Interpretation of satellite retrievals of PM_{2.5} over the Southern African Interior

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Abstract

A case study is presented for using an unsupervised classification (Self-Organizing Map) of a global PM_{2.5} data product assembled from satellite retrievals (SeaWIFS, MODIS Terra and MODIS Aqua) and ground observations. The PM_{2.5} data products are available, on a daily basis, from August 1997 to the present, with 10 km resolutions and global coverage. In this study, a sub-set of the PM_{2.5} retrievals (collected over the southern African Interior) has been averaged over ten-day intervals for a period of ten years. These averaged sub-sets have been clustered using self-organizing maps to generate spatial and seasonal “PM_{2.5} climates” and air quality interpretations over southern Africa. Results are an indirect validation of the satellite based data product against available regional ground-based and airborne studies. The final PM_{2.5} aerosol climatology shows that the data product provides credible PM_{2.5} estimates for a region that is lacking routine aerosol monitoring data.

Keywords: Regional air pollution, PM_{2.5} particulate matter, aerosol retrievals, aerosol climatology; SeaWIFS, MODIS

Introduction

Particulate matter less than 2.5 μm diameter ($\text{PM}_{2.5}$) suspended in the atmosphere is important because of both its impact on human health when inhaled, and its effect on the global energy budget (e.g. climate change). $\text{PM}_{2.5}$ has a predicted negative forcing on global radiation budget, with an uncertain magnitude. Networks of ground-based sensors routinely measure the near-surface concentration of $\text{PM}_{2.5}$. However, the spatial coverage on regional scales of $\text{PM}_{2.5}$ monitoring is fragmentary because health-related and compliance requirements tend to concentrate monitoring sites within urban areas. Numerous studies have sought to overcome the spatial coverage limitation by using remote sensing and satellite-derived aerosol optical depth (AOD) data, coupled with regression and/or numerical models, to estimate the ground-level concentrations of $\text{PM}_{2.5}$ (Engel-Cox and others 2006, 8056-8067; Van Donkelaar and others 2012, 11971-11978; Van Donkelaar and others 2013, 5621-5636; Paciorek and Liu 2009, 904-909; Liu and others 2011, 508-513; Munchak and others 2013, 1747-1759; Liu and others 2007, 33-44; Lee and others 2011, 7991-8002; Hoff and others 2009, 980-989; Weber and others 2010, 574-585; Kumar 2013, 34-49). These studies have shown that a relationship between $\text{PM}_{2.5}$ and AOD is not easily established by using simple regression models. This is because the relationship is a non-linear function of a number of parameters – including: humidity; temperature, boundary layer height; surface pressure, population density; topography, wind speed; surface type, surface reflectivity; season; land use; normalized variance of rainfall events; particle size spectrum and the phases of cloud particles; cloud cover; cloud optical depth; cloud top pressure; proximity to identified particulate sources (Levy and others 2009, 2942-2956; Lee and others 2011, 7991-8002; Weber and others 2010, 574-585; Liu and Daum 2002, 580-581; Paciorek and Liu 2010, A110-A111; Reid and others 2008; Hu and others 2013, 1-10; Muchoney and Williamson 2001, 1969-1977; Choi, Park, and Ho 2009; Choi and others 2009, 5654-5660; Zhang, Hoff, and Engel-Cox 2009, 1358-1369; Zhang and others 2014, 665-671). Further complications are introduced by biases present in the satellite AOD products because they assume that there is a linear relationship between the total column and ground level particulate concentrations (e.g. Lary and others 2009, 694-698; Lary 2013a; Zhang and others 2014, 665-671; Hyer, Reid, and Zhang 2011, 379-408; Reid and others 2013,

403-468; Shi and others 2013, 949-969), differences in spatial scales of the *in situ* point PM_{2.5} observations, the scale of remote sensing retrievals (several kilometers per pixel), and, finally, the steep PM_{2.5} gradients that can exist across urban boundaries, both vertically and horizontally, which impact on the success of AOD and similar data products.

