Using infrared geostationary remote sensing to determine particulate matter ground-level composition and concentration

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Abstract

Speciated ground-level aerosol concentrations are required to understand and mitigate health impacts from dust storms, wildfires, and other aerosol emissions. Globally, surface monitoring is limited due to cost and infrastructure demands. While remote sensing can help estimate respirable (i.e. ground level) concentrations, current observations are restricted by inadequate spatiotemporal resolution, uncertainty in aerosol type, particle size, and vertical profile. One key issue with current remote sensing datasets is that they are derived from reflectances observed by polar-orbiting imagers, which means that aerosol is only derived during the daytime and only once or twice per day. Newer quantification methods using geostationary infrared (IR) data have focussed on detecting the presence, or absence, of an event. The determination of aerosol composition or particle size using IR exclusively has received little attention. This manuscript summarizes four scientific papers, published as part of a larger study, and identifies requirements for (a) using infrared radiance observations to obtain continual (i.e. day and night) concentration estimates; (b) increasing temporal resolution by using geostationary satellites; (c) utilizing all infrared channels to maximize spectral differences due to compositional changes; and (d) applying a high-pass filter (brightness temperature differences) to identify compositional variability. Additionally, (e) a preliminary calibration methodology was tested against three severe air quality case study incidents, namely, a dust storm, smoke from prescribed burns, and an ozone smog incident, near Sydney in eastern Australia which highlighted the ability of the method to determine atmospheric stability, clouds, and particle size. Geostationary remote sensing provides near-continuous data at a temporal resolution comparable to monitoring equipment. The spatial resolution ($\sim 4 \text{ km}^2$ at NADIR) is adequate for large sources but coarse for localized sources. The spectral sensitivity of aerosol is limited and appears to be dominated by humidity changes rather than concentration or compositional changes. Geostationary remote sensing can be used to determine the timing, duration, and spatial extent of an air quality event. Brightness temperature differences can assist in qualifying composition with an order of magnitude estimate of concentration.

Keywords Aerosol · Remote sensing · Himawari-8 · Ground-level concentrations

Introduction

Climate change-induced drought, across large regions of Australia, has contributed to severe dust storms and the loss of soil and vegetation moisture (McTainsh et al. 1998). Recent extreme temperatures, combined with vegetation desiccation, has ignited wildfires across vast regions of

eastern Australia, resulting in destruction of property and life (Benali et al. 2016). Secondary effects of smoke and dust inhalation are poorly measured because of cost and infrastructure demands. Speciated ground-level aerosol concentrations are required to understand and mitigate health impacts from dust storms, wildfires, and other aerosol emissions (Bell and Adams 2008; Delfino et al. 2009). These air quality incidents can occur at night, and pre-dawn inversion conditions can result in high concentrations, and it is vital that elevated concentration levels are continuously measured (Tran and Mölders 2012).

These severe air pollution concentrations may have fatal consequences, and consequently, six commonly occurring criteria air pollutants (CO , O_3 , SO_2 , NO_2 , Pb, and particles)

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are routinely monitored to protect health and the environment (Zhao et al. 2016). Particulate matter (PM) is of concern due to its ubiquitous nature as urbanization, coupled with increased affluence, leads to an increase in vehicles and industrial activities with concurrent increases in ambient particulate levels that, together with geogenic emissions from fires and wind-blown events, contribute to PM being present in most populated, arid, and forested regions (Begum et al. 2013). Health impacts of PM depend on particle size and composition (DSD 2010), and it is therefore vital that PM monitoring provides speciated concentrations in order to assess health risks.

Ambient monitoring using fixed locations provides reliable concentration data. However, monitoring sites may be sparse outside of metropolitan centres, because of cost and infrastructure, and sited according to population numbers rather than at areas of risk in arid or mining regions (NSW 2019). Methods to determine concentration must have sufficient spatial and temporal resolution to accurately represent an event, typically hourly, and 1 km² resolution is required (Zhao et al. 2016). In regions without dedicated monitoring, it may be possible to estimate concentrations using dispersion modelling or remote sensing (Li et al. 2015).

