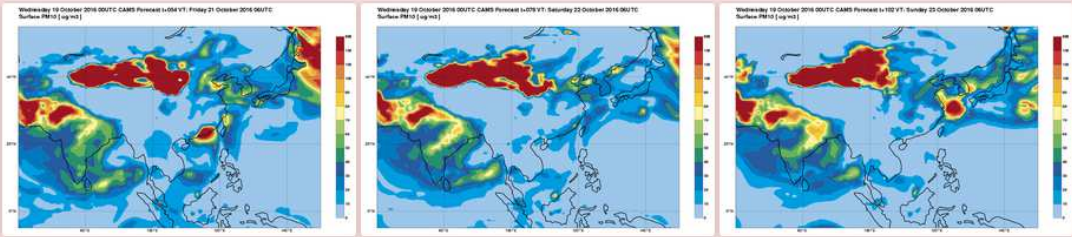
In addition to the regional forecasts for a selection of cities, air quality forecasts covering the entire region of East Asia are provided at the toolbox: The C-IFS and SILAM models are run daily to provide atmospheric composition forecasts for several chemical species in China and large areas of South and Southeast Asia. C-IFS provides maps valid for 2pm local time (CST), while SILAM provides maps of the maximum concentrations during a 24-hour period (00 to 24 UTC). Figure (4) shows as an example the forecast of ozone and PM10.

C-IFS

In the images below, forecasts from the C-IFS model are shown. More information and plots can be viewed on the MACC page of C-IFS forecasts for the PANDA project.



Ozone forecast for several days into the future, at 6am UTC (i.e. 2pm CST). Click images to enlarge.



PM10 forecast for several days into the future, at 6am UTC (i.e. 2pm CST). Click images to enlarge.

Figure 4: Ozone and PM10 forecast from the C-IFS model.

(2) Model Results:

A selection of atmospheric composition models have been run for China and a larger Asian domain in the past, focusing on model evaluation and specific air pollution episodes of the past. Some results are shown here. Details about the model evaluation of the histrocial cases are presented in the Section Model Evaluation.

The EMEP/MSC-W model has been run on 0.5 × 0.5 degree resolution for 2010 and the global domain, using HTAPv2 emission data. Figure 5 shows examples zoomed in on an Asian sub domain for PM2.5 in different seasons.

The WRFchem model (version V3.6/MOZART chemical scheme) has been run for an Asian domain on 60km x 60km resolution with MACCity emissions for January and July, and a smaller domain (sub-regional) on 20km x 20km resolution with HTAPv2 emissions (also January and July). Figure 6 shows examples of modeled PM2.5 for January and surface ozone for July 2010.

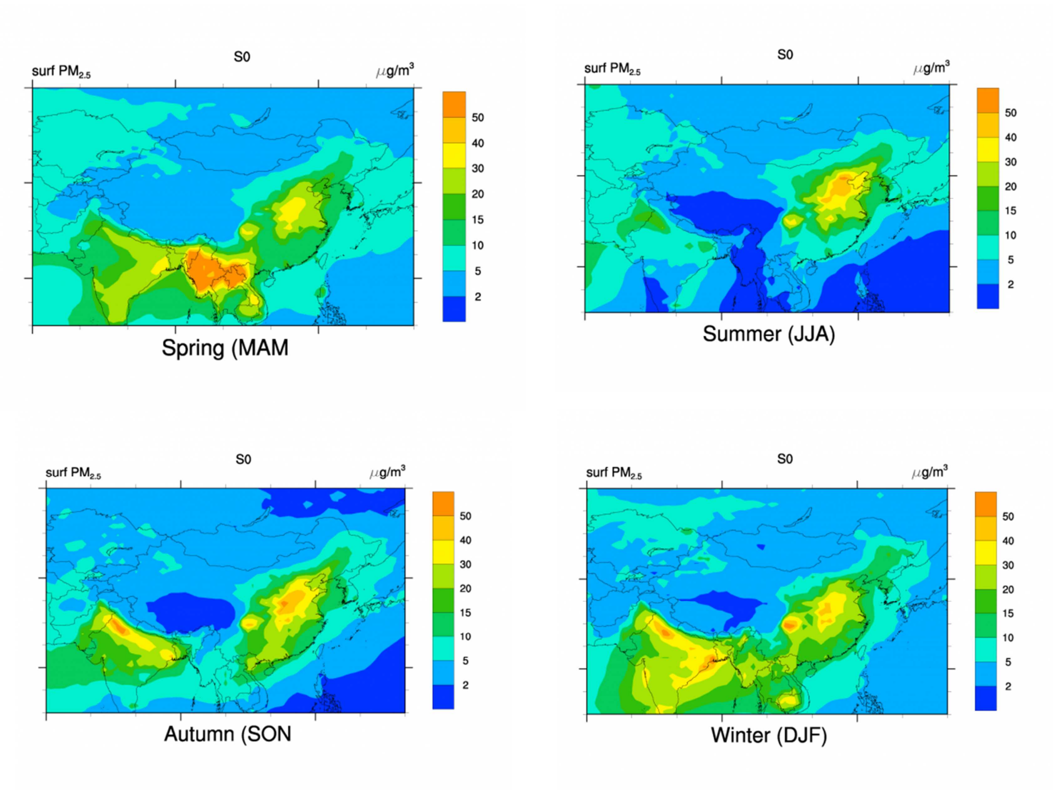


Figure 5: Historical case simulation of the EMEP model for 2010.

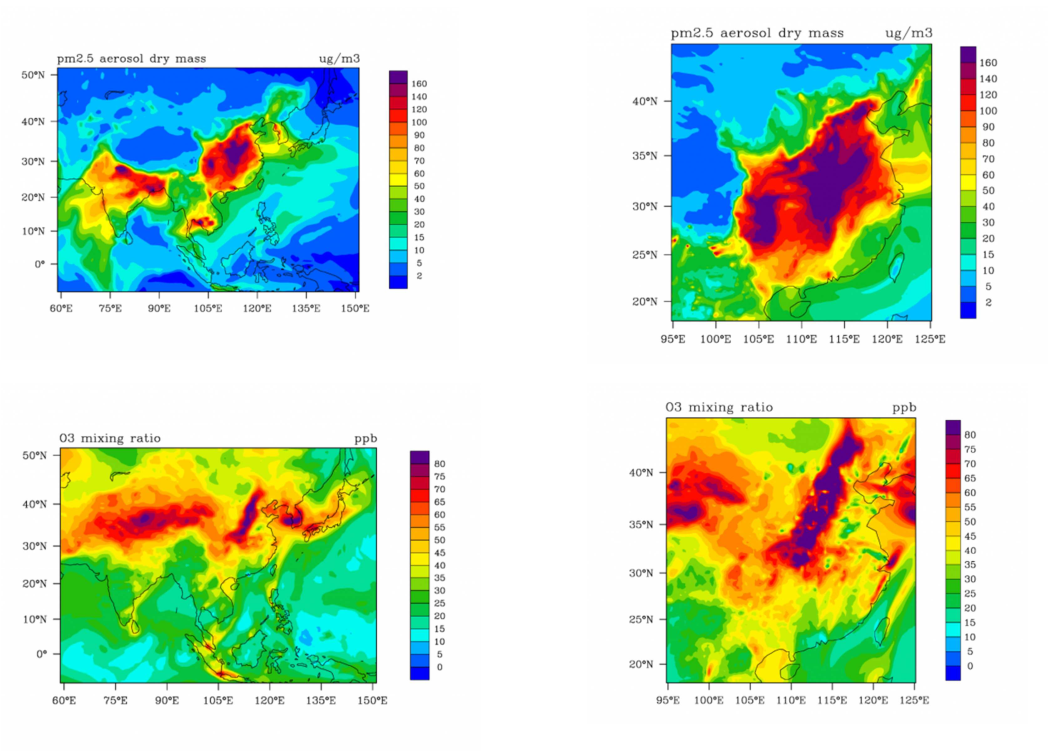


Figure 6: Historical case simulation of the WRFchem model for 2010

EMEP Source-Receptor calculations

The EMEP MSC-W model has been run for an Asian domain extending from 5°N to 55°N in the latitude direction and from 62°E to 134°E in the longitude direction, i.e. including China, India, Japan and other major emitting countries in Asia. Lateral boundary conditions are taken from ECMWF C-IFS. In the Base run, all emissions are included in full, while in the perturbation runs anthropogenic emissions are reduced by 15% either within the city or outside the city in consideration. By differencing the perturbation runs with the Base run, the bar charts in the Figures below are created. The charts visualize the effect of emission changes on concentrations of various chemical species. Comparison between Figures 7 and 8 gives hints on the efficiency of local measures and on whether measures outside the region are necessary to meet air quality standards.