Machine learning has recently been used to create a global daily PM_{2.5} surface abundance data product, with an associated uncertainty at 10 km resolution, between 1997 and 2013 (Lary 2013b). The PM_{2.5} data product was created using machine learning to evolve the mapping from *in situ* hourly PM_{2.5} observations at more than 8 000 sites in 55 countries; using approximately forty different global data products from remote sensing (aerosol optical depth, multi-wavelength surface reflectivity, satellite viewing geometry, solar illumination geometry, quality flags), meteorology (wind speed, humidity, surface temperature, boundary layer height, etc.) and demographics. Computational intelligence (or machine learning techniques) use massive data sets and iterative mathematical algorithms to “train” the computer to predict the values of the desired variable/s at known locations, thus revealing subtle multi dimensional non-linear mathematical patterns in the data possibly not be apparent in more constrained analyses. These patterns are used to compute probable values for the variables at unknown and test locations. Success at correctly predicting values at test locations is taken as an indication that predictions at the unknown location may also be reliable.

The purpose of this case study was to test the practical application of this PM_{2.5} data product in a region with limited spatial coverage for long-term monitoring. A rectangular area over the southern African Interior (22.5°S to 32.5°S; 22.5° E to 31.5°E) was selected for the study (Figure 1). The region included both monitored city regions and large tracts of unmonitored space (where the regional short-term studies have provided good basic indications of likely PM_{2.5} concentrations and the effects of changes in season). For the purposes of this investigation, the region selected has the advantage of being remote from other source regions of PM_{2.5} – in contrast with the industrialized northern hemisphere where the plumes from major conurbations and industrial regions often merge into one another. The reduction in complexity in

the location patterns of the emissions makes it practical to track pollutants upwind to source and downwind to impact area, a task which is less understandable when pollutant emissions are not associated with very specific locations. The climatology and transport of air masses from these regions over the sub-continent is well studied (Tesfaye and others 2011; Swap and others 2003b, 336-345; Annegarn and others 1996a, 548-550; Ross and others 2003; Stein and others 2003; Zunckel, Piketh, and Freiman 1999, 445-463; Winkler and others 2008, 5569-5578; Terblanche and others 2000, 15-21; Swap and others 2002, 125-130; Reason and others 2006, 35-45; Queface and others 2003; Piketh, Annegarn, and Tyson 1999, 1597-1607; Piketh, Tyson, and Steffen 2000, 244-246; Piketh and others 2002a; Piketh and others 1999, 35-43; Maenhaut and others 1996, 23631-23650; Kowalkowski, Piketh, and Cukrowska 2008, 705-713; Freiman, D'Abreton, and Piketh 1998, 561-566; Formenti and others 2002, 11-32; Formenti, Annegarn, and Piketh 1998a, 948-954; Annegarn and others 1996b, 548-550). The benefit of using locally distinct sources is the ability to link seasonal emission patterns (with similar patterns in the estimated $PM_{2.5}$ concentrations) with minimal interference caused by long-range transport of pollutants and overlapping pollutant paths from other regions that might confound the trends.

To assess the practical use of this new $PM_{2.5}$ data product, an unsupervised classification of the $PM_{2.5}$ data product was performed on ten-day average predictions over 10 years. The seasonal $PM_{2.5}$ patterns were then compared with the known climate, transport and emission patterns obtained from previous research. This classification allowed an adept characterization of the distinct $PM_{2.5}$ “climates” that exist in South Africa. This was particularly useful for examining the seasonal $PM_{2.5}$ “climate” in locations where data from ground-based measurements does not exist.

