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IOCCG Report Number 17, 2018

Earth Observations in Support of Global Water Quality Monitoring

Edited by:

Steven Greb, Arnold Dekker and Caren Binding

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Preface

Declining coastal, estuarine and inland water quality has become a global issue of significant concern as anthropogenic activities expand and climate change threatens to cause major alterations to the hydrological cycle (UNEP 2002; Bates et al. 2008; UNESCO 2012). The measurement of water quality variables via radiometric measurements of the water's optical properties has grown rapidly over recent years. Improvements in algorithms and product development, sensor technology and maturity, and data accessibility and provision have led to demonstrated confidence in remotely-sensed data with potential applications to water resources management. Management agencies, however, have been slow to embrace satellite-derived measurements to date even though important parameters such as chlorophyll-*a*, c-phycocyanin, suspended solids, coloured dissolved organic matter (CDOM), light attenuation, Secchi Disk transparency and turbidity have been quantified with required accuracies using remotely sensed data.

An IOCCG working group on "Earth Observations in Support of Global Water Quality Monitoring" was formed in 2014 to support the implementation of a global water quality monitoring service that contributes to the broader implementation of the Global Earth Observation System of Systems (GEOSS) under the auspices of the Group on Earth Observations (GEO). The goal of the working group was to provide a strategic plan that incorporates current and future Earth Observation (EO) information into national and international near-coastal and inland water quality monitoring efforts. This can be accomplished by promoting best practices, coordination of efforts and partnerships, and proposing specific new linkages between data providers and data end users. The members of the working group brought a diverse range of backgrounds and perspectives to this task and included individuals from space agencies, local and national management agencies, as well as the scientific community (see list of contributing authors on front page).

Purpose of This Report

This report provides an overview, as well as background and detailed information needed to support the development of an EO-based global water quality monitoring service. The objectives of this report are to assess current knowledge and gaps regarding coastal and inland water quality and associated use of remote sensing data, and to assess existing space-based and *in situ* observing capabilities. This report also identifies user needs and requirements, new observing capabilities, new and improved data streams and products, mission requirements, supporting research and development activities, and best practices. Finally, this report explicitly discusses user engagement and outreach with the objective to strengthen linkages between data providers and end users.

Who should read this report?

This report is intended to reach a broad audience, particularly targeting 1) water resources management end users; 2) the global aquatic remote sensing science community; and 3) aquatic and ocean colour radiometry (OCR) data providers. The goal of targeting these audiences is to build a community of practice and strengthen linkages between the groups for broader "downstream" end-user utilization of aquatic colour data.

How to read this report

The chapters in this report are grouped into three sections, aimed respectively at the audiences identified above, and ends with recommendations for each of the three groups.

- ❖ **Earth Observations in Support of Water Quality Monitoring and Assessment for Stakeholders**: The first four chapters are written for the end user and provide a background on water quality monitoring frameworks and available tools. These chapters include a discussion of the accuracies, uncertainties and representativeness of the tools and also describe the fundamentals of remote sensing, what can and cannot be measured with remote sensing, the complementary role of remote sensing and *in situ* measurements, and where to find further information and decision support tools.
- ❖ **Remote Sensing Science in Support of Water Quality Monitoring and Assessment**: Chapters 5 and 6 are directed towards the science community and focus on the current understanding of the water and atmospheric satellite signal over inland and coastal waters, current methodologies for deriving optical properties and derived water quality products, and current and future sensor requirements, constraints and applications.
- ❖ **Perspectives for Space Agencies in Support of Water Quality Monitoring and Assessment**: Chapters 7 and 8 are directed towards space agencies with responsibilities associated with space or ground segments. Chapter 8 also explores concepts in data processing and applications, and will be of interest to a wider audience.

The report is also organized from a time-frame perspective: the first four chapters examine the immediate needs (<1 year) of the end-user; chapters 5 and 6 address the research and development questions with a 1–5 year timeframe, and Chapters 7 and 8 have a long-term perspective with recommendations for future programmes.

Chapter 1

Water Quality Monitoring and Assessment: Needs, Benefits and Frameworks

Blake A. Schaeffer, Steven Greb, Caren Binding and Erin A. Urquhart

1.1 Introduction

Chapters 1 to 4 of this report target water quality managers and other stakeholders interested in monitoring and assessing coastal and inland waters with satellite remote sensing. Water quality managers are identified as anyone who is responsible for protecting the designated, or beneficial, uses of water for any purpose. Water quality is defined as the biological, physical, and chemical characteristics required to maintain these uses. Broad categories of designated uses may include drinking water, recreation, irrigation, and food supply. Stakeholders are more broadly defined as any person or entity that may have interest in, interact with, or benefit from, the uses of a waterbody. An end-user of the satellite remote sensing information may include both water quality managers and stakeholders.

It is important to have a robust scientific understanding of environmental processes to inform stakeholders when addressing biological, physical, and chemical water quality dynamics that impact designated uses. Management of water quality generally focuses on watersheds and the connected inland and coastal waters. Here, we focus on surface inland waters in wider rivers, lakes, reservoirs, estuaries and coastal marine waters that can be adequately resolved by current or planned future satellite remote sensing technology (Figure 1.1).