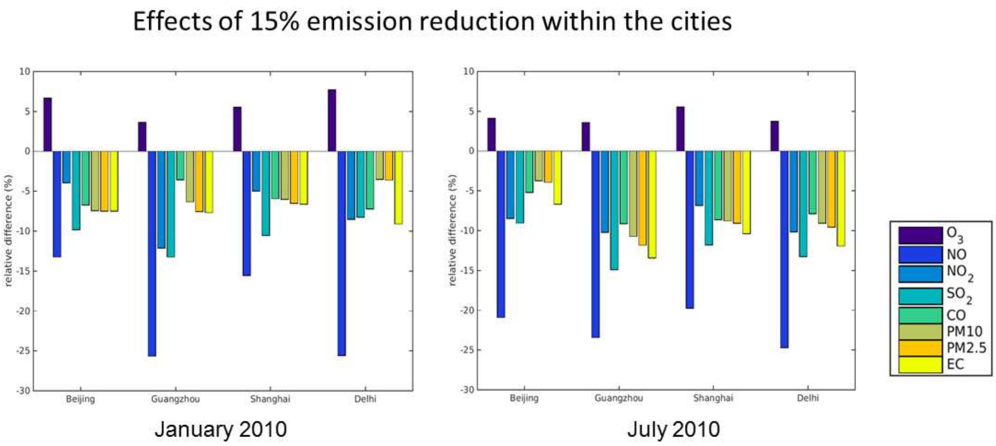


Figure 7: Effect of emission reduction of 15% with in the cities on concentrations of various chemical species

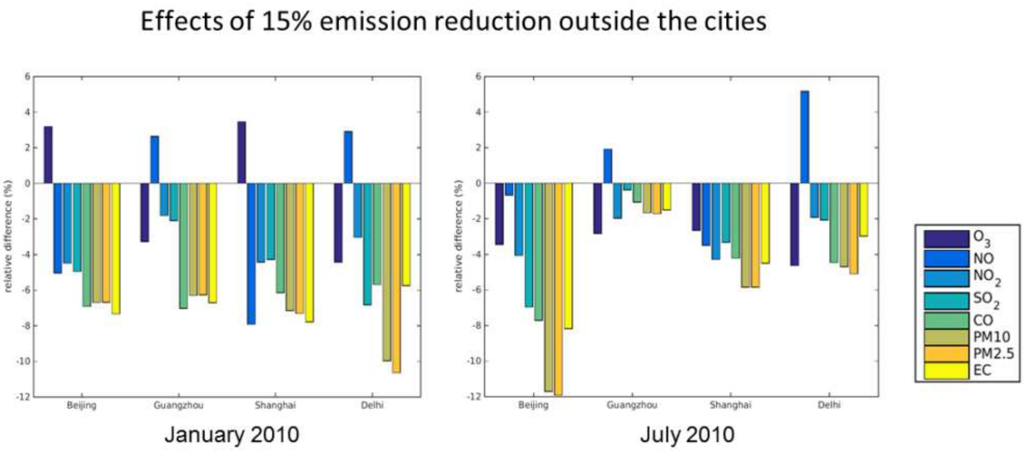


Figure 8: Effect of emission reduction of 15% outside in the cities on concentrations of various chemical species.

A 15% reduction in anthropogenic emissions within different cities on air pollutant concentrations within these cites (upper figure) give large reductions in NO, while ozone increases (an effect known as titration). In some cases NO can decrease by even more than 15%, due to shifts in the NO/NO2 ratio related to changes in the chemical regime. A 15% reduction in anthropogenic emissions outside the cities leads, in January, to large impacts on particulate matter in Delhi, as well as to an increase in ozone in Beijing and Shanghai. In July Beijing is largely impacted by external emissions. Increases in NO are related to shifts in the NO/NO2 ratio.

Source-receptor calculations scientifically underpin international emission reduction agreements and help policy makers in assessing the efficiency of local versus national/international emission reduction measures. As the effects of emission reductions in different regions depend on factors that vary in space and time, calculations have to be made repeatedly for different regions and with current meteorology, in order to make accurate assessments for any given situation.

(3) Model Evaluation

In order to provide a toolbox for model evaluation, the Panda projects links to the Aerocom website. The AerocCom project is an open international initiative of scientists interested in the advancement of the understanding of the global aerosol and its impact on climate. A large amount of observational data and model results have been assembled to document and compare state of the art modeling of global aerosol. The AeroCom tool is hosted by MET Norway and can be used to visualize observational data and to evaluate models globally, but also regionally for the region of East Asia. A link is provided to the AeroCom project toolbox.
Apart from the toolbox for model evaluation, the Panda project performed a detailed model intercomparison exercise for model evaluation, presented in the following section.

PANDA model Intercomparison exercise

We present in this section an overview of the performance of the regional models involved in the second phase of the modeling intercomparison exercise. In addition to comparison of modeled monthly mean surface concentrations of chemical and aerosol species relevant for air quality, model results are also compared to in-situ measurements. Detailed analyses with the interpretation of differences between models and observations are being prepared for publications in a peer-reviewed journal.

The detailed evaluation of the different periods has been distributed to different teams:

- case1: January 2010 (led by MPI)
- case 2: January 2013 (led by NUIST)
- case 3: July 2010 (led by SCUEM and Met. Norway)

All the data has been stored by ECMWF to facilitate the distributed collaborative work.

Figure 9 displays monthly mean surface PM2.5 concentrations calculated by the different models for January 2010. The models show some similar patterns with high PM2.5 concentrations in the North-Eastern regions and in the Sichuan Basin in the South-Western part of China. The results show however interesting differences among the models despite using the same anthropogenic emissions. The EMEP and SCUEM model simulations show quite similar low values compared to the models of NUIST and SILAM. SILAM shows the highest concentrations all over China.

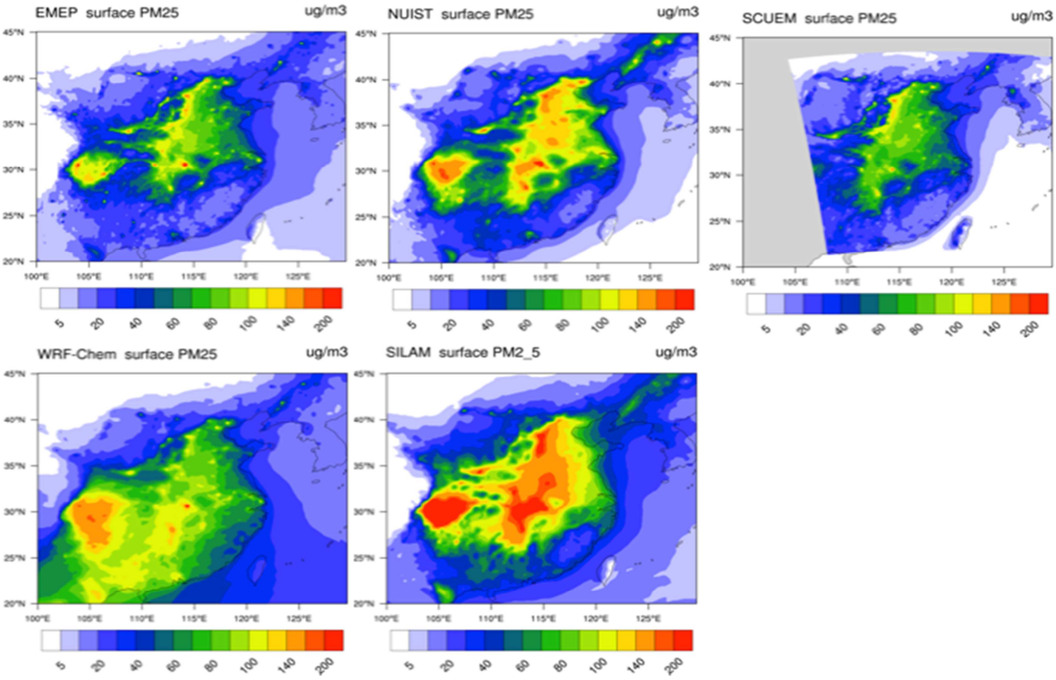


Figure 9. Modeled monthly mean surface PM2.5 concentrations for January 2010

Figure 10 displays model results during the haze event that took place in northern China in January 2010. During this event, high concentrations of several pollutants including NOx, CO, PM10, PM2.5 and SO2 were observed in several stations in Beijing and surrounding regions for several days around mid-January. This can be observed in Figure 7 which shows increasing values of PM2.5 from 50 µg m^{-3} in 15 January to around 300 µg m^{-3} in 18 January followed by a decrease in the concentrations to again to less than 80 µg m^{-3} after 20 January. This event is found to be due to a combination of low wind speed and a temperature inversion which led to accumulation of pollution in the lower troposphere. Consistent with the results displayed on Figure 9, the SILAM model results from FMI show the highest PM2.5 concentrations and tend to overestimate observed values. SCUEM and EMEP modeled values are close and better capture the PM2.5 concentrations during the haze event. MPI and NUIST results tend to underestimate PM2.5 during this event but overall all the models capture well the daily variability of observed PM2.5 concentrations in January 2010.

Comparison with measurements of meteorological fields such as temperature, wind speed and relative humidity (not shown) showed that all models capture quite well the observed values. This could explain why the models show reasonable skills during the haze event. Differences in the complexities of the aerosol schemes used could explain the differences observed among the models.