The significance of this study is that, by demonstrating the reliability of the $PM_{2.5}$ data product for estimating concentrations in this region, it can be extrapolated that this $PM_{2.5}$ data product can be used, with confidence, in other regions also lacking long-term ground based monitoring. Atmospheric aerosols are characterized by marked spatial and temporal variability, not adequately characterized by the localized ground based sampling stations. By giving a global daily data product, at 0.1 decimal degrees

latitude/longitude resolution (approximately 10 km x 10 km), a voice through an unsupervised classification technique, which is able to handle highly multivariate non-linear data sets, predictions of the PM_{2.5} concentrations can provide information about local spatial and temporal particulate levels in the vast areas without using ground based measurements.

Data and Processing Methods

The data product - Satellite Based Daily PM_{2.5} Estimates and Calibration

Retrievals from three satellite instruments were used for this study: The *Sea-viewing Wide Field-of-view Sensor* (SeaWiFS) launched on August 1, 1997 (Melin, Zibordi, and Holben 2013, 1185-1189); *Moderate-resolution Imaging Spectroradiometers* (MODIS), both part of the NASA A-Train (Remer, Kaufman, and Kleidman 2006, 537-540) – i.e. MODIS on NASA Terra (EOS AM), launched in 1999, and MODIS on NASA Aqua (EOS PM), launched in 2002.

Inclusion of additional ground data (sites indicated in Figure 1) from Europe and North America together with recent additions from the southern hemisphere (Chile, Brazil, South Africa, Australia and New Zealand) and Asia (China, India, Japan, Taiwan, and Hong Kong) dramatically improved the quality of the global machine learning estimates of PM_{2.5}.

The development and description of the PM_{2.5} aerosol data product has been covered in detail by Lary *et al.* (Lary and others 2014, S611-S630; Lary, Lary, and Sattler 2015, 41-41-52). Neighborhood scale variability was examined using multiple days at meter scale over an area of 100 km², as described by Harrison *et al.* (Harrison and others 2015). The length scale of variability was typically 1.6 km (ranging between 0.8 and 5 km) indicating that very small resolution effects are also important at local health levels.

Figure 1. PM_{2.5} measurement site locations from 55 countries (black and red squares) that were used to calibrate the daily PM_{2.5} estimates over the period 1997-2013. Background color scale shows the global topography and bathymetry (Lary 2013b). Case study region demarcated by the red rectangle.

Seasonal Patterns: Southern African Interior Case Study

To produce a regional PM_{2.5} climatology (or seasonally representative time series), a rectangular area was demarcated [22.5°S to 32.5°S; 22.5° E to 31.5°E], centered on the main emission areas of the South African Highveld plateau, extending outwards for 5° in each direction to the eastern continental coastline. Daily PM_{2.5} estimates were extracted from the global PM_{2.5} aerosol data product, then averaged over ten-day periods. Ten-day averages of satellite retrievals have been used for derived data products (such as NDVI, GOMES Ozone estimates etc.) because the period covered is longer than most synoptic weather patterns and thereby compensates for days lost to cloud cover. Conversely, ten-day averages consistently provide more detail than monthly averages. The process produced an array of data points, consisting of 36 ten-day annual periods, each averaged over 10 years, for each of the 9 456 segments within the defined study domain.

Source Type - Cluster Analysis

Self-organizing maps (SOMs) are a data visualization and unsupervised classification technique, developed by Kohonen (Kohonen 1982, 59-69; Kohonen 1984, 3-12; Kohonen 1987, 4910-4918), that reduces the dimensions of data through the use of self-organizing neural networks, making no *a priori* assumptions. Once a SOMs classification is complete, characteristic time series signatures for each class can be defined and interpreted.