As there are numerous definitions of coastal marine waters that depend on boundaries delineated scientifically, politically, or through other mechanisms, a single definition of coastal waters is not practical (IGOS 2006). This report considers coastal marine waters to cover the interface between land and sea toward the furthest ocean extent necessary, dependent on the stakeholder requirements for specific local, regional, or national interests. Historically, ocean colour satellite sensors focused on the global oceans (McClain 2009) and these same sensors are re-purposed for coastal marine and inland water quality monitoring (Mouw et al. 2015). Therefore, there is no limit as to how far these capabilities can be applied into the ocean beyond any single definition of coastal marine waters.

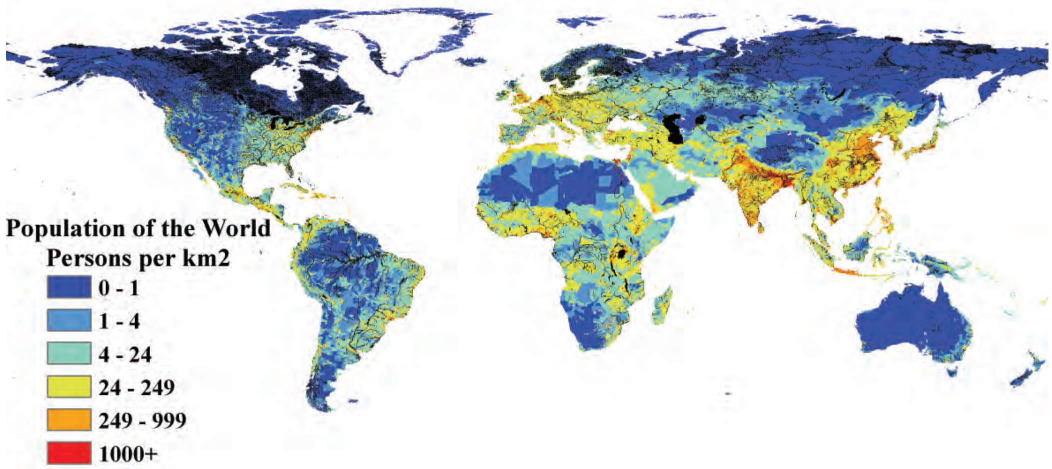

Figure 1.1 Global map of population density projected for 2015 (CIESIN 2005) with world-wide lakes, reservoirs, rivers and permanent open water bodies with a surface area $\geqslant 0.1$ km^2 (black points) from the World Wildlife Foundation.

1.1.1 The need for protecting water designated uses

Managing the demand for finite water resources to support societal uses requires information on the quality of the water so that stakeholders can make sustainable decisions. Population growth, climate change and variability (Vörösmarty et al. 2000), and changing land use practices (Meyer and Turner 1992) all contribute to the stress of national water quality. Water quality can be measured in terms of biological, physical, and chemical indicators such as turbidity, chlorophyll-*a*, harmful algae, pollution-sediment, submerged habitat, temperature, metals, dissolved oxygen, nutrients (primarily phosphorus and nitrogen), and many other contaminants. Here, we focus on core water quality indicators that can be derived directly from satellite remote sensing including turbidity, chlorophyll-*a*, harmful algae, pollution-sediment, submerged habitat, and temperature (Muller-Karger 1992). These six core indicators enable water quality managers and stakeholders to link anthropogenic stressors to water environmental responses that may impact designated uses.

1.2 Benefits of Maintaining Water Designated Uses

The world population was estimated at over seven billion people in 2016 (U.S. Census Bureau 2016). An estimated 30% to 70% of this population live within 100 km of a marine coastline, and 90% live within 10 km of a freshwater body (UNEP 2007; Wilson and Fischetti 2010; Kummu et al. 2011). Sustainable water management practices are critical for ensuring overall environmental stewardship, human health and well-being, and continued economic growth.

1.2.1 Environmental stewardship

Since the last century, water use has exceeded long-term supply and the status of these water resources are inadequately monitored to inform stakeholders of change in quality (Millennium Ecosystem Assessment 2005a; UNESCO 2006). The decline in the quality of water resources is causing extinction of freshwater species and putting many ecosystems at risk, including a loss of biodiversity (Millennium Ecosystem Assessment 2005a). Coastal zones, among the most productive aquatic ecosystems on Earth, are particularly vulnerable and are linked to human and animal life, as well as entire ecosystem health (Barbier et al. 2011; Day et al. 2012; UNEP 2012). In recent decades, increasing pollution from land, along with loss of coastal habitats that filter pollution, has led to extensive "dead zones" — or areas with low amounts of oxygen, where aquatic animals are unable to survive, such as in the Black Sea (Sorokin 2002), Baltic Sea (Conley et al. 2009), and the Gulf of Mexico (Diaz and Rosenberg 2008) (Figure 1.2). Ecosystem function is known to be of major importance to the well-being of humans, and the conservation of biological diversity is one key element in maintaining ecosystems in good condition (Millennium Ecosystem Assessment 2005b).