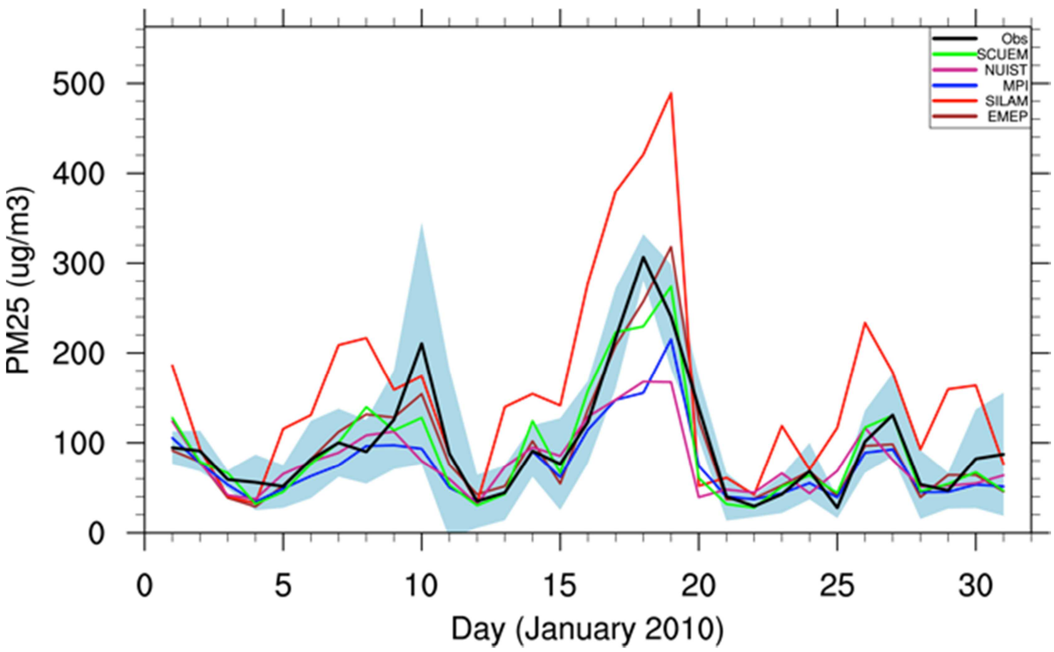


Figure 10. Time series of modeled and observed PM2.5 concentrations in the northern China plain in January 2010.

Figure 11 shows modeled monthly mean PM2.5 concentrations for the case of January 2013. There are similarities in the modeled patterns but still differences can be observed among the models. In particular, SILAM results from FMI still show higher concentrations compared to other models while both MPI and EMEP show lower values. SCUEM simulated much higher PM2.5 concentrations in some regions west of Beijing.

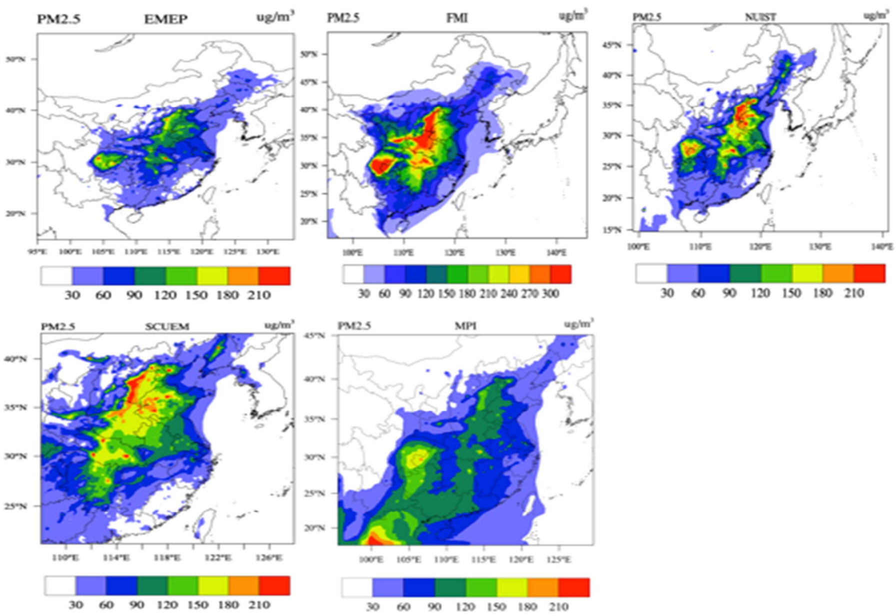
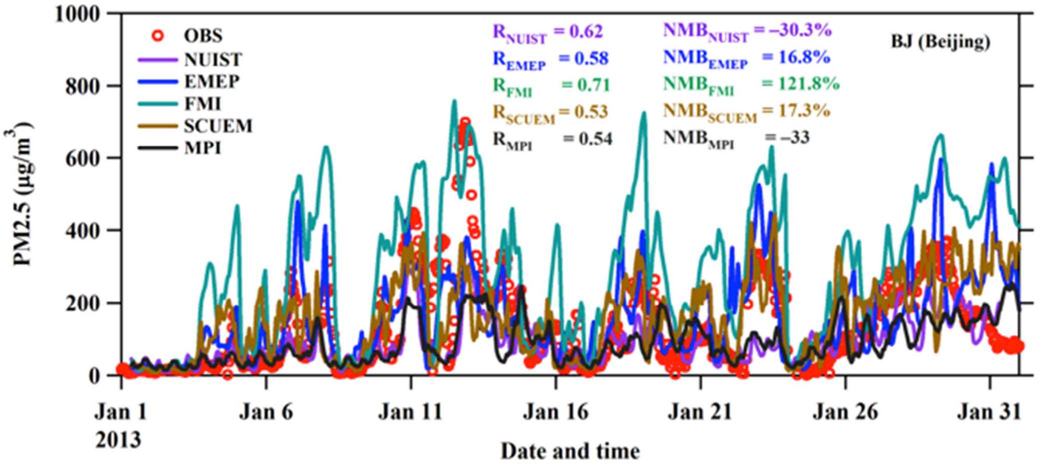


Figure 11. Modeled monthly mean surface PM2.5 concentrations for January 2013.

Figure 12 shows model results during January 2013 in Beijing and in the Xinglong station located in the North-West of Beijing. A major pollution event happened during the second week of January 2013 and is considered as one of the most important pollution events of the last decade in China. During this event, PM2.5 concentrations of up to 600 and 200 µg.m^{-3} were observed respectively in the 2 stations in 11-13 January. Several other smaller pollution events but still with higher pollution concentrations occurred also during other days in this month.

The models reproduce generally well the variability of the observations in both stations and are able to capture the increases in the concentrations during the different pollution events. This is illustrated also by the correlation coefficients displayed on Figure 12 which show reasonable skills (0.5-0.7).

As for the case of January 2010, the SILAM model shows also a general overestimation of PM2.5 with normalized bias values (NMB) of 121% and 157% respectively in the Beijing and Xinglong. It is however the only model who is able to capture the 600 µg.m^{-3} PM2.5 values observed in Beijing around 12 January 2013. In Beijing, EMEP and SCUEM show the lower positive NMB skills (ca. 17%) while NUIST and MPI show negative bias (ca. -30% and -33% respectively) indicating underestimation of the observations. In Xinglong however, NUIST and MPI show higher correlation with the observations and lower NMB followed by EMEP and SCUEM.



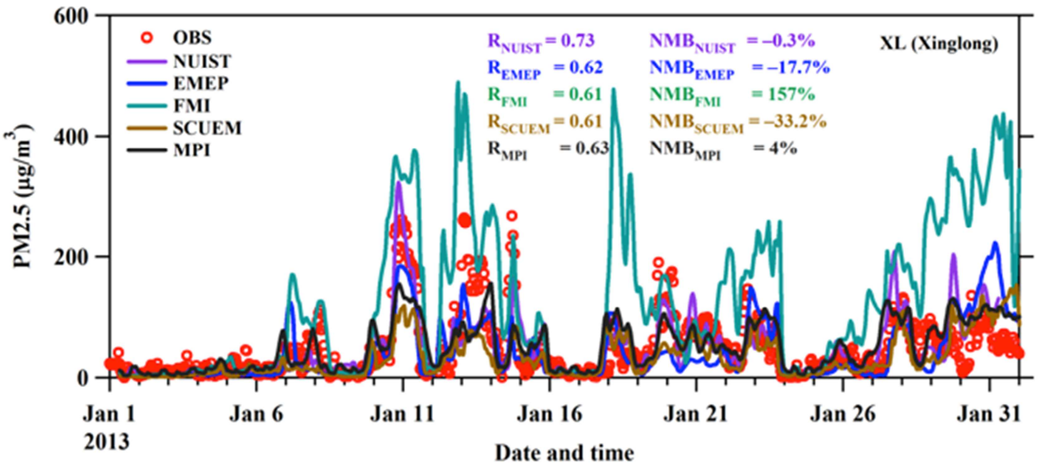


Figure 12. Time series of modeled and observed PM2.5 concentrations in Beijing and Xinglong stations in January 2013.

(4) Observations

The MarcoPolo and Panda projects have collected observational data, both in-situ and from satellites. The satellite data browser developed by MarcoPolo contains data from GOME, SCIAMACHY and other instruments on a number of relevant species. A link to additional satellite and in-situ data provided by the partners of Panda can be accessed via the Panda toolbox.

The toolbox for observational data contains items labelled 'satellite data browser', 'satellite data links', 'in situ data links', and 'combined datasets'.

(a) Satellite data:

As MarcoPolo and PANDA joined forces ('MarcopoloPANDA' toolbox), satellite data are now provided by both MarcoPolo and PANDA partners through a browser (interface created by MarcoPolo partner KNMI) at the MarcoPolo-PANDA website via 'Products' – 'Observational data' – 'Satellite data browser'. The satellite data from PANDA have been provided by IUP-UB, based on observations from GOME and SCIAMACHY. Figure 13 below shows a screenshot of SCIAMACHY data on NO_2 tropospheric columns for one specific day. Users can select the species, the instrument and the date. A link to direct data access is provided.