The regional time-series of PM_{2.5} concentrations extracted for this study was classified using a number of different SOM configurations. Specifically, SOMs will classify the supplied data array into a set of n classes, where the user specifies n . Neural network results from this type of analysis are not identical when repeated because of inbuilt randomness and varying initial conditions. The effect of changing the number of classes was tested, ranging between 20 and 100. Classifications, using 30 to 40 classes, assigned the pixels representing the same locations to a single class in the course of a number of different runs. Classification using less than 30 classes did not separate all the groupings into logical time series plots. Conversely, classification using more than 40 classes divided similar time patterns into multiple classes, where individual locations with similar patterns were not always classified into the same group. The classification using $n=40$ produced almost identical results under various initial conditions and configurations, indicating an appropriate dimensionality. Classification where additional data was used, by including minimum and maximum information with the seasonal average, were also of interest for highlighting local episodic events – such as nearby vegetation fires and other intermittent activities that were not annual or seasonal – an aspect that not discussed within the scope of this paper.

No geographic information on the location of the PM_{2.5} abundance was present in the data set used in the classification. So the way the classification highlighted appropriate regions, in a spatially appropriate and coherent manner (Figure 2), became an indication of the effectiveness of the unsupervised SOM classification, allowing the data to “speak freely.”

Figure 2. Map of the 40-class classification of $PM_{2.5}$ abundance, with each class assigned a distinct color. The white area, lower right, is the southern Indian Ocean which was excluded from the classification; the blue line is the Orange River.

To simplify the display, Google Earth® Keyhole Markup Language (KML) files were generated and imported into Google Earth®. The clusters were then superimposed over Google Earth's high-resolution imagery. With the image transparency set to 50%, it became possible to match the classification overlay with the terrain and land cover associated with each $PM_{2.5}$ class's seasonal trends (Figure 3).

Results and Interpretation

Looking first at the whole region, followed by specific examples of local patterns (based on emission, land use and weather patterns), the utility of the regional data set and its application are demonstrated in the selected results discussions.

Overlaying the classification image in Google Earth (Figure 3), caused a number of interesting features to immediately become apparent: the circular class just south of Pretoria (white center, blue halo) is the city of Johannesburg, which was assigned a separate class of its own; two subtler classes seem to surround the Johannesburg metropolitan area. Also, the country of Lesotho can be identified as a separate class.

Figure 3. Google Earth image with the PM_{2.5} classification (40x1) version superimposed. Classes defined on the ten-day average time-series patterns, created using ten-year seasonally averaged PM_{2.5} concentrations.

Zooming in for additional detail, it is apparent that the circular feature south of Pretoria (Figure 3) corresponds to the industrial and residential regions of the City of Johannesburg and the adjacent suburbs of the greater metropolitan area (Figure 4). PM_{2.5} sources in this region are numerous and include: vehicle emissions; extensive wood and coal-burning for domestic heating and cooking; numerous light industries and several gold mine tailing storage facilities. This urban conglomeration is the commercial and industrial hub of southern Africa, with five million inhabitants. It is acknowledged to have the most polluted atmosphere in Gauteng Province and in South Africa. The classification and the time series seasonal climatology developed was compared with information collected from numerous short- and long-term local air pollution monitoring campaigns. (Ojelede, Annegarn, and Kneen 2012, 477-486; Annegarn and others 2000, 3-6; Wentzel and others 1999, 141-145).

Figure 4. Higher resolution Google Earth Image of the Johannesburg metropolitan conglomerate (southern Gauteng Province), with the classification colored and draped over a Google Earth satellite image, with partial transparency of the classes.

Definition of a class that approximates the borders of a country using this technique was not expected, but overlaying the image in Google Earth shows the mountainous, high elevation terrain of Lesotho (altitude: 1 800 m to 3 000 m above mean sea level) underlies the light blue $PM_{2.5}$ classification layer (classes 13 and 14) (Figure 5). The mountainous terrain was a contributory factor in the political formation of Lesotho – the early challenges in travelling within this region led to it being excluded from the original British Cape and Natal colonies. The mountains lead to a localized microclimate, subject to frequent ventilation by air masses travelling in the mid-troposphere not exposed to anthropogenic or natural emissions that occur in the boundary layer of the Highveld plateau (elevations 1 300 to 1 800 m). It is these weather conditions, combined with the pastoral nature of the subsistence farming lifestyle of the people living in these mountains, which defines the $PM_{2.5}$ climatology (low $PM_{2.5}$ loading) at this location.