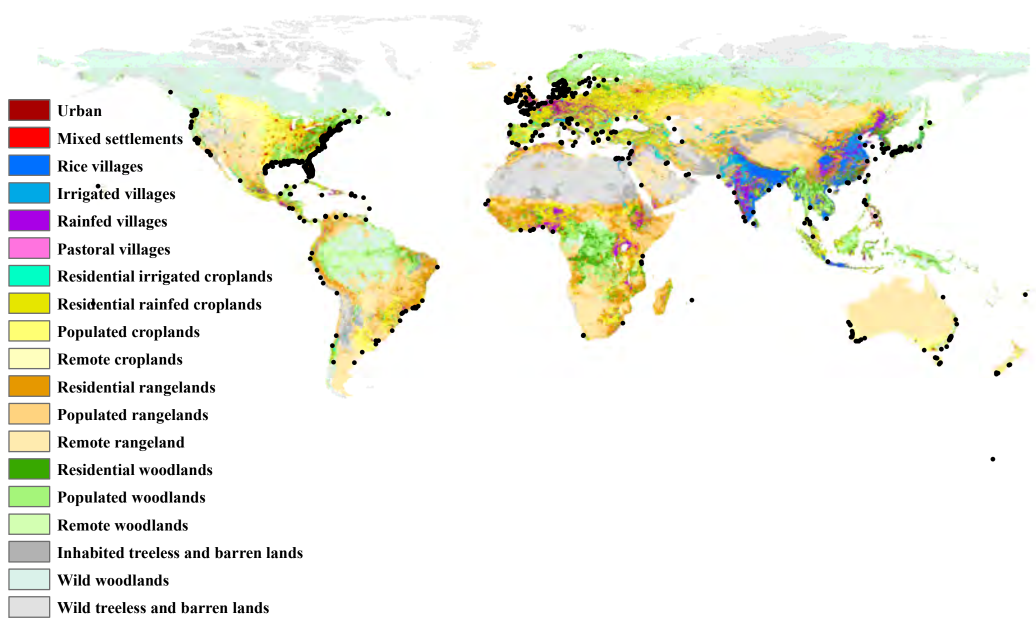

Figure 1.2 Global estimates for anthropogenic biomes (Ellis et al. 2013) with distribution of 476 hypoxic zones (black points), as of 2011, from the World Resources Institute (Diaz et al. 2011).

1.2.2 Human health and well-being

Coastal and inland water recreation benefits human well-being and quality of life due to increased contact with the natural environment (Cox et al. 2006). Furthermore, all socioeconomic levels associated with human health increase with living proximity to the coast (Wheeler et al. 2012). And yet, by far the largest causes of water quality degradation and subsequent decline of aquatic systems originate from anthropogenic activities, impacting both human and ecosystem health. More than 80% of the global health burden is water related, and at any given time, people suffering from water illnesses occupy more than half of the world's hospital beds. The lack of access to clean water and adequate sanitation remains the world's largest health problem, resulting in the death of an estimated 3 million people per year, the majority of which are children under the age of five (DFID et al. 2002; WHO 2006).

1.2.3 Economic growth

Water quality impacts economies through, for example, changes in property valuation and visitor decisions, which in turn impact tax revenues (Dodds et al. 2009). Eutrophication in lakes has historically been identified as a cause for appraisal declines in residential property, especially in proximity to the degraded waterbody (Michael et al. 1996; Gibbs et al. 2002). Additionally, visibility of coastal waters has provided a premium for homes with waterfront views (Major and Lusht 2004). In freshwater systems, total eutrophication-related losses in the U.S. are estimated at $4.6 billion annually (Dodds et al. 2009), in the UK $105–160 million (Millennium Ecosystem Assessment 2005c), in South Africa $250 million (Frost and Sullivan 2010) and Australia A$200 million (Atech Group 2000). Cyanobacterial blooms in Lake Taihu during 1998 resulted in economic losses of $6.5 billion (Le et al. 2010). Global economic losses due to water pollution, eutrophication, and declining water quality are estimated at $6–$16 billion (Millennium Ecosystem Assessment 2005c; OECD 2012). Combined global ecosystem benefit estimates were $18 trillion USD per year for coastal waters and $2.3 trillion USD per year for lakes and rivers (Costanza et al. 2014). Therefore, the value of satellite data to inform decisions for water quality management could be significant based on a value of information calculation (Macauley 2006).

1.3 Frameworks for Monitoring and Protecting Designated Uses

A global overview from the perspective of the United Nations (UN), World Health Organization (WHO), and World Bank are provided to describe the context of water designated uses and their related challenges that cross all continents. Select examples of water quality frameworks are presented to demonstrate the common goals for monitoring and protecting water uses within each continent. These frameworks define needs and requirements, some of which could be addressed with satellite remote sensing of water quality to assist in monitoring and maintaining the designated uses of water.

1.3.1 Global challenges related to water designated uses

The WHO's primary water focus is the prevention of waterborne and water-related diseases under the World Health Assembly resolution 64.24 of May 2011. There are five objectives through 2020: (1) collect information on water quality and health; (2) provide water quality management guidelines; (3) strengthen capacity to manage water quality; (4) facilitate implementation; and (5) monitor the impact on policies and practice. The Water Quality and Health Strategy 2013–2020 will support public health, socioeconomic development and well-being. This WHO strategy also supports the UN's previous Millennium Development Goals which promotes human rights to sustainable water access (WHO 2013), and the new Sustainable Development Goals.