The use of remote sensing has been limited in the past because single daily snapshots from polar-orbiting satellites can miss high-intensity short-duration events and may not be representative of daily average concentrations (Guo et al. 2017). Second-generation geostationary earth-orbiting (GEO) satellites such as Himawari-8 (Yumimoto et al. 2016)

and GOES-R (Wang et al. 2014; Schmit et al. 2018) can detect these temporal changes, as these satellites supply sub-hourly data. Aerosol optical depth (AOD) (Levy et al. 2013) is a measure of the extinction of electromagnetic radiation by dust and haze, which absorbs and scatters light. AOD is dimensionless and is related to the total amount of aerosol in the vertical column of the atmosphere over a location.

Remote sensing has been beneficial in understanding global aerosol movements of large-scale dust events (Duncan et al. 2014), such as the Sydney storm during September 2009 (De Deckker et al. 2014) and other dust storms (Yao et al. 2012; Karagulian et al. 2019), fires and smoke plumes (Chung and Kim 2008), and tracking inactivation times of the SARS coronaviruses (Herman et al. 2020). Despite its potential benefits, the general scientific community has been reluctant to use remote sensing data for monitoring surface atmospheric concentrations, citing difficulties in accessing, processing, and interpreting the data (Duncan et al. 2014). The potential benefit of remote sensing is demonstrated in Fig. 1, which shows a major fire near Denmark, along the southern coastline of Western Australia which contributed to dense smoke being observed in Perth (~400 km to the north).

The locations of the fires were detected with a resolution of 1 km² in the MODIS thermal anomalies product known as MOD14 (Mouillot et al. 2014; Benali et al. 2016). The MODIS AOD product is spatially averaged, to remove cloud interferences, and is computed to 100 km² (collection 5) (Levy et al. 2009) or 9 km² (collection 6) (Levy et al. 2013) spatial resolution. However, neither the fire location, the

Fig. 1 MODIS visible (left) and Aerosol optical depth (right) data from 5th Jan 2014 over South Western Australia. Both “visible” and AOD products are generated using multiple bands. The figure shows

fires in the south and smoke plume travelling westward and then re-crossing the coast to the north over Perth

AOD, nor indeed any other MODIS product directly supplies aerosol ground-level concentrations (GLCs) of aerosols relevant for air quality.

Figure 1 highlights several problems in comparing the true colour against the AOD imagery from MODIS. The observational swath does not cover the globe instantaneously, and multiple observations need to be joined. These joints created discontinuities and gaps along the boundaries due to differences in the timing of the observations, difference in solar illumination, view geometry, and other effects. Cloud masking is especially noticeable over land, and the AOD 9 km² aggregation creates pixelation and a loss of detail in the smoke plumes. A lack of temporal resolution creates a disjoint between the smoke plume near the source of the fire and the stagnant plume 500 km to the north, over the ocean. While it is probable that the high AOD over the sea arose from the smoke plume, there is no definitive smoke trail showing this. Lastly, while the AOD plume over the ocean is well defined, the AOD over land is pixelated and poorly defined because of the need to account for surface reflectance.

In addressing the health impacts of PM, there is a need to extrapolate the total AOD column amount into respirable ground-level concentrations (GLCs) using simple linear approximations or by including secondary effects such as humidity, temperature inversions, and increased wind speeds (Sotoudehian and Arhami 2014). While daily AOD measurements have been extrapolated to surface concentrations, short-term events such as fires and inversion weather conditions may be inactive during infrequent satellite observations, or clouds may obscure the scene, leading to the event being missed. Therefore, the rate of data acquisition should match the rate of compositional change in order to determine exposure levels (O’Loingsigh et al. 2015; Philip et al. 2016).

