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Radiometric Validation of Multi-spectral Ocean Colour Satellite Data in High Biomass Southern Benguela Waters

Elisabeth Robertson

Thesis presented for the degree
Master of Science
in the Department of Oceanography
University of Cape Town
September 2009
Declaration:

I know the meaning of plagiarism and declare that all work in this document, save that which is properly acknowledged, is my own.

E.J. Robertson

September 2009
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All those from UCT and MCM who made the fieldwork so enjoyable and the Lambert's Bay Madness survivable. Special thanks to Andre du Randt for all his hard work and great patience at sea.

My family.

And Nick, for constantly insisting that I back up my work.
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Abstract

This study forms the first step towards a comprehensive ocean colour satellite validation strategy for the Southern Benguela region, and underlines the value of a statistical radiometric validation as a prerequisite to any geophysical validation exercise. A radiometric validation exercise was performed using co-incident MERIS RR data and in situ radiometer data from a mooring in the Southern Benguela near Lambert's Bay during the late summer bloom seasons of 2005 and 2006. The data are typified by very high biomass conditions. Sources of error associated with the in situ data are assessed and the magnitudes quantified. The satellite data is examined with particular reference to uncertainty derived from the atmospheric correction processes, which perform unreliably in many of the matchup instances. Results show that the accuracy of the atmospheric correction does not appear to be related to the in-water constituents and is more likely due to atmospheric variability or aerosol features that are not addressed in the models employed by the correction processes. It is also shown that while the radiometric data display a consistent bias in the red region of the spectrum, good correlation with the satellite measurements is observed here under high biomass conditions, underlining the importance of the red wavebands for coastal remote sensing. Recommendations towards the development of a comprehensive regional validation strategy include the establishment of low-cost measurement protocols for high biomass conditions, as well as further investigations into regional atmospheric variability to improve confidence in the atmospheric correction procedures.
# Notation and Units

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<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tr>
<td>Chl a</td>
<td>Chlorophyll a</td>
<td>mgm⁻³</td>
</tr>
<tr>
<td>R搦</td>
<td>Remote Sensing Reflectance</td>
<td>sr⁻¹</td>
</tr>
<tr>
<td>Eₓd</td>
<td>Downwelling Irradiance</td>
<td>µW cm⁻²nm⁻¹sr⁻¹</td>
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<tr>
<td>Lᵤ</td>
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<td>µW cm⁻²nm⁻¹sr⁻¹</td>
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<td>Water-leaving radiance (measured by remote sensing)</td>
<td>µW cm⁻²nm⁻¹sr⁻¹</td>
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<tr>
<td>nLₙw</td>
<td>Normalised water-leaving radiance</td>
<td>µW cm⁻²nm⁻¹sr⁻¹</td>
</tr>
<tr>
<td>ρᵤ</td>
<td>Normalised water-leaving reflectance</td>
<td>sr⁻¹</td>
</tr>
<tr>
<td>λ</td>
<td>Lambda (signifying wavelength)</td>
<td>nm</td>
</tr>
<tr>
<td>Iₒ(λ)</td>
<td>Solar irradiance at sun's surface</td>
<td>µW cm⁻²nm⁻¹</td>
</tr>
<tr>
<td>a(λ)</td>
<td>Total absorption coefficient</td>
<td>m⁻¹</td>
</tr>
<tr>
<td>bₒ(λ)</td>
<td>Total backscattering coefficient</td>
<td>m⁻¹</td>
</tr>
<tr>
<td>Kᵤ</td>
<td>Diffuse attenuation coefficient</td>
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</tr>
<tr>
<td>τₐer</td>
<td>Aerosol Optical Thickness</td>
<td>dimensionless</td>
</tr>
<tr>
<td>p</td>
<td>Atmospheric pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>A</td>
<td>Ozone column abundance</td>
<td>DU</td>
</tr>
<tr>
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<td>Wavelength-dependent ozone absorption coefficient</td>
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1. Introduction and Background

1.1 Rationale and Objectives

The study of Harmful Algal Blooms (HABs) in the Southern Benguela can be regarded as pushing the science of ocean colour to its underexplored edges, where very high biomass conditions and complex in-water optics are combined with the challenges of coastal remote sensing. Ocean colour remote sensing offers considerable potential for the observation of HABs (Bernard et al., 2008), but whereas open ocean applications are well established, coastal applications present significant difficulties which still need to be addressed if ocean colour data are to be properly beneficial to this field.

Ocean colour satellite data validation is an essential step in the process towards establishing confidence in coastal remote sensing. Validation activities for sensors such as ESA's MEdition Resolution Imaging Spectrometer (MERIS) generally take place in oligotrophic North Atlantic and Mediterranean waters, and high biomass coastal waters are dramatically under-represented. The Benguela Calibration (BENCAL) cruise (2002) has been the only validation activity undertaken in the Southern Benguela (Aiken et al., 2007). Protocols for performing such activities in high biomass bloom conditions are not well established, and there are many additional considerations (such as addressing biomass patchiness, for example) that differentiate procedures from those suitable for measurements in comparatively stable, clear, and deep waters.

Currently, local efforts are being concentrated towards an ongoing, operational HAB monitoring system on the West Coast, using near-real time MERIS RR data together with an in situ monitoring buoy, the value of which was ably demonstrated by the BOB mooring between 2005 and 2008 (Fawcett, 2006). The successfully low-cost, lightweight approach to the mooring has shown promise for future endeavours of a similar nature, and the potential for this system to double as a validation site is apparent. This exercise, performing a basic validation of the satellite data using radiometric data from the mooring, is a first step towards the establishment of a proper satellite validation strategy and
measurement protocols for the high biomass, spatially heterogenous conditions of the Southern Benguela.

The objectives of this study are to evaluate the utility of the MERIS RR radiometric data used for the operational HAB monitoring system, and to comment on circumstances in which it should be regarded with caution. The reasons behind any divergence will be investigated and discussed. It is well known that atmospheric corrections over high biomass coastal waters are challenging and a good understanding of the problems was sought. New ideas from current research were investigated with a view to possibly generating a new, region-specific solution to this problem. Problems with atmospheric corrections in these conditions will be discussed in detail, and recommendations will be made for future work in this direction.

While the protocols and data processing discussed are relevant to the validation of any available ocean colour satellite data, the focus for this study is on MERIS data. It has been observed that MERIS generally outperforms MODIS in the study area\(^1\), and MERIS RR data are available in near-real time (whereas the definitive MODIS processing incurs a delay of a few days) so it is MERIS that is used operationally for HAB monitoring in the area. A full satellite validation strategy would address the different responses of various sensors in a more comprehensive approach.

1.2 Thesis Organisation

Section 1, Introduction and Background (this section), serves as an introduction to HABs and Ocean Colour Remote Sensing. A short section on the hyperspectral and the future of remote sensing is accompanied by a few details on the South African context for such sensors. The last part of this section focuses on the various requirements for a successful validation activity.

Section 2 presents the validation exercises themselves, accompanied by some introductory material on local conditions and some comments on the results.

---

\(^1\) The MERIS overpass occurs between 08h30 and 11h00, and MODIS between 13h00 and 15h00, approximately. Prevailing weather conditions result in more MODIS data being lost to cloud cover. Negative water-leaving radiances are also more frequently observed in the MODIS data.
Methods and comments pertaining to the formulation of the dataset are dealt with first in the subsection 2.2 'Introducing the Validation Dataset'. A detailed look at the errors associated with the Trios-derived $R_{rs}$ is undertaken in section 2.3.

Section 3 focuses on the Atmospheric Correction as an important source of error in the validations, and various techniques are presented and some of the problems with them are explored further. A short investigation into local Aerosol Optical Thickness (AOT) conditions is reported on in this section.

Finally in section 4, the key findings of this study are presented. Recommendations are made for the way forward with regards to approaching the design of a comprehensive regional satellite validation strategy and its plan of implementation.

1.3 Remote Sensing of Harmful Algal Blooms (HABs)

In productive regions of the world’s oceans, single celled phytoplankton are able to grow in large quantities. They are the primary producers, forming the fundamental basis of the marine food web. When conditions are favourable, this algal growth can be dense and extensive, forming an algal bloom.

The harmful impacts of algal blooms can be two-fold: firstly the bloom itself may be composed of toxic species (commonly dinoflagellates), or the ecosystem is negatively impacted when a high biomass bloom collapses as a result of the exhaustion of available nutrients, which can result in hypoxic events and even the production of hydrogen sulphide ("black tide") in extreme cases (Dierssen et al., 2006). Effects are both ecological and economic as the region supports subsistence and commercial fishing operations as well as recreational interests.

Chlorophyll $a$ is the pigment present in all photosynthesising organisms, and so is the chosen proxy for phytoplankton biomass via ocean colour. Cells may also contain a wide range of other pigments, absorbing light to different extents in different parts of the spectrum. It is the complex combination of all of the absorption and backscattering characteristics of these pigments within the cell structure, and the nature of the other in-water constituents (and their own
absorption and backscattering properties), as well as with the surrounding light field, that gives the bloom its colour in the water (Dierssen et al., 2006). Because each phytoplankton cell contains Chl \( a \), even a highly varied population with a complex mixture of optically significant constituents can be measured in terms of its total biomass per unit volume.

1.3.1 **HABs and Ocean Colour Satellites**

It is essentially the presence of Chl \( a \) in each cell that enables the remote sensing of phytoplankton and HABs by satellite. This has been undertaken with the use of ocean colour satellite data since the launch of the first proof-of-concept ocean colour satellite, the Coastal Zone Colour Scanner (CZCS) in 1978 (Gordon et al., 1983, in Bailey & Werdell, 2006). It provided radiometric data from 6 bands in the visible, near infra red (NIR) and thermal parts of the spectrum. From this proof-of-concept instrument, the value of ocean colour satellite data was readily recognised by oceanographers. It soon transpired that sustained time series and more spectral information would be welcomed by the ocean colour community, and so this sensor was followed by SeaWiFS and MODIS from NASA (launched in 1997 and 2002 respectively), and MERIS (launched 2002) from ESA, among others.

Ocean colour data yields not only spectral information of the first order, but can be used to provide Chlorophyll \( a \), suspended sediment, CDOM etc. products with the use of specialised algorithms. In this way, satellite remotely sensed data is well suited to applications with complex optically significant constituents, such as HABs. In addition to challenging the science of ocean colour with very high biomass, because HABs occur in productive coastal upwelling systems the satellite remote sensing of HABs incorporates all the difficulties inherent to coastal ocean remote sensing. These include light reflected off adjacent land, unusual atmospheric aerosols in the form of desert dust or from anthropogenic sources; and in shallow water, the effect of light reflected off the sandy or rocky bottom. HABs are the extreme case in phytoplankton production inferences from ocean colour satellite data, and satellite validation activities in high biomass conditions are all the more important as a full understanding of in-
water and atmospheric optical influences, as well as of instrumentation and measurement protocols, is necessary.

1.3.2 The hyperspectral future of coastal ocean remote sensing

Traditional ocean colour sensors collect light in a small number of relatively broad spectral bands (varying from 8 bands for SeaWiFS to 15 bands for MERIS and 16 bands for MODIS). This is adequate for mapping phytoplankton (typically represented by Chlorophyll $a$ concentration) in oceanic waters (Chang et al., 2004). However, the complexity of the coastal oceans means that more sophisticated analytical algorithms are required to retrieve the relevant geophysical and optical parameters (e.g. Roesler & Boss, 2003 and Roesler & Perry, 1995), and as much spectral information as possible is needed to distinguish unambiguously between the various optically significant substances (van Mol & Ruddick, 2004 and Davis et al., 2007). The theoretical basis and computational demands of analytical algorithms, and the necessity of moving away from a more empirical approach, has influenced the development of reflectance inversion algorithms which can equally be used in a hyperspectral system, thus addressing complexity not only in the optical theory but also radiometrically.

Technical and computational limitations have long been a hindrance to the full exploitation of the resulting large volumes of data, but recently high resolution, high sample rate sensors have been developed and employed in both coastal and open ocean studies (Chang et al., 2004), although not yet deployed routinely from space. Computational advances have enabled simplified data storage and more rapid processing capabilities.

The first generation of "hyperspectral" imaging sensors was airborne. These optical remote-sensing systems can provide image data with detailed spectral resolution over a stipulated part of the electromagnetic spectrum, using many narrow bands (about 10nm) that are usually adjacent. However, airborne image spectrometry has some disadvantages compared with satellite-based image spectroscopy of which the reduced swath is one (van Mol & Ruddick, 2004).
Other significant disadvantages include the irregularity of viewing opportunities (i.e. no regular, routine image acquisitions), and the expense.

The next step from a technology perspective was the deployment of hyperspectral sensors on satellites for the remote sensing of the coastal and ocean environment (Chang et al., 2004).

The successful demonstration of the CHRIS hyperspectral imager on board the small and low-cost Proba satellite (ESA) has introduced a new aspect to coastal satellite remote sensing. Its low-earth orbit allows a high-resolution view of coastal areas, and the resulting 17 by 17 km images have a Ground Sampling Distance (GSD) of about 30m in Mode 4 (optimised for water targets). Thus the gap between airborne and space-borne imagery is narrowed (van Mol & Ruddick, 2004) and small features can now be detected. This has remarkable consequences for coastal and near-shore environments, which can now be detected and monitored on a finer scale than ever before.

There remain some unresolved issues with spaceborne, high resolution hyperspectral sensors. The narrowing of wavebands to around 10 nm has consequences for the signal to noise ratio (SNR), which is often not high enough for ocean studies where great sensitivity is needed, particularly in the blue where most atmospheric scattering occurs. Another issue with high-resolution sensors on small satellites is that the revisit times are usually not adequate for highly dynamic coastal environments.

The optical complexity of coastal waters and their overlying atmosphere drives a need for much greater spectral resolution than is available on current ocean colour sensors, e.g. to detect large changes in the spectral characteristics of phytoplankton types, or to perform accurate atmospheric correction for turbid waters. The frequent proximity of HABs to the shore can be a hindrance when using space borne sensors to study them, as pixels are frequently contaminated by the small angle forward scattering of photons reflected from nearby land surfaces (the “adjacency effect”). There is also a possible component from bottom reflectance, which cannot be completely ruled out in the shallowest
waters (van Mol & Ruddick, 2004). For these reasons too, it is becoming clear that the future for coastal and inland waters is hyperspectral (van Mol & Ruddick, 2004 and Davis et al., 2007).

Experiments by Lee & Carder (2002, in Chang et al., 2004) using hyperspectral techniques and modelled IOPs have exposed potential weaknesses in ocean colour Chl \(a\) algorithms, for example, where bottom effects from two different substrate types reveal significant spectral differences in the 500-600 nm range. However when these scenes are viewed only with the SeaWifs wavebands the spectra appear identical. Hydrolight was used to model various combinations of 9 different sets of IOPs, 32 different bottom reflectances, and 22 depths between 5.5 and 50m. These spectra are clearly unique (ibid.). However each spectrum has nearly the same remote sensing reflectance ratio of 490/555 – which is used in the SeaWifs OC2 chlorophyll determination algorithm. So in the presence of bottom effects, the OC2 algorithm is likely to fail.

Experiments of this type demonstrate possible weaknesses in algorithms used for the retrieval of ocean colour constituents using multi-spectral waveband data in contrasting water types. Additional spectral information could herald a new approach to the production of standard satellite data products (Davis et al., 2002).

Although ocean colour focuses on the visible wavelengths as these are most significant in terms of penetration beneath the ocean surface (Davis et al., 2002) and the resulting emitted radiation from the ocean, the opportunity presented by hyperspectral sensors for the simultaneous measurement of wavelengths on either side of the visible is a valuable one. On multi-spectral sensors NIR and IR wavebands have traditionally been included in order to perform the atmospheric correction. More recently, the value of UV measurements has been acknowledged for the determination of aerosol types (Holler et al., 2004, Herman, 2005). Retrieval of atmospheric products and hence the correction can be greatly improved with the use of additional spectral information from these regions. This is discussed in detail in Section 3.
Johnson & Coletti (2002, in Chang 2004) have shown that routine spectral measurements of nutrients are possible from the unique spectral characteristics of nitrates and sulphides, for example, in the UVA and UVB. With spaceborne sensors, this would mean the ability to resolve nitrate concentrations at temporal and spatial scales consistent with temperature and salinity concentrations, representing a huge advance in biogeochemical investigations (Chang, 2004).

Currently, ESA’s CHRIS imager and NASA’s Hyperion are the only two non-military fully hyperspectral space-borne instruments in operation, despite plans for other sensors that have not yet been realised: notably a proposal to mount the HICO system (Hyperspectral Imager for the Coastal Ocean, under the auspices of the Naval Research Laboratory of the USA) on board the International Space Station (Corson et al., 2003).

1.3.3 **MSMI: Integrated Hyperspectral, Multispectral and Video Imager for Microsatellites**

The South African Department of Science and Technology has revealed plans for a series of South African-built microsatellites. The first of these is currently awaiting launch in anticipation of the launch details being finalised.

Second in the ZASAT series is a microsatellite proposing to house the MSMI sensor (Integrated Hyperspectral, Multispectral and Video Imager for Microsatellites) (Schoonwinkel et al., 2005). This push-broom imager comprises 3 components, namely hyper- and multi-spectral sensors together with a video recorder for real-time motion detection (Schoonwinkel et al., 2005). The imager is designed for use on microsatellites, and as such is design-limited by the relevant weight and size requirements. The MSMI in total weighs in around 60kg, and of this the hyperspectral subsystem comprises about 22kg. It is intended for a 660 km altitude, sun-synchronous orbit and a lifetime of 5 years (ibid.).

Such an orbital configuration would result in a ground sampling distance of 4.6 m in the multispectral and 14.5 m in the hyperspectral, with a swath of 27.6 km and 14.9 km respectively. The hyperspectral images would thus be comparable
in terms of coverage and resolution, with that from the CHRIS imager aboard the Proba satellite, currently in operation.