The UN has 17 "Sustainable Development Goals" that include the relevant issues of clean water and sanitation, taking action on climate change and sustainable use of oceans, marine resources and wetlands. Eradication of hunger, clean water and sanitation, clean energy, climate action, life below water, life on land, and strengthening partnerships are all supported with water quality measures in wide rivers, lakes, reservoirs, estuaries and coastal marine waters (GEO 2017). Global assessments on the status and trends of freshwater resources is supported by the UN's Global Environment Monitoring System Water Programme. The goal of sustainability is directly dependent on safe and clean environments for social and economic growth and development.

Case Study 1: Aquawatch

❖ The Group on Earth Observations (GEO) is a global network of governments and organizations, established in 2005, with a focus on providing coordinated, comprehensive and sustained Earth observations and information. AquaWatch, a water quality community of practice within GEO (https://www.geoaquawatch.org/), was formed in response to the need for an international operational water quality information system. The mission of AquaWatch is to deliver timely, consistent, accurate, and fit-for-purpose water quality data products and information to support water resource management and decision making in coastal marine and inland waters. AquaWatch aims to develop international operational water quality information systems based on EO because the extensive nature of many surface water resources and the lack of suitable measurement or access infrastructure inhibit intensive *in situ* water quality sampling networks.

The World Bank views water management as essential for continued human development, food and energy security, and job creation (Radstake and Tuinhof 2003). Water management is an important aspect for human lives, and continued economic and social growth. Maintaining beneficial water uses for growth and development support agriculture, energy production, and overall reduction in poverty. Water demand has increased and is expected to continue increasing in the future, which may threaten human health, agriculture, industry, and biodiversity. The World Bank has historically focused on sanitation, treatment, and nutrient pollution to protect water resources and mitigate the economic consequences.

1.3.2 Africa

The National Water Act 36 of 1998 established the national framework for South Africa water management, protection, and use to benefit the public interest. The National Water Act required the development of the National Water Resource Strategy, with the objective to manage water resources for sustainable social and economic development. This strategy must provide information on water requirements and propose management actions. The National Environmental Management Act 107 of 1998 states everyone has the right to an environment that is not harmful, while supporting sustainable development to serve current and future generations. The Integrated Coastal Management Act 24 of 2008 ensures that the coastal zone is socially, economically, and ecologically sustainable; and to protect against adverse effects on the coastal environment. The National Eutrophication Monitoring Programme and the National Aquatic Ecosystem Health Monitoring Programme are aimed at maintaining the quality of surface water, such as reporting trophic status and related problems such as harmful algal blooms.

1.3.3 Asia

The Water Environment Partnership in Asia includes 13 countries and looks to achieve sustainable socio-economic development and manage water resources. In Japan, the Water Pollution Control Law preserves public water areas to protect human health and the living environment, and is managed by the Ministry of Environment. The Mekong River Commission is comprised of China, Burma, Laos, Thailand, Cambodia, and Vietnam to support sustainable management and development of water and related resources to balance economic development, environmental protection, and social sustainability. The Environment Programme conducts monitoring activities to report water quality results to the involved nations, and the objective is to provide up-to-date environmental and social knowledge and efficient environmental management cooperation mechanisms for basin management and development (MRC 2010).

1.3.4 Australia

The National Water Quality Management Strategy is the primary water quality management policy in Australia, overseen by the Natural Resource Management Ministerial Council and the Environment Protection and Heritage Council, and is implemented by state and territory governments. The objective is to protect and enhance water quality while maintaining economic and social growth. The Water Act 2007 and the Water Regulations 2008 implemented key water management reforms in Australia, such as giving the Bureau of Meteorology water information functions for the nation. Under the Water Act 2007 the Bureau is required to collect, hold, manage, interpret, and disseminate information on Australia's water. The Water Regulations 2008 requires all individuals, trusts companies, corporations, and agencies of state, territory or Australian governments to give water information, including water quality information, to the Bureau. The Bureau of Meteorology provides regular reports on the status of water resources and use, which may be used for reporting on inland water quality and condition under the Environment Protection and Biodiversity Conservation Act of 1999. This Act requires a State of the Environment report to Parliament every five years on Australia's biophysical, ecological, social, and culturally related environmental issues. The most recent Australian State of the Environment report at the time of writing is from 2016 with a section dedicated to inland waters. Each of these acts and regulations are regularly updated to reflect current societal, economic, and environmental settings.

1.3.5 Europe

The European Union (EU) Water Framework Directive provides protection of aquatic ecology, drinking water resources, and bathing water across EU member states. This directive is also complimented by a number of other directives such as the Marine Strategy Framework Directive 2008. The objective of the Water Framework Directive is to protect human health, water supply, natural ecosystems, and biodiversity by maintaining good ecological and chemical status of all ground and surface waters. Ecological status indicators are measured by the departure from the biological community that would be expected in conditions under no anthropogenic influence. The ecological status includes measures of the aquatic flora and fauna, nutrients, salinity, temperature, and chemical pollutants.

The Oslo Paris Commission (OSPAR Commission 2010) consisting of 15 European nations, focuses on protecting land-based sources, ecosystems, biodiversity, and economic development in the North-East Atlantic. Relevant strategies to this topic include a Biodiversity and Ecosystem Strategy and an Eutrophication Strategy as part of the North-East Atlantic Environment Strategy. The overall goal is to manage anthropogenic activities that impact the maritime area, maintain healthy ecosystems, safeguard human health, and restore marine areas.