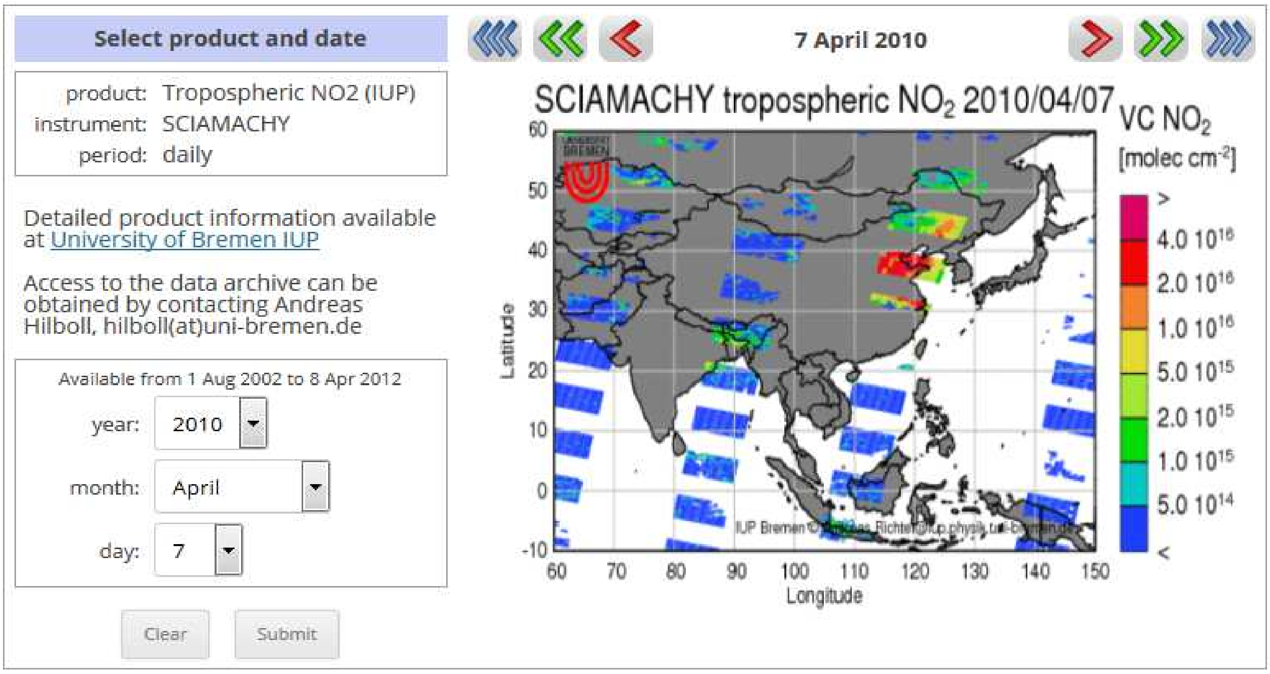


Figure 13: Screenshot of SCIAMACHY data set on NO2 tropospheric columns for one specific day.

Improvement of retrieval

The main achievement of the Panda project for the satellite observations is the improvement of the retrievals.
The first version of satellite data was based on existing retrievals and was provided in the first reporting period. During the course of the project, validation and retrieval improvement attempts finally lead to the second version of satellite data.

NO2 retrieval

In general, UV/Vis satellite retrievals comprise the following steps, in which changes and improvements were applied:
The second version of satellite data delivered by the Partner IUP-UB is improved in:

- Optimized DOAS fit parameters
- Comprehensive AMF LUT
- Surface Albedo (climatologies)
- Surface elevation
- Apriori profiles
- Tropopause height
- Temperature correction
- Cloud correction
- Aerosol treatment
- Stratospheric correction

The satellite data with the improved retrieval has been validated using independent ground based data. Highlighted here can be the collaboration established with the MarcoPolo Partners, providing additional validation data (MAX-DOAS from Xianghe). The improved data set shows a better agreement with ground based data than the first data set. This is shown in the Figure 14:

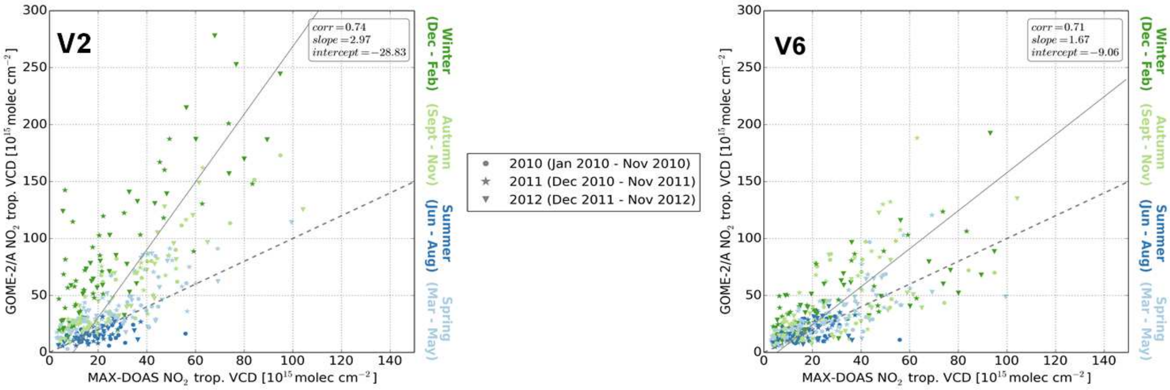


Figure 14: Scatterplots of GOME NO2 with the old retrieval (left panel) and the improved retrieval (right panel) versus ground-based MAX DOAS NO2 from Xianghe.

The Partner ULB-LATMOS provided satellite data of O3, NH3 and CO from the IASI satellite and improved the data during the project**.** Based upon the results of the validation/inter-comparison exercises a new version of IASI retrievals has been developed and tested:

O3 and CO retrieval

Several important changes/corrections have been implemented in the FORLI processing. The updated FORLI-O_3 and CO products (v20151001) are being validated. While preliminary comparisons show negligible differences for the total CO columns between the two FORLI versions, important improvements are found for the total and the partial O_3 columns. The FORLI-O_3 total column product from the two versions (v20140922 and v20151001) have been inter-compared to that from GOME-2 in Figure 15 for evaluating the improvements bring to the FORLI software. A much better agreement is observed between the updated FORLI (v20151001) and GOME-2A on a global scale (although local differences still remain especially in the Antarctic region) with a global mean bias between FORLI-O_3 against GOME-2A which decreases from 6.5±7.3% (with v20140922) to 2.1±9.0% (with v20151001).

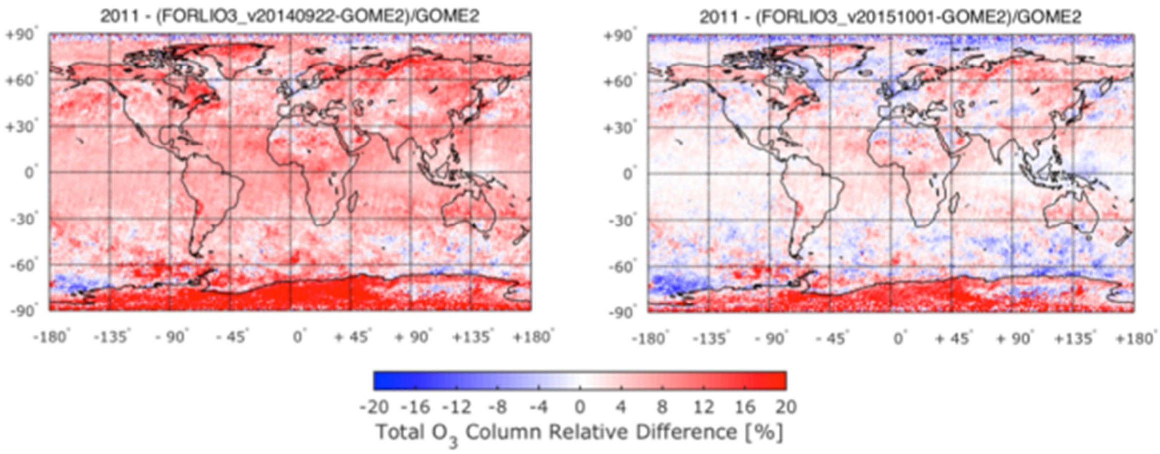


Figure 15: Global distribution of the relative differences (in %) between FORLI v20140922 (left panel) and FORLI v20151001 (right panel) against GOME-2A (O3M-SAF) TOCs averaged over 12 days of 2011 (on the 15th of each month) and over a 1° x 1° grid. The relative difference is calculated as: 100 x (FORLI-O3 – GOME-2) / GOME-2 (Boynard et al., 2016).

NH3 retrieval

A new retrieval algorithm for NH_3 based on a supervised artificial neural network (NN) approach has been developed to improve the conversion of the hyperspectral range index (HRI) from the IASI spectra to NH_3 columns and is found to strongly reduce the bias. The NN-based method inherits the advantages of the LUT-based HRI method (computational efficiency, consideration of full spectral range, low dependency on the forward model, no a priori information) whilst providing several significant improvements, such as:

- A better sensitivity at lower concentrations due to the consideration of full temperature, pressure and humidity vertical profiles in the retrieval.
- A reduction of the reported positive bias of LUT retrieval at low concentrations.
- The possible consideration of NH_3 vertical profile information from third party sources.
- A full uncertainty characterization of the retrieved column

In Figure 16, a distribution over Eastern Asia and a time-series of daily mean values over the Beijing area and the North China Plain (black box, left panel) for 2013 is provided. High daily mean values are observed in spring and summer months, with total columns above 4.10^{16} $molec.cm^{-2}$ measured in this area in July. The right panel of Figure 16 also compares the historical dataset with the second version, highlighting the reduction of the bias-high identified for the LUT-based product.