The MSMI sensor is able to sample at more than 200 spectral bands, from 400 to 2350 nm in 10 nm bins. The multispectral imager has a target signal to noise ratio (SNR) of >30 at 20% reflectivity, but SNR figures over low albedo surfaces are not yet available for the hyperspectral instrument. Required SNR for such a sensor would be around 120 in the blue spectral region where the signal of coastal water dominates, and of the order of 30 in the red, the requirement dropping slightly in the NIR (Davis et al., 2002).

The MSMI is not specifically designed to satisfy the stringent demands of a spaceborne ocean colour sensor and so its performance as such is not anticipated. However it is discussed here from a perspective of technology development and as an indication of the level of local capability in satellite sensor design and manufacture. With more defined user requirements emerging from the marine science community, future hyperspectral ocean colour sensors may well be possible.

It is quite clear that in the open ocean the use of high-resolution satellite imagery for oceanographic purposes is impractical. But in the coastal oceans, both geographic and radiometric features need to be resolved at a much finer scale. Davis et al (2002) report on experiments conducted in New Jersey under the auspices of HyCODE (Hyperspectral Coastal Ocean Dynamics Experiment) where the simultaneous acquisition of airborne PHILLS hyperspectral data of 1.8m and 9m resolution took place, together with AVIRIS (also airborne) 20m GSD data, and SeaWiFS and MODIS imagery at 1km GSD. At the same time, in situ measurements were collected in multiple locations (Davis et al., 2002).

Overall, results showed that the SeaWiFS and MODIS 1km data are ideal for imaging the larger scale coastal features on the continental shelf. But for back bays and estuaries a higher spatial resolution is required. In terms of spectral resolution, they found that for deep water, 20 nm bins from the in situ radiometers provided equivalent spectral sensitivity to the 5 nm measurements. However in shallow water where bottom effects are not negligible, the 20 nm
data performed better than the satellites' wavebands but not as well as the 10 nm data. This is an indication that for oligotrophic or open ocean waters, increased spectral resolution may well be redundant (Davis et al., 2002). The real advantage of hyperspectral data is its use in optically complex waters.

The investigation concluded with the opinion that the larger spatial and radiometric scales of current multi-spectral ocean colour satellites are sufficient for use in the open ocean beyond the continental shelf. Inshore of the shelf, however, requires better spatial and radiometric sensitivity (Davis et al., 2002). Depending on the radiometric sensitivity and spectral calibration of the MSMI, it may be a useful source of coastal data in the future.

1.4 Ocean Colour Remote Sensing Fundamentals

Gordon & McCluney (1975) demonstrated that 90% of the remotely sensed water-leaving radiance originates in the upper layer, described by $Z_{90}$, corresponding to the first optical attenuation depth as defined by Beer's Law (in Werdell & Bailey, 2005). This contribution to the surface optical characteristics from the vertical water column means that certain conclusions can be drawn about the euphotic zone from a surface (or satellite) measurement. However, the ocean environment is very dynamic and a proper understanding of the above- and in-water contributions to the emergent light field is essential. Conclusions regarding water constituents at depth must be made with care. In this study of high biomass waters it is likely that the first optical depth is small, and variable according to its constituents.

1.4.1 Radiance, Reflectance and Remote Sensing

Marine light fields are complex and variable, and there exist a number of different approaches to characterise them. The properties easily measureable in-water are different from those measureable from space, and so each must be manipulated to provide analogous data that can be used for radiometric validation. The spectral remote sensing reflectance, $R_{rs}(\theta,\phi;\lambda)$, is a useful quantity in optical remote sensing as it can be derived from in situ or from satellite measurements. It is defined as (Mobley, 1994):
\[ R_{\text{s}} = \frac{L(\theta, \phi; \lambda)}{E_d(\theta, \phi; \lambda)} \left( sr^{-1} \right) \]

(1.1)

where \( L \) is the spectral radiance (just above the water's surface) with angular dependences \( \theta, \phi \) and at wavelength \( \lambda \). \( E_d \) is the downwelling plane irradiance at wavelength \( \lambda \) (just above the surface). All radiances, irradiances and reflectances are spectrally dependent. \( R_{\text{s}} \) is a measure of how much of the downwelling light that is incident onto the water surface is returned through the surface in direction \( (\theta, \phi) \), such that it can be detected by a radiometer pointed in the opposite (downward) direction (Mobley, 1994). These quantities are represented schematically in Figure 1.1, below.

**Figure 1.1** Schematic of fundamental properties of the light field at the ocean/atmosphere interface

The desired quantity of \( R_{\text{s}} \) can be derived from \textit{in situ} radiometric measurements using the reflectance approximation (Zaneveld, 1995), which relates the radiometric quantities to the absorption and backscattering coefficients in the upper optical depths:
but variability in this parameter should be acknowledged by analytical reflectance models in order to account properly for these effects (e.g. Roesler & Boss, 2003, and Bernard, 2005). Bidirectional effects (BDRF) are dependent on the IOPs and other factors such as the solar zenith angle and surface roughness (Albert and Mobley 2003, in Bernard, 2005). Thus an uneven surface, such as a wind-roughened ocean, might have different illumination geometries across one scene. This can also be affected by shadowing, either topographically by waves, or by clouds or dust in the atmosphere, which may be spatially heterogenous (Robinson, 2004).

As previously noted in Section 1.4.1, all measurements must be normalised to an overhead sun and standard illumination conditions in order to be comparable from day to day and between in situ and remotely sensed.

1.5 Satellite Validation and vicarious calibration

1.5.1 Satellite Validation

Satellite validation studies are essential to the appropriate use of satellite data, as they establish the relationship between satellite measurements and their ground-based or modelled equivalents, quantifying the quality and accuracy of the data or products for a specific site (Bailey & Werdell, 2006). Validation activities comprise two main aspects: establishing the relationship between measurements made in orbit and measurements made on the ground, and the verification of models, algorithms and derived products. Validation in the form of “ground truth measurement” is performed for a specific site, which can then be extrapolated to an appropriate geographical region or within limits of certain parameters e.g. low chlorophyll concentrations, or high zenith sun angles, for application of the image data with reasonable confidence (Desa et al., 2001).

Regional validation exercises are important from many perspectives. Ocean systems are enormously variable in terms of in-water constituents and the driving physical processes. Atmospheric variability, too, is important on the regional scale and may not coincide with the generally demarcated oceanic regions. Understanding regional variability in both ocean and atmospheric processes is therefore necessary to perform a sound validation appropriate to
the area. Local variability on a finer spatial scale should also be understood. Historically the focus has been on open ocean validation studies, concentrating on the consistency of satellite measurements over oceanographically stable sites. Many ocean colour satellites’ radiometric capability in the open ocean is well established. Now, the increased need for specialised coastal applications has seen renewed interest in coastal validation activities.

As part of any good satellite validation strategy, a thorough radiometric validation must be undertaken first as it is the basis of all the downstream products. No comprehensive satellite validation has been undertaken for this region before, so this validation activity will focus on radiometric validation rather than that of the geophysical satellite products. It forms a first attempt to quantify the errors associated with the in situ radiometric measurements and to extract, compare and analyse the necessary satellite data for validation. The need for the validation of geophysical products is acknowledged but this is a much more complex undertaking as uncertainties in the geophysical products depend on the radiometric retrievals and algorithm performance, and they will not be addressed here due to the scope of the study and data availability.

In radiometric validation activities the goal is to quantify the confidence with which all relevant radiometric measurements are made as well as to understand their limitations. For example, the stipulated radiometric accuracy of MERIS in the visible wavelengths is to better than 2 % at Level 1b (i.e. Top of Atmosphere radiances) (ESA, 2008). It is therefore essential to understand the measuring procedure, and the conditions in which the measurement is performed, as well as under what conditions it can be expected to be accurate and under what conditions it becomes insufficiently so. This applies to both space-borne and in situ measurements. Also in both cases, the processing of the data will again have an influence on the results and the quality, and this needs to be assessed carefully. In the case of space-borne data the atmospheric correction is a major source of error because approximations have to be made (Neumann, 2001) e.g. regarding the spatial homogeneity of gases and aerosols, and the vertical structure of atmospheric layers.
1.5.2 Vicarious Calibration

If a comprehensive and sufficiently accurate dataset can be collected, the validation activity may be extended to perform a vicarious calibration. This refers not to the physical calibration of the satellite sensor itself, but rather to the radiometric closure of sensor values (top of atmosphere radiances or TOA) with those made from the ground (bottom of atmosphere radiances or BOA) (Neumann, 2001). This can be done either by using BOA measurements to compute TOA values and compare with satellite data (producing closure at TOA), or alternatively by atmospherically correcting satellite data and comparing to BOA measurements (producing closure at BOA). In both approaches, the forward or inverse atmospheric calculation respectively is done with radiative transfer models.

1.5.3 Practical Validation Requirements

The design and requirements for a rigorous validation approach (particularly if to be used for vicarious calibration) are quite stringent, and some of them are outlined below, according to Bailey et al. (2001). While current validation activities on the West Coast do not undertake to be of such accuracy, it is useful to assess their position in the wider context. Examples of other validation efforts are the Marine Optical Buoy (MOBY) in the North Pacific (Clark et al., 2003) and BOUSSOLE in the Mediterranean (Antoine et al., 2006). MOBY is positioned off the Hawaiian islands in very stable oligotrophic Case 1 waters and is therefore an ideal candidate as a source of data for vicarious calibration (Clark et al., 2003). Coastal sites, particularly with high biomass concentrations, are too dynamic to be suitable for vicarious calibration. However the value in performing regular validation is clear for the sake of accurately characterising the radiometric data, even where the errors may be large. Responses to the issues below with respect to the validation activities undertaken on the South African West Coast are covered in Section 2.2.2.1.

1. The ground measurements must be performed at the same time as the satellite overpass takes place (or within an acceptable time window).
2. Differences in viewing geometry must be addressed e.g. measuring optical thicknesses from earth to sun is different from the satellite's measurement from itself to the study location.

3. Problems of spatial resolution or scale must be addressed: the satellite has to integrate over a larger area on the surface in order to get a clear enough signal to measure. However, the ground measurement is being made at one point.

4. Problems of radiometric resolution or the comparability of measurements: e.g. an in situ radiometer may be measuring upwelled radiance at 488 nm with a band pass of 10 nm, while the satellite may be measuring at 490 nm with a 20 nm band pass.

5. A sufficient number of synchronous measurements is necessary to perform any statistical operations, and thus validation and calibration, with confidence.

6. Out-of-bounds conditions or exclusion criteria must be set to ensure the comparison is being performed under conditions where all measurements can be expected to be resolved adequately.

(Adapted from Bailey et al., 2001).

A long-term validation and vicarious calibration strategy forms a vital part of an ocean colour satellite mission and these are well documented and easily available. Hooker et al. published a plan for a strategy for NASA’s ocean biogeochemical satellite data in 2007, and emphasised that the most challenging aspect of validation and vicarious calibration activities is the requirement of making high-quality observations in the harsh marine environment – that is, "measurements with a documented uncertainty in keeping with established performance metrics" (p.25). For this reason the authors ultimately conclude that a “rather basic and low-cost approach [to these activities] appears tenable and worth investigating” (p. 25). A primary motivation for the validation activities on the West Coast is to ascertain the utility of the existing low-cost, lightweight monitoring system for this very precise scientific approach.
1.5.4 Validation, Vicarious calibration and Atmospheric Correction

A satellite validation exercise is an important step in improving the understanding of regional uncertainty associated with satellite measurements, and the results can be used to determine the best approach to reducing these errors. In the case of the coastal Southern Benguela, it is evident from preliminary validation data that the atmospheric correction is an important source of error. A comprehensive validation exercise may be able to determine under what conditions the correction can be expected to perform well as opposed to under which conditions it may fail.

Where in situ validation data can be determined within known error levels and for certain matchup criteria, and it does not compare well with cloud-free satellite data, it can usually be assumed that there is a problem in the atmospheric correction of the satellite-measured radiances (Neumann, 2001). It is evident that a better understanding of regional atmospheric conditions and variability is required to reduce these errors. The nature of satellite measurements provides the opportunity to treat the ocean and atmosphere as a coupled system in order to better understand the limitations of the atmospheric correction, and this is proposed as a sensible approach to validation activities in the Southern Benguela.
2. Validation Activities in the Southern Benguela

2.1 Introduction

2.1.1 HABs in the Southern Benguela

Smayda & Reynolds (2001) write that it is generally accepted that globally, near-shore blooms of benign, noxious and toxic flagellate species are on the increase, and are now commonplace in annual successional cycles.

In the Southern Benguela, Harmful Algal Blooms (HABs) are certainly a frequent occurrence (Pitcher & Calder, 2000), which often result in severe negative impacts to the marine ecosystem as well as to the local community.

“Red tides” are common and usually attributed to members of the Dinophyceae phytoplankton group, some of which are toxic. The Benguela upwelling system is very much wind driven and is typified by periods of upwelling followed by a quiescence phase which may allow blooms to develop. Blooms occur most commonly from January to May, during the latter half of the upwelling season. Each red tide is associated with synoptic weather patterns, which dictate the onshore and offshore movement of dinoflagellate-dominated frontal blooms. There is also interannual variation, thought to be related to weather pattern changes (Pitcher & Calder, 2000).

The harmful impacts of such phytoplankton blooms are either associated with specific toxic species or with the high biomass that these blooms can attain (Dierssen et al., 2006).

Toxic species cause mass mortalities of fish, shellfish, marine mammals, seabirds and other animals. Human illness is caused by contaminated seafood when toxic phytoplankton are filtered from the water by shellfish that accumulate toxins to levels that are potentially lethal to humans and other consumers. Of these shellfish poisoning syndromes, Paralytic (PSP) and Diarrhetic Shellfish Poisoning (DSP) are common in the Benguela. Confirmed cases of PSP have been attributed to the dinoflagellate *Alexandrium catenella* (Pitcher & Calder, 2000).
The collapse of high biomass blooms through natural causes such as nutrient exhaustion can lead to hypoxic events and sometimes, in extreme cases, the production of hydrogen sulphide. This can also cause extensive mortalities of marine organisms, and the area is well known for mass walkouts of West Coast rock lobster escaping near-shore low oxygen conditions (Cockroft et al., 2000). In addition to the damage to the local marine ecosystem and obvious health risks, the consequent negative impacts on the local economy can be significant during the bloom season as a result of the collapse of fish stocks and also due to the loss of income from tourism.

2.1.2 Multi-Platform Ocean Colour data for HAB monitoring

Marine and Coastal Management (MCM), in conjunction with the University of Cape Town (UCT), and under the auspices of the Benguela Current Large Marine Ecosystem Programme (BCLME), have made significant progress towards the establishment of a near-real-time HAB identification and monitoring system, with the use of satellite ocean colour data as well as in situ data from a mooring near Lambert's Bay. In addition to this, annual field campaigns yield a more extensive suite of data used for the development and testing of regional algorithms, which contribute to a deeper understanding of the system dynamics.

A regional inversion algorithm (Bernard, 2005) is used to derive seven in-water constituent parameters (Chl $a$ concentration, algal effective diameter, the relative concentration of three representative algal groups, combined gelbstoff and detrital absorption, and small particle backscattering) from an input of in situ $E_d$ and $L_u$ radiometric measurements, or alternatively from MERIS atmospherically-corrected multi-spectral normalised water-leaving reflectances, $p_w$. During the demonstration-of-concept period between 2005-2008, in situ data from a high frequency, multi-sensor buoy were available on demand to use in conjunction with the processed satellite data to identify blooms and investigate their dynamics.

The UCT/MCM system, while challenging to maintain operationally, successfully demonstrated the validity of ongoing efforts towards this goal. Indications are that a significant weakness in the current system is the reliance on
atmospherically corrected Level 2 satellite data. The failure of the atmospheric correction is frequently confirmed by the appearance of negative water-leaving reflectances. A failure of the atmospheric correction could also lead to the overestimation of water-leaving reflectances in the blue. These effects are discussed more thoroughly in Section 3. The introduction of unquantified errors associated with the atmospheric correction in the Level 2 data obviously has significant effects on any downstream products.

\[ R_{rs} = \frac{L_u(0^+, \lambda)}{E_d(0^+, \lambda)} = \frac{f}{Q} \frac{b_a(\lambda)}{a(\lambda) + b_b(\lambda)} \]  

(1.2)

where \( L_u(0^+, \lambda) \) is the upwelling radiance just above the sea surface, \( E_d(0^+, \lambda) \) is the downwelling irradiance just above the sea surface, \( f/Q \) describes the angular structure of the light field, and \( a(\lambda) \) and \( b_b(\lambda) \) are the total absorption and backscattering coefficients respectively (Zaneveld, 1995).

In practice when performing the necessary in situ radiometric measurements, it is necessary to measure \( L_u \) at some depth below the surface rather than just above as is required by the approximation above. So a propagation scheme is required to describe the attenuation of the upwelled radiance as it is propagated to the surface. This is performed using the formulation of \( K_u \), the diffuse attenuation coefficient for upwelling radiance, of Albert & Mobley (2003) (as described in Bernard, 2005) and there may be regional uncertainties associated with this (discussed further in section 2.2.2.2).

A satellite receives not only the spectral reflectance of the surface, of course, but measures all light arriving at its sensor: a complex relationship of spectral solar irradiance \( (I_o) \) interacting with the atmosphere on both its downward journey to illuminate the surface and penetrate the water, and on its upward return journey to the sensor.

MERIS radiometric satellite products are delivered as normalised water-leaving reflectances (after section 3).
possible figures, a sample period between February and June 2005 was examined, chosen for when BOB was working fairly consistently and so a high number of the MERIS images were sought out. Out of 126 days during this period where BOB had recorded data, 72 MERIS RR images were available and of these, 34 were acceptable in terms of cloud cover and high glint flags. Taken as an indication of general conditions, this translates to approximately 57% coverage by the satellite, or a 27% success rate in terms of getting a clear image. These figures, while not comprehensive, can be regarded as meaningful in terms of an operational monitoring system because the sample period does include that which is most important for HAB monitoring i.e. the late summer. There may be a possible bias in this selection due to bad weather in the autumn/early winter.

