MODIS AND OMI SATELLITE OBSERVATIONS SUPPORTING AIR QUALITY MONITORING

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Within the framework of air quality monitoring, measurements by Earth-observing satellite sensors are combined here with regional meteorological and chemical transport models. Two satellite-derived products developed within the QUITSAT project, regarding significant pollutants including PM2.5 and NO2, are presented. Estimates of PM2.5 concentrations at ground level were obtained using moderate resolution imaging spectroradiometer (Terra-Aqua/NASA) aerosol optical properties. The semi-empirical approach adopted takes into account PM2.5 sampling and meteorological descriptions of the area studied, as simulated by MM5, to infer aerosol optical properties to PM projection coefficients. Daily maps of satellite-based PM2.5 concentrations over northern Italy are derived. Monthly average values were compared with in situ PM2.5 samplings showing good agreement. Ozone monitoring instrument (OMI) (Aura/NASA) NO2 tropospheric contents are merged using the GAMES chemical model simulations. The method employs a weighted rescaling of the model column in the troposphere according to the OMI observations. The weightings take into account measurement errors and model column variances within the satellite ground pixel. The obtained ground-level concentrations of NO2 show good agreement with the environmental agencies’ in situ.

The capabilities of Earth observation satellites have greatly improved over the last few years, with gradual improvements in temporal and spatial resolutions and enhancements in radiometric accuracy, thus encouraging further studies on the use of satellite data to assess air quality (AQ).

Within this context, the synoptic view and the daily repetition cycle of satellite-based measurements strengthen the potential for monitoring air pollution transport and directly evaluating the spatial distribution of various air pollutant concentrations. These evaluations are in compliance with the regulations of the European Community (1).

Great attention has been paid to data analysis on the correlation between aerosol optical depth (AOD), provided on a daily basis at 10 × 10 km2 resolution by the moderate resolution imaging spectroradiometer (MODIS) sensors onboard NASA’s Terra and Aqua satellite, and surface concentrations of PM2.5 (particulate matter with diameter <2.5 μm)(2–4).

Similarly, with the ozone monitoring instrument (OMI) onboard NASA’s Aura satellite, the tropospheric loading of polluting trace gases, such as nitrogen dioxide (NO2), is provided once per day at 13 × 24 km2 resolution (5).

The processing of satellite-calibrated spectral radiance data provides estimates of the columnar contents of various atmospheric constituents. However, in order to derive satellite-based concentrations of pollutants at ground level, it is necessary to integrate satellite data with ground-based measurements and/or modelling simulations.

The QUITSAT project, funded by the Italian Space Agency (ASI), is based on this concept aiming at the implementation of a prototype system with AQ monitoring, forecasting and planning functionalities. This system is devoted to assess AQ in northern Italy (from 43.15 to 46.65°N and from 6.32 to 14.38°E) through the synergy of satellite observations with ground-based data provided by DOAS spectrometers, multispectral sunphotometers, lidars and chemical transport models (CTM). Regional environmental protection agencies (ARPs) of Emilia Romagna and Piedmont take part in the project to check the suitability of the results for AQ assessment and management. The principal QUITSAT functionalities are (1) PM and gas monitoring, with production of maps of surface-level PM and gas concentrations, maps of AQ index and categories and extreme aerosol transport events; (2) PM and gas concentration forecasting, including the forecast of AQ scenarios and above-threshold events; (3) planning and providing emission

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reduction costs and impact evaluations of emission scenarios for the environmental decision-makers\(^6\).

In the following, methods and results regarding two user products processed by the QUITSAT monitoring system (v. 2.0) are presented, including estimates of PM\(_{2.5}\) and NO\(_2\) concentrations at surface, based on MODIS and OMI data, respectively.

**MODIS-BASED ESTIMATES OF PM CONCENTRATIONS AT SURFACE LEVEL**

Values of columnar AOD can be retrieved from the radiance measurements performed by satellite sensors within the spectral range 400–2100 nm\(^7\). AOD estimates over land can be assumed as being mainly due to PM atmospheric loading from anthropogenic activities\(^8\), especially in heavily polluted areas and in the absence of natural aerosol transport (such as desert dust) towards the monitored area.