While traditional methods on quantifying aerosol use the daytime-only visible portion of the electromagnetic spectrum (Levy et al. 2013), more recent studies favour revising and utilizing older dust detection methodologies (Ackerman 1997; Park et al. 2014) using infrared to provide continuous monitoring (i.e. 24 h a day) (She et al. 2018). Land, sea, and clouds comprise most of the satellite observation, and trace constituents of air pollutants have a marginal impact on the overall spectral result due to their lower concentration. These methods use brightness temperature differences (BTD) between two infrared wavelengths as a high-pass filter that enhances the spectral differences (from trace constituents) between two similar wavelength bands while minimizing commonality (land, sea, and cloud) to enable aerosols to be distinguished from clouds (Hu et al. 2008; Lensky and Rosenfeld 2008). However, these dust detection methodologies provide a qualitative, not quantitative assessment of concentration (Ackerman 1997), and there is a need to improve the methodology to provide speciated GLCs across unmonitored regions.

This article (a) highlights the deficiencies of current remote sensing of ground-level concentrations (monitoring frequency, measurements at night, and the columnar/ground-level ratio); (b) provides a critical overview and summary of four of the author’s recent papers on the topic; and (c) provides a very limited “proof of concept” validation using three case study incidents.

Material and methods

Data sources

Data files of all ten infrared bands from the Himawari-8 satellite were obtained from the Australian Bureau of Meteorology (BOM). These data files were cropped to the study domain and analysed using the “Climate Data Operators” (CDO) (CDO 2018). The satellite data were augmented with meteorological and ambient air quality data across the greater Sydney region in eastern Australia downloaded from the New South Wales (NSW) government office of Environment and Heritage (OEH 2019) website <https://www.environment.nsw.gov.au/AQMS/search.htm>. The Australian Nuclear Science and Technology Organization (ANSTO) supplied fine PM_{2.5} characterization, which was used to quantitate aerosol by source type (Cohen et al. 2016).

Methodology

A literature review of surface particulate monitoring of dust events using geostationary satellite remote sensing was undertaken to understand the theory and limitations in the current methodology (Sowden et al. 2018). The review identified, amongst other findings, the reliance on visible reflectances and the lack of temporal resolution in polar-orbiting satellite data. As a result of this study, a dust storm was investigated to determine how rapidly the storm passed and what temporal data resolution is required to monitor these and other similar events (Sowden et al. 2019). Various dust indices were investigated to determine which are optimum in determining spectral change (Sowden and Blake 2020). These indices were then used to qualify and quantitate dust events (Sowden et al. 2020), and the methodology was tested against all three severe air quality events described on the OEH website of a dust storm; smoke from prescribed burns; and an ozone smog incident.

Results and discussions

Literature review (Atmospheric Environment 183:154–164)

The literature review therefore looked at the deficiencies of current AOD techniques against air quality requirements

regarding the need for continuous, speciated aerosol GLCs. In the review, it was clear that the current AOD product does not meet the needs of the air quality community in that the temporal and spatial resolutions of polar-orbiting satellites are too coarse, the predicted AOD over land (especially bright surfaces) is dubious and misses plumes, the remote sensing aerosol “type” does not represent aerosol composition, and the AOD is fundamentally the wrong metric (a dimensionless, full-column property) for describing GLCs needed for health studies. The review found that:

- i. The new “second-generation” geostationary satellites provide excellent temporal resolution (10 min) but coarse spatial resolution (4 km^2 at nadir).
- ii. The lack of temporal resolution has historically constrained the wider adoption of remote sensing for atmospheric studies. Therefore, there is a need to understand if the temporal resolution requirements are driven by chemical transformations, health criteria, hardware (scan time), big data (volume, network, processing), or meteorological (turbulence) drivers.
- iii. Continuous wavelengths (such as IR) are required to quantify sporadic dust events throughout the day. AOD methodology has focussed on the stronger visible spectra. However, there has been renewed interest in using dust indices for the detection of aerosol events. These dust indices were developed previously, but, presumably due to the predominance of visible AOD studies, limited attention has been paid to determining which IR indices are optimal for identifying spectral changes from aerosols, prompting an evaluation of three index types subtraction (BTD), normalized differences (NDDI), and ratio (RAT) across three types of samples (spectral database of pure soils, potential aerosol plumes from a dust storm, and annual variance at a surface monitoring site).
- iv. There is a need to change the AOD methodology to include infrared wavelengths to obtain temporal coverage and, following on from the identification of suitable indices, a calibration of those indices against surface monitored compositional data.