2.2.1.2 Buoy Data

A multi-instrument buoy, BOB, was moored at approximately 32° 05.067' S 18° 16.146' E, about 3 km east of Lambert's Bay harbour, between 2005 and 2008. Hyperspectral radiometric data has in fact been available for this site from 2004, when a prototype buoy, Bokkom, was deployed to demonstrate the utility of such a mooring for operational HAB detection and monitoring.

The design requirements of BOB were, amongst others, for a lightweight, low cost in-water optical mooring that could provide real-time remote sensing reflectance data and that could withstand the challenges of being submerged in an inhospitable coastal environment (Bernard & Fawcett, 2004). The spar buoy design experiences reduced tilt and roll compared to a surface following buoy (Detrick et al., 2000 in Fawcett, 2006), and following this design, the bulk of the buoy's weight is located as far below the surface as possible. While this provides more stability in terms of its vertical orientation, a compromise in terms of sensor depth had to be effected, although efforts were made to keep the sensor as close to the surface as possible and thus minimise the necessary extrapolation to the surface of the radiance measurements. The mooring houses a RAMSES-ARC hyperspectral subsurface radiance sensor (TriOS, Germany) measuring \( L_u(z) \) with \( z \approx 0.2 \) m, as well as an irradiance sensor (TriOS RAMSES-ACC) on the mast, measuring \( E_d \). TriOS radiometers are not only well priced compared to
similar instruments, but have shown themselves to be robust and able to withstand prolonged exposure to a harsh ocean environment (Fawcett, 2006). Both radiometers sample from 320 to 950 nm with 3.3 nm per pixel. The spectral accuracy is 0.3 nm (ibid.). It was also a key design requirement that the mooring's radiometers should have sensors capable of being field calibrated (Bernard & Fawcett, 2004), and the drift of the radiometers is tested regularly using a field calibration instrument (FieldCAL, TriOS, Germany) (Fawcett, 2006).2

The radiance sensor is attached to a vertical arm extending about a metre outwards from the flotation device in order to prevent instrument shading from the structure itself (Fawcett, 2006). A PDCR 1830 pressure sensor (Druck, UK) is positioned adjacent to the radiance sensor for depth data, while an inclinometer incorporated into the radiance sensor records tilt and roll data for each radiometer measurement (Mueller et al., 2003, in Fawcett, 2006). Other instrumentation includes a fluorometer, a thermistor chain and an ADCP.

The TriOS radiometric data are processed with the background, calibration and wavelength files that accompany each radiometer (Fawcett, 2006). Median values from the 3-minute sampling period are used to derive a single spectrum for each radiometer, which are then resampled to a wavelength resolution of 5 nm. Once this has taken place, $L_u(z)$ can be extrapolated to the surface using the diffuse attenuation coefficient $K_u$. $L_u(0^+)$ is then normalised to $E_d$ and $R_{rs}$ is calculated using the reflectance approximation (Eq. 1.2). The propagation of $L_u$ to the surface and through the air-sea interface and the conversion to $R_{rs}$ are performed as part of a locally developed regional reflectance inversion algorithm (Bernard, 2005).

2005 and 2006 were the best operating years of BOB. Over this 2-year period, 227 days of data were recorded (the mooring was removed for the winter period of each year). However it should be noted that this does not imply a complete suite of measurements on each day.

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2 The immersion factor coefficient was calculated from the refractive index of the Trios lens, with the same result as seen in Ohde & Siegel (2003).
The BOB dataset is difficult to characterise accurately as there are only short periods where all the sensors worked to their full capacity. Where some sensors performed, others did not, and hardly ever at the same time. It is not a simple question of the sensor either functioning or not, but variability within days is also present (i.e. sensors working intermittently). As the value of the dataset is not only in its completeness, but also in the selected satellite matchup dates and times, evaluating it becomes complicated. For simplicity, the details given here disregard the ancillary data (ADCP, thermistor chain, and fluorometer) in favour of an accurate representation of the status of the radiometric data, which is relevant for satellite validation purposes.

When considering future plans for validation activities at this site, there are advantages to above-water radiometry rather than in-water sensors now that the capability of the former has been shown to be equivalent if not advantageous (Zibordi et al., 2004 in Hooker et al., 2007). An above-water sensor is not nearly as vulnerable (to ships and severe weather, for example), and does not suffer any bio-fouling (except possibly from birds). However the construction of a suitable platform at the study site would be required which would involve a sizeable financial consideration. A SeaPRISM system (manufactured by Cimel, France e.g. Zibordi et al., 2002) mounted on a split structure at a fixed angular orientation, together with an automated sunphotometer, would provide an excellent opportunity for high biomass coastal validation exercises. However with constraints on budget and personnel, a small in-water buoy provides a cost-effective first step in establishing a proper validation site.

2.2.1.3 Field Data

Field data from Lambert's Bay has been collected annually during the late summer bloom season since 2004. Depending largely on the resources of MCM, including the use of vessels Ecklonia (2004-2007) and Catenella (2008), this is a joint effort by UCT and MCM in pursuit of quality field data for multi-disciplinary HAB research and ocean colour satellite validation.

During each field campaign, water samples and radiometric measurements are taken daily at the site of the mooring. In addition, occasional transects are
undertaken as needed. The daily station is sampled as close to the MERIS overpass (between 9 and 11 am) as the tides and other logistic constraints allow, usually within half an hour of the overpass.

A Hyperspectral Tethered Surface Radiometer Buoy (H-TSRB: Satlantic, Halifax, Canada) is deployed to provide radiometric data in addition to the Trios radiometers on the mooring. The instrument consists of two linked 256-channel spectrographs connected to an upward looking cosine corrected irradiance sensor and a downward looking 8.5° field of view radiance sensor (Bernard, 2005). The spectral range is from 400 to 800 nm at a resolution of 3.3 nm and an accuracy of 0.3 nm (ibid.). Upwelling radiance is measured at a nominal depth of 0.66 m, and the downwelling irradiance is measured just above the surface. Care is taken to perform the measurement as close as possible to the mooring to get good agreement between the radiometers, particularly in high biomass conditions when the water can be very patchy. While avoiding any shading by the vessel, the instrument is left to collect data for a minimum of 3 minutes while the surface water samples are taken, and is then retrieved. Data are processed using the relevant proprietary software (Satlantic: Halifax, Canada). As detailed in Bernard (2005), a median $L_u(z)$ and $E_d$ are calculated, giving the full spectrum of the wavelength-dependent light fields above and below the surface of the water. As for the TriOS processing, the $L_u(z)$ values are then extrapolated upwards to the air-sea interface by means of the diffuse attenuation coefficient $K_u$. $L_u(0^+)$ is then normalised to $E_d$ and $R_{rs}$ is then calculated from the reflectance approximation (Eq 1.2). The propagation of $L_u$ to the surface and through the air-sea interface and the conversion to $R_{rs}$ are performed as part of a locally developed regional reflectance inversion algorithm (Bernard, 2005).

A hand-held Microtops (Solar Light Inc., Pennsylvania, USA) was used in 2007 and 2008 to perform aerosol optical thickness measurements. Due to persistent fog in March/April 2007 the data from this period are not very reliable. The difficulties of deploying hand-held sunphotometers at sea are not insignificant. A ship-based measuring protocol suggested by Porter et al. (2001) and further developed by Knobelspiesse et al. (2003) was employed to reduce the bias
observed in AERONET's database of hand-held sunphotometer measurements. Where there are errors in sun pointing, a direct path to the solar disk cannot be measured and hence unrealistically large AOT values are computed. The protocol suggests using only the highest voltage measured at each scan to perform this calculation, and later to iteratively remove outliers from the dataset in order to remove variability due to sun-pointing errors. However it must be acknowledged that this procedure is somewhat subjective, and also that a ship will be somewhat more stable than a smaller vessel such as Ecklonia or Catenella. Thus the Microtops measurements should be regarded with caution. Comments on the 2007 data by Smirnov (pers comm, 2007) indicate that they are within the expected range, but with a concerning increase in the 500 nm channel that may be an artefact of pointing error or of haze. However, the possible presence of absorbing aerosol necessitates further spectral investigation before any conclusions are made in this regard.

Fluorometric chlorophyll measurements from 5 depths are made (Parsons, 1984), as are High Performance Liquid Chromatography (HPLC) pigment concentration determinations from the water samples, using a reverse phase procedure outlined by Barlow et al., 1997 (in Bernard, 2005). Total suspended particle matter (Roesler, 1998), gelbstoff (Mueller & Austin, 1995) and detrital absorption measurements (Kishino et al., 1985) (all in Bernard, 2005) are also performed using a spectrophotometer but are not explicitly used in this study.

For this study the decision was made to use fluorometric Chl a measurements only, as problems with the chromatography in 2005 resulted in an incomplete HPLC dataset over this period.

2.2.2 Compiling the Validation database

2.2.2.1 Addressing Concerns regarding the Validity of Match-ups

The considerations for an appropriate validation field strategy as outlined by Bailey et al. (2001) (see Section 1.5.2) are addressed below.

1. The ground measurements must be performed at the same time as the satellite overpass takes place.
In practice, exactly synchronous measurements are logistically difficult to undertake, given the station’s distance offshore as well as variable conditions at sea. Bailey describes the acceptable time difference for validation activities as dependent on the stability of the geophysical parameter being studied. For the 2001 study at Monterey Bay, this was determined as within 2.5 to 3 hours of the overpass. Zibordi et al. (2006, in the Baltic Sea) and Desa et al. (2001, in the Eastern Arabian Sea) define an acceptable time difference of not more than 2 hours. In the highly dynamic Southern Benguela, a best effort is made to perform the station measurements well within an hour of the overpass. In the case of the BOB radiometric data, samples can be extracted on the hour and half hour straddling the overpass (i.e. within half an hour of the overpass) and these are then averaged (see Section 2.2.2.2).

2. Differences in viewing geometry must be addressed e.g. measuring AOT from earth to sun is different from the satellite’s measurement from itself to the study location.

For this reason the measurements must be normalised and BDRF effects addressed. Water-leaving radiances from the satellite are normalised as a matter of course to an overhead sun to standardise measurements in this way (to enable day to day comparisons). Both sets of in situ radiometric data are converted to $R_{rs}$ for comparison hence are adjusted for angular dependencies.

3. Problems of spatial resolution or scale must be addressed: the satellite has to integrate over a larger area on the surface in order to get a clear enough signal to measure, but the ground measurement is being made at one point.

It is noted that the ocean’s surfaces are some of the darkest on earth and their highest reflectances are in the same wave bands as those wavelengths mainly scattered by the atmosphere (i.e. the blue). For this reason satellite sensors usually need to increase their collection of radiation over larger areas spatially and/or radiometrically to get the
required signal-to-noise ratios over water. This is inherent in the nature of the measurement due to the technological constraints of the sensors.

Bailey et al. (2001) determined that a box of $5 \times 5$ pixels (assuming $1$km satellite resolution) was adequate for their Monterey Bay study. As with the question of the acceptable time lag, recognition of the highly dynamic conditions in the Southern Benguela should underly this judgement. There are often visible, fast-moving fronts; the tension lies between selecting a large enough area to have some confidence in the satellite's measurement, and avoiding the dampening of smaller-scale but dramatic features by averaging too many pixels. A comparative study of 1, 5 and 9 pixel averages was performed to test this sensitivity. It was decided that a 5-pixel average is a reasonable compromise, adequately addressing patchiness concerns without generating too much noise in the averaged data. Some allowance must of course be made for the fact that a point measurement is being compared to an area one.

The other concern regarding pixel selection is that sometimes there will be no data available for the chosen pixel, or for a few pixels in the desired box. This is frequently due to negative water-leaving reflectances where the atmospheric correction has failed. Sometimes there are simply no data available at all. In all of these cases a strategy has to be devised to cater for the complexities of comparing an average of, for example, six pixels (if three are invalid) to an average of 9.

4. Problems of radiometric resolution or the comparability of measurements:
   An in situ radiometer may be measuring upwelled radiance at 488 nm with a band pass of 10 nm, while the satellite may be measuring at 490 nm with a 20 nm band pass.

In this investigation these differences are not quantified but are simply acknowledged as a possible source of variability when comparing measurements. The Satlantic and Trios data can be processed to 5 nm intervals between 400 and 750 nm with some confidence. The visible MERIS bands are centred at 412.5, 442.5, 489, 509, 559, 619, 664, 681.25,
and 708.75 nm and so must be rounded to the nearest 5 nm for intercomparison with the *in situ* radiometer data. The MERIS bands are all 10 nm wide except around 681.25 nm, which is 7.5 nm wide. Differences between a band measurement and a point measurement are acknowledged but are not addressed here.

5. *A sufficient number of synchronous measurements is necessary to perform any statistical operations, and thus calibration, with confidence.*

As described later in section 2.3.3 a total of 34 complete satellite/*in situ* radiometric matchups was achieved. Any statistical operations are performed with acknowledgement of the size of the matchup dataset.

6. *Out-of-bounds conditions or exclusion criteria must be set to ensure the comparison is being performed under conditions where all measurements can be expected to be resolved adequately.*

Exclusion criteria for satellite data:

- Although this study is not a validation of geophysical products, the range for which a Chl *a* algorithm is validated would provide grounds for the exclusion of data outside of this range. The regional inversion algorithm used on the West Coast and discussed in this study is validated (from an in-water perspective) for chlorophyll *a* concentrations from 0.5 to 300 mg/m³ (Bernard, 2005).

- Another set of exclusions is the presence of cloud. In cloudy conditions satellite data cannot be used at all and this greatly reduces the number of successful match-ups on the West Coast where persistent fog can be a real setback. Hazy conditions are known to be problematic but in this exercise are not addressed due to the inability to quantify this easily. However it is acknowledged that particularly where AOT measurements are concerned, confidence can be greatly reduced in the presence of haze.
- Sun-glint contaminated pixels were also rejected according to the high and medium glint flags.

Exclusion Criteria for *in situ* data:

- The tilt-roll sensor on the mooring, when properly operational, provides enhanced confidence in the radiometric measurements as data can be filtered to include only those taken within certain tilt angles. However during periods where the sensor was faulty or non-operational, confidence can be reduced in this way as well. Because the sensor was so frequently non-operational, it was decided that radiometric data unaccompanied by tilt/roll data would not be excluded from this study, although a more stringent study would require this.

- Low ambient light conditions would reduce confidence in the *in situ* radiometric data and would form the basis of exclusions where appropriate. As the MERIS overpass is between 9 and 11 am in full daylight, any time-related exclusions (e.g. dawn, dusk) need not be made. Likewise, the presence of cloud renders the matchup invalid so days with significant cloud cover will already have been removed from the dataset according to the cloud flag criteria described above.

### 2.2.2.2 Data Processing

1. The BOB dataset was assembled first and it was ensured that the full dataset was processed consistently to $L_u$ and $E_d$ values. There are intermittent radiometer data from January 2005 until December 2006. Due to a combination of technical problems with the radiance sensor and the Ocean-i controller, and bad weather, there were no MERIS/Trios matches in 2007 or 2008. As there is a much higher volume of Trios data than Satlantic, it was decided to base the validation exercise on the former and use the Satlantic only as a measure of confidence in the Trios data (see section 2.3.2.1).
ii. MERIS data was collected for the dates where the BOB data were at least partially intact, and a list was made of the date and time of each overpass. The MERIS archive at UCT is not complete and this process of data collection was very time consuming as each image had to be downloaded from MERCI or requested from the EOLI archive. To avoid downloading images that would not be useful for validation purposes, a very conservative preliminary cloud-screening inspection was performed on each quick-look image.

iii. Using the list of overpass times, the BOB data for the half hour before the overpass and the half hour after the overpass were extracted from the data files. (The Trios radiometers attached to BOB were programmed to sample for 3 minutes on the hour and on the half hour during daylight hours. So if the overpass was at 10h20, the radiometer data for 3 minutes from 10h00 to 10h03 and for 10h30 to 10h33 was extracted and stored.)

iv. An inventory was created detailing which data are available for which dates. The matchup radiometer data for each day were inspected, and rejected if there were no data, or data from a sampling burst of less than 1 minute (a complete sampling burst is 3 minutes). Due to the small volume of data with an accurate tilt/roll or depth measurement, these were not regarded as exclusion criteria and consequently none of the Trios data used for the validation exercise is tilt/roll filtered or processed with an actual depth measurement. An approximate depth of 0.2 m is used, as recommended by Fawcett (2006).

v. All Trios data was processed to $R_{rs}$ using a reflectance inversion algorithm (Bernard, 2005) as detailed later in this section.

vi. The MERIS N1 files were converted to HDF files using an EnviView (European Space Agency) 1.2.1.2 tool. As the mooring had been removed and re-deployed several times, accurate positional data was needed to identify the closest pixel to the mooring at the time of the satellite overpass. The following procedure was undertaken for each image using custom scripts written in Matlab (Version 7.5, The MathWorks, Mass. USA): radiances and both Chl a products (Algal 1 and Algal 2) for one pixel were extracted (the pixel closest to the specified BOB position), then
5 (the pixels horizontally and vertically adjacent) and then 9 (all adjacent pixels to the first):

![MERIS pixel selections](image)

**Figure 2.1 Schematic of MERIS pixel selections for the validation dataset**

vii. The mean and standard deviation of each set of pixels were calculated and stored. During this procedure each image was inspected using the Basic ERS & Envisat (A)ATS & MERIS Toolbox (BEAM) (Brockmann Consult, Germany) with a positional marker and a closer look was taken at the data for the relevant pixels. Images were rejected completely in the presence of cloud or high glint at the site of the buoy.

viii. Further rejection criteria were applied to the satellite validation data:
   a. 2 or more pixels with more than half negative values for all (visible) \( R_{vis} \)
   b. Any pixel with \( R_{vis} \) at 410nm < -0.1
   c. Any pixel with \( R_{vis} \) at 410nm >0.015 i.e. possible cloud

ix. The set of Trios/MERIS validation matchups was compared to the set of field measurements and cross-referenced. The cloud-screened Trios/MERIS/field measurement matchup dataset is presented in Table 1 below.

x. All MERIS \( \rho_w \) values were converted to \( R_{vis} \) using Eq. 1.3.
Table 2.1 The Validation Dataset 2005-2006. The presence of Satlantic data implies the full suite of field measurements.