Figure 5. Higher resolution Google Earth Image of the Lesotho highlands region with the classifications transparently draped over the satellite earth image.

Regional PM_{2.5} Climatology

PM_{2.5} climatology can be defined for class regions (groups of same-color pixels in Figure 3), allowing interpretation of important processes affecting particulate concentration bands and transport pathways. To make this evaluation, a *seasonal profile* (time-series of ten-day averages over an annual cycle) or *climatology* for the PM_{2.5} aerosol pattern for each of the 40 classes was defined. Box-whisker plots allow visual discrimination of statistically distinct classes, and, when combined with location of pixels falling into that class, allow the interpretation of geographic influences.

Assessment of the results included: considering the maximum and minimum values compared with previous studies where available (mismatches in time of data collection meant that this was qualitative more than quantitative); identifying the seasonal trends and average concentrations (in the light of known data about the emissions, wind patterns, rainfall, population distribution and regional climate).

Five examples of this approach are used below to illustrate the potential uses for this information in locations currently without routine air quality monitoring stations and for discerning regional-scale influences.

The first example is over Greater Johannesburg/Gauteng (Figure 4). When examining the classes prevalent over Johannesburg – classes 1 (Red) and 2 (Blue) – $\text{PM}_{2.5}$ levels exceed $50 \mu\text{g m}^{-3}$ during September and October, and are the highest concentrations in the entire set. This is as expected, since this is the densest conurbation and the most polluted region in the study rectangle (Figure 3). The trends of seasonal patterns for these classes are similar, however, with distinctly different concentration ranges, justifying the statistical separation into separate classes. Class 1 (red) represents the city and class 2 (blue) the immediate surroundings. Both classes show concentrations above WHO guidelines ($25 \mu\text{g m}^{-3}$) and US EPA standard 24 hour average levels ($35 \mu\text{g m}^{-3}$), with the highest concentrations closest to sources (class 1) from which the $\text{PM}_{2.5}$ would be transported into the surrounding areas; but as dilution of the polluted air occurs, by mixing with cleaner air masses during transport, the surrounding locations experience reduced aerosol concentrations (class 2).

Lower concentrations during the early part of the year (periods 1 to 15 – equivalent to January through May) and the end of the year (periods 31 through 36 – equivalent to November and December) correspond to the rainy season, extending from early summer to late autumn. Domestic heating emissions are absent in the summer, and $\text{PM}_{2.5}$ from other sources is efficiently diluted by moderate velocity gradient winds or washed out of the air by frequent rains. Higher concentrations between June and August (austral winter, periods 16-24) are associated with domestic coal burning for space heating, coinciding with calmer wind conditions and the absence of rainfall. The continuation of the high $\text{PM}_{2.5}$ values through September and October are linked to high wind speeds, associated with aeolian dust generation in the absence of rainfall, and extensive smoke from both urban grass fires (deliberate and accidental) and regional wildfire biomass burning. The monitoring stations used in the product calibration fall within the city of Johannesburg and additional information about this network can be found most recently in a paper

by Hersey, S. P., and others, 2015. They provide an “An overview of regional and local characteristics of aerosols in South Africa using satellite, ground, and modeling data.” and report average ground based $PM_{2.5}$ measurements between 20 and $70 \mu g m^{-3}$. Similarly to Hersey, S. P., and others, 2015, the $PM_{2.5}$ satellite product showed higher concentrations in the beginning of October than in the ground based monitoring data. At locations where domestic burning from heating and cooking dominate emissions, ground monitoring shows a rapid drop in particulate concentration following the cooler winter months. Similarly, in locations where industrial and traffic emissions are the major aerosol sources, we find a reduction in particulate concentration in October, again following the winter months. The domestic burning locations, however show a faster reduction in concentration.