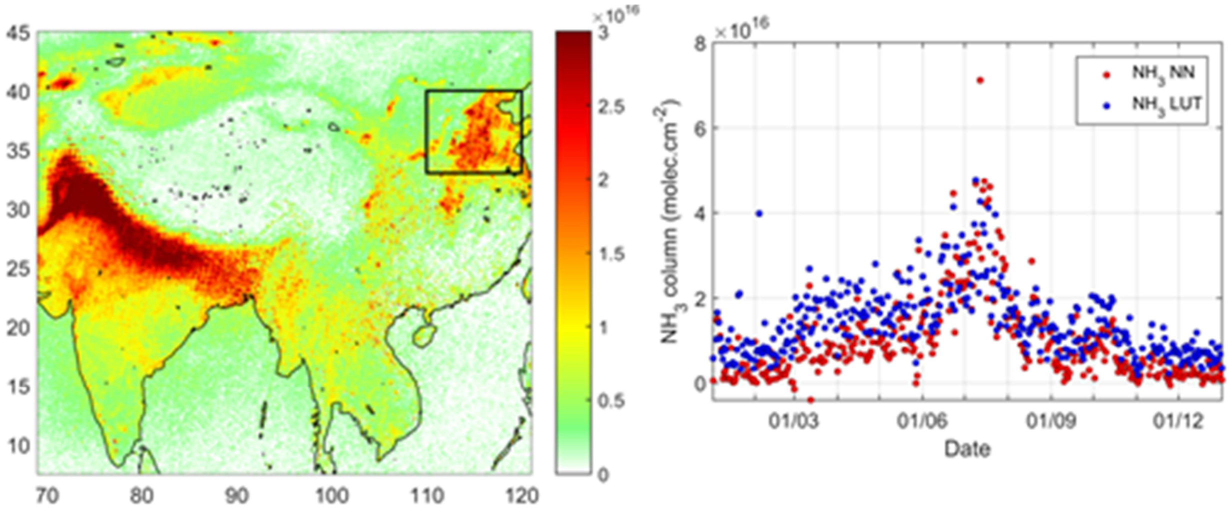


Figure 16: (Left panel) Mean NH_3 total column (molec.cm^{-2}) distribution over Eastern Asia for the year 2013. The black rectangle highlights the area considered for the calculation of the time series in the right panel. (Right panel) Daily mean NH_3 total columns (molec.cm^{-2}) in 2013 for the region of Beijing derived from the LUT-based (blue dots) and the NN-based method (red dots).

This reduction of the bias is also well shown in Figure 13 (right panels) (Whitburn et al., 2016). Top panels present the evaluation of the NH_3-NN dataset (D1.4 and D1.5) while the evaluation of the first version of historical NH_3 dataset (NH_3-LUT, D1.2 and D1.3) is presented at the bottom row, pointing to a clear improvement of the second version of the IASI-NH_3 dataset. The mean error between the real states and the retrieved columns is also lower with the NN approach, especially for low thermal contrast conditions. This results from the better sensitivity achieved thanks to the increased number of input parameters the neural network is able to cope with (such as full temperature, pressure and humidity profiles, emissivity, etc.).

Evolution of NO2 in China

In Figure 17, the tropospheric NO_2 column time series over Central East China is shown for SCIAMACHY, GOME2a, and GOME2b combining V6 and V6.1 data. SCIAMACHY columns are larger than those retrieved from GOME2a in winter, either because of instrumental differences or because of the earlier overpass time of GOME2a. The GOME2b data series is nearly perfectly consistent with that of GOME2a in the time period of overlapping measurements in spite of the difference in spatial sampling which results from the orbital differences (half an orbit shift) and the changes in coverage and spatial resolution following the reduced GOME2a swath width after July 15, 2013. Differences between V6 and V6.1 for GOME2a are small relative to absolute values as already pointed out.

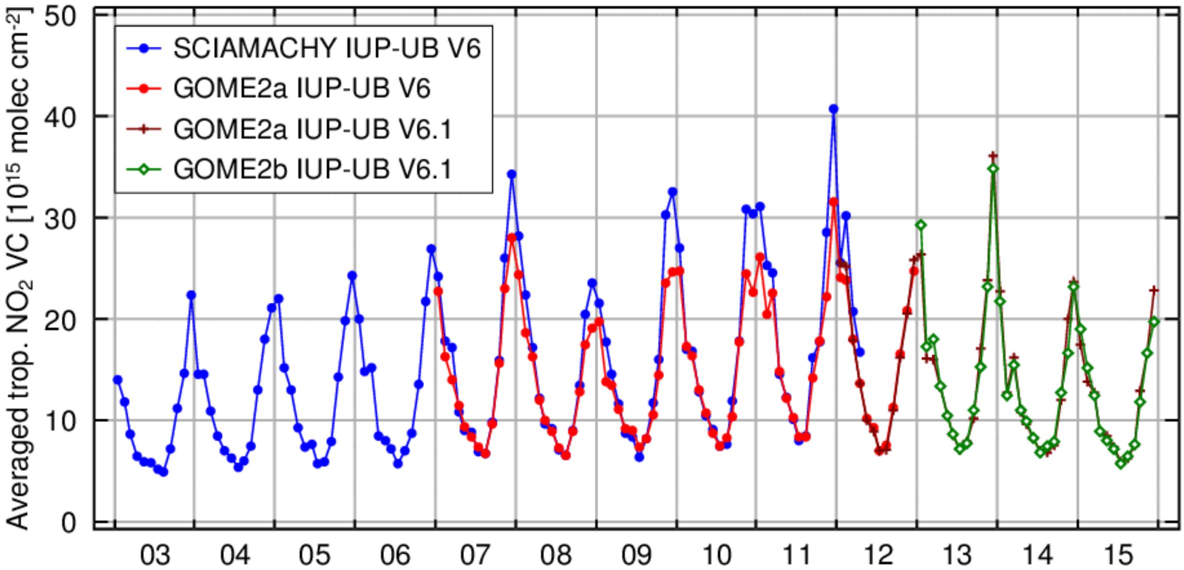


Figure 17: Combined IUP-UB V6 and V6.1 data sets of tropospheric NO_2 columns over Central East China for SCIAMACHY, GOME2a, and GOME2b data. For 2012, GOME2a data is shown in both data versions for comparison.

It is apparent from Figure 17, that after many years of increasing NO_2 columns starting with the GOME era (Richter e al., 2005), values have significantly decreased from 2012 onwards, most notably in winter but also in summer. In 2015, values were already back to SCIAMACHY observed values from 2006 but some care needs to be taken because of the difference between GOME2a and SCIAMACHY observations in winter. This change is very rapid and once again demonstrates the dynamics of the Evolution of emissions in China, which are driven by economic and technological development but also by strict environmental politics and legislation.

(b) In situ data:

A comprehensive table of observational data was established by MET Norway ECMWF and ULeic containing information on where to get observational data through bilateral agreements. This has turned out to be very useful in the end and the data have been used extensively for model evaluation. The table is not available at the toolbox, but has been distributed among interested partners of PANDA.
The toolbox lists publicly available measurement data sites, which are used, inter alia, for the evaluation of the city air quality forecast tool.
http://www.marcopolo-panda.eu/products/in-situ-data/

(c) Combined data sets:

A harmonised, high-resolution (0.01°) surface NO_2 dataset from PANDA partner ULeic has been made available at the toolbox of PANDA. Physically the data are stored at MET Norway (met.no).
Surface concentrations have been calculated ULeic by combining in-situ measurements with OMI tropospheric columns as part of a Land Use Regression model (see Panda deliverable report D2.2). Data is presented for the North China Plain (ppb) and the Pearl River Delta (µgm-3) regions for January and July 2010/2013, and for Hong Kong SAR for the period 2005 to 2015. Fine-scale information has been derived by correlating the in-situ data with known covariates from other datasets (e.g. urban area coverage from MODIS and OMI, surface elevation from ASTER, and road networks from OpenStreetMap). The Land Use Regression model was validated using in-situ data sampled by 5-fold cross-validation; overall, the modelled data shows good agreement with surface concentration measurements over both regions (R2 = 0.54 and 0.70 for the North China Plain and Pearl River Delta, respectively). However, insufficient OMI coverage from excessive cloud cover and degradation caused by the row anomaly has caused nonphysical artifacts to appear due to sampling biases.

The data are freely available on the Marcopolo-PANDA website via 'Products' – 'Observational data' – 'Combined data sets'. The direct link is:
http://www.marcopolo-panda.eu/combined-datasets/

Daily OMI observations allow for the measurement of the mean NO_2 field and daily spatiotemporal variations caused changes in local meteorology and emissions. As well as this, it is known that major emission sources are closely correlated with features such as road networks and urban areas, which in turn can be processed using publically available datasets such as OpenStreetMap and population density statistics.

A mixed effects model can therefore be used to infer daily surface NO_2 concentrations from these datasets. The model we propose is based on the mixed effects modelling approach discussed in Lee and Koutrakis (2014). It can be assumed that the surface concentration of a trace gas (*S*) at a location *i* and day *j* can be expressed as a linear sum of the daily OMI-measured column (Ω), and several additional parameters ($X_1, X_2, \ldots, X_n$):

$$\ln\left(S_{i,j}\right) = a + u_j + \left(\beta_1 + \upsilon_j\right)\Omega_{i,j} + \sum_n \beta_n X_{i,n} + \varepsilon_{i,j} \quad (1)$$

In this equation, *a* and u_j are fixed and random intercepts, respectively. β_1 and υ_j are the fixed and random coefficients of Ω, respectively. The fixed intercept and coefficient of Ω represent the average relationship between surface concentration and the satellite column during the whole time period. The random intercept and coefficient of Ω represent the daily variation in this relationship, which may be the result of difficult to model parameters, such as changes in the vertical profile or seasonal influences.