<table>
<thead>
<tr>
<th>YEAR</th>
<th>DATE</th>
<th>MERIS RR</th>
<th>RR Trios</th>
<th>Satlantic</th>
</tr>
</thead>
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<td>-</td>
</tr>
<tr>
<td></td>
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<td>27-Feb</td>
<td>X</td>
<td>X</td>
<td>-</td>
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<tr>
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<td>X</td>
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<tr>
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<td>22-Mar</td>
<td>-</td>
<td>X</td>
<td>X</td>
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<td>X</td>
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<td>07-Dec</td>
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<td>16-Mar</td>
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<tr>
<td></td>
<td>22-Mar</td>
<td>X</td>
<td>X</td>
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</tr>
</tbody>
</table>
Notes on the reflectance approximation and the use of $K_u$

The reflectance approximation, commonly used for reflectance inversion algorithms, expresses the light leaving the sea surface in terms of the absorption and backscattering properties of the water column. As seen previously in Eq. 1.2, the reflectance approximation for $R_{rs}$ (Zaneveld, 1995) describes the relation between the absorption and backscattering coefficients in the upper optical depths and measurements of the upwelling radiance and downwelling irradiance (Gordon & McCluney, 1975 in Bernard, 2005).

A locally developed hyperspectral reflectance inversion algorithm forms the basis of the processing chain for both the Trios and the Satlantic radiometer systems with respect to extrapolating the upwelling radiance and downwelling irradiance measurements to the surface (Bernard, 2005). $L_u$ and $E_d$ are related to $R_{rs}$ via the use of $K_u$, the diffuse attenuation coefficient for upwelling radiance. It is dependent on the total absorption and backscattering coefficients and the solar zenith angle, using the formulation of Albert & Mobley (2003) (in Bernard, 2005):

$$K_u = (a + b_a) \left[ \frac{b_b}{a + b_a} \right]^{3.452} \left( 1 - \frac{0.2786}{\cos \theta_s} \right)$$  \hspace{1cm} (2.1)

The use of $K_u$ is unavoidable given that in this optical measuring system a subsurface measurement of $L_u$ is performed. In the absence of direct measurements of $K_u$, such an approximation as used by Bernard (2005) is the only viable solution. Alternative characterisations of $K_u$ e.g. Morel (1988), are appropriate only for relatively low biomass waters and are therefore of limited use here.
2.3 Validation Exercises

2.3.1 MERIS processing updates

The validation matchups selected for this exercise are all from the summer and autumn of 2005 and the summer of 2006, as can be seen in Table 2.1. The MERIS RR processing changed in April 2006 so all of these data were processed using IPF 4.10 (the current IPF is version 5.02). Many improvements to the processing were made in the upgrade to IPF 5.02, including a revision of the Turbid Water Correction Algorithm. The Aerosol Database was also revised, enabling the improved detection of dust-like aerosols. The Case 2 Neural Network was implemented and the Algal 1 index was refined (Bourg & Oblensky, 2006). These changes will have a significant impact on any validation exercise performed with Level 2 MERIS data from April 2006 onwards. It is unfortunate that the highest frequency of validation data here does not occur more recently, when the atmospheric correction and constituent retrieval algorithms are much improved, as the usefulness of this exercise is thus limited in terms of its relevance to the current performance of MERIS ocean colour products. However as an exercise it provides a good training in validation techniques and considerations, and once this approach has been assessed and critiqued, the forthcoming MERIS reprocessing (expected in 2009) will provide the opportunity to repeat the exercise with the expectation of more current results.

2.3.2 Sources of Error in the in situ derived $R_s$

It has been established in section 1.5 that a good understanding of the sources and quantities of error in all the measurements, but particularly in the in situ data, is fundamental to a radiometric validation activity.

Table 2.2 below outlines the most important sources of error in the $R_s$ derived from the in situ data and provides nominal estimates of their magnitude. The errors are expressed as a percentage of the fully processed $R_s$ signal.
Table 2.2 Sources of error in the Trios-derived $R_{rs}$, and estimates of their magnitude

<table>
<thead>
<tr>
<th>Source of Error in $R_{rs}$</th>
<th>Estimated magnitude (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_u$ and $E_o$ measurement uncertainty (including instrument calibration accuracy)</td>
<td>5</td>
</tr>
<tr>
<td>Use of $K_u$ to extrapolate $L_u(z)$ to surface</td>
<td>10</td>
</tr>
<tr>
<td>Bidirectionality</td>
<td>2</td>
</tr>
<tr>
<td>Biofouling of in-water sensors</td>
<td>1</td>
</tr>
<tr>
<td>Instrument Self-shading</td>
<td>1</td>
</tr>
<tr>
<td>No tilt/roll filtering or depth adjustment</td>
<td>10</td>
</tr>
<tr>
<td>Scale differences with satellite matchups</td>
<td>2</td>
</tr>
</tbody>
</table>

Using composite RMS error formulation

$$RMS\ error = \sqrt{a^2 + b^2 + c^2} \ldots$$ \hspace{1cm} (2.2)

where $a$, $b$ and $c$ are the individual estimated errors, these estimates give a total error of approximately 15% of the $R_{rs}$.

In the following sections some of these errors will be examined more closely to assess their spectral dependence and better characterise their size. It should be noted that some of these figures are first order estimates (e.g. 2% for differences in scale between satellite and in situ data). Errors for bidirectionality and instrument self-shading are taken from Antoine et al. (2006) (although it is acknowledged that self-shading effects do increase with biomass as described in Leathers et al. 2004).
2.3.2.1 Trios/Satlantic “Vicarious Calibration” exercise

Method

There are good quality co-incident or nearly co-incident (within 30 minutes) data for the Trios and Satlantic radiometers for 23 days during the field campaigns of 2005 and 2006. In order to compute a reasonable estimate of error associated with the Trios data for the satellite/in situ radiometric validation, the agreement between the two in situ radiometers is calculated and used as a minimum error estimate for uncertainty in the Trios measurements. It should be noted that this selection of Trios data is not tilt/roll filtered (and neither are the Satlantic data). 6 days of data were rejected for this study, as they had anomalously high errors in the blue (more than 30%). They corresponded to days of Chl a concentrations of over 150 mg/m$^3$ according to the regional retrieval algorithm (Bernard, 2005).

Bernard & Fawcett (2004) report that a less than 5% drift in Trios measurements (in absolute radiometric units) was observed. Here it is assumed that the Trios radiometers are therefore measuring $L_u$ and $E_d$ to within 5% accuracy (see table 2.2).

The computation was performed using the Trios and Satlantic $R_{rs}$ as opposed to the $L_u$ or $E_d$ values because the Trios $L_u$ is measured at about 0.2 m whereas the Satlantic $L_u$ is measured at about 0.66 m depth. Converting them both to $R_{rs}$ allows the assessment of the whole processing chain’s effect on the relative error.

To keep the comparison relevant to the MERIS validation exercise, reflectances at these wavelengths were selected for this statistical exercise. The radiometer data are only processed to the nearest 5 nm, so the following wavelengths were selected: 410, 440, 490, 560, 620, 665, 680, and 710 nm.

In order to overcome the assumption of a normal probability distribution of the data within each dataset, a Bootstrapping technique was used to determine the relevant correlations. A Fisher transform was then executed on the correlation data (in turn to avoid assuming the correlation coefficients are normally
distributed) (Fisher, 1921) and each wavelength’s dataset was thus resampled 1000 times and the variation in the resulting correlation coefficients was considered.

The average relative percentage errors by wavelength were calculated using the formula:

\[
\% \text{error} = \left| \frac{R_{rs(Satlantic)} - R_{rs(Trios)}}{R_{rs(Trios)}} \right| \times 100
\]

The dataset was then divided into 3 biomass categories to determine whether the biomass has any effect on the magnitude of the relative error between the Trios and Satlantic R_{rs}.

Results and Comments

Table 2.3 Median Correlation Coefficients resulting from the Bootstrapping Technique (n=1000)

<table>
<thead>
<tr>
<th>Wavelength</th>
<th>Median Correlation Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>410 nm</td>
<td>0.96</td>
</tr>
<tr>
<td>440 nm</td>
<td>0.94</td>
</tr>
<tr>
<td>490 nm</td>
<td>0.96</td>
</tr>
<tr>
<td>510 nm</td>
<td>0.98</td>
</tr>
<tr>
<td>560 nm</td>
<td>0.98</td>
</tr>
<tr>
<td>620 nm</td>
<td>0.95</td>
</tr>
<tr>
<td>665 nm</td>
<td>0.97</td>
</tr>
<tr>
<td>680 nm</td>
<td>0.92</td>
</tr>
<tr>
<td>710 nm</td>
<td>0.83</td>
</tr>
</tbody>
</table>

The median correlation coefficients resulting from the Bootstrapping technique (Table 2.3) show a very good correlation across the spectrum, highest from 410 to 680 nm and dropping slightly in the red although still highly significant at the 95% confidence level. This means a high degree of variability in the dataset is explainable.

Figure 2.2 shows an average percentage relative error as computed with Eqn. 2.3 of approximately 10% between 400 and 720 nm, after which the errors rise to a maximum of 70%. This rise is partly attributable to error magnification (as a percentage of the measurement) where the R_{rs} values are small.
The dataset was divided into 3 biomass categories of high (more than 30 mgm$^{-3}$ of Chl $a$), intermediate (between 5 and 30 mgm$^{-3}$) and low (less than 5 mgm$^{-3}$). Some examples from each category are shown below. It is expected that there will be some correlation as when the biomass is very high, the water is patchy and therefore the distance between the sampling areas becomes critical even if it is small. The large errors in the rejected days' data are very likely attributable to patchiness.
Figures 2.3 (a-c) Example of Trios/Satlantic derived $R_\text{rs}$ spectra for high (Chl $a > 30 \text{mg m}^{-3}$), intermediate ($5 < \text{Chl } a < 30 \text{ mg m}^{-3}$) and low biomass (Chl $a > 5 \text{ mg m}^{-3}$).
These examples of Trios and Satlantic derived $R_n$ for high, intermediate and low biomass show generally very good agreement between the sensors. The high biomass examples display the typically low $R_n$ in the blue due to the sum of water absorption and massive phytoplankton absorption here. The elevated fluorescence peak and the “red shift” of this peak towards 709 nm in very high biomass (Dierssen et al., 2006), is also evident. The largest differences between the radiometers were observed in this biomass category but this is much more likely to be due to the patchiness of the water at very high Chl $a$ concentrations than for radiometric reasons.

The intermediate biomass category is typified by large variability in the radiometric matchups, due to the large variability of conditions between 5 and 30 mg/m³ of Chl $a$. The low biomass examples exhibit some differences between the radiometers in the region 560 - 570 nm, but these are small.

### 2.3.2.2 Tilt/roll and Depth Adjustment Exercise

**Method**

Ideally each Trios measurement should be accompanied by a tilt/roll angle and a measured depth, so that measurements performed outside of a 5 degree angle can be excluded, and to enable a more accurate $K_u$ calculation by using a measured depth rather than an estimate. In practice these sensors only functioned intermittently, so the largest body of available data is unfiltered and must be processed using an estimated depth. The following exercise was carried out in order to assess the percentage relative error introduced when the Trios radiometer data could not be processed using the additional tilt/roll and depth data.

Data were chosen from 26 days in February 2005 when the tilt/roll and depth sensors were both functioning consistently.

In order to reduce error originating from differences in solar zenith angle at the time of measurement, for each day only data sampled between 10 and 11 am were selected. They were processed as per the default Trios processing (see
section 2.2.2.2), so as to ensure an accurate comparison. These data are not tilt/roll filtered or depth adjusted, and form the “default” dataset.

To create the comparison dataset of filtered and depth adjusted data, all measurements falling within a 5° tilt/roll angle were extracted for between 10 and 11 am each day. Out of a total of an average 112 samples, about 8 fell within this criteria per day.

As for the default Trios processing, the median of these data was taken for both the radiometers and the depth sensor. Using these as inputs to the reflectance inversion algorithm (Bernard, 2005), the Rs were calculated for each day’s sampling. A second batch was processed without using the depth as an input, and using an approximate depth of 0.2 m instead. (This is based on the most representative depth as reported in Fawcett, 2006). A third set was processed using only the actual depth, and were not tilt/roll filtered. This process yielded three datasets:

1. Fully tilt/roll filtered and depth adjusted data
2. Tilt/rolled filtered but not depth adjusted (using instead an approximation of 0.2 m depth)
3. Not tilt/roll filtered but using the measured depth as input into the reflectance algorithm

For each day the percentage relative errors were calculated by wavelength as indicated in Eq. 2.3b, in each case using the filtered and depth adjusted data as the best estimate to determine their contribution to the total error. A mean percentage relative error (unsigned) over all the days was then calculated.

\[
\% \text{error} = \frac{|R_{A,appr} - R_{A,cor}|}{R_{A,cor}} \times 100
\]  

(2.3b)
Results and comments

The results of this experiment show a total error of between 4 and 20% introduced by not using an angular filter or using a measured depth to perform the extrapolation to the surface and the conversion to $R_0$ of the Trios data. The error magnitude is largely wavelength-dependent, with the errors being...
substantially larger in the red. Figure 2.4(b) shows the standard deviations of the average relative percentage error by wavelength, revealing considerably less variability (and thus higher confidence) in the errors calculated between 550 and 600 nm than elsewhere in the spectrum. It is noted in the main radiometric validation (section 2.3.3) that this is the region of the spectrum in which *in situ* and satellite radiometric measurements agree best.

![Graph](image)

**Figures 2.5 (a, b) Contributions of Depth and Tilt/Roll filtering to the total relative error, for a selection of data from February 2005.**

It should be noted that the contributions of the tilt/roll filtering and the depth measurement are not independent (high angle data will be at a shallower depth...
and vice versa) and may even serve to counteract each other, explaining the higher relative errors when one refinement to the processing is made and not the other. It is remarkable that the use of an accurate tilt/roll measurement with which to filter the data affects the error much more, and more variably in terms of wavelength, than the use of an accurate depth measurement, although both are significant (see figures 2.5 a and b). Errors are consistently largest in the red, particularly without the use of an angular filter (Fig 2.5b), but are considerable throughout the spectrum. Larger percentage errors in the red can be expected due to the increased amount of backscatter at these wavelengths, particularly in high biomass conditions. Thus the angular response will be more sensitive so more variability is expected. Reflectances are very small at these wavelengths so errors are quickly magnified.

This study shows the importance of having functional tilt/roll and depth sensors on the instrument at all times. From this exercise it is concluded that the standard error in the Trios measurements due to the lack of tilt/roll and depth adjustment is in the order of 5% for the 400–680 nm range and up to 18% in the red (680–750 nm).

2.3.2.3 Contribution of Ku to error propagation

An attempt was made to quantify the error introduced to the calculation of the Trios-derived \( R_{rs} \) by the use of \( K_u \). \( L_u \) spectra from two measured depths (the minimum and maximum depths from a 3 minute sampling burst) were used to calculate an average \( K_u \) using the approximation of Kirk (2003). This \( K_u \) was then multiplied by the average depth of the two \( L_u \) spectra and propagated to \( L_u(0^\circ) \). However the results were inconclusive due to the radiometric data being very noisy.

A simple error propagation exercise was thus undertaken to determine to what extent a sizeable error in \( K_u \) affects the \( R_{rs} \).

Using the approximation

\[
R_{rs} = \frac{L_u(z) - K_u z^*}{E_d(0^\circ)} \times 0.554
\]
it can be calculated that for example $L_a \sim 1.5$ at a depth of 0.15m and $E_d \sim 1350$ (in $\mu W \, cm^{-2} \, nm^{-1} \, sr^{-1}$) (both reasonable values in the Benguela system), varying $K_u$ from 0.1 to 2 yields $R_{rs}$ that vary between 0.0041 and 0.0047 (sr$^{-1}$). This means that large errors in the $K_u$ (2000%) result in relatively small errors in the $R_{rs}$ in this example approximately 14%.

An average error estimate of 10% due to the use of $K_u$ should therefore be appropriate.

2.3.2.4 Total RMS Error Calculation

Using the spectral error results from the Trios/Atlantic experiment and the tilt/roll and depth experiment, an average RMS error for the Trios-derived $R_{rs}$ was calculated across the spectrum, using the remaining error estimates as fixed where no spectral information was possible.

![Graph showing average percentage RMS errors across the spectrum for the Trios-derived $R_{rs}$](image)

**Figure 2.6** Average percentage RMS errors across the spectrum for the Trios-derived $R_{rs}$. 
The spectral RMS errors show a steady error of around 10% in the 400 - 650 nm range, rising steeply to a maximum of just under 80% in the red. As can be seen in the Trios/MERIS matches (in the Appendix), the small $R_4$ values in the red mean the associated absolute errors are small even though the percentages are large.

2.3.3 Trios/MERIS RR Validation

Out of the 245 days of BOB data acquired between January 2005 and December 2006 (the mooring was removed for the winter months each year), only 12% (or 30 days) had a successful matchup with MERIS Reduced Resolution images. The low matchup rate can be attributed to the following 4 factors:

i. No MERIS overpass
ii. Contamination by cloud
iii. High glint in the study area
iv. Technical problems with the radiometers resulting in incomplete sets of measurements

As efforts were concentrated over the fieldwork periods of March/April each year, 15 of these days have additional geophysical data available – for validation purposes the important ones being measurements of Chl a and other intracellular pigments via HPLC and fluorometry.