The relationship between AOD and PM at surface varies with region and season as well as with vertical profiles and microphysical properties of aerosols. In this regard, it is important to take into account the fact that PM concentrations are usually sampled at relative humidity (RH) lower than 50 %, and both aerosol optical properties and AOD begin to differ considerably from those of dry air only in cases where ambient RH is >60–70 %, depending also on aerosol composition.

In this analysis, covering northern Italy, aerosol is considered being well mixed within the mixing layer of height \(H_{\text{mix}}\) during the diurnal hours of summer clear-sky days, considering that the planetary boundary layer (PBL) is usually affected by intense convective conditions. The parameter \(H_{\text{mix}}\) was estimated to provide reliable evaluations also of the thermal inversion ground-layer depth in winter, when stable conditions of the atmosphere are often present in the Po valley both day and night. In summer, the thermal structure of the atmosphere becomes gradually more stable during the nocturnal hours, favouring the formation of multilayer aerosol extinction profiles at altitudes above the PBL. Under these conditions, \(H_{\text{mix}}\) provides realistic estimates of the PBL depth during both diurnal and nocturnal hours throughout the year.

Dependence features of AOD and PM on RH conditions at surface and within the mixing layer were also considered, examining the variations of the RH vertical profile simulated by MM5 meteorological model\(^9\) within the atmospheric boundary layer at various Po valley sites and the evolutionary patterns of lidar profiles at Milan and San Pietro Capofiume ground stations. Within this context, particular attention was paid to the variations of RH and aerosol profiles during the day with respect to those measured at the two MODIS satellite overpass times, i.e. at around 10:00 (Terra) and 13:00 (Aqua) local time. MM5 simulations, performed under clear-sky conditions over urban and rural Po valley sites, indicated that only limited variations in RH occurred, ranging typically between 45 and 60 % in summer and between 55 and 65 % in winter, at the different altitudes within the mixing layer.

Discrepancies of 5–10 % were found between the surface value of RH and its mean value calculated over the mixing layer, which are expected to cause only slight effects on the growth of aerosol particles suspended in air for RH values of \(\sim 60\) %.

Comparisons between the time patterns of PM\(_{2.5}\) and AOD measured at some QUITSAT sites with optical techniques and sun-photometers have shown that the MODIS AOD values agree very closely with the daily average values of AOD measured from sunrise to sunset (with sun-photometer measurements) and over the 24-h period (with nephelometer measurements). These results confirm that ‘instantaneous’ values of MODIS AOD are consistent with the ground-based measurements of PM sampled on a daily basis.

In addition, on the basis of chemical composition analysis of PM at different Po valley sites for different seasons, it was found that the mass percentages of water soluble and organic carbon vary considerably with season. This implies that a marked fraction of particles generated by local sources is present during long periods of a month or more, presenting stable composition features during the same seasonal period. Therefore, it is important to take into account that a large fraction of PM\(_{2.5}\) consists of PM originating from anthropogenic sources in the Po valley, having stable composition characteristics. On days without the presence of residual layers of continental aerosols or of desert dust, the major part of airborne aerosols is suspended within the PBL with chemical characteristics defined substantially by local emissions.

On the basis of these remarks, the following points can be made: (i) the estimates of the \(H_{\text{mix}}\) parameter at MODIS overpass times are suitable for the conversion of AOD into estimates of ground-level PM\(_{2.5}\) concentration; (ii) the instantaneous values of PM\(_{2.5}\) derived from MODIS AOD are usually close to the 24-h average PM\(_{2.5}\) values obtained from sampling measurements; (iii) the corresponding values of surface RH can be used to realistically evaluate the growth of aerosols within the whole mixing layer; and (iv) the chemical composition and microphysical properties relative to the satellite overpasses vary considerably with season. These variations are more limited over shorter periods of a few weeks, because such short-time variations are closely related to the evolutionary patterns of atmospheric transport episodes.