Temporal resolution requirements (Atmospheric Environment 216:116,914)

Remote sensing of surface PM concentrations has been shown to be invaluable for regional areas which have limited ground-based monitoring. However, there is a requirement for a high temporal resolution to detect sporadic dust events and use other wavelengths, i.e. apart from the visible wavelength spectrum, to detect events that occur in the evening. It was identified that the probability of a polar-orbiting satellite overpass coinciding with a cloud-free aerosol event

is low. Therefore, polar-orbiting satellites such as MODIS are unsuitable for detecting rapidly changing aerosol events, and geostationary satellites are required to provide suitable, temporally resolved data.

Principal component analysis of BTD IR indices for a large dust storm in the Pilbara region of Western Australia identified that each aerosol phase of the dust storm lasted between 30 min and 2 h and that compositional change is driven by atmospheric turbulence — which suggests that 5 to 10 min scan times are optimal for detecting sporadic effects.

Selection of dual-band indices (Atmospheric Environment 241:117,620)

Having identified suitable IR wavelengths, the study identified how these wavelengths can be combined, using different ratio methods to develop indices to determine specific air quality events. The results showed that BTD was marginally better than NDDI at identifying aerosol changes and recommended that all ten of the Himawari-8 infrared bands should be used with five dual-band combinations (BTD_{3.9–6.2 μm} , BTD_{11–12 μm} , BTD_{9.6–13 μm} , BTD_{8.6–10 μm} , BTD_{6.9–7.3 μm}) to maximize the identification of compositional changes. Using the five dual-band indices enhances quantification across diverse regions and different aerosol species, and this was illustrated by comparing index differences across the entire Himawari-8 monitoring region. Figure 2 depicts these dust indices across the full Himawari monitoring hemisphere on the morning of the Pilbara dust storm. These indices, therefore, improve the ability to identify spectral changes from aerosols at a high temporal (10 min) and spatial (4 km^2 at nadir) resolution.

Calibrating aerosol change using the five BTD indices (Atmospheric Environment 229: 117,435)

To understand the efficacy of the indices, they were tested against GLCs data where the indices were calibrated against surface monitored compositional data using seventeen ground-level monitoring sites in the greater Sydney region in New South Wales, Australia. These monitoring sites measured NO, NO₂, SO₂, PM_{2.5}, PM₁₀, and O₃, and this data was augmented with positive matrix factorization aerosol source apportionment data (soil, sea-spray, smoke, auto, and secondary sulphates) at five collocated sites.

While it was not the intention to consider gaseous species in this study, ground-level ozone had the highest compositional correlation, while aerosol speciation correlation was weak. It has been suggested by Ackerman (1997) that the BTD differencing results in a lack of sensitivity and poor correlation to concentration. Multilinear regression was used to determine a pollution index from the five BTD indices

Fig. 2 Dust indices over the full Himawari monitoring hemisphere, with cloud masking, 10:30 AM (UTC+8) 8 Mar 2017. **a** $\text{BTD}_{3.9-6.2 \mu\text{m}}$ (with cloud); **b** $\text{BTD}_{3.9-6.2 \mu\text{m}}$ aerosol/moisture; **c** $\text{BTD}_{11-12 \mu\text{m}}$ particle size index; **d** $\text{BTD}_{9.6-13 \mu\text{m}}$ O_3 – CO_2 photochemical/oxidation; **e** $\text{BTD}_{8.6-10 \mu\text{m}}$ sulphate–crustal and H_2O ; **f** $\text{BTD}_{6.9-7.3 \mu\text{m}}$ atmospheric (in)stability. (Note, zenith angles greater than sixty degrees are not recommended for qualitative analysis due to the poor spatial resolution at large angles). Captions based on band characteristics (Schmit et al. 2018)

that predicts particle size, humidity, and species probability, and it is suggested that the predicted concentrations should be multiplied by the probability derived from the pollution index to reduce the high predictions at low probabilities.