The Helsinki Commission is responsible for protecting the Baltic Sea in a multi-national effort between Baltic countries. There are four main segments to the Baltic Sea Action Plan: eutrophication, hazardous waste, biodiversity, and maritime activities (HELCOM 2007).

1.3.6 North America

Mexico's National Water Law is administered by the National Water Commission (CONAGUA) to preserve water and associated services to achieve sustainable use. The 2030 Agenda includes protecting water quality of rivers and lakes to meet the needs of the population. One of the principles defined in the 2030 Agenda is to meet society's needs with an adequate water quality and quantity to maintain public health. In Canada, the responsibility for water quality is shared between federal, provincial/territorial, and municipal levels of government, developing various governance mechanisms to protect and enhance the quality of Canada's water resources, promote the wise and efficient management and use of water, and develop guidelines for water quality standards. Several federal departments and agencies (including Environment and Climate Change Canada, Health Canada, and the Department of Fisheries and Oceans) work closely to address nationally significant freshwater concerns, ensuring national policies and guidelines are in place on environmental and health-related water issues, and are responsible for administering federal legislation such as The Canada Water Act, Canadian Environmental Protection Act, and Fisheries Act.

Canada and the United States share many waterways, including the Great Lakes which are among the world's largest bodies of freshwater, and as such the two countries maintain several treaties and agreements (e.g., the International Boundary Waters Treaty Act) which provide a mechanism for cooperation and coordination in managing these trans-boundary waters. The Great Lakes Water Quality Agreement (GLWQA) between Canada and the United States identifies shared priorities and coordinates actions to restore and protect the chemical, physical, and biological integrity of the waters of the Great Lakes.

In the United States, the Clean Water Act, Safe Drinking Water Act, and Harmful Algal Bloom and Hypoxia Research and Control Act provide the basic structure for monitoring and maintaining water quality standards. Specifically, the Clean Water Act established the structure for water quality standards in surface waters, and the Safe Drinking Water Act allows for standards to ensure the quality of drinking water. The Harmful Algal Bloom and Hypoxia Research and Control Act is primarily focused on detecting, predicting, controlling, mitigating, and responding to marine and freshwater harmful algal bloom and hypoxia events.

Case Study 2: Numeric Water Quality Criteria

❖ In the United States, the Clean Water Act requires states to identify designated uses of their waters and, when necessary, to develop science-based water quality criteria to ensure protection of the designated uses. Numeric water quality criteria are concentrations or levels of a pollutant that, if achieved, provide an expectation that designated uses will be supported. The U.S. Environmental Protection Agency established a national strategy for the development of numeric criteria identifying chlorophyll-*a* as a nutrient-related response variable. Schaeffer et al. (2012) and Schaeffer et al. (2013a) developed an approach to numeric criteria using satellite remote sensing to derive chlorophyll-*a*. This approach is illustrated using data from the State of Florida coastal waters (Figure 1.3). The Sea-viewing Wide Field-of-view Sensor (SeaWiFS) satellite was used to determine a quantitative reference baseline to protect coastal waters from eutrophication impacts. Briefly, the 90^{th} percentile of annual geometric means between 1998 and 2009 from the SeaWiFS mission was used to determine the criteria value (Figure 1.4). In addition, approaches to enable transition of assessments from the SeaWiFS to newer platforms such as the Sentinel-3 Ocean and Land Colour Imager (OLCI), were established.

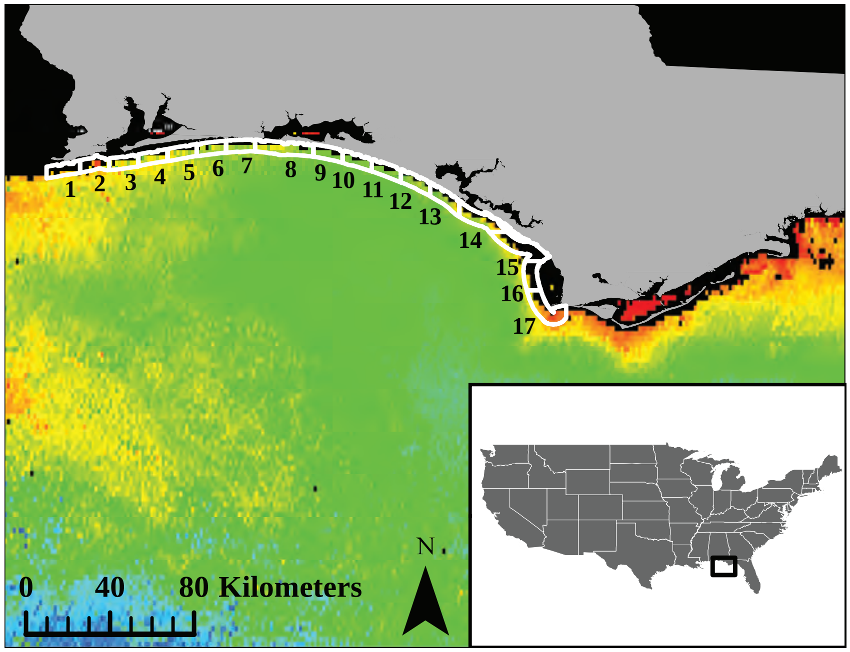

Figure 1.3 Fixed coastal segments used in the numeric criteria approach for the Florida Panhandle. Numbers are coastal segment numbers ranging from 1 through 17. From Schaeffer et al. (2012).