On this basis, reliable estimates of surface PM\(_{2.5}\) (\(\mu g\ m^{-3}\)) can be derived from satellite-based
estimates of AOD at 550 nm, provided that the meteorological characterisation of the $H_{\text{mix}}$ parameter and surface RH conditions in the atmospheric boundary layer are also taken into account, as simulated by a meteorological model\(^{(4)}\).

MODIS/Terra-Aqua aerosol level 2 data (C005) provided by NASA at 10 × 10 km\(^2\) resolution\(^{(10)}\) for the whole of 2004, three summer months (May–July) in 2007 and three winter months (January–March) in 2008 were selected.

The MM5 model has been employed to simulate meteorological fields—at 12 × 12 km\(^2\) resolution over the QUITSAT domain—from which hourly values of $H_{\text{mix}}$ and RH at surface were extracted for the analysis of MODIS aerosol parameters.

Both gravimetric PM\(_{2.5}\) data provided by ARPA Piedmont and those sampled at several sites in Lombardy during 2004 were examined, and gravimetric samplings taken by ARPA Emilia Romagna and Lombardy in summer 2007 and winter 2008 were used. Additional data recorded during sampling campaigns at six dedicated sites of the QUITSAT project were analysed, as obtained from measurements performed at urban (Bologna and Milan), rural (San Pietro Capofiume and Oasi Bine) and background sites (Mt Cimone and Bormio).

For each month and each sampling site, corresponding spatio-temporal data from the three data sets consisting of satellite aerosol data, modelling meteorological simulations and PM\(_{2.5}\) gravimetric samplings were grouped together. These data were then used to derive relationships between satellite-based AOD and in situ PM\(_{2.5}\) sampling data at the various sites, on a monthly basis, considering the dependence on physical parameters such as $H_{\text{mix}}$ and aerosol growth factor, $F(\text{RH})$, expressed in terms of surface RH.

More precisely, the intercept and slope coefficient parameters of the monthly regression lines between the daily values of AOD/($F(\text{RH}) \times H_{\text{mix}}$) and in situ PM\(_{2.5}\) were calculated for each measurement site.

Once best regression parameters had been determined for each sampling site and month, a spatial interpolation function over the whole QUITSAT domain—based on an average weighted by the inverse of the square of the distance between each sampling site and the current geolocation—was employed to define the spatial distribution of these regression parameters.

The obtained monthly maps of these coefficients were finally used to estimate daily maps of PM\(_{2.5}\) at 10 × 10 km\(^2\) resolution from daily satellite AOD maps, MM5 simulated fields of $H_{\text{mix}}$ and RH at surface.

Figure 1 shows an example of daily maps based on MODIS/Terra data for two clear-sky days of summer and winter. High values of PM\(_{2.5}\) are evident in winter and frequently exceed thresholds of 25 µg m\(^{-3}\) in summer at several Po valley locations. In general, mainly due to clouds, winter daily maps show a deficit of data. For a nominal repetition cycle of 1 per day for MODIS onboard each platform, about 15 useful overpasses for aerosol retrieval are available in a summer month and no more than about 10 in a winter month.

The maps of average PM\(_{2.5}\) presented in Figure 2 were derived using MODIS/Aqua data, as represented by average concentrations of at least 10 PM\(_{2.5}\) values per pixel in June and August 2004.