Severe event case studies

OEH provides an annual report of severe incidents (dust, smoke, and ozone), and these three incidents were analysed using the methodology developed and compared to OEH's analysis of the three events. During one of these events (24 Sept 2017), a dust storm crossed over eastern Australia, and

this is depicted in Fig. 3. The validation studies reflect that water vapour is a strong absorber of infrared, and consequently, atmospheric stability (vertical movement of water vapour), cloud height (and phase), and relative humidity are determined with high confidence. However, the strong absorption of water vapour negatively impacted the calibration of GLCs, and therefore, it is suggested that the calibration process should be repeated according to atmospheric stability and cloud height categorizations. Secondly, the validation studies did not detect plausible plumes from aerosol species (soil, sea-spray, smoke, auto, and secondary sulphates), and this was attributed to the daily aerosol

Fig. 3 Analysis of dust event on 24 Sep 2017 showing **a** stability; **b** cloud height; **c** NO₂; **d** PM_{2.5}; **e** PM₁₀ and O₃. Video available at <https://tinyurl.com/DustEvent>

speciation and cloud spectral interference. Both PM_{2.5} and PM₁₀ concentrations depict plausible plumes that began at a consistent “source” and disperse according to normal plume behaviour. Potential methodologies to determining atmospheric stability, cloud height, and smoke from fires using infrared wavelengths are discussed below.

Atmospheric stability

Atmospheric stability is an essential parameter in dispersion modelling that should be considered in determining GLCs. Rapidly rising air is termed unstable, while stagnate (inversion) conditions are termed stable. The BTD_{6.9–7.3 μm} index reflects the difference between mid- and lower-level moisture and is therefore a measure of stability. If the index is positive, i.e. mid-level moisture is greater than lower level, this indicates rising unstable air as depicted in Fig. 4. This method is not dependent on thick clouds but on moisture differences between the levels. Good spatial and temporal agreement was obtained between the low-pressure isobars in the synoptic chart (Fig. 4a) and the stability estimations Fig. 4b (red/yellow colouring).

Cloud height

Clouds show the movement of air which is critical to both emissions and dispersion of atmospheric pollutants with high pollutant concentrations typically collocated at the cold/hot front boundary. It is vital that the methodology be

developed which allows collocated cloud and aerosol to be determined — even though the infrared signal is dominated by water. Cloud dynamics are important in determining GLCs and are reproduced in Fig. 5 (indicating water phase changes at the inflexion points in the graph) (Sowden and Blake 2020), and cloud height (approximation of mixing height) is estimated in Fig. 6 using the adiabatic lapse rate of 9.8 °C/km.

Smoke from fires

Fire observation and burn scars are an excellent mature product that uses visible and near-infrared wavelengths. However, the detection of fires needs to be modified at night to use infrared wavelengths and, more importantly, determine smoke GLCs. Figure 7 depicts estimated PM_{2.5} and PM₁₀ concentrations emitted by a fire and shows that incomplete combustion and coarse PM predominates in the smoke near the fire, while finer particles are transported greater distances. Using five indices may allow components that are not visible in one index to be observable in the other indices.

While not typically used to detect smoke plumes due to the wavelength and non-detectable particle size of smoke, this study demonstrates that IR wavelengths may be able to be used to detect smoke plumes as these indices are not detecting aerosol types but the resultant spectral differences. A hot rising plume of smoke could initially have low moisture, due to the temperature of the fire, but these particles could absorb moisture from the atmosphere and be identified

Fig. 4 a MSLP synoptic chart and b atmospheric instability 5 PM AEDT 12 Feb 2017

Fig. 5 Cloud phase and temperature

Fig. 6 Estimate of cloud height 5 PM AEDT 12 Feb 2017

by the spectral response to $\text{BTBD}_{3.9-6.2 \mu\text{m}}$. Furthermore, the rising air could affect the vertical air movement, identified by $\text{BTBD}_{6.9-7.3 \mu\text{m}}$, despite potentially being transparent at $\text{BTBD}_{11-12 \mu\text{m}}$. Rising ash (large particle size) may indicate

the initial spatial distribution of the smoke surrounding a fire as the larger ash particles would dissipate near to the fire.