![Figure 2.7 MERIS/Trios/Satantic matches 2005-2006](image)
2.3.3.1 Methods for MERIS data

The rejection criteria for validation matchups, as detailed in section 2.2.2.2 are:

1. 2 or more pixels with more than half negative values for all (visible) $R_{rs}$
2. Any pixel with $R_{rs}$ at 410nm $<-0.1$
3. Any pixel with $R_{rs}$ at 410nm $>0.015$ i.e. possible cloud

The challenge is to filter the satellite data appropriately: without wanting to select only good matches and hence introducing a positive bias, it is necessary to reject some obvious outliers (Figs 2.8 a and b), so as to prevent a negative bias. While every effort has been made to conduct the filtering in a systematic manner and reject only those pixel reflectances well outside of any realistic $R_{rs}$ value, it is acknowledged that there is an element of subjectivity present in the statistical part of this exercise. Some examples of rejected matchups are shown below. In the case of Fig. 2.8 a, 4 pixels have all negative values. In Fig. 2.8 (b) only the 710 nm band has positive $R_{rs}$ values for any of the pixels. (Note that the appearance of only 4 pixels on the chart means that two have identical $R_{rs}$ values).
Figures 2.8 (a, b) Examples of rejected MERIS 5 pixel selections
Following this method of filtering, each matchup instance had 5 “acceptable” pixels and could therefore be averaged in the same way throughout the dataset in order to keep the processing consistent. The total was reduced to 34 “acceptable” matchups according to these criteria. Each matchup instance is available graphically for inspection in the Appendix.

As for the Trios/Satlantic comparison exercise, a Bootstrapping technique (Fisher, 1921) was used to overcome the need to make assumptions about the probability distribution of the Trios and MERIS data points. The data were resampled 1000 times and resulting correlation coefficients were considered.

The data were then plotted as scatter plots (Figs 2.11 a-i) for each relevant wavelength and the bias (signed average relative percent difference, indicated by $\Psi$) and uncertainty (unsigned average relative percent difference, indicated by $|\Psi|$) were calculated for each wavelength’s matchups.

2.3.3.2 Sample matchups

As detailed in Fawcett et al. (2007), the 2005 bloom (Figs 2.9 a-d) consisted of a narrow inshore band of high phytoplankton biomass dominated by the dinoflagellate *Prorocentrum triestinum*, with small components of the toxic species *Dinophysis acuminata*, *D. fortii* and *Protoceratium reticulatum*.

In 2006 (Figures 2.10 a-d) the water column water was cooler and more mixed, and a spatially extensive diatom bloom was co-dominated by *Pseudo-nitzschia spp* and *Chaetoceros spp* (Fawcett et al., 2007).

The MERIS spectra show the mean of 5 “acceptable” pixels and the associated errorbars show the standard deviation of the mean at each relevant wavelength. The Trios data are processed using the default method (as detailed in section 2.2.2.2), and the errorbars show the uncertainty associated with the Trios-derived $R_{rs}$ at each wavelength, as determined in section 2.3.2.1. The first two Chl $a$ values in the title of each image are those retrieved from the MERIS Algal 1 and Algal 2 algorithms respectively. The third is the Chl $a$ value retrieved by the regional algorithm (Bernard, 2005) performed on the Trios data, and is marked with an asterisk. All are in mg m$^{-3}$. 
Figures 2.9 (a,b) Trios/MERIS $R_\text{f}$ matchups from 30/03/2005 and 02/04/2005. The Chl $a$ values shown in the titles are from Algal 1, Algal 2 and the regional algorithm (marked with a *). All Chl $a$ values are in mg m$^{-3}$. 
Figures 2.9 (c,d) Trios/MERIS R<sub>s</sub> matchups from 03/04/2005 and 05/04/2005. The Chl a values shown in the titles are from Algal 1, Algal 2 and the regional algorithm (marked with a *). All Chl a values are in mg m<sup>-2</sup>.
Figures 2.10 (a,b) Trios/MERIS $R_\alpha$ matchups from 12/03/2006 and 15/03/2006. The Chl $a$ values shown in the titles are from Algal 1, Algal 2 and the regional algorithm (marked with a *). All Chl $a$ values are in mg m$^{-3}$. 
Figures 2.10 (c-d) Trios/MERIS $R_n$ matchups from 19/03/2006 and 21/03/2006. The Chl \(a\) values shown in the titles are from Algal 1, Algal 2 and the regional algorithm (marked with a *). All Chl \(a\) values are in mg m\(^{-3}\).
Matchups from the 2005 bloom (Figures 2.9 a-d) show good agreement in terms of spectral shape, while there appears to be a tendency by MERIS to overestimate generally throughout the spectrum. The matchup from 03/04/2005 (Figure 2.9 c) shows massive underestimation in the blue, probably indicative of the presence of absorbing aerosols, which can perturb the atmospheric correction process (Hooker et al., 2007).

The 2006 matchups (Figures 2.10 a-d) show a more significant overestimation in the blue rather than elsewhere in the spectrum, probably also indicative of a problem with the aerosol model selection during the atmospheric correction process.

It can be seen from Figures 2.9 (b) and 2.10 (d) that the matchup can occasionally be very good. Further investigations should shed some light on whether good matchup results are biomass-related or not.

| Table 2.4 Biomass conditions for the Trios/MERIS matches from the 2005/6 blooms. All Chl \(a\) values in mgm\(^{-3}\), using the fluorometric method. |
|-----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| MERIS Algal 1   | 30            | 10            | 30            | 30            | 25            | 5             | 2             | 9             |
| MERIS Algal 2   | 27            | 6             | 32            | 29            | 19            | 10            | 9             | 14            |
| Regional Algorithm | 128         | 33            | 44            | 65            | 42            | 20            | 22            | 8             |
| Measured chl \(a\) [0m] | 148         | 6             | 20            | 35            | 57            | 8             | 11            | 9             |
| Measured chl \(a\) [5m] | 31           | 35            | 43            | 47            | 34            | 28            | 15            | 11            |

The validation of in-water constituent products is not an aim of this study, however the relevant measurements and products are presented in Table 2.4 for interest. Neither Algal 1 or 2 appears to perform consistently well in this region, with the regional algorithm (Bernard, 2005) showing the closest agreement with the measured Chl \(a\) (fluorometric method, Parsons 1984). The data are typified by very high biomass conditions.
2.3.3.3 Statistical Results and Comments

The median correlation coefficients are generally much lower for the smaller wavelengths, with a maximum of 79% variability explainable at 710 nm, and 71% at 560 nm. This confirms the critical importance of these two bands in the remote sensing of high biomass waters.

Table 2.5 Median Correlation Coefficients resulting from Bootstrapping Technique (n=1000)

<table>
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<th>Wavelength</th>
<th>Coefficient</th>
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<td>410 nm</td>
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<tr>
<td>440 nm</td>
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<tr>
<td>490 nm</td>
<td>0.42</td>
</tr>
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<td>510 nm</td>
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<td>560 nm</td>
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<tr>
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<td>680 nm</td>
<td>0.56</td>
</tr>
<tr>
<td>710 nm</td>
<td>0.79</td>
</tr>
</tbody>
</table>

Figs 2.11 a-i show the scatter plots for Trios vs MERIS $R_s$ for all 34 matchups. Ψ indicates the bias (calculated by a signed average relative percentage difference) and the uncertainty (unsigned average relative percent difference) is indicated by $|Ψ|$. The vertical errorbars show the standard deviation of the $R_s$ for the MERIS pixels at the relevant wavelength (the point plotted is the mean). The horizontal errorbars are the total estimated spectrally-dependent RMS errors for the Trios-derived $R_s$ (the calculation is described in section 2.3.2.4).

The bias is positive at all wavelengths, indicating a consistent overestimation, on average, by MERIS. The resulting uncertainties on the matchups are typically very large, but a reasonable uncertainty of 28% at 560 nm is achieved. The best performing matchups are at 560 and 620 nm, and the worst at either end of the visible spectrum. The dependence on wavelength of these results correlate fairly well with those of Park et al. (2006) and Zibordi et al. (2006b), with higher correlation coefficients at 560 nm and in the red, and lower correlations in the blue. Interestingly, correlation coefficients at the appropriate wavelengths are all
smaller for the Southern Benguela except in the blue, where Park *et al.* (2006) have an $R^2$ of 0.04 at 412 nm and the local result is 0.1 at 410 nm. (However Zibordi *et al.* (2006b) report a correlation of 0.63, which is larger even than theirs at 443 nm).

Comparing the sizes of the uncertainties and the biases with those of Zibordi *et al.* (2006b), the local results are much larger in magnitude across the spectrum. As reported in Zibordi *et al.* (2006b), the bias is positive in all cases. However their magnitudes range from a maximum of 73% at 412 nm to a minimum of 9% at 665 nm whereas local biases range from a maximum of 83% at 410 nm to a minimum of 16% at 560 nm.

These results show that the MERIS response is good even in the presence of high levels of uncertainty. The 709/710 nm band is shown to be critically important in these high biomass conditions. It is promising to note that the causal relationship holds well in the MERIS data; that is, even where the bias is large, the response remains sensitive. These results highlight the potential utility of this band in high biomass studies.
Figures 2.11 (a,b) Scatter plots of Trios vs MERIS $R_{rs}$ at 410 and 440 nm. Vertical errorbars indicate the standard deviation of the 5 MERIS pixels from which a mean was taken, horizontal errorbars indicate the total calculated uncertainty associated with the Trios $R_{rs}$. 

$\Psi = 94\%$

$|\psi| = 148\%$

$\Psi = 89\%$

$|\psi| = 134\%$
Figures 2.11 (c,d) Scatter plots of Trios vs MERIS $R_{rs}$ at 490 and 510 nm. Vertical errorbars indicate the standard deviation of the 5 MERIS pixels from which a mean was taken, horizontal errorbars indicate the total calculated uncertainty associated with the Trios $R_{rs}$. 

$\Psi = 68\%$  
$|\psi| = 94\%$  

$\Psi = 60\%$  
$|\psi| = 80\%$
Figures 2.11 (e,f) Scatter plots of Trios vs MERIS $R_{rs}$ at 560 and 620 nm. Vertical errorbars indicate the standard deviation of the 5 MERIS pixels from which a mean was taken, horizontal errorbars indicate the total calculated uncertainty associated with the Trios $R_{rs}$. 

$\Psi = 28\%$ 
$|\psi| = 34\%$

$\Psi = 34\%$ 
$|\psi| = 54\%$
Figures 2.11 (g,h) Scatter plots of Trios vs MERIS $R_{rs}$ at 665 and 680 nm. Vertical errorbars indicate the standard deviation of the 5 MERIS pixels from which a mean was taken, horizontal errorbars indicate the total calculated uncertainty associated with the Trios $R_{rs}$. 

$\Psi = 48\%$

$|\Psi| = 65\%$

$\Psi = 49\%$

$|\Psi| = 59\%$
Figure 2.11 (i) Scatter plots of Trios vs MERIS $R_{rs}$ at 710 nm. Vertical errorbars indicate the standard deviation of the 5 MERIS pixels from which a mean was taken, horizontal errorbars indicate the total calculated uncertainty associated with the Trios $R_{rs}$.
Table 2.6 shows the retrieved Algal 1 and Algal 2 Chlorophyll $a$ products, as well as those retrieved by the locally developed reflectance algorithm (Bernard, 2005) performed on the Trios data for each match up instance. Algal 1 is calculated using the Black Pixel Assumption and an arrangement of 3 band-ratios. Algal 2 uses an inverse modelling technique parameterised by a multiple non-linear regression (neural network) technique. (Full details can be found in Morel & Antoine (2000) and Doerffer & Schiller (1997) respectively). Algal 1 is designed for Chl $a$ retrieval in the range 0.01 to 30 mg/m$^3$. Algal 2 is expected to perform in the range 0.003 – 50 mg/m$^3$.

Each figure (for Algal 1 and 2) represents the average of the 5 pixels used to determine the $R_{rs}$. From the results of the previous examination of selected MERIS imagery (section 2.3.3.2) it is known that neither of these products is completely reliable in the study area, and also that they can be expected not to perform well in very high biomass conditions for which they were not developed or tested. As noted previously, most of these chlorophyll products will be flagged due to anomalous scattering. There is some discrepancy between the retrieved products, both between the MERIS products and in comparison to those retrieved by the reflectance algorithm.

The bold figures in this table indicate when an Algal 1 or 2 product agrees with the local derived product to within 20%. While no firm conclusions can be drawn, it appears that in low biomass conditions (less than 10 mg/m$^3$) Algal 1 outperforms Algal 2 using the local algorithm as a benchmark. Measured chlorophylls (fluorometric: Parsons, 1984) are shown where available from the surface and 5m. The best agreement with the measured values is with those of the local algorithm, so the categorisation of high, medium and low biomass was performed according to that.
Table 2.6 Comparison of Chlorophyll $a$ products MERIS Algal 1, Algal 2, Chl $a$ retrieved from local algorithm and measured Chl $a$ at 0 and 5m (fluorometric, where available).

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<th>Algorithm (mg/m$^3$)</th>
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2.3.3.4 Relative Errors for each wavelength according to Chl a content

The percentage relative errors for each MERIS wavelength were calculated and arranged according to biomass, retrieved by the regional algorithm (Bernard, 2005).

The results (in Figures 2.12 a-i) show large errors (more than 50% of the data have errors of more than 50%) at 410, 440, 490 and 710 nm. In the blue region (at 410, 440 and 490 nm) the errors appear to be largest in high biomass conditions, while at 710 nm the inverse appears true and the largest errors are seen in the lower Chl a concentrations. This feature can be interpreted, again, as indicative of the importance of the 709/710 nm band in high biomass conditions.

Generally the errors are smallest at 560 nm, and this wavelength also has the lowest variability in the errors.

Intermediate Chl a values seem to yield the best results, but apart from the large errors associated with the sample at 118 mg/m³, there does not appear to be a clear correlation between the magnitude of the errors and the Chl a concentration. At 710 nm however, the errors are larger at lower concentrations.

From these results that there is no clear correlation between the Chl a concentration and the performance of MERIS, it can be concluded that the failure of the atmospheric correction is unlikely to be due to the failure of the black pixel assumption and is more likely to be an aerosol problem (see section 3 for further discussion).
Figures 2.12 (a,b) Percentage relative errors for Trios vs. MERIS $R_s$ arranged according to Chl $a$ concentration for 410 and 440 nm.
Figures 2.12 (c,d) Percentage relative errors for Trios vs MERIS Rrs, arranged according to Chl a concentration for 480 and 510 nm.
Figures 2.12 (e,f) Percentage relative errors for Trios vs MERIS $R_\alpha$, arranged according to Chl $a$ concentration for 560 and 620 nm.
Figures 2.12 (g.h) Percentage relative errors for Trios vs MERIS $R_s$ arranged according to Chl $a$ concentration for 665 and 680 nm.
It is evident from this investigation that aside from a problem with the atmospheric correction in a number of cases, the MERIS retrieved $R_s$ can be useful in the monitoring of high biomass blooms when used in conjunction with local in situ radiometric data. Although the data are routinely flagged by the MERIS processing, this should not mean they are completely unreliable, as has been shown here. The similarity in spectral shapes is very encouraging, and the potential for better results with the use of a locally appropriate atmospheric correction is promising.
3. Discussion

The radiometric results shown are encouraging but do seem to indicate persistent problems with the atmospheric correction, although no clear relationship between a failure of the atmospheric correction and the in-water constituents was observed. The proximity of the mooring to the coast almost certainly results in adjacency contamination (light reflected off land into the path radiance above the desired pixels). But the presence of inland semi-desert (and thus the possibility of dust which can contain absorbing aerosols) could also indicate a more serious problem with aerosol type determination, and hence the selection of an appropriate aerosol model during the atmospheric correction procedure. In order to start the process of investigating a possible solution to this problem a full understanding of the techniques used to perform atmospheric corrections was sought, and the possibility of generating a new solution to this problem was researched.

3.1 Atmospheric Correction Techniques

One of the largest potential sources of error in regarding the ocean surface from space is that light from the ocean must travel through another medium - the atmosphere - before it is received by the satellite. The atmosphere is opaque to electromagnetic radiation at many wavelengths, and there are only certain wavelength windows through which radiation may be fully or partially transmitted (Robinson, 2004). The composition of the atmosphere (made up largely of gas molecules, water droplets and suspended aerosol particles) has a profound influence on its transmission properties.

Even in ideal viewing conditions (clear atmosphere, small solar zenith angle and good viewing angle), the water-leaving radiance represents only about 10% of the total TOA radiance (Antoine & Morel, 2005).

Sensors using the visible and IR parts of the spectrum cannot view the ocean through cloud at all. When handling data from such sensors the first step after sensor calibration is to detect which pixels are obscured by cloud and which are clear. There are various levels of complexity in performing this operation, from
simply flagging contaminated pixels, to indicating which of several different cloud detection tests has been positive (Robinson, 2004). The atmospheric correction techniques discussed below all assume a clear atmosphere i.e. pixels containing clouds have been successfully flagged and will not be dealt with.

Top-of-atmosphere (TOA) radiances measured by the satellite contain both the water-leaving radiance (which is the target signal) and the atmospheric interference on this signal. The processes of atmospheric interference are both additive and subtractive (Robinson, 2004): some of the water-leaving signal is scattered or absorbed so that it does not get to the sensor. At the same time atmospheric emission or scattering into the path radiance may introduce additional components to the detected signal.

There are various approaches to compensating or correcting for these atmospheric effects. For the most accurate results, an atmospheric correction on a pixel-by-pixel basis should be applied before any geometric correction that might involve resampling of pixels, smoothing or averaging of values.

3.1.1 Physical Models

As detailed in Robinson (2004), radiance arriving at the sensor \( L_s \) is made up of the atmospheric path radiance \( L_p \) plus the proportion of water-leaving radiance not scattered out if the field of view \( TL_w \) plus the proportion of surface radiance scattered into the field of view \( TL_r \) i.e.

\[
L_s = L_p + TL_w + TL_r
\]

\( T \), the proportion of \( L_w \) and \( L_r \) reaching the sensor, can be expressed as a function of the attenuation coefficient, \( K \) and the optical thickness \( \tau \) (dimensionless). \( \tau \) represents the amount of attenuation caused by absorption and scattering between the surface and height \( z \). \( K \) and \( \tau \) are due to the collision of photons with air molecules and with aerosols. The latter are small solid or liquid particles, which may have been lifted by wind from the Earth’s surface, or may be sublimated and condensed gases from the atmosphere (all in Robinson, 2004, p 60).
Under the assumption of the separability of radiances, contributions made by different components in the atmosphere can be identified. Since the molecular composition of the atmosphere is generally uniform and well known (Robinson 2004) it is convenient to treat molecular effects separately from aerosol effects, which are much more variable in space and time.