Moving further away from the densely populated city, class 12 (green) illustrates further reductions in the particulate concentration but maintains a similar seasonal pattern (Figure 6). Based on the wind direction analysis, the prevalent transport of the urban plume would be southwards, carried by northerly winds. Class 15 (yellow) (Figure 6) shows this trend but the concentrations were lower – specifically in September (periods 25 – 28). While initially counter-intuitive (because of the wind direction) for the concentrations to be lower in the south than in the north, it is important to realize that other contributing sources exist in the northern part of this region. Additional urban developments to the north and west of Johannesburg (Pretoria metropolitan municipality, Krugersdorp, Rustenburg platinum and chrome mining belt) also contribute to the $PM_{2.5}$ atmospheric burden.

Class 15 (yellow) also includes most of the eastern Highveld – the major energy generating region. Industrial activities in this region include iron and steel refineries and seven large coal-fired power plants, each of 3 600 MWe generating capacity. The ground level $PM_{2.5}$ concentrations are not extensively affected by these activities because stack design (mean stack height of 270 m) results in the emissions from these large commercial entities being injected above the boundary layer and therefore ground concentrations are insulated from the peaks in this pollution – except when plume downwash conditions

occur (typically in the summer months) – but mixing from the upper air contributes to high regional concentrations.

Despite the Self-Organising Maps algorithm having identified a distinct, coherent class covering the Lesotho highlands, the seasonal pattern is similar to that over Johannesburg (Figure 7). Lower concentrations are associated with both the lower lying edges of the region and the center (class 13) compared with the rest of the high region (class 14). Similarity with Johannesburg is to be expected because much of the $PM_{2.5}$ will be transported in well-mixed regional air masses from source regions, with little local contribution. Terrain-induced turbulence, when gradient winds encounter the mountainous landscape, will further induce uniform mixing of aerosol loading.

Figure 6. Box-whisker plots of the seasonal variations of classes 1, 2, 12 and 15 representing Johannesburg and a penumbra surrounding Johannesburg respectively; location of cells falling into each class shown in the legend maps.

Recirculation of the air masses over the region has been shown to recycle the natural and anthropogenic pollutants around the region. A number of studies on the air transport into and out of the Highveld (Annegarn and others 1996c, 548-550; Formenti, Piketh, and Annegarn 1999, 332-338; Freiman and Piketh 2003, 994-1002; Terblanche and others 2000, 15-21) have tracked the air masses and the chemical pollutant traces associated with these emissions. 33% of the time air masses circulate over the sub-continent in an extensive counter-clockwise gyre; with a further 39 % frequency, air masses flow away from the Highveld towards the south east, passing over Lesotho and KwaZulu-Natal (Freiman and

Piketh 2003, 994-1002; Piketh and others 1999, 35-43; Piketh and others 2002a). The only other contributory pollution source in this region would be domestic wood burning for cooking and heating. The local weather, combined with cold conditions and high altitude, requires wood burning for heating purposes (greatest for periods 13-24), but as most of the population is sparsely distributed across rural areas, the resultant emissions are not concentrated over one locality. Regional spring winds produce peak concentrations (periods 24-30). The region fell into two similar classes: the lower outskirts and central ruggedly protected terrain exhibit slightly lower concentrations than the highland mountainous areas in the path of the air masses carrying urban pollution away from the Highveld.

Figure 7. Box-whisker plots of the seasonal variations of classes 13, and 14 representing Lesotho; location of cells falling into each class shown in the legend maps.

Another grouping of classes are of particular interest, because of a bi-modal seasonal aerosol pattern (Figure 8) that differs markedly from the patterns discussed for Johannesburg and Lesotho. The classes have been identified for two localities that are not spatially connected but which share an important climatic setting. The first is represented by classes 3 (red) and 4 (blue); the second, represented by classes 21 (green), 22 (yellow) and 23 (cyan). These groups of classes

show double peaks in the PM_{2.5} levels (February–March and September–October), with lower concentrations in the winter (May through August) and summer (November through January).