Conclusions

Four papers were examined that (a) evaluated current deficiencies in remote sensing of respirable particles; (b) identified the need for temporally resolved remote sensing data to be at least comparable to hourly data; (c) experimentally identified five BTBD indices, during periods of elevated particulate matter surface concentrations, which maximized the detection of spectral change; and (d) attempted to correlate the BTBD indices to the surface speciated concentrations.

GEO satellites have improved the temporal data resolution from daily (e.g. MODIS) to 10 min (e.g. Himawari-8). This data frequency, and reduced latency, is comparable to real-time monitoring and thus suitable for air quality studies. However, working with big data presents challenges, and cloud gaps require adjustment of the methodology to minimize cloud spectral contamination. More should be done to leverage speciated surface ambient air concentrations from infrared measurements, which provide near-continuous data — but at the cost of lower spectral sensitivity to changes in composition.

The lack of spectral infrared resolution between compounds makes determining composition and concentration challenging. However, as speciation appears to be correlated with humidity and particle size, this may potentially be used as a proxy for speciation — especially given the enhanced spectral sensitivity of IR to water. Correlations between aerosol species and gaseous components were noted. The reasons for the correlation are unknown and could be based on aerosol products or related to humidity. However, the correlations imply that both aerosol species and gaseous

Fig. 7 $PM_{2.5}$ and PM_{10} emitted from a fire depicting size discrimination with downwind distance

pollutants can potentially be estimated from geostationary remote sensing data. Therefore, that which is measured is potentially not the IR components of NO_2 or smoke aerosols but the resulting spectral changes, possibly related to the uptake or loss of water, rather than the radiative properties of the gaseous or aerosol species directly.

Five indices were chosen that use all ten Himawari-8 IR bands ($BTD_{3.9-6.2 \mu m}$, $BTD_{11-12 \mu m}$, $BTD_{9.6-13 \mu m}$, $BTD_{8.6-10 \mu m}$, $BTD_{6.9-7.3 \mu m}$). Using five indices increases the probability of detecting all aerosol types and is an improvement over current IR methods, which use fewer indices. The pollution index that was developed correlates to aerosol species, relative humidity, particle size, ozone, and vertical stability, and it is this correlation that has potentially improved the qualitative assessment and ultimately quantitative analysis of the method.

Quantifying surface concentration by scaling the predicted concentrations by the probability of the aerosol type is a compromise that produces an order of magnitude estimate and which requires further studies to improve the quantification. High-pass filtering using BTI indices, from all IR bands, has improved the qualification of aerosol species but diminished quantification. Quantification might be improved by calibrating aerosol species against the raw spectra as suggested by Ackerman (1997). Further verification, beyond the limited three severe incident case studies, is required to extend the applicability of the method. The three incident case studies demonstrated plausible plumes and established a preliminary methodology to determine ground-level concentrations of particulate matter, speciated by particle size ($PM_{2.5}/PM_{10}$ ratio), source type (soil, sea-spray, smoke, auto, and secondary sulphates), and gaseous composition (NO , NO_2 , SO_2 , O_3 , $PM_{2.5}$, PM_{10}).

Studies are in progress to further analyse the past Australian spring's dust storms and fires, which were reputed to be the worst on record with almost daily exceedances of ambient guidelines, to improve the methodology. Geostationary

satellite data has increased the temporal resolution to enable severe dust events to be identified at sub-hourly timeframes. The spatial resolution, $\sim 4 km^2$ at NADIR, is coarse, and localized events smaller than this scale may be indistinguishable at that spatial resolution. The spectral sensitivity of aerosol plumes at infrared wavelengths is dominated by water vapour and may suggest that quantification of aerosol species may be attributed to humidity changes within the aerosol plumes rather than correlation with concentration.

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Author contribution Co-authors assisted with review and editing of the manuscript.

Data Availability Not applicable, large TB size.

Code availability Not applicable.

Declarations

Competing interests The authors declare no competing interests.

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