The optical thickness of molecular effects alone is due largely to scattering by air molecules and depends little on absorption except by ozone, which absorbs light around 600 nm (Hansen & Travis 1974). Since molecular scatterers are small with respect to the wavelengths of visible light, Rayleigh scattering theory applies, and the Rayleigh optical thickness can be calculated from the wavelength in question and the respective atmospheric pressures of the sea surface and the satellite:

\[
\tau_{\text{Rayleigh}} = \left( \frac{p}{p_0} \right) \left( \frac{0.008569}{\lambda^4} \right) \left( 1 - \frac{0.0113}{\lambda^2} - \frac{0.00013}{\lambda^4} \right) 
\]

(3.2)

where \( p \) is the atmospheric pressure at the point of measurement, \( p_0 \) is the atmospheric pressure at sea level in Pa and \( \lambda \) is the wavelength in micro meters (\( \mu \)m) (from Hansen & Travis, 1974).

Ozone optical thickness is then calculated from a database of known observations (e.g. McClatchey et al. 1972, Sturm 1981) (in Robinson 2004). Unless relatively current data are available, this is potentially a significant source of error. The 2005/6 MERIS processing used a TOMS climatological estimate for ozone concentration (Antoine & Morel, 2000).

The aerosol optical thickness (AOT or \( \tau_{\text{aer}} \)) is more difficult to calculate. In this case Mie scattering applies, as the particles are much larger than the molecular sizes. Aerosols are highly variable in time and space (Smirnov et al., 2002). AOT is wavelength dependent and this dependence can usually be approximated with the use of the Angström exponent as a first order parameter indicative of the general size distribution and the relative dominance of fine vs. coarse particles (ibid.). AOT typically increases with decreasing wavelength. The difficulty in
determining the aerosol concentration and type remotely means that an atmospheric correction approach from a physical model alone is impractical.

Model packages such as MODTRAN (Berk et al., 1999), and 6S (Simulation of the Satellite Signal in the Solar Spectrum: Vermote et al., 1997b) evaluate atmospheric transmission at the required fine spectral resolution across the visible, short wave and thermal IR parts of the spectrum but they still depend on detailed information about aerosols if they are to specify precisely the atmospheric contribution to the satellite measured radiances.

Whichever approach is used, the problem of determining the aerosol type and concentration remains a primary concern. This information is most reliably (Smirnov et al., 2002) derived from simultaneous ground-based AOT measurements coupled with the use of a radiative transfer model to account for Rayleigh scattering and ozone and other gas absorption. It can also be derived from spectral information from the colour sensor itself and approximated with the use of the Angström exponent to calculate the effects on other wavelengths through the selection of one of number of possible atmospheric models with varying humidity and aerosol type (ibid.). The first approach has problems of practicality, and the second makes critical assumptions, which may not hold true for the relevant regional environmental conditions.

3.1.1.1 Ground Based Aerosol Measurements

Remote sensing from ground-based sun/sky radiometers measures both the spectral attenuation of sunlight and the spectral-angular properties of scattered light - sky brightness. These measurements provide the most accurate and comprehensive long-term measurements of the optical properties of the ambient aerosol (Holben et al. 2001, Dubovik et al. 2001, in Smirnov et al., 2002) in the entire atmospheric column, in specific instrumented locations.

The total optical depth (dimensionless) between the top of the atmosphere and the instruments is calculated using Beer's law:
\[
\tau_{\text{total}}(\lambda, t) = - \frac{1}{m} \log \left( \frac{I_{\text{meas}}(\lambda, t)}{I_0(\lambda)} \right)
\]

(3.3)

where \( m \) is the air mass between the sun and the instrument (dimensionless), \( I_{\text{meas}}(\lambda, t) \) is the measured direct normal irradiance (\( \mu W \ cm^{-2} \ nm^{-1} \)) at time \( t \); and it varies with wavelength \( \lambda \). \( I_0(\lambda) \) (\( \mu W \ cm^{-2} \ nm^{-1} \)) is the sun’s irradiance at the top of the atmosphere. In this equation both \( I_{\text{meas}} \) and \( I_0 \) need to have been corrected for the eccentricity of the earth’s orbit (Flynn et al., 2002).

Once \( \tau_{\text{total}} \) is found, the AOT is calculated by subtracting the following from \( \tau_{\text{total}} \): (a) the optical thickness associated with Rayleigh scattering, \( \tau_{\text{Rayleigh}} \) (Hansen & Travis, 1974), and (b) the optical thickness of ozone and NO\(_2\) absorption, \( \tau_{\text{ozone} + \tau_{\text{NO2}}} \). The optical thickness of NO\(_2\) absorption is often very small in the visible wavelengths (e.g., less than 0.001 nm at 500 nm, see Schmid & Wehrli 1995 in Flynn et al., 2002), and it is often neglected in optical thickness calculations. So the AOT is given as:

\[
\tau_{\text{aer}} = \tau_{\text{total}} - \tau_{\text{ozone}} - \tau_{\text{Rayleigh}}
\]

(3.4)

While calculation of the \( \tau_{\text{aer}} \) using the above equation is simple in principle, in practice it is fraught with difficulty because of inaccuracies in the measurements. Small calibration and/or measurement errors, of the order of a few percent, will cause errors of similar magnitude in total optical thickness but much larger relative errors in \( \tau_{\text{aer}} \). Specifically, an error of 1% in the measurements translates into an error of about 0.01 in total optical thickness at 415 nm (with \( m \approx 1 \)).

Under conditions of low aerosol loadings, a typical total optical thickness at 415 nm is 0.35 (at sea level) (Flynn et al., 2002), and a calibration error of 1% corresponds to a percentage error in total optical thickness of about 2%. This may seem small but when aerosol loadings are low, an error magnification occurs because \( \tau_{\text{aer}} \) is obtained from subtracting two relatively large numbers from one another, \( \tau_{\text{total}} \) and \( \tau_{\text{Rayleigh}} + \tau_{\text{ozone}} \), leaving a small remainder. For example, at sea level, \( \tau_{\text{Rayleigh}} + \tau_{\text{ozone}} \) is about 0.31 nm at 415 nm, and if the total
optical thickness is 0.35, $\tau_{aer}$ is about 0.04. A calibration error of 1%, which induces a 2% error in $\tau_{total}$, translates into a relative error of 25% in AOT (Flynn et al., 2002). Therefore when determining $\tau_{aer}$, the need for accurate measurements is critical.

There are various reasons why field data of this nature are difficult to collect. Data collection is expensive, takes time and is labour intensive. Instrumental and methodological difficulties (such as balancing on a small vessel) add to these concerns.

The first systematic experiments at sea were conducted in the early 1980s, and since then significant progress has been made (Smirnov et al., 2002). Unfortunately, many experiments that have taken place have been opportunistic and hence neither systematic nor extensive, employing only a few wavelengths and the accuracy of measurements is sometimes unknown (Smirnov et al., 2002). A large number of these efforts, whether systematic or not, have been consolidated in the AERONET project, which makes this data available to the public (Holben et al., 1998). (The closest AERONET site to Lambert’s Bay is at Swakopmund in Namibia. This was judged to be too far away for the measurements to be of use in this study).

Smirnov et al (2002) have reported comprehensively on ground-based aerosol optical depth data spanning the last 3 decades. They describe aerosol optical depth over the Atlantic Ocean as showing large temporal and spatial variability; in fact that the largest optical variability occurs in the Atlantic Ocean. This is largely attributable to the diverse contributions of a variety of continental aerosol sources (urban/industrial pollutants from Europe and North America, dust and biomass burning from Africa and South America). The enrichment of maritime air by "stationary" and "fresh" sea-spray aerosol components (Gathman, 1983) is an additional source of variability (in Smirnov et al. 2002).

They also note that the spectral behavior of $\tau_{aer}(\lambda)$ is more selective over the Atlantic than over the Pacific (higher Angström parameter values correspond to
generally higher extinction contributions from smaller particles). In the oceanic areas influenced by Saharan dust, high turbidity (high $\tau_{\text{aer}}(\lambda)$) corresponds to small values of Angström parameter $\alpha$, since in that case large particles of non-maritime origin (dust) are dominant (ibid).

A brief investigation into the appropriateness of the use of the Angström exponent, and the contribution of aerosol optical thickness to the total optical thickness was performed for local conditions, and is reported on in section 3.4.

3.1.1.2 Space Based Aerosol Measurements

Space-borne remote sensing of aerosol particles is based on an assumed relationship between the spectral aerosol optical thickness and the spectral path radiance. (Path radiance is the radiance detected by a space-borne sensor above a non-reflective surface and is the result of backscattering to space by particles and molecules in the atmosphere) (Kaufman, 1997). Assumptions about the particle homogeneity, sphericity, composition, and size distribution used in remote sensing models and in estimates of the radiative effects of aerosol are common but not validated (ibid.). The easiest way to extract aerosol information from the path radiance is to examine radiances in the NIR wavelengths on the assumption that there is no water-leaving radiance in this spectral region. However this “black pixel assumption” does not hold in many coastal regions as is discussed in Section 3.2.2. Furthermore, aerosol spectral characteristics are commonly retrieved using the Angström exponent and there is some dispute over the validity of this approximation as not all optical depth spectra are well represented by an Angström fit (Knestrick et al. 1962; King & Byrne 1976; Kaufman 1993; Villevalde et al. 1994; Eck et al. 1999; O’Neill et al. 2001; all in Smirnov et al., 2002). In the case of the 2008 data for the mooring site, it will be shown to a reasonable approximation of the spectral dependence of the AOT (see Figure 3.1).

The problem of determining aerosol type and concentration is an inherent one due simply to the variability of these parameters (Kaufmann et al., 1997). The
risk involved in approximation is less in stable atmospheric conditions. Over the open oceans, far removed from anthropogenic aerosol inputs, the maritime models may be perfectly adequate. It is a complication of coastal remote sensing that these areas are typically subject to both anthropogenic aerosol effects as well as continental sand and dust transport, both in highly variable quantities (ibid.). Without an operational system for the measurement of optical thickness at suitable sites providing continuous data for atmospheric corrections, assumptions have to be made to compensate for the aerosol effects whether the full radiative transfer approach is used or whether a simpler spectral adjustment solution is employed (as seen in Section 3.1.2).

The use of a comprehensive model of atmospheric radiative transfer addressing all known theoretical aspects of the problem, in combination with aerosol optical thickness measurements from the ground, would thus be the most reliable method of performing the correction accurately. But due to such models' theoretical complexity and required computational resources, as well as the practical difficulties in acquiring such in situ data, it is more usual to employ a simpler method whose accuracy is compromised by the necessity of making many assumptions and approximations. In the particular case of low-cost research in the Southern Benguela, the challenge is to develop a satisfactory atmospheric model incorporating the necessary variability but which does not rely on intensive ongoing measurements. The measurements required depend on the approximation techniques employed. Some of these approaches are outlined in the next section.

3.1.2 Atmospheric Correction Approximation Techniques

The simplest approach is not to attempt a separate atmospheric correction at all but rather to calibrate each scene with ground data, incorporating both sensor and atmospheric effects into a calibration valid for that image only. This can be satisfactory for land but is generally not for ocean images for reasons of practicality and accuracy (atmospheric composition varies with space and time and ocean images tend to be of a scale which reduces confidence in such an approach) (Robinson, 2004). This is sometimes called a “known pixel” approach,
and essentially forms the basis of a calibration/validation activity. Significant confidence in the ground measurements is required.

Ocean applications do lend themselves, however, to a multi-spectral atmospheric correction in a way that land applications do not. The “black pixel assumption” method is routinely used in colour sensor data processing. It is assumed that in certain NIR bands it is unlikely that there will be any upwelling radiation from the sea, and so what is recorded by the satellite sensor is exclusively due to atmospheric effects. These values are then fed into a model of the spectral dependence of atmospheric transmission in order to extrapolate atmospheric contributions to other wavebands. This enables a pixel-by-pixel correction rather than one correction for the whole scene. For this approach a suitable transmission model is needed, requiring assumptions or observations to be made concerning the optical properties of the local atmosphere (Robinson, 2004).

A third strategy is to mount an atmospheric sounding sensor on the same satellite as the oceanographic sensor for which the correction is required e.g. a microwave sensor is capable of detecting water vapour in the atmosphere and thus provides a means of correcting an IR radiometer for thermal-IR absorption and emission by water vapour. In the case of ocean colour and aerosol determination, a co-incident optical thickness measurement at multiple wavelengths may reduce uncertainty in the assumptions made in atmospheric model selection (Kaufmann et al., 1997).

The “multi angle approach” is to view the same piece of sea twice, along different paths through the atmosphere (e.g. from nadir and then from an oblique angle). Provided that sea conditions have not changed significantly between observations, the differences between these two measurements can then be related to the magnitude of the atmospheric effects in either of them (Robinson, 2004). This method again relies heavily on a suitable atmospheric model for the region in question.
The "dark pixel approach" assumes that the darkest pixel in the image corresponds to clear water-leaving radiances, which can be estimated. Thus the atmospheric effects for that pixel can be identified and removed from other pixels. Even if allowance is made for viewing geometry, there is no way to address the assumption that aerosol is uniform across the scene (Robinson, 2004). This method is not appropriate for coastal waters where backscattering from suspended particles brightens pixels to the extent that the presence of a clear water pixel cannot usually be assumed. This is the method used for the 2005/6 Case 1 MERIS data (Antoine & Morel, 2005).

The 2005/6 Case 2 MERIS data were processed using a turbid water ("bright pixel") correction by Aiken & Moore (2000). TOA radiances in 3 NIR bands are used as inputs into an iterative process whereby estimated contributions by the ocean and the atmosphere at these wavelengths are fitted with associated Suspended Particulate Matter (SPM) concentrations, scan- and sun-angles, by the means of look-up tables. The SPM may be of terrestrial (sediment) or biogenic (coccolith) origin.

The majority of the 2005/6 data used for the validation exercises in this study are flagged as bright pixels (Case 2 turbid water flag) and will therefore have had the Case 2 atmospheric correction Aiken & Moore (2000) performed on them. Resulting MERIS spectra with over- or underestimations at the blue and red ends will therefore be more likely to stem from an aerosol problem than from the failure of the black pixel assumption (because the Case 2 correction does not require this assumption to be made).

Recently, procedures using a neural network approach have been applied to the atmospheric correction problem with some success e.g. Jamet et al. (2005) and Schröder et al. (2002). (In 2006 the MERIS Bright Pixel Atmospheric Correction was replaced with a neural network scheme that performs the simultaneous retrieval of atmospheric parameters and in-water constituents.)
3.2 The failure of atmospheric corrections over coastal waters

The MERIS remotely sensed reflectances fall largely within the standard deviation of the Trios data. However due to the lack of filtering for tilt/roll and precise depth processing, the standard deviations are admittedly quite large. The most frequent large disagreements between Trios and MERIS $R_{rs}$ occur in the blue region of the spectrum, which likely signals a problem with the atmospheric correction as errors in the atmospheric representation would be most evident in the blue where most of the scattering occurs.

There is a fairly consistent overestimation overall by MERIS, but particularly in the red and often by approximately the same amount over the 620 to 710 nm range. This could be interpreted as an atmospheric under-correction (Zibordi et al., 2002).

3.2.1 Case 1/Case 2 Classification

Morel & Prieur (1977) suggested the use of a simple theoretical classification scheme to distinguish broadly between two fundamentally optically different water types – the open oceans and coastal waters. Case 1 waters were thus defined as where "the chlorophyll concentration is high relative to the scattering coefficient" (p. 715) i.e. where the water itself is very clear. Case 2 illustrates waters that are relatively higher in inorganic particles than in phytoplankton.

Case 1 waters were further described as displaying a decreasing Reflectance ratio $R$ (as a function of $\lambda$) in the ultraviolet region with a defined minimum at 440 nm, corresponding to the maximum absorption of chlorophyll (Morel & Prieur, 1977). The maxima appear between 565 and 570 nm, where pigment absorption is at its smallest and the absorption of water at its highest simultaneously. The spectral reflectance of Case 2 waters, however, is marked by higher $R$ values throughout, no 440 nm minimum, and a convex curve between 400 and 560 nm. The curve is flattened throughout as a result of increased backscattering that is not compensated by an increase in absorption, as in Case 1 (Morel & Prieur, 1977).
Over time these definitions have evolved and changed, and this initial classification has been used more generally to represent the basic optical differences between oceanic and coastal waters. Morel & Prieur acknowledged in their initial paper that the scheme is theoretical – an ideal Case 1 would be a pure culture of phytoplankton, and an ideal Case 2 a suspension of nonliving material with a zero concentration of pigments (p. 715, 1977). Of course water bodies around the globe cannot simply be divided into these two categories, neither of which in fact occurs naturally at all.

The idealised concept of Case 1 water in particular proved very useful for the development of the first generation of bio-optical models. The driving force behind the development of ocean colour satellites was the simple Case 1 idea that phytoplankton can be estimated from optical measurements (Mobley et al., 2004). However, the use of algorithms designed for Case 2 waters frequently fail, partly due to the natural variability in optical properties (an issue unrelated to the classification of those properties), but also due to the now commonplace inaccuracy of holding Morel & Prieur’s Case 2 classification as generally representative of coastal waters (ibid.): a practice not suggested by the authors of that original paper.

The productive waters of the coastal southern Benguela, for example, are of a category that cannot even be described as mid-way between the cases. Very high chlorophyll absorption combines with the high scattering typical of turbid coastal waters, and the scattering may be due to a high density of phytoplankton cells rather than inorganic particles. Consequently spectral reflectances are atypical in terms of the Case 1/Case 2 classification, and it cannot be assumed that either case will describe the dominant optical characteristics adequately. The Case 1/2 classification is often dealt with under a working definition of Case 1 having covarying optical constituents, whereas Case 2 does not. But even this operational classification is not always applicable in very high biomass systems where there is increased scattering by particles. The MERIS processing flags these anomalously scattering pixels as Case 2, and applies the Case 2 product
algorithms to them, which may not necessarily be appropriate. All the MERIS pixels used for the matchups are flagged for invalid algal 1, invalid algal 2, Case 2 turbid water and Case 2 anomalous scattering in recognition of the expected failure of the constituent retrieval algorithms.