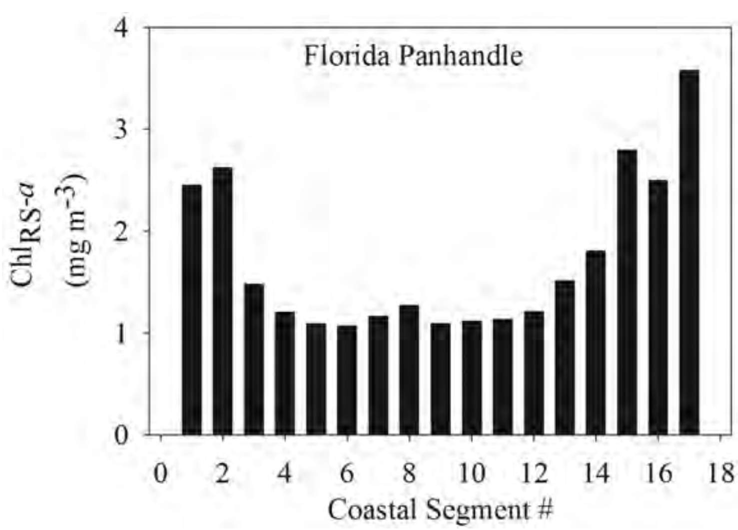

Figure 1.4 Candidate criteria for each coastal segment calculated on the basis of the 90th percentile of the annual chlorophyll-*a* geometric means for the Florida panhandle. Coastal segment numbers correspond to segments identified in Figure 1.3 above. From Schaeffer et al. (2013a).

1.3.7 South America

Brazil Law No. 9,433 of January 1977 established the National Water Resource Policy and National Water Resource Management System, which is implemented by the Brazil National Water Agency to ensure sustainable use of rivers and lakes. The Argentina National Constitution states people should have access to a healthy environment for human uses. The provinces of Argentina have developed specific environmental laws that regulate water quality. The Peru Water Resources Law established the National Water Authority (ANA) to manage water resources for sustainable use. In 1981, Chile enacted its new Water Code (later reformed in 2005) that guarantees the right of citizens to live in an environment free from contamination. Since then Chile's National Commission on the Environment have made improvements in wastewater and industrial water treatment.

1.4 How Satellite Remote Sensing Can Contribute

Data from satellite remote sensing can address and inform communities on water quality changes that impact societal uses (Vörösmarty et al. 2015). Mechanistic models are necessary for water quality management, but current models cannot resolve ecological and human health-related events because of limitations on knowing when and where these events occur. Satellite data provides information on dynamic and ephemeral events over extensive spatial and temporal scales. Feasibility of incorporating satellite information into water quality monitoring has been demonstrated, and operational applications are expanding. Local and national government and non-government organizations conduct field-based activities with limited resources to provide information on water quality conditions. Satellites have the potential to help address the limitations of geographic extent and temporal coverage of traditional sampling approaches. When coupled with field-based observations, satellite data provide a more comprehensive ability to monitor, assess, and forecast changes in the environment. Satellite information can be used to assess baseline conditions and to understand trends for water quality management. Furthermore, inland and estuarine waters present a challenge due to complex hydrologic connections and spatial separation, variable ecological drivers, and anthropogenic stressors. Satellites provide an integrated and synoptic approach that will be beneficial as extreme events increase (IPCC 2012).

1.5 Challenges and Why Now?

Technology, tools, and methodological approaches required for satellite remote sensing of water quality will continue to mature over the coming decade and will be addressed throughout this report. However, other challenges to integrating satellite remote sensing into water quality management still exist and can only be solved with open and effective discussion and forum between scientists, stakeholders, and water quality managers. Schaeffer et al. (2013b) found four main challenges inhibited the consideration of satellite remote sensing data in water quality management including perceived cost of purchasing data, lack of understanding regarding the accuracy of satellite products, questions about data continuity between missions, and programmatic support and understanding. This report is intended to begin addressing some of these challenges and is one of many forms of communication to continue an effective dialogue between the scientific community and stakeholders, for example, the 2015 International Ocean Colour Science (IOCS-2015) meeting breakout session *"Tools to Harness the Potential of Earth Observations for Water Quality Reporting and Management"* (IOCS 2015), and the IOCS-2017 breakout session on *"Remote Sensing of Inland and Coastal Waters: Current Status, Challenges, Research Priorities, and End-User Engagement*" (IOCS 2017).