Comparisons between in situ sampling and satellite-based PM\(_{2.5}\) data sets were routinely performed. Figure 3 shows the time patterns of satellite-based and in situ daily PM\(_{2.5}\) data sets were routinely performed. Figure 3 shows the time patterns of satellite-based and in situ daily PM\(_{2.5}\) data sets were routinely performed. Figure 3 shows the time patterns of satellite-based and in situ daily PM\(_{2.5}\) data sets were routinely performed. Figure 3 shows the time patterns of satellite-based and in situ daily PM\(_{2.5}\) data sets were routinely performed. Figure 3 shows the time patterns of satellite-based and in situ daily PM\(_{2.5}\) data sets were routinely performed. Figure 3 shows the time patterns of satellite-based and in situ daily PM\(_{2.5}\) data sets were routinely performed. Figure 3 shows the time patterns of satellite-based and in situ daily PM\(_{2.5}\) data sets were routinely performed. Figure 3 shows the time patterns of satellite-based and in situ daily PM\(_{2.5}\) data sets were routinely performed. Figure 3 shows the time patterns of satellite-based and in situ daily PM\(_{2.5}\) data sets were routinely performed. Figure 3 shows the time patterns of satellite-based and in situ daily PM\(_{2.5}\) data sets were routinely performed.

These results comply with the European Community rules\(^{(1)}\). Within this context, satellite-based monthly average estimates of PM\(_{2.5}\) can be exploited as parameters useful for monitoring the AQ over the whole year and individuate the periods within the year with the highest risks of exceeding threshold.

Figure 4 presents the scatter plot of monthly average values of PM\(_{2.5}\), with their standard deviations, as derived from MODIS, onboard Terra and Aqua, and in situ measurements performed at the QUITSAT sites, in summer 2007 and winter 2008. There is good agreement between these monthly values, with $R^2 > 0.7$ for both Terra and Aqua data, showing a tendency of satellite-based AOD values to underestimate the PM\(_{2.5}\) monthly average values by nearly 20 %. This kind of comparison serves to identify sites and months for which the risk of exceeding threshold is highest. Thus, this information derived from satellite observations over the entire Po valley area provides a valuable contribution for the application of EC Directives.

**NO\(_2\) CONCENTRATION ESTIMATES AT SURFACE LEVEL USING GAMES SIMULATIONS AND OMI OBSERVATIONS**

Tropospheric columnar satellite observations of trace gases, such as NO\(_2\), are widely used to assess anthropogenic emissions and their long-range transport\(^{(11)}\). One of the main challenges of columnar content use in AQ applications is to derive from them an estimate of trace species' ground-level concentration. This represents one of the main aims of the QUITSAT project pursued with observations
from the OMI sensor onboard Aura\(^{(5)}\) (level 2 data kindly provided by the TEMIS project) and CTM simulations from the GAMES model\(^{(12)}\) on a regional scale (northern Italy domain) at 10\(\times\)10 km\(^2\) resolution.

The main goal of merging modelling data and satellite observations was to obtain a procedure to improve the accuracy of modelled NO\(_2\) simulations within the context of AQ monitoring. This is achieved using OMI measurements to directly correct model output. A similar approach has been proposed by Lamsal \textit{et al.}\(^{(13)}\)

The model developed in QUITSAT uses satellite NO\(_2\) column values \((C_S)\) to correct the time-corresponding model column \((C_M)\) re-gridded and averaged over the OMI ground pixel \((13 \times 24\, \text{km}^2)\) according to the following formula:

\[
C_C = \left( \frac{C_S^2}{\Delta C_S} + \frac{C_M^2}{\Delta C_M} \right) \left( \frac{C_S}{\Delta C_S} + \frac{C_M}{\Delta C_M} \right)^{-1}, \tag{1}
\]

where \(\Delta C_M\) and \(\Delta C_S\) are the standard deviations of the modelled column within the OMI ground pixel.

\[\text{Figure 1. Maps of MODIS-based PM}_{2.5} \text{concentrations over northern Italy on 10 February 2008 (upper part) and 17 July 2007 (lower part).}\]
and the error on NO$_2$ retrieval, respectively. The latter depends on several factors such as DOAS processing, air mass factor simulations, NO$_2$ actual vertical profile, etc. and is supplied by the OMI level 2 data. Details on the calculation of the tropospheric vertical column density error of NO$_2$ can be found in Boersma et al.$^{14}$ The corrected column is thus a weighted average of the model, and measured columns weighted according to the reciprocal of the respective relative errors.