Equation (1) is solved using mixed effects linear regression, using the daily average concentrations measured by each in-situ station (*S*) coinciding with a cloud-free OMI overpass measurement (Ω). Other parameters were chosen from variables including road length, urban area cover, and surface elevation. These variables were selected iteratively based on their influence on the model R^2 and statistical significance, using a stepwise regression technique similar to the approach employed by the ESCAPE project (Beelen et al, 2013). Further information about this approach is summarised in D2.2.

Because of a lack of additional observation data, the models developed in this work were validated using five-fold cross-validation. This method has been applied for three different regions: North China Plain (ppb) and the Pearl River Delta (µgm-3) regions for January and July 2010/2013, and for Hong Kong SAR for the period 2005 to 2015.

Figure 18 shows the combined dataset (first row) for North China Plain, Pearl River Delta and the Hong Kong area and the modeled NO2 surface concentrations from the WRFchem MPI (2nd row), WRFchem SCUEM (3rd row), EMEP (4th row) and the WRFchem SYSE (5th row) for January 2010.

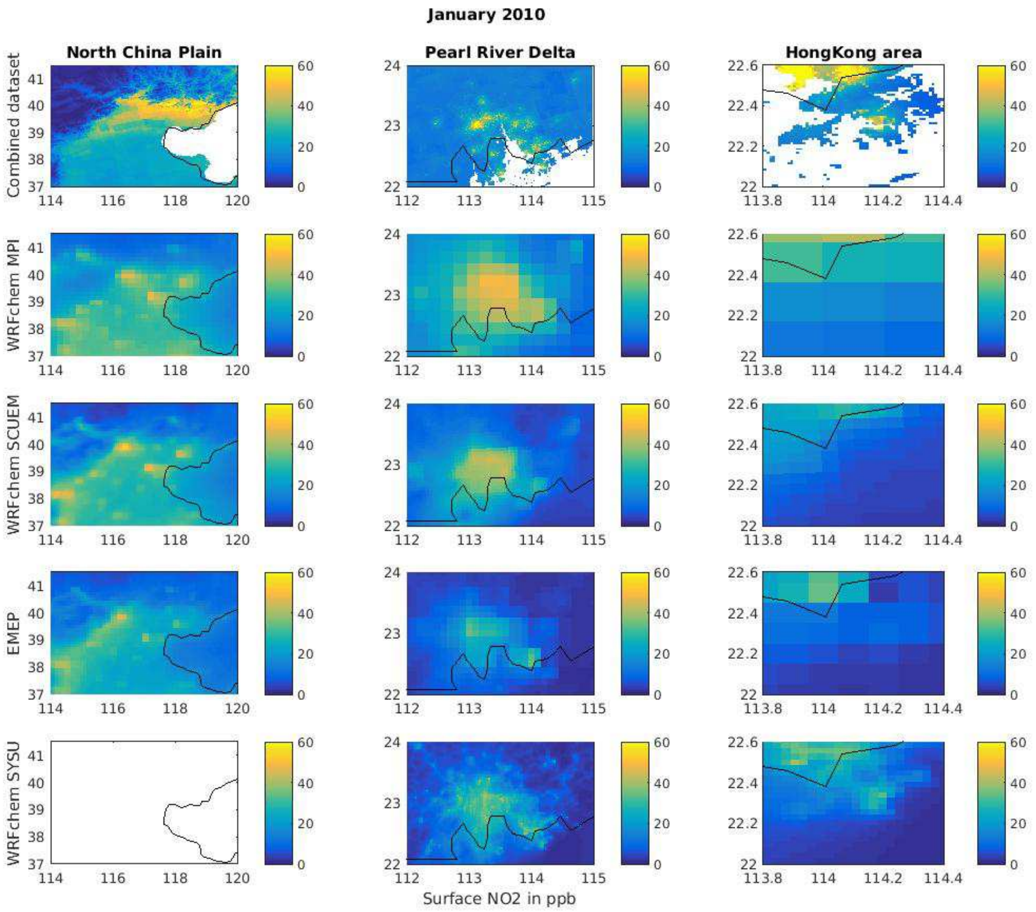


Figure 18: Combined dataset (first row) for North China Plains (left), Pearl River Delta (middle) and Hong Kong area (right) and the modeled NO2 surface concentrations from WRFchem MPI (2nd row), WRFchem SCUEM (3rd row), EMEP model (4th row) and WRFchem SYSE (5th row) for January 2010.

(5) Emissions

The MarcoPolo and Panda projects have collected emission data for different air pollutants. A comprehensive list, linking to data on both anthropogenic and natural emissions, can be found in the toolbox.
The Emission data base contains the MarcoPolo Inventory for East China, Satellite-derived emission estimates for NOx (OMI-based, GOME2-based), for SO2 (OMI-based), anthropogenic VOC, Isoprene, aerosols, anthropogenicPM2.5 and wildfire PM2.5 as well as bottom-up inventories from the MEIC emission data base and the ECCAD emission database.

The MEIC emission inventory

Anthropogenic emissions in China have been developed based on the MEIC framework using technology-based methodology. The MEIC (Multi-resolution Emission Inventory for China) model is a bottom-up emission inventory model framework developed and maintained by Tsinghua University, which uses technology-based methodology to calculate air pollutant and CO_2 emissions for more than 700 anthropogenic emitting sources for China. With a detailed source classification, the MEIC model can represent emission characteristics from different sectors, fuels, products, combustion/process technologies, and emission control technologies. Emissions are provided for 2008 and 2010 (MEIC 1.0) and for 2008, 2010 and 2012 (MEIC 1.2).

Power plant emissions in MEIC are derived from the China coal-fired Power plant Emissions Database (CPED), in which emissions are estimated for each generation unit based on unit-specific parameters including fuel consumption rates, fuel quality, combustion technology, and emission control technology. For on-road transportation sector, MEIC uses an approach which estimates vehicle emissions at a high spatial resolution by using vehicle population and emission factors at county level. County-level emissions are further allocated to high-resolution grids based on a digital road map and weighting factors of vehicle kilometers traveled by vehicle and road type.

MEIC provides lumped speciated NMVOC emissions for different chemical mechanisms, e.g., SAPRC99, SAPRC07, CBIV, CB05, and RADM2. Emissions of individual NMVOC species are calculated for each source category by splitting total NMVOC emissions with corresponding source profiles. Emissions are then assigned to various mechanisms using species mapping tables.

MEIC delivers monthly emissions at various spatial resolutions. Monthly variations and gridded emissions are generated by sector using different temporal profiles and spatial proxies. Users can define the metadata, calculate gridded emissions, and download data from the website. Emissions are aggregated to five sectors: power, industry, residential, transportation and agriculture. The emissions can be downloaded from the MEIC model website (available at http://www.meicmodel.org).

Emissions of NOx and PM2.5 in 2012 as given by MEIC1.2 are shown in Figure 19.

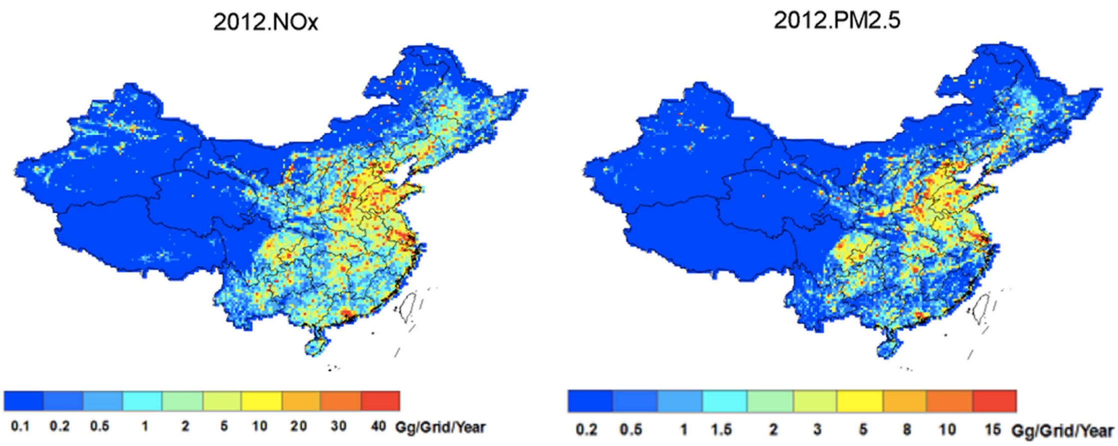


Figure 19: Emissions for 2012 of NOx and PM2.5 from the MEIC1.2 emissions dataset

The PanHaM inventory

After discussions with the PANDA WP4 partners, it was decided that WP3 partners will develop a consistent emissions dataset for the simulations performed for the period past-January 2013. The most desirable solution was identified as a merge of the MEIC 2012 inventory for China and the HTAPv2 global inventory for 2010. The PanHaM inventory was developed using the methodology shown in Figure 20: this inventory was then used by the PANDA modelers for their simulations.