Recent technology advances in cloud-based infrastructure now allow for coordinated data sharing with centralized, open access, publicly available data (Mouw et al. 2015). For example, the Committee on Earth Observation Satellites (CEOS) is planning for the creation of analysis-ready data cubes to reduce the barrier and costs of data integration, analysis, interpretation and applications between large volumes of satellite data and end-users. Analysis-ready data cubes assign satellite data, quality assurance information, and metadata to a common spatial grid that covers the necessary spatial and temporal extent of observations (Lewis et al. 2016). Advances in these technologies will help address the increased demand from local and national government and non-governmental organizations in the ability to monitor water quality, by re-purposing ocean colour and land imaging satellites. Significant progress has been demonstrated in deriving water quality information from inland and coastal marine waters using satellite ocean colour sensors such as the Moderate resolution Imaging Spectroradiometer (MODIS) and MEdium Resolution Imaging Spectrometer (MERIS). Due to the coarse spatial resolution of these ocean colour sensors (1-km and 300-m respectively), water quality science and applications also depend on terrestrial sensors such as the Landsat series and Sentinel-2 MultiSpectral Instruments (MSI) (Mouw et al. 2015; Palmer et al. 2015b). The relatively new Copernicus programme series of Sentinel-3 OLCI (Ocean and Land Colour Imager) and Sentinel-2 MSI sensors will also improve temporal resolutions, approaching those associated with ocean colour missions of multiple images per week at the same location (Berger et al. 2012; Donlon et al. 2012; Hestir et al. 2015). Understanding the capabilities and limitations of these satellite sensors is critical to maximizing the potential of EO data and is further detailed in the following chapters.

Chapter 2

Introduction to Deriving Water Quality Measures from Satellites

Caren Binding, Richard P. Stumpf, Blake A. Schaeffer, Andrew Tyler and Peter Hunter

2.1 Introduction

Remote sensing of water quality is based on the concept that measurable changes in the colour of the water caused by variations in the concentrations of key water quality constituents may be detected from a remote platform such as a satellite or aircraft. Chapter 1 defined water quality as those biological, physical, and chemical characteristics of natural water required to maintain beneficial use of a water body. There are several recurring basic needs of water quality monitoring programmes which may include observations of water clarity (transmittance, turbidity, Secchi disk depth), algal biomass (chlorophyll-*a*), harmful or nuisance algal blooms (HNABs), trophic status, suspended sediments, temperature, nutrients, dissolved oxygen, organic/inorganic pollutants and microbial contamination. Some of these parameters have a definite and well-defined influence on the colour of water, some do not, and it is this distinction that determines whether or not they may be directly measurable using aquatic colour remote sensing. In this chapter we present a broad summary of the theoretical basis for remote sensing of water quality, including a discussion of what key water quality parameters can and cannot be measured, an introduction to platforms and algorithms, and advantages and limitations of the remote sensing approach.

Historically, *in situ* measurements and the collection of water samples for subsequent laboratory analyses have been the conventional protocols for water quality monitoring programmes. While providing accurate information for particular points in space and time, acquiring such information in the required frequency and geographic coverage to adequately characterize spatial heterogeneity and temporal variability in water quality is often prohibitively expensive and logistically challenging. Remote sensing offers one of the most cost-effective, spatially and temporally comprehensive tools for observing often highly dynamic water quality phenomena in coastal and inland waters, and is particularly beneficial for monitoring previously undersampled locations and areas with limited access. New and improved sensor technologies, novel algorithm development, and considerable improvements in data availability, image processing capabilities and product dissemination, have resulted in major advancements in remote sensing of coastal and inland waters, and a demonstrable increase in the confidence in, and uptake of, derived water quality products. Many examples now exist where remote sensing is contributing routinely to programmes of water quality monitoring and reporting, delivering prompt, reliable, synoptic maps of water quality in support of lake and coastal zone management. A subset of these will be included here and in other chapters throughout this volume as case studies to demonstrate the state of the art in fit-for-purpose water quality remote sensing applications (i.e., those products of sufficient quality that they may be useful in fulfilling a water quality monitoring or assessment need).

2.2 Theoretical Basis of Water Quality Remote Sensing

When sun and skylight reaches a water body, some of it is reflected directly off the surface, but most of the light penetrates into the water column and interacts not only with water molecules, but also with organic and inorganic materials which are dissolved and suspended within the water column (Figure 2.1). Materials that interact with light, termed optically-active constituents (OACs), do so through the processes of light absorption and scattering. These OACs have measurable, often unique, absorption and scattering signatures, referred to as inherent optical properties (IOPs). For practical purposes, OACs are often grouped into four main components: pure water, phytoplankton (containing chlorophyll-*a* and other pigments), non-algal particles (NAP, including organic detritus and inorganic mineral sediments), and coloured dissolved organic material (CDOM). By preferentially absorbing or scattering light at different wavelengths across the visible and near-infra-red portions of the spectrum, OACs determine the magnitude and spectral shape of light scattered upwards and back through the air-water interface (the water-leaving radiance, L_w). It is these variations in spectral L_w, as detected by sensors mounted on a remote platform such as a satellite, which can be interpreted in terms of key water quality parameters.

The depth to which sufficient sun and skylight penetrates (and therefore the depth the satellite signal represents) depends on both the wavelength of light (blue and green light penetrates further than red light in pure water) and the composition of the water through which it travels. In highly turbid waters, the satellite signal may be representative of only the upper few centimeters of the water column, while in clearer waters, up to tens of meters depth. In shallow, clear waters, sunlight may penetrate to the bottom substrate and be reflected back to the surface making bottom-reflectance an additional contributor to the water-leaving radiance. In such waters, bottom substrate type, submerged vegetation and water depth may be estimated (Lee et al. 2007a; Leiper et al. 2014).