Such problems of classification have had a profound influence on the approach to in-water constituent retrieval algorithms as well as atmospheric correction algorithms over coastal waters (Mobley et al., 2004).

3.2.2 The Black Pixel Assumption

In clear, open ocean water, the water is usually optically black in the near infrared (NIR) i.e. it is a perfect absorber and no NIR radiation is emitted (Hooker et al., 2007). One of the simplest, widely used, atmospheric correction techniques is to examine the aerosol radiance levels in the NIR, armed with the knowledge that there is no water-leaving radiance at these wavelengths. From these, using empirical algorithms or simply an Angström exponent calculation, the aerosol optical thickness can be computed and thus an appropriate selection of atmospheric aerosol model can be made (often based on Shettle & Fenn’s of 1979) (Hooker et al., 2007). This assumption of zero water-leaving radiance in the NIR is termed the “Black Pixel Assumption”.

In very productive or turbid waters, however, the black pixel assumption fails because backscattering from particles is not insignificant. There is, or may be, non-zero water-leaving radiance at the NIR wavelengths. Even in cases where the assumption holds, current atmospheric correction techniques tend to overcorrect for aerosols (Siegel et al., 2000, Bailey et al., 2003, McClain et al., 2004 in Hooker et al., 2007).

As the atmosphere scatters mainly in the blue, this is where the largest errors in the atmospheric correction occur. Negative $nL_{ws}$ or $\rho_w$ s are an indication of this, but so are large overestimations in the blue. This can indicate the presence of
absorbing aerosols, a problem which extends much further than coastal waters (Hooker et al., 2007).

The difficulty in performing in situ measurements in the NIR means there is no data confirming the suspicion that the Black Pixel Assumption does not hold true for these conditions. But this is a very likely cause of the failure of the atmospheric correction particularly when errors in the red are also evident. This would explain why the size of the error in the red is within a certain range while an appropriate spectral shape is maintained.

3.2.3 Bi-Directional Reflectance Function (BDRF) and Adjacency Effects

Often, retrieval algorithms are concerned only with the removal of atmospheric attenuation due to molecular, gaseous, and aerosol scattering, and absorption. However, there is an interaction between the surface and the atmosphere, as a result of multiple scattering, that is affected by surface BRDF properties. This could impact the accuracy of surface reflectance retrievals where the surface is not Lambertian (i.e. not flat reflecting). Computations show that errors of approximately 5% in average aerosol loading conditions can be introduced as a result of neglecting BDRF interactions at the ocean surface (Trischenko et al., 2000).

The advantage of using greater spatial resolution data in coastal applications is that where the resolution is higher and so the scene size is smaller, assumptions about the uniformity of atmospheric conditions may be less problematic. However when pixels represent larger areas, nearshore pixels of interest may be adjacent to pixels containing some (or all) land. The multidirectional reflectance off land can thus contaminate the coastal pixels, particularly where the resolution is fairly high and land pixels are therefore very bright. This is where the effect is most obvious but it in fact occurs everywhere. For satellite data with high spatial resolution, multiple scattering makes the pixel adjacency effect important for all pixels, although for data with a pixel size larger than 1 km, this effect is much less significant (Vermote et al., 1997).
Another challenge with respect to atmospheric correction techniques is addressing the contribution to this effect of the vertical distribution of aerosols (Minomura et al., 2001).

3.2.4 Absorbing Aerosols

Absorbing aerosols present a further challenge to the standard atmospheric correction approaches i.e. via the selection of an aerosol model based on one or more waveband relationships. Dust and smoke particles tend to absorb in the blue and the UV with the result that radiances in the red and NIR cannot easily be extrapolated to shorter wavelengths, even with the addition of specific aerosol models (Kaufman et al., 1997). Generally, atmospheric correction algorithms assume that aerosols are located only in the boundary layer, or distributed vertically according to some climatology. For non-absorbing aerosols the influence of vertical structure is negligible, but it cannot be neglected in the presence of absorbing aerosols above 7 – 8 km (Ding & Gordon, 1995 in Kaufman et al., 1997). Unfortunately it is not easy to detect absorbing aerosols so it is uncertain as to whether these influences may be of concern to a specific region. Dust particles are non-spherical and as such their optical properties are not well known (Smirnov et al., 2002). Simple strategies to identify absorbing aerosols from the visible and infrared bands usually available on ocean colour satellites require known water-leaving radiances at 550 nm (e.g. Fukushima & Toratani, in Kaufman et al., 1997), which is often problematic.

In the 2006 examples a more serious overestimation by MERIS is evident in the blue. Also frequently seen in the study area (although not in this particular selection of data) are negative $\rho_w$'s. Large errors in both directions can be indicative of the presence of absorbing aerosols, which interfere with standard atmospheric aerosol models (Hooker et al., 2007).

As mentioned before, the vast majority of MERIS pixels used for the matchups are flagged for invalid algal 1, invalid algal 2, Case 2 turbid water and Case 2 anomalous scattering. A large number are also flagged for uncertain aerosol type.
3.3.2 Validity of Aerosol Models

Atmospheric correction schemes often require a set of candidate aerosol models usually taken from the work of Shettle & Fenn (1979). These models are built from ground-based physicochemical analysis of aerosol samples and therefore must be validated in terms of phase function, optical thickness and single-scattering albedo, including the variables that directly affect path radiances. This can be accomplished with spectral solar transmission and sky radiance measurements (Kaufman et al., 1997). A investigation by Martiny & Santer (2002) into the validity of the standard Shettle & Fenn models over coastal waters found that aerosol spectral dependencies in their study sites in Italy and Spain fell between two of the standard models. An interpolation scheme was thus employed to improve the extrapolation of the optical parameters into the visible for a more accurate atmospheric correction (Martiny & Santer, 2002).

In the case of a region-specific problem such as that under investigation in this paper, appropriate measurements (such as AOT and aerosol type) could lead to such an adjustment scheme or even the development of new seasonal regional atmospheric aerosol models, which could be used with confidence.

3.3 New methods to address the Aerosol Issue

The IOCCG Report on Remote Sensing of Ocean Colour in Coastal and Other Optically Complex Waters (ed. Sathyendranath, 2000) acknowledges that algorithms used for water leaving reflectance retrievals in Case 1 waters break down in Case 2 situations where the optics are more complicated. The report calls for a “completely new family of algorithms for dealing with both atmospheric correction and with retrieval of oceanic constituents” (p. 24). The report envisages the development of successful Case 2 algorithms involving a movement away from a focus on two or three waveband ratios to multi-waveband algorithms “designed for retrieval of multiple variables” (p. 24). In the days of simple instruments like the CZCS this was not possible, but with the advent of a new generation of hyperspectral sensors, the opportunity for the development of such algorithms has presented itself.
High concentrations of scattering constituents may cause the water-leaving signal in the NIR (more than 700nm) to be significantly greater than zero, that is turbid waters are not "black" in the NIR as is generally assumed for AC procedures. This non-zero water-leaving signal results in the overestimation of aerosol optical thickness (typically derived from the signal in the NIR), and therefore, an "atmospheric over-correction" in the visible parts of the spectrum (p. 56). Some more recent correction algorithms for Case 2 waters therefore account for the non-zero water-leaving signal in the NIR by applying a coupled approach to the separation of atmospheric and aquatic contributions to the signal.

It has been shown that the performance of standard Case 1 atmospheric correction algorithms can be improved if the procedures are modified to account for non-zero $\rho_w$ in the NIR (Hu et al., 2000, Ruddick et al., 2000). Other approaches have included iterative techniques (Arnone et al. 1998, Land 1999, Lavender & Groom 1999) and an integrated approach (Krawczyk et al., 1993, Kopelevich et al. 1998). The IOCCG calls for more extensive research into reliable AC procedures.

Standard Case 1 algorithms also fail in the presence of strongly absorbing aerosols e.g. wind blown mineral dust and anthropogenic aerosol. The presence of such aerosol can only be inferred from the visible, where multiple scattering is high. It is quite likely that this is the case in the Benguela with adjacent semi-desert. In such a situation the two-step process of atmospheric correction followed by a bio-optical algorithm to estimate water properties is no longer feasible. Instead a single step process is required that retrieves atmospheric and water properties simultaneously. Chomko & Gordon (1998) have proposed a spectral optimisation algorithm to deal with this problem, while Gordon et al. (1997) used a spectral matching algorithm, in which the optimisation is achieved by a systematic variation of all the unknown quantities in the model. (Note at present these are used with the assumption of NIR $= 0$. This can be relaxed with the added cost of processing time).
Research is also progressing on one-step ocean colour algorithms which retrieve the atmosphere and water properties at the same time, by inverting a complete model of the end-to-end light flow from the sea to the sensor e.g. Gordon, 1997, Chomko & Gordon, 2001, Chomko et al., 2003 (all in Robinson 2004).

3.3.1 Aerosol Models

The crux of the matter in all of these methods is the application of a suitable method by which to detect aerosols in one or more wavelengths or bands, and the selection of an appropriate aerosol model through which to extrapolate aerosol contributions to other wavelengths.

Wherever atmospheric correction schemes rely on spectral information in order to derive aerosol properties and hence model selection, there is some discussion about the best way to compute aerosol optical properties and thus the about the atmospheric models usually available for selection during the atmospheric correction process.

Shettle & Fenn’s 1979 tropospheric, coastal, maritime and urban aerosol models have been used extensively in the atmospheric correction of ocean colour imagery (Stamnes et al., 2003). They each consist of a multicomponent mixture of dry aerosol particles that will grow when exposed to a humid environment. To compute the optical characteristics associated with the models, assumptions must be made about how the particles grow and mix (internal versus external mixing) when exposed to enhanced humidity (Stamnes et al., 2003). Results from Yan et al. (2002) show that the internal mixing rule adopted by Shettle & Fenn leads to atmospheric corrections that differ significantly from those obtained with the more realistic external-mixing approach. For relative humidities of 90% or more, the differences in retrieved aerosol optical properties and chlorophyll concentrations, incurred by application of the internal-mixing approach, become unacceptably large (Yan et al., 2002). These conclusions, however, are contested by Gordon (2003), yielding an animated debate clearly indicative of the complexity of this modelling approach.

Hsu et al. (2004) propose a method for the retrieval of aerosol properties over bright reflecting pixels. This is designed for use over land where there is high
reflectance in the red and NIR, and low reflectance in the blue and shorter wavelengths. Optical thickness and aerosol type are calculated simultaneously using look-up tables to match the satellite-observed spectral radiances. This method could also be extended to the UV for ocean applications (where there is significant reflectance in the blue).

3.3.2 Determination of Aerosol Characteristics from the UV

Information from the UV wavelengths can be used to flag and improve atmospheric correction algorithms where the black pixel assumption fails (i.e. in productive or turbid water, or in the presence of absorbing aerosols). To address the failure due to absorbing aerosols, a combination of UV and longer NIR (>1um) bands may provide an alternate source of information upon which to base an aerosol model selection (Wang 2007, Hooker et al., 2007).

Herman (2005) has proposed a method of atmospheric correction for satellite remote sensing of coastal oceans using both visible and UV wavelengths. He explains that current atmospheric techniques for MODIS and SeaWIFS fail in the coastal ocean (that is, yield negative water-leaving reflectances) as anthropogenic atmospheric aerosols can absorb strongly in the blue. He proposed the use of the UV and visible bands to improve a correction in the presence of both absorbing and scattering aerosols. He proposed combining data from AURA/OMI (260 – 500 nm) and AQUA/MODIS (412 nm to IR), which view the same scene only 15 minutes apart. The same technique will be applied to SeaWIFS (412 nm to NIR). A UV extension to Hydrolight will be used to develop the radiative transfer corrections needed for retrieval techniques applicable to the visible and UV.

The Total Ozone Mapping Spectrometer (TOMS) (also on board NASA’s AURA spacecraft) has seen the development of a method using the UV to characterise aerosol scattering and absorption properties (Torres et al., 2002). It is based on spectral contrast in the near UV that results from the interaction of Rayleigh scattering, particle scattering and absorption. This interaction produces spectral variations of the backscattered radiances at the top of the atmosphere that can be used to separate aerosol absorption from scattering effects.
The usual method of characterising aerosols using path radiances in the NIR only works effectively over dark ocean surfaces. Even then, the aerosol reflectance is proportional to the product of the single scattering albedo and the aerosol optical thickness (Torres et al., 2002). Therefore at small optical depths there is no way to distinguish non-absorbing aerosols at a given optical depth from absorbing particles and a larger optical depth. The low surface radiance in the near-UV is a unique advantage that allows the retrieval of aerosol information over both land and water surfaces (Vasilkov et al., 2005, Höller et al., 2004). The interaction of aerosol absorption and multiple Rayleigh scattering in the near UV can be used for this retrieval. The length of photons’ paths through an absorbing aerosol layer is increased by multiple Rayleigh scattering so the chance of aerosol absorption is enhanced (Torres et al., 2002). The sensitivity to aerosol height is largest for strongly UV-absorbing aerosols and decreases rapidly with increasing single scattering albedo. Thus knowledge of the location in the atmosphere of the absorbing aerosol layer is required for UV remotely sensed aerosol.

The in-water UV light field has been characterised further by Vasilkov et al. (2005) with the aim of improving UV aerosol sensing. TOMS aerosol and ozone products are derived using the monthly global database of minimum Lambert equivalent surface reflectance derived from the Nimbus7/TOMS measurements. An actual estimate of the ocean reflectance in the UV can improve the retrieval of total column ozone and aerosol from the TOMS and OMI observations. A global model was developed which yields IOP properties and UV irradiances with accuracies approaching those in visible wavelengths (Vasilkov et al., 2005).

Calibration in the UV is exceptionally difficult and is a limiting factor in whether or not such measurements may be routinely performed in the field to a required precision.

Incidentally, the addition of UV wavelengths on an ocean colour sensor could also provide useful information for the detection of HABs such as red tides, because they produce UV absorbing compounds called mycosporine-like amino acids (Laurion et al., 2003, in Hooker et al., 2007).
3.3.3 Potential of SWIR bands for Aerosol Determination

Wang (2007) investigates the possibilities of using the SWIR bands as opposed to the near IR for aerosol property identification. The standard black pixel in the NIR fails in turbid waters but in SWIR wavelengths (>1000 nm) the ocean absorbs significantly more strongly, meaning the black pixel assumption in the SWIR is generally valid for turbid waters.

Including the UV bands on sensors allows (apart from better inorganic and organic constituent retrievals) the detection of absorbing aerosols and deriving their optical properties for use in the AC (Torres et al., 1998). In the UV region the useful radiance with the shortest wavelength for ocean colour remote sensing is at around 340 nm due to extremely strong absorption by ozone for wavelengths less than 340 nm. Wang (2007) derives the UV radiance at 340 nm using various models and NIR waveband ratios and assesses the success of the approaches. There is significantly less reflectance by aerosols in the UV so these UV radiances can be derived quite accurately. There are two main factors affecting the performances of atmospheric correction with various band combinations i.e. the wavelength distance needed to be extrapolated from the NIR (or SWIR) band, and secondly the aerosol reflectance dispersion provided between two NIR or SWIR bands. Thus the aerosol reflectance can usually be more accurately extrapolated for the shorter wavelength distance than for the longer one, meaning the NIR method is slightly better than the SWIR (except of course where the black pixel in NIR fails). On the other hand, larger dispersion of aerosol reflectance between two NIR (or SWIR) bands with various aerosol models for atmospheric correction has a better sensitivity in deriving aerosol optical properties, leading to a better result in the derived water-leaving reflectances.

He concludes that an atmospheric correction using SWIR band combinations 1000, 1240; 1240, 1640; 1240, 2130 can generally produce results similar to NIR 765, 865. In particular, the water-leaving reflectance at 340 can be derived accurately. Aerosol optical thickness at 865 nm can be retrieved to within 5-10% accuracy. In turbid coastal waters these figures improve as the NIR method’s
over-estimation of aerosol optical thickness is addressed by the use of the SWIR (Wang, 2007).

Franz et al. (2006) also explore the possibilities of using MODIS land bands for ocean applications, particularly the SWIR as Wang did above. The additional spectral channels in the SWIR provide an opportunity to explore a variety of new atmospheric correction options that may be of particular value in highly reflective, turbid waters. The standard aerosol correction algorithm (Gordon & Wang, 1994) used by the Ocean Biology Processing Group (OBPG) for global MODIS ocean processing makes use of the NIR bands at 748 and 869 nm to determine aerosol type and concentration. The method requires a priori knowledge of the water-leaving radiance in these longer wavelengths to separate the aerosol and water contributions to the total radiance. The OBPG employs an iteration scheme (Stumpf et al., 2003) to model and predict the water-leaving radiances in the NIR from retrieved water-leaving radiances in the visible, but the modelling approach is based on empirical relationships that may not be valid in all waters. In contrast, water is so strongly absorbing in the SWIR spectral regime that even highly reflective turbid waters appear black. Following work by Wang & Shi (2005), where the SWIR bands at 1240 and 1640 were used to determine aerosol type and concentration, optional aerosol correction methods were developed for MSL12 (the radiative transfer code used for MODIS) to allow the determination of aerosol concentration and/or aerosol type using any combination of NIR and SWIR bands. As with Gordon & Wang (1994), this information can then be extrapolated to the visible wavelengths via aerosol models. It should be noted, however, that the signal-to-noise in the SWIR bands is generally quite low, and this may be a limiting factor in any advantage gained by using the SWIR, especially where the aerosol signal is low (Wang, 2007).

3.3.4 Estimating Aerosol Optical Properties from Sunglint

Glint brightness varies mostly with changes in sea surface roughness and cannot be estimated with the required 1% accuracy to evaluate aerosol attenuation, although the spectral properties of glint are well known (Cox & Munk, 1954 in Kaufman et al., 2002). In order to account for the glint reflection at least one
spectral channel with negligible aerosol absorption is needed. Dust absorption, for example, is near zero in the NIR, and this measurement of path radiance over glint can therefore be used to derive dust absorption in shorter wavelengths. While this method could be useful on a global scale for evaluating aerosol climatology, the fact that the aerosol signal is derived from an image whose radiometric value is limited (due to the glint) is problematic for an ocean colour monitoring application.