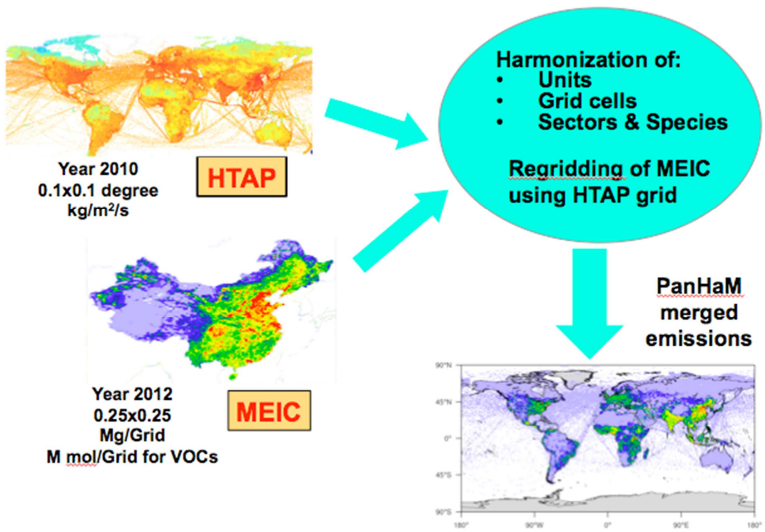


Figure 20: Methodology used to develop the PanHaM emissions.

The PanHaM emissions represent a merge of the emissions provided by the MEIC inventory described in the previous section and the HTAPv2 global inventory. The HTAPv2 emissions dataset was developed by the Joint Research Center (JRC, Ispra, Italy). It consists of gridmaps at a 0.1x0.1 degree resolution, and provides emissions for CH_4, CO, SO_2, NO_x, NMVOCs, NH_3, PM10, PM2.5 and BC (black carbon) and OC (organic carbon), for the years

2008 and 2010, on a monthly basis. HTAPv2 uses nationally reported emissions combined with regional scientific inventories in the format of sector-specific gridmaps.

The PanHaM inventory provides emissions for different sectors, i.e. transportation, residential use, energy/power, industry, ships, aviation, agriculture (NH_3 only). Each emissions are provided at a 0.1x0.1 degree resolution, as kg/m2/s. Emissions of nitrogen oxides from the PanHaM inventory at the global scale and for China are shown in Figure 21.

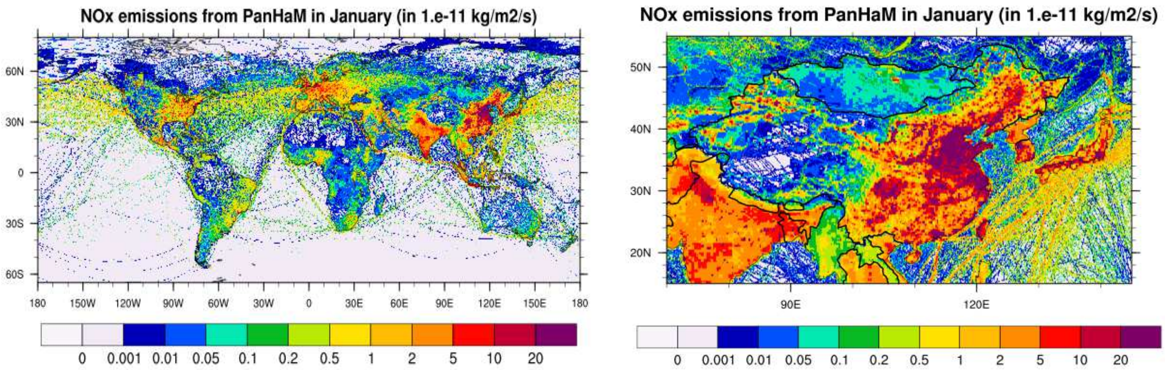


Figure 21: NOx emissions from the PanHaM inventory

Evaluation of anthropogenic emissions in China

Comparisons from a large number of datasets providing emissions for the past four decades were performed. The list of all the inventories considered in this intercomparison is provided in the deliverable describing this work. Both global and regional datasets are considered in the evaluation. The comparisons of the emissions of NOx and VOCs also include the emissions determined through inverse modeling techniques in the MarcoPolo project. Figure 22 shows the comparison of the emissions of NOx and VOCs in China. The different inventories used in the comparisons are indicated below each graph.

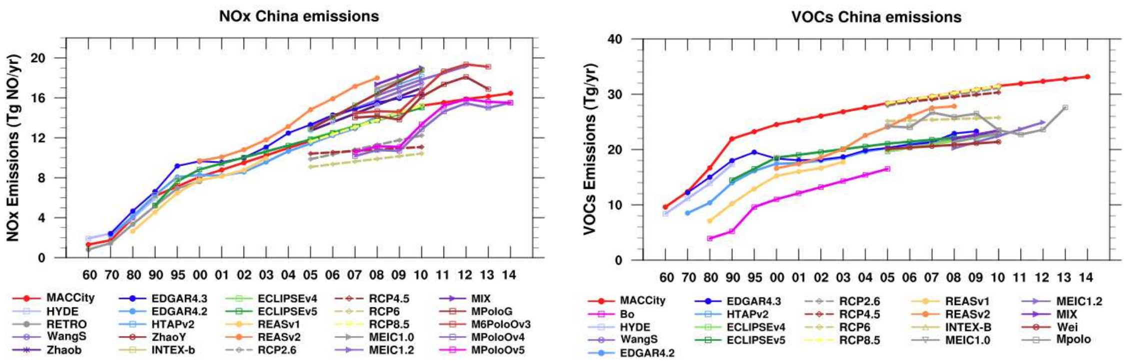


Figure 22: Comparisons of NOx ans VOCs emissions in China, as provided by different global and regional inventories.

NO_x is the compound for which the best agreement between different inventories is found. The emissions optimized using inverse modeling as part of the MarcoPolo project are in close agreement with the other inventories. They show a slight decrease after 2012 and such a feature will have to be confirmed in the coming years, when more recent data on emissions and more satellite observations will be available. It should be noted that the emissions optimized by inverse modeling techniques have large differences among themselves, which are as large as the differences between all the different inventories. Such differences are related to the disparities between the satellite data used to constrain the emissions.

Total NMVOCs emissions show a constant increase in all datasets, except for the emissions optimized with inverse modeling techniques, which show rather constant values since 2005: the decrease obtained in 2011-2012 is not present in the 2013 emissions. It should also be noted that the MACCity inventory provides emissions significantly higher than all the other datasets.

Emissions of biogenic volatile organic compounds in China

A methodology was developed to determine the emissions of terpenoid compounds at a 4-km resolution in the Pearl River Delta (PRD), China. It combines a distribution of plant functional types and observed emission potential of biogenic volatile organic compounds (BVOC) from local plant species and high-resolution meteorological outputs.

Accurate estimation of BVOC emissions highly relies on the accurate description of land use/land cover, i.e. plant functional types (PFT). Four PFTs are considered in the study: broadleaf trees, needle leaf trees, shrubs and bushes, and grasses and crops. The model default PFTs distribution based on 1-km Moderate Resolution Imaging Spectroradiometer (MODIS) data in 2003 that can be downloaded from http://cdp.ucar.edu/acd/megan. These data were merged with PFT distributions based on local datasets obtained from (1) the Thematic Mapper (TM) images for 2006 with 30-m resolution, (2) a dataset from Guangdong Forestry Bureau, which collects the total vegetation coverage for each county and identifies the dominant tree species and vegetation categories and (3) from field surveys conducted by the Sun Yat-sen University. The survey team made 50 visits to places where the TM data differs from the Forestry Bureau statistic data.

Figure 23 shows presents the BVOC estimates for July and October 2006. As temperature and solar radiation increases in the summer, isoprene emissions reach their annual maximum values. In October, isoprene emissions start to decrease due to lower temperature and radiation. The ratio of biogenic isoprene emissions between summer and winter is very large (about 10.6). The spatial distribution of monoterpene emissions is different from that of isoprene emissions, especially in southern Huizhou where needle leaf trees are dominant, which have higher emission factors of monoterpenes than broadleaf trees. The dominant monoterpene species are α- pinene and β-pinene which account for 55% of the total emissions.

The spatial distribution of sesquiterpene emissions is similar to the monoterpene emissions, except that their emission amount is smaller. The highest emission occurs in summer, responding to the highest temperature and incoming solar radiation. The ratio of biogenic sesquiterpene emissions between summer and winter is about 9.3. The sesquiterpene emissions in the PRD are about 10 times lower than monoterpene and isoprene.

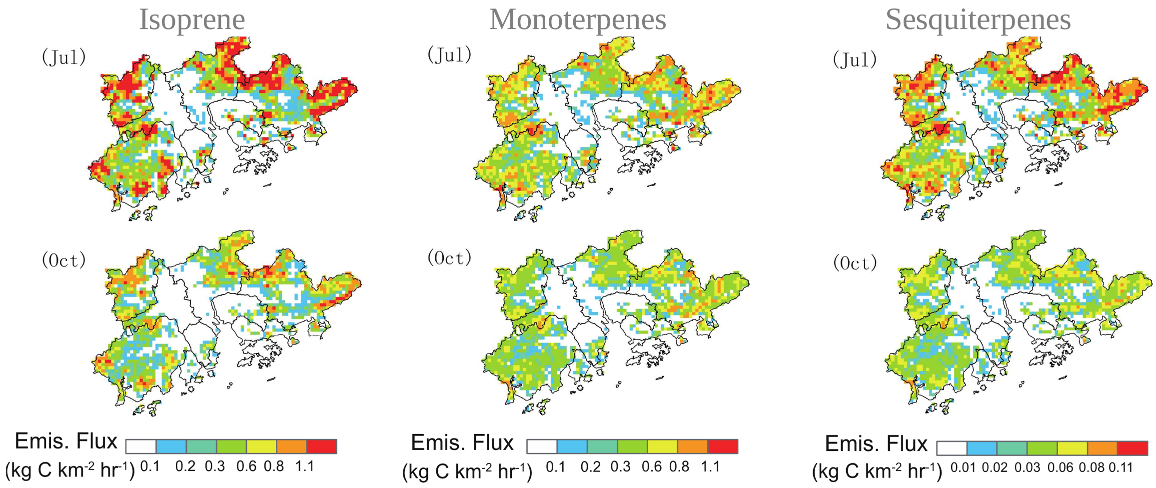


Figure 23: BVOC emissions estimates for July and October 2006

Emissions of particle from biomass burning in China

The burning of crop residues at the end of the harvest season leads to emissions of gaseous and particulate compounds. A study was conducted to evaluate the spatial-temporal variation of biomass burning in June during the wheat harvest season in Northern China. The occurrences of fires exhibit temporal changes with a minimum in 2008 (during the Beijing Olympics) and a peak and explosive growth in 2012. Under high relative humidity and south winds, fire emissions from straw burning combined with high urban/industrial emissions to produce intensive regional haze pollution in the North Plain. Figure 24 shows the location of active fires (black dots) for different days in June, averaged from 2005 to 2012, at a spatial resolution of 500m.