The averaged NO$_2$ GAMES vertical profile ($p_{NO_2}(z)$) within the OMI pixel is thus normalised to the new corrected column ($C_C$). The respective ground concentrations (QUITSAT ground concentration, QGC) represent the main result of this procedure, being obtained from the following formula:

$$QGC = p_{NO_2}(10\,\text{m}) \frac{C_C}{C_M},$$

(2)

where 10 m is the height (above ground) of the first GAMES layer.

In Figure 5, NO$_2$ QGCs are presented as averages for summer 2007 and winter 2008. These seasonal averages are calculated over more than 30 d, in each
Figure 3. Comparison between daily satellite-based and in situ sampling PM$_{2.5}$ values at San Pietro Capofiume in February–March 2008.

Figure 4. Comparison between monthly averaged MODIS-based and in situ samplings PM$_{2.5}$ values at the six measurement sites in the QUITSAT project. Data are related to summer 2007 and winter 2008.

Figure 5. OMI-based average NO$_2$ concentrations at ground level during summer 2007 (up) and winter 2008 (down).
season, singled out for the best meteorological conditions. The seasonal trend and the local pattern related to anthropogenic and natural emission are clearly recognisable from the plot showing the summer minimum and the winter maximum related mainly to human activity. Major city emissions (Milan, Bologna, Florence, Turin) and highway patterns also become evident on observing individual day maps.

The procedure described herein for correcting CTM simulations according to equations (1) and (2) was tested by comparing the resulting NO$_2$ QGC with corresponding \textit{in situ} measurements.

In Figure 6a, ARPA \textit{in situ} measurements of ground-level NO$_2$ are set against NO$_2$ QGC estimates for summer 2007 and winter 2008.

When several ARPA measurements were available within one OMI pixel, those measurements were averaged. The overall agreement is good, data being scattered around the bisector of the first quadrant (expected as best result), but the correlation is not satisfactory ($R^2 = 0.23$, and the RMSE = 32.5 \text{\mu g cm}^{-2}$). Actually, this plot is made up of several days (>60 as mentioned earlier) each corresponding to one of the two case studies plotted in Figure 6b and 6c. The last one (11 February 2008) is characterised by optimal horizontal mixing conditions, and the correlation coefficient is $\approx 0.69$, while the first one does not match this situation as confirmed by the error bars in the ARPA measurements (standard deviation of the average value within the OMI pixels). High errors mean low horizontal homogeneity in NO$_2$ concentration, and as result, the correlation coefficient decreases. In fact, the NO$_2$ QGCs value its concentration relative to a $13 \times 24$ km$^2$ area and could be interpreted as an average concentration over this area, and thus a comparison with \textit{in situ} sampling performed by ARPA may not always be appropriate.

**CONCLUSIONS**

Results shown on MODIS-based PM$_{2.5}$ and OMI-based NO$_2$ estimates at surface level, with auxiliary modelling simulations and \textit{in situ} measurements, confirm the potential for using satellite remote sensing within the AQ monitoring context. The possibility of daily and spatially distributed

Figure 6. (a) Comparison between \textit{in situ} ARPA measurements of NO$_2$ and satellite-based values during summer 2007 and winter 2007–2008; (b) case study for 11 February 2008; (c) case study for 12 July 2007. Error bars on ARPA values are the standard deviations of the average concentrations and are available only for ground pixel matching with more than one ARPA station.
monitoring of the pollutants complies with the regulations of the new EC Directive on AQ.

In QUITSAT version 3, information from lidar and balloon measurements will be used to take better into account the atmospheric aerosol vertical structure. At the same time, data analysis of the ground-based radiometric measurements will allow better study of how RH affects aerosol hygroscopic growth in the Po valley. Ground-based DOAS data will also be used to evaluate the differences observed in several cases between NO$_2$ in situ measurements and the horizontal gradient within the OMI pixel for the NO$_2$ QGC product.

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