Figure 8. Box-whisker plots of the seasonal variations of classes 3, and 4 (representing Kalahari) and classes 21, 22 and 23 (representing Karoo), location of cells falling into each class shown in the legend maps.

The first locations (Figure 8) fall in Botswana and in the northern regions of South Africa's Northern Cape Province – areas with low population and minimal industrial activity. The second set of classes are also sparsely populated and without significant industrial activity. What is most interesting about the similarity in these patterns is that these regions represent the Kalahari and Karoo semi-deserts respectively. Both have very low rainfall (Karoo 190 mm/a; Kalahari 110–200 mm/a) and low populations; therefore minimal influences from local human activities. Both deserts are vegetated by sparse low scrub bushes (i.e. not totally barren). Because of calm atmospheric conditions at this latitude (under the descending branch of the Hadley cell circulation), the land itself is not a specific source of dust during the dry winter months.

Because of the lack of local anthropogenic emissions, the two most likely explanations are aeolian processes and the import of regional plumes from natural or anthropogenic sources (including biomass burning from wildfires north of the region – i.e. Congo, Angola, and Zambia). Biomass burning smoke is mostly condensed hydrocarbons comprised of $<1 \mu\text{m}$ particles that travel great distances in dry air because they remain suspended until removal by rain events (Swap and others 2003a; Andreae and others 1998, 32119-32128; Winkler and others 2008, 5569-5578; Queface and others 2003; Annegarn and others 2002, 111-113; Swap, Annegarn, and Otter 2002, 119-124). Both deserts are surrounded by semi-arid regions where vegetation renewal is based on fire regeneration ecology (Staver, Archibald, and Levin 2011, 1063-1072; House and others 2003, 1763-1777). The high background concentration portion of the $\text{PM}_{2.5}$ is also likely to have been imported into these sparsely populated areas from those surrounding regions with high industrial or domestic emissions. Residence time in suspension of $\text{PM}_{2.5}$ is from one to ten days – during which period, even at moderate wind speeds, air masses can move between 40 and 1 000 km distant, enabling a mixed background of all natural and human produced $\text{PM}_{2.5}$ to be imported into regions without local emission sources. The low annual rainfall in these regions allows the residence time of the regional aerosols to be extended, leading to the higher concentrations in locations far from any anthropogenic sources.

The cleanest classes (lowest average $PM_{2.5}$ concentrations), estimated by the machine learning algorithm for this region during this ten-year period, are associated with the rural coastal regions of the south eastern KwaZulu-Natal coast. These regions – excluding the coastal port cities – represent sub-tropical regions with relatively low population concentrations (extensive rural population but minimal urban development) and minimal industrial activity. The major explanations for the cleaner air include: the incursion of moist ocean air masses along the coastal zones; frequent incursions of clean marine air; and topographically induced precipitation that washes the air and reduces the average aerosol concentrations.

Figure 9. Box-whisker plot of the seasonal variations of class 40 representing clean rural coastal regions, location of cells falling into each class shown in the legend map.

Discussion

Extrapolation of regional and global particulate aerosol distributions from often-sparse ground-based measurements is often difficult, especially in less-developed regions like sub-Saharan Africa. The satellite based neural network and machine learning based estimates and classification of seasonal patterns developed and demonstrated above are especially helpful in areas such as South Africa, with strongly

localized particulate pollution, combined with a lack of regional monitoring to quantify natural effects. An understanding of natural background signals is crucial for establishing reasonable and achievable mitigation approaches. Similarly, projection of aerosol changes under various climate change scenarios will greatly benefit from understanding regional correlations between climate, seasonality, and particulate mobilization. The satellite-neural network machine learning approach used here is likely to be the most practical way to derive appropriate correlations over much of the Earth. In South Africa, clear regional correlations emerge. The generated classes are spatially and temporally reasonable. Further distinct seasonal and spatial patterns are summarized in Figure 10.