3.3.5 The continued problem of Absorbing Aerosols

The methods outlined above, while promising in terms of better aerosol model selection and avoiding the problem of non-zero water-leaving radiance in the NIR, are still unable to account for the presence of strongly absorbing aerosols without empirical ground-based data.

Gordon et al. (1997) present an algorithm that uses the whole available ocean colour satellite spectrum (i.e. from 412 to 865 nm) to retrieve in-water biophysical properties and aerosol optical properties in atmospheres containing both weakly and strongly absorbing aerosols. In their paper the algorithm uses a bio-optical model of Case 1 waters together with the Shettle & Fenn models. The relevant parameters of both the ocean and atmosphere are systematically varied to find the best root-mean-square fit to the measured TOA spectral reflectance (Gordon et al., 1997). Although this work was not extended for use in Case 2 waters, this could possibly be addressed using a more recent bio-optical model that accounts for the demands of large amounts of in-water backscattering.

Nobileau & Antoine (2005) also propose a solution which uses ocean colour data in the visible and near infra-red. Essentially, estimation of an error budget at 510 nm using a maritime model atmosphere enables the identification of blue-absorbing aerosols when the budget demonstrates a significant over-correction of the atmospheric signal when using models of non-absorbing maritime aerosols (Nobileau & Antoine, 2005). It is based on a “reasonable hypothesis” about the water-leaving signal at 510 nm, however, which may not be appropriate for all waters.
3.3.6 Coupled Ocean-Atmosphere Solutions

One way to overcome the difficulties of separating the ocean signal from the atmosphere is to introduce a coupled ocean-atmosphere model for simultaneous retrievals of in-water and aerosol parameters. The disadvantage of such approaches is that they are computationally demanding on resources and time, so their use operationally is limited. However the opportunity does exist to refine such a model with regionally appropriate parameter values in order to expedite the processing.

Much progress has been made in the domain of coupled models in the last decade since the improvements to the commonly used atmospheric radiative transfer codes such as DISORT (Discrete Ordinate Radiative Transfer: Stamnes & Swanson, 1981; Stamnes et al., 1987), and MODTRAN (Berk et al., 1999). Amendments account for non-Lambertian surfaces (i.e. not flat reflecting), improved multiple scattering, Bidirectional Reflectance Distribution Functions (BRDF) and adjacency effects (Matthew et al., 2000).

3.3.6.1 Ocean Atmosphere Radiative Model (OARM) (Gregg 2002)

Developed as an input to ocean biogeochemical models, OARM evaluates irradiance availability and quality in the water column to support phytoplankton growth and drive ocean thermodynamics.

The atmospheric component incorporates spectral and directional effects of clear and cloudy skies as a function of atmospheric optical constituents, and spectral reflectance across the air-sea interface. The atmospheric radiative model is based on the Gregg & Carder (1990) spectral model for clear skies, and relies on Slingo (1989) for spectral cloud transmittance (in Gregg, 2002). This model is extended for OARM from the PAR spectral domain to the entire solar spectrum, from 200 nm to 4 μm, representing more than 99% of the total solar irradiance present at the top of the atmosphere (Gregg, 2002). For computational efficiency, the spectral resolution is degraded from 1 nm used in Gregg & Carder (1990). A modification to the clear sky model is the use of spectral surface reflectance in the presence of sea foam based on observations by Frouin et al., 1996 (in Gregg 2002).
The oceanic component evaluates the propagation of spectral and directional irradiance through the water column as a function of water itself, five phytoplankton groups, and coloured dissolved organic matter. It tracks the direct and diffuse streams from the atmospheric component, and a third stream, upwelling diffuse irradiance (Gregg, 2002).

### 3.3.6.2 Coupled Ocean Atmosphere Radiative Transfer (COART)

Developed by Jin et al. (2006), COART is an online tool to calculate radiances and irradiances at individual wavelengths or spectral bands defined by the user at any level in the air or water. It can also generate water-leaving radiances at the ocean surface.

The model is based on the Coupled DISORT code (Jin & Stamnes, 1994) distributed freely by NASA. CDISORT improves on DISORT (Stamnes & Swanson, 1981; Stamnes et al., 1988) by including the refractive index at the air/water interface into the radiative transfer equation. However DISORT is based on a flat reflecting surface, which is very rarely the case in reality. So in COART wind-blowed surface roughness is included as a function of windspeed. Sun glint as a function of surface roughness is included as well. In this model the ocean is treated as simply another atmospheric layer, but with significantly different optical properties. It treats scattering and absorption in ocean and atmosphere explicitly, so unlike other models where the ocean surface has a given reflectance, COART can simulate the ocean reflectance.

The discrete ordinates method entirely avoids any interpolation at the ocean/atmosphere interface, and the radiation field can efficiently be solved for both the ocean and the atmosphere at once. Vertical heterogeneity can be accounted for with the use of different homogenous layers within each stratus, so that vertical profiles of optical properties may be incorporated or neglected at will (Jin & Stamnes, 1994).

The discrete ordinates model has been tested successfully in terms of energy conservation (Jin & Stamnes, 1994), but comprehensive in situ datasets are required to validate the model and this has been a hindrance (Jin et al., 2006).
3.4 **Aerosol Optical Thickness Investigation**

In order to investigate the prevailing atmospheric conditions in Lambert's Bay for the purposes of identifying problems with the atmospheric correction, sunphotometer measurements have been included in the suite of field data since 2007. Unfortunately no AOT data is available for the validation matchups from 2005/6. However this experiment is relevant to the current study as it reports generally on the contribution of uncertainty in the aerosol determination processes to the characterisation of the atmosphere locally, and hence to the atmospheric correction procedure.

### 3.4.1 Methods

Optical thickness measurements were acquired using a hand-held Microtops sunphotometer (Solar Light Inc., Pennsylvania, USA) during the 2007 and 2008 field campaigns. Persistent fog in 2007 and few MERIS overpasses during the field campaign meant no cloud free satellite validation opportunities, but 2008 was better, and saw 4 successful MERIS matchups as well as two with CHRIS Proba. The MERIS FR data were requested from this time period as well, so a full dataset awaits further analysis.

The Aerosol Optical Thicknesses are calculated automatically by the Microtops software. To investigate whether the use of the Angström exponent to calculate the spectral dependence of AOT is suitable for the study area, a short exercise was undertaken to examine the possible error introduced. The Angström exponent is used in the MERIS atmospheric correction procedures to extrapolate the spectral dependence of aerosol scattering, after an initial estimate of the AOT is deduced from radiance in the 870 nm band, where it is assumed that all radiance is path radiance because there is no water-leaving radiance at these wavelengths. While error may be introduced by the failure of this black pixel assumption, it could be propagated further by an extrapolation method (i.e the use of the Angström exponent) that may not be robust.

To investigate this, the Angström exponent $\alpha$ was calculated as follows from each Aerosol Optical Thickness product:
\[ \alpha = - \frac{\ln(\tau_{\text{aer}}(\lambda_1)/\tau_{\text{aer}}(\lambda_2))}{\ln(\lambda_1/\lambda_2)} \]  

(3.5)

where \( \tau_{\text{aer}} \) is the AOT at adjacent Microtops wavelengths \( \lambda_1 \) and \( \lambda_2 \).

The exponent was calculated for each adjacent pair of AOT products. A mean of these for each acquisition was taken, and compared to the Angström exponent calculated over the interval 440/870 nm. The results will enable a comparison of a mean Angström exponent calculated using all the measured AOTs, with an Angström exponent calculated only from the measured AOTs at the shortest and longest wavelengths.

**Contributions to Total Optical Thickness by atmospheric components**

To discover the relative contributions of the optical thicknesses of ozone, Rayleigh scattering and aerosols to the total optical thickness, they were computed individually as follows, from Equation 3.4:

\[ \tau_{\text{aer}} = \tau_{\text{total}} - \tau_{\text{ozone}} - \tau_{\text{Rayleigh}} \]  

(3.4)

it follows that

\[ \tau_{\text{total}} = \tau_{\text{ozone}} + \tau_{\text{Rayleigh}} + \tau_{\text{aer}} \]  

(3.4b)

Rayleigh scattering is assumed constant throughout the atmosphere, and can be calculated from the atmospheric pressure (Hansen & Travis, 1974):

\[ \tau_{\text{Rayleigh}} = (p / p_0) (0.008569 / \lambda^4) (1 - 0.0113 / \lambda^2 - 0.00013 / \lambda^4) \]  

(3.2)

where \( p \) is the atmospheric pressure at the measurement site (in Pa) and \( p_0 \) is the atmospheric pressure at sea level (in Pa) and \( \lambda \) is the wavelength in micrometers (\( \mu \)m).

The ozone optical thickness can be calculated as follows (King & Byrne, 1976):

\[ \tau_{\text{ozone}} = A \ast C(\lambda) / 1000 \]  

(3.6)
where $A$ is the ozone column abundance in Dobson Units and $C(\lambda)$ is the wavelength-dependent absorption coefficient (in DU$^{-1}$) as described in King & Byrne (1976).

In this case we have no direct way of measuring $A$, so a TOMS climatology average for the West Coast in March 2008 was used (250 DU) (TOMS, NASA, 2008*).

$\tau_{aer}$ was calculated from the Microtops sunphotometer measurements by the Microtops software (Solar Light Inc., Pennsylvania, USA).

* TOMS data is available at http://jwocky.gsfc.nasa.gov/ozone/ozone_v8.html

3.4.2 Results and Comments

![Angstrom Exponent: Averaged Ratios vs 440/870](image)

Figure 3.1 Correlation between mean Angström Exponents of adjacent wavelength ratios and the Angström Exponents of 440/870 ($n = 27$ sets of aerosol measurements, $\rho = 0.92$)

A correlation of 0.85 was observed, indicating that the use of the Angström exponent is a good approximation for the spectral dependence of AOT, although not without the introduction of some error.
The variability of the calculated exponents, from less than 0.5 to 2.5 over a period of 20 days, is of some concern as it could indicate periodic movements of dust or sand over the mooring site, providing further difficulties for a consistently good atmospheric correction.

As discussed in section 3.1.1.1, the largest optical variability occurs in the Atlantic Ocean (Smirnov et al., 2002), and this is mostly due to the diversity of continental aerosol sources (urban/industrial pollutants from Europe and North America, dust and biomass burning from Africa and South America), as well as sea-spray. Higher Angström parameter values generally correspond to smaller particles, and small values of Angström parameter indicate the presence of large particles of non-maritime origin (dust) (Smirnov et al., 2002). Most of the calculated Angström exponents in Fig. 3.1 lie between 0.75 and 1.5, and of the 4 that rise above this, 3 are on consecutive days. It seems reasonable to assume that an Aeolian event of some sort caused the elevated exponent on those days.

From these two examples there does not appear to be much difference in the contributions to AOT of ozone, Rayleigh scattering and aerosols according to variations in atmospheric pressure in the range that was experienced in Lambert’s Bay in March 2008 (1011 to 1024 Pa). What can be clearly seen is the dominant contribution to Total Optical Thickness of the aerosols, particularly in the longer wavelengths where Rayleigh scattering is not as strong. Therefore if an accurate atmospheric correction is to be performed, appropriate modelling of the aerosols and the spectral dependence of the aerosol optical thickness is essential.
Figure 3.2 (a,b) Contributions to Total Optical Thickness by Ozone, Rayleigh scattering and Aerosols under clear skies at (a, above) 1011 and (b, below) 1024 Pa at the mooring site near Lambert's Bay on the West Coast of South Africa.
4. **Conclusions and Recommendations**

This study is the first step in the development of a regional ocean colour satellite validation programme. The value of a statistical radiometric validation as a prerequisite to any further geophysical validation studies has been emphasised. The *in situ* radiometric measurement system has been examined and the magnitude and sources of error have been discussed. Corresponding satellite data have been inspected across a range of in-water and atmospheric conditions and their overall performance has been evaluated. Some important results from this first radiometric validation have been shown:

i. The matchup data show no consistent relationship between high phytoplankton biomass and the accuracy of the atmospheric correction. An improved understanding of the regional atmospheric variability is therefore required before real progress can be made in terms of properly evaluating the performance of the MERIS atmospheric corrections over a range of in-water conditions.

ii. While the in-water constituents do not appear to affect the performance of the atmospheric correction, their influence on the red portion of the spectrum has been demonstrated. As the signal-to-noise ratio increases in the red with increasing biomass, confidence in this spectral region increases too. This could prove to be important in the remote sensing of high biomass waters, and geophysical product retrieval algorithms that exploit this feature in the 709 nm waveband should be developed.

iii. The lack of tilt/roll and accurate depth data has been identified as a major source of error in this investigation. Cumulative errors are largest in the red due to the small signal in this region of the spectrum. However, given the importance of this region to high biomass studies, these errors should be reduced by whatever means possible in order to exploit this spectral region fully. Consistent tilt/roll and depth data would reduce errors here by up to 20%.
The development of a comprehensive regional ocean colour satellite validation strategy is highly recommended for the ongoing use of remote sensing data in this area, and should be undertaken with the following recommendations in mind:

i. There are currently no standardised technical protocols for validation in very high biomass waters. Specific issues to be considered would include those concerning the remotely sensed component (e.g. sub-pixel variability and atmospheric characterisation), as well as the in situ and theoretical components (e.g. the characterisation of \( K_u \) in high biomass conditions). The development of such protocols, particularly for use with low-cost, lightweight systems, is necessary. The relative merits and constraints of above- vs in-water systems should be considered in light of renewed interest in investing in coastal monitoring systems in Southern Africa. It is clear from this preliminary study that constructive engagement with the validation problem is still possible from a coastal ocean remote sensing perspective, despite the large errors generally associated with data in these optically complex systems. The newly formed GEO Coastal and Inland Waters Algorithm Development group provides a good opportunity to develop and formalise these protocols.

ii. Due consideration should be given to the extrapolation of radiometric validation results onto the calculation of the geophysical parameters used in coastal ocean process studies. The results of a statistical radiometric validation, as described in this study, are fundamental to identifying and quantifying downstream errors in the derivation of geophysical parameters. MERIS geophysical products rely inherently on the sensor's radiometric performance, and on the accuracy of every stage in the data processing from level 0. On top of these error budgets, the performance of the retrieval algorithm and the suitability of the retrieval algorithms for regional conditions must be assessed. Identifying the sources and magnitudes of these errors would enable the use of these data for time series analysis, opening up a whole new area of opportunity for coastal scientists in this region.
iii. An in-depth investigation into the satellite data processing is also recommended to identify where efforts should be concentrated in the initial stages of the development of a full validation strategy – including the development of a regional atmospheric model, for example. A detailed assessment of the “anomalous scattering” and the atmospheric flags (frequently raised in these conditions) should be performed as this may reveal useful clues to poorly understood regional ocean-atmosphere optical effects. Efforts in this regard should lead towards the development of a 'regional processing template', which would establish appropriate data processing options for regional users.

iv. Finally it should be stressed that all protocols developed, systems deployed and strategies established should be fully applicable or adaptable to any major ocean colour satellite sensors (e.g. MERIS, MODIS, OCM) and observing networks (e.g. ChloroGIN). Potential collaboration with AERONET OC (Ocean Colour) should be explored as an opportunity to increase monitoring capability and data gathering, both in-water and atmospheric. Collaboration and synergy with these organisations would encourage and ensure strong regional participation in projects of a wider scope, and sound contribution to the scientific knowledge of the global ocean.
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Appendix: Trios/MERIS Validation Matches

Each figure’s title displays the Chl α values retrieved by the MERIS Algal 1, MERIS Algal 2 and the regional algorithm respectively (marked with a *).

The MERIS R<sub>rs</sub> depicted are the mean of 5 pixels. The errorbars associated with the MERIS spectra are the resulting standard deviations.

The Trios R<sub>rs</sub> are those resulting from the default processing scheme (see section 2.2.2.2). The errorbars are the uncertainty in the Trios-derived R<sub>rs</sub> as determined in section.
01/02/2005: Chlorophyll a...30...33...63...

04/02/2005: Chlorophyll a...16...4...12...
30/03/2005: Chlorophyll a, 18, 25, 128

02/04/2005: Chlorophyll a, 11, 5, 33

R^0 (sr^-1) vs. wavelength (nm)
08/04/2005: Chlorophyll a, 15, 26, 59°

09/04/2005: Chlorophyll a, 21, 12, 48°
12/04/2005: Chlorophyll a. 25...14...40°

15/04/2005: Chlorophyll a...24...8...36°

R (sr⁻¹)

wavelength (nm)
18/04/2005: Chlorophyll a...12...18...116°

22/04/2005: Chlorophyll a...26...31...133°
25/04/2005 Chlorophyll a 20...6...17

28/04/2005 Chlorophyll a 25...4...20

Wavelength (nm)
07/05/2005: Chlorophyll a \( \lambda \) 15 \( \lambda \) 41°

\[ R_{15} (sr^{-1}) \]

\[ \text{wavelength (nm)} \]

08/05/2005: Chlorophyll a \( \lambda \) 10 \( \lambda \) 16 \( \lambda \) 52°

\[ R_{10} (sr^{-1}) \]

\[ \text{wavelength (nm)} \]
17/06/2005: Chlorophyll a. 3...24...4*

24/06/2005: Chlorophyll a. 2...10...2*
27/06/2005: Chlorophyll a.2 11 19°

30/06/2005: Chlorophyll a.1 13 9°
01/07/2005: Chlorophyll a...

04/07/2005: Chlorophyll a...

University of Cape Town
07/12/2005: Chlorophyll a...

$R_{IS} \text{ (sr}^{-1})$

wavelength (nm)
18/03/2006: Chlorophyll a: 0.32...10...39°

19/03/2006: Chlorophyll a: 0.2...9...22°
21/03/2006: Chlorophyll a, 9, 14, 8°

22/03/2006: Chlorophyll a, 7, 1, 8°