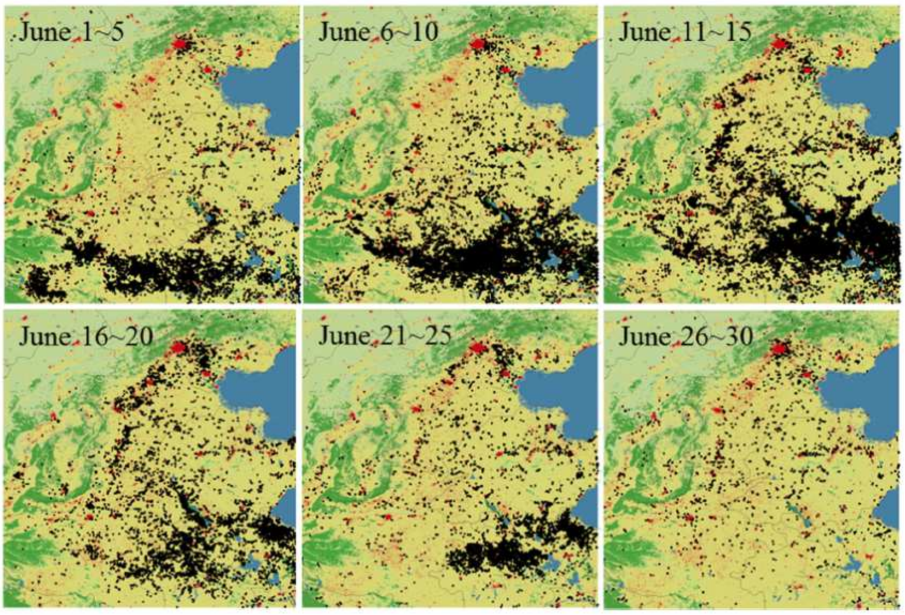


Figure 24: Distributions of fire points in June in Northern China (32-41°N, 111-120°E).

Potential Impact:

The PANDA Project provides the scientific basis required for meeting the newly defined standards designed by the Chinese authorities, specifically the regional and local environmental agencies to implement measures needed to improve air quality. To bring the scientific research beyond state-of-the-art, and useful for users and for decision-makers, progress has been accelerated in several areas:

(a) **Improvement of monitoring methods:** Best-practice on the development and delivery of in-situ measurement networks has been exchanged between the European and Chinese partners. Exchange of knowledge between Europe and China reinforce the existing cooperation between the two regions in the area of space observations.

b) Accurate knowledge of the magnitude of primary emissions, as well as their distributions in space and time, is required to evaluate the impact of chemical pollution on air quality, climate, ecosystem viability and human health. Adequate and accurate emission inventories needed therefore to be established. One expected outcome of the present project was to improve the cooperation between European and Chinese scientists on the development of emission inventories for Asia, and to evaluate existing emission data.

c) Combination of remote-sensing and in-situ observations for improvement of air quality analysis and forecasting: With the availability of observational data and of different models including assimilation techniques, systematic studies have been performed in cooperation with Chinese scientists. Observations provided by space instrumentation and from surface sites together with global and regional models help improve our representation of multi-scale processes in chemical transport models.

PANDA provides new data, methods and applications related to:

- The forecasting of air quality and its dependence on (near real time) observations of atmospheric composition ("air quality and health").
- Surface emissions of gaseous and particulate compounds and their improvement on the basis of observations.
- The distribution of short-lived climate forcing species (black carbon and ozone), which play a key role not only in air pollution reduction but also in climate change protection and sustainable development.
- The impact of sand and dust storms, which are crucial for the forecasting of pollution events in China.
- Reactive nitrogen, trends, variability/climatology (integral to food production).

Dissemination:

Toolbox

In an effort to disseminate information and data to a broad community and to the public, the project has produced a so-called toolbox for easy access to information, and developed related educational activities. The toolbox of the PANDA project is located at the joint MarcoPolo-Panda web portal hosted by the MarcoPolo partner KNMI. It gathers available measurements and observations, emission inventories and model data on atmospheric compositionas well as the system for the prediction of air quality for China.

They can be accessed from the main page http://www.marcopolo-panda.eu/ via the main menu item ‘Products’. An overview is provided in the same menu item, both in English and in Chinese. Direct links to the overview:
http://www.marcopolo-panda.eu/products/toolbox/ (English version)
http://www.marcopolo-panda.eu/products_cn/toolbox_cn/ (Chinese version).

The toolbox contains six sections: (1) Air quality Forecasts, (2) Model Results, (3) Model Evaluation, (4) Observations, (5) Emissions, and (6) Tutorials, presenting the main results of the Panda project and making them available to the scientific community and the public.

Scientific Presentations

Apart from the dissemination of results through the toolbox, the Panda Project and its results have been presented at several international conferences and meetings, among them the most important international conferences in Geoscience (at the European Geosciences Union, The American Geophysical Union, and others). A scientific session by the PIs of the Panda and MarcoPolo projects, Guy Brasseur and Ronald van der A, has been organized at the AGU fall meeting (A009: Analysis and Numerical Forecast of Air Quality in Asia **(Session ID#:** 13625)), presenting the results of the projects and from recent research acitvities. Ying Xie (Partner SCUEM) and Trissevgeni Stavrakou (MarcoPolo Partner BIRA) presented invited talks. Six oral presentations have been presented by Partners from the MarcoPolo and Panda projects and 8 poster presentations.

Workshop and Proceedings book

During the Panda Project, two meeting have been organized, financially supported by the ISSI (International Space Science Institute, Bern, Switzerland) and ISSI-Beijing, with the objective to bring together a group of experts, many of them from the Panda and MarcoPolo projects, to address the problem of the formation of large haze episodes in Asia from different perspectives (space observations, surface monitoring, profiling, laboratory approaches, data analysis, modeling and impacts). Two meetings, one in Beijing (Feb. 29 to March 04, 2016: ISSI-BJ, Beijing) and one in Bern (17-20 May 2016 at ISSI, Bern) provided the opportunity to discuss in detail the different issues related to haze formation and to develop a synthesis that lead to the production of a proceedings book, presented here: The Book will be published in 2017 under the title “**Air Pollution in Eastern Asia**” **(***Guy Brasseur, Xuemei Wang and Idir Bouarar, Editors),* Springer Verlag, 2017.

Policy User Workshop

A Policy User workshop was organized by SYSU and PANDA on 25 February 2016. The purpose of the workshop was to develop a dialogue with potential users of the tools and products developed by the MarcoPolo and PANDA projects.

Several presentations highlighted some of these products. A long and very fruitful discussion took place during the workshop to help identify the needs and wishes of users, and to provide the opportunity for the projects to develop additional tools and to align them with the needs of stakeholders. About 100 participants attended the workshop. The detailed agenda of the workshop is available at: http://www.marcopolo-panda.eu/wp/internal/wp-content/uploads/2014/04/Joint-workshop-agenda-2016.2.20.pdf

The Policy user workshop was successful in making the MarcoPolo-PANDA products well-known among a large community of potential policy users in China. The conclusion from the workshop was that after a careful evaluation of the air quality forecasts, further use could be considered.
A new user workshop is planned by MarcoPolo for March 2017 to promote use of the evaluated products. PANDA partners will be present as well.

Summer schools

Finally, the organization of two very successful summer schools, one in Bremen and one in Guangzhou has provided the opportunity to make a large group of junior scientists familiar with the Panda products and models, and to provide background information on the science related to the European Panda project.

The first summer school was held from 23 August to 29 August 2015 at the Institute of Environmental Physics (IUP), University of Bremen, Bremen, Germany. The topic of the European summer school was “Remote Sensing of the Atmosphere, Emissions and Modeling”. Within this summer school, training courses with interdisciplinary lectures, practical work and field excursions were offered to 41 students in total with 13 of them from China and others from Europe. Some of the students are enrolled at one of the partners of PANDA or MarcoPolo projects but other motivated students with a background in atmospheric chemistry or meteorology were also welcomed to participate to the summer school.

The second PANDA / MarcoPolo Summer school “International Summer School on Air Pollution Monitoring and Forecast: Space observations and Air Quality” took place from 04 to 08 July 2016 at the School of Atmospheric Sciences (SAS), Sun Yat-sen University in

Guangzhou, China. Within this summer school, training courses with interdisciplinary lectures, practical work and field excursions were offered to 75 students in total with 10 of them from Europe and others from China. Some of the students are enrolled at one of the partners of PANDA or MarcoPolo projects but other motivated students with a background in atmospheric chemistry or meteorology were also welcomed to participate to the summer school.