Similar problems and experiences, arising through using any remote-sensing-based measurement methods, continue to affect/influence the applicability of the results. One major concern, raised when coordinating the training of the machine learning algorithm with the existing ground-based sampling systems, is the site selection for most of the monitoring campaigns. Limited resources and budgetary constraints cause many ground-based monitors to be located in the projected worst air quality locations. This is certainly true for the City of Johannesburg sampling sites, whose locations include the busiest highway intersection and the center of the largest domestic coal-burning suburb. Biases in ground monitoring location sites are recognized as the greatest probable source of variations in the results. The implication of the bias issue is a relatively constant inflation in the calculation of the concentrations. Seasonal trends, local problems and long-range transport paths can all be derived from the product – without negative effects from the probable bias in the calibration sites.

Figure 10. Summary of seasonal trends and average $PM_{2.5}$ concentrations (all plotted at same scale) as predicted using machine learning.

An additional concern is the representativeness of the single value for $PM_{2.5}$ concentration for such large grid locations (10 km x 10 km) – both in the vertical and in the horizontal. Ground-based and remote control unmanned aircraft-based measurements are currently underway in Dallas to quantify both horizontal and vertical distribution of $PM_{2.5}$ concentrations within specific grid/cells. Further updates will include adjustments to the calibration, based on the distribution of concentrations within the three-dimensional grid cells. Additionally this calibration project will quantify the levels of possible inflation of the concentrations caused by worst-case site selection – issues common to most monitoring run by regulatory networks.

Conclusions

Daily retrievals of $PM_{2.5}$ from satellites were processed using neural network based machine learning to derive regional $PM_{2.5}$ seasonal trends/ $PM_{2.5}$ climatologies for the South African Highveld and surrounding regions. The results show seasonal trends in the estimated $PM_{2.5}$ concentrations that are compatible with results of surface and airborne monitoring campaigns.

Aerosol trends match seasonal patterns identified by field-based and long-term monitoring campaigns conducted in this region, as detailed for the five regions being investigated. Regional air mass movements and mixing provides a viable justification that the results and interpretation given are applicable and valid for remote locations where ongoing monitoring data are not available.

The cleanest areas are those most frequently exposed to onshore oceanic air masses, and without significant residential or industrial emissions. The higher frequency of rainfall events provides a secondary mechanism explaining locations where there is lower $PM_{2.5}$.

Desert locations in the interior of the sub-continent show similar seasonal trends and particulate levels despite the considerable distances between these regions. The similarity between these patterns was unexpected but confirms that the SOM techniques are capable of identifying contrasting patterns, and of producing useful insights and data.

In Greater Johannesburg, the daily $PM_{2.5}$ estimates have been compared with the historic and short term ground-based measurements: from numerous studies (Reason and others 2006, 35-45; Annegarn and others 1983, 489-498; Annegarn and others 1991, 46; Annegarn and others 1990, 1-14; Annegarn and others 1981, 435-440; Annegarn and Przybylowicz 1993, 582-587; Formenti, Annegarn, and Piketh 1998b, 948-954; Kirkman and others 2000, 423-431; Maenhaut and others 1996, 23631-23650; Piketh and others 2002b; Swap and others 2002, 125-130; Winkler and others 2008, 5569-5578, Hersey and others 2015, 4259-4278) and also with the long-term monitoring stations within this region (which were

also included in the original neural network calibration). However, these monitoring stations are few and are located only within the major urban area.

The absence of viable data, on suspended particulate matter in the unmonitored regions, has been a challenge for researchers in a number of fields as diverse as human health and climate change. This regional case study proves that this PM_{2.5} satellite-derived aerosol product can provide a valid and viable alternative to *in situ* measurements for locations where local monitoring is not available.

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