As a passive remote sensing device, an aquatic colour satellite sensor measures the response of the water body to solar illumination, and so provides meaningful data only during daytime, under cloud-free conditions. Sensor scanning capabilities produce a two-dimensional array of pixels which, combined with the orbit of the satellite and the Earth's rotation, allow instantaneous, synoptic images over the satellite path projected on the globe. Imagery is geolocated such that for each pixel, one can obtain a measure of the water-leaving radiance

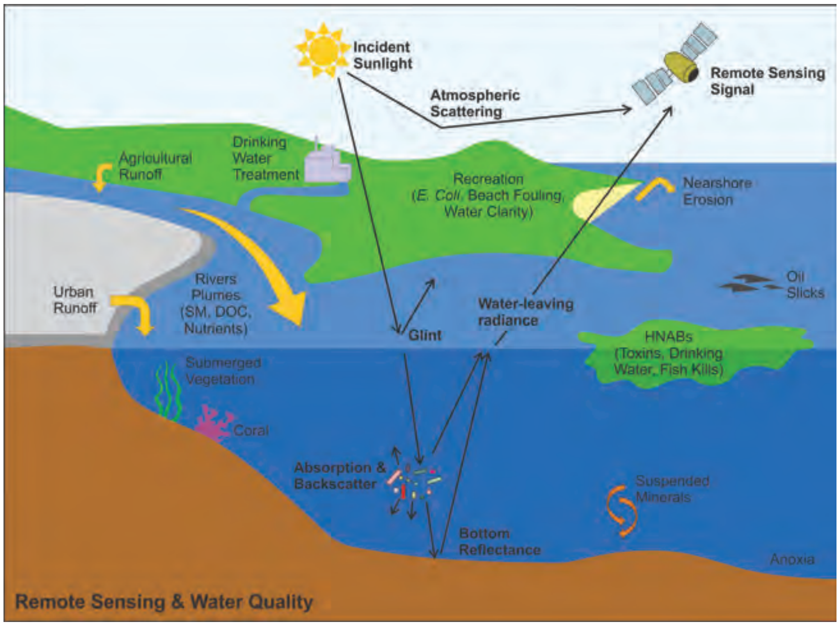

Figure 2.1 Schematic describing key water quality concerns for coastal and inland waters in relation to satellite remote sensing of water colour. Image credit: Environment and Climate Change Canada.

(or the derived water quality parameter of interest) along with its location. Repeat imagery allows for the tracking of seasonal cycles, long term trends, or episodic events over time for any specified area of interest.

For a more detailed technical introduction to remote sensing and aquatic optics relevant to observations of coastal and inland waters the reader is directed to Chapters 5 and 6 within this report, as well as IOCCG Report 3 (IOCCG 2000).

2.3 What Can be Measured Using Remote Sensing?

The primary measure from an aquatic colour sensor is the top-of-atmosphere (TOA) radiance at a number of discrete wavelengths in the visible-near-infra-red domain. The majority of the TOA radiance is light reflected by air molecules and aerosols in the atmosphere, as well as sun glint and sky radiance reflected by the water surface (see Figure 2.1). Removal of those contributions allows the retrieval of water-leaving radiance or remote-sensing reflectance products. Often a suite of in-water optical properties (e.g., absorption, backscatter) can also be derived. It is these primary optical products (Section 2.3.1) which form the basis of any subsequent water quality determinations.

Water quality parameters that can be measured directly from these primary optical parameters are those that have a measurable effect on water colour through their ability to absorb or scatter light and in some instances fluoresce (Section 2.3.2). There are additional water quality properties of interest that cannot be directly measured from space, but rather may be derived by combining remotely-sensed data with *in situ* or other ancillary data (Section 2.3.3). Integrated approaches based on assimilation of remotely-sensed data into diagnostic and prognostic models have expanded the potential of remote sensing beyond retrieval of directly measurable quantities, for example, in studies of primary productivity, carbon budgets and biogeochemical cycles. Other, non-optically active water quality parameters of interest (such as nutrients, organic/inorganic pollutants, microbial contamination, dissolved oxygen), although impossible to measure directly with remote sensing, have been estimated through inference using proxy relationships and empirical models. Such relationships cannot, however, be relied upon as physics-based solutions; they may not be causal, and may have a limited validity range, both spatially and temporally. The use of proxies depends strongly on the spatial/temporal robustness of the proxy relationship with a directly measurable water quality parameter. As such, proxy-based observations may be appropriate for regional, often qualitative applications more so than quantitative, global applications, unless linked to more mechanistic modelling approaches and ancillary data.

2.3.1 Primary optical parameters

- ❖ Radiance/reflectance — TOA radiance/reflectance, water-leaving radiance or remote-sensing reflectance are required with adequate accuracy to minimize uncertainty in derived water quality products.
- ❖ Derived IOPs (absorption, backscatter) — an essential first step in many analytical methods to derive water quality constituents (IOCCG, 2006).

2.3.2 Water quality parameters directly measurable from space

- ❖ Water clarity — many empirical or analytical approaches are available for estimating diffuse attenuation, Secchi disk depth, or euphotic depth (Lee et al. 2005, 2007b; Doron et al. 2007, 2011; Olmanson et al. 2008; Binding et al. 2015).
- ❖ Chlorophyll-*a* (as an indicator of total phytoplankton biomass) — a variety of algorithms suitable for wide-ranging coastal and inland water conditions are now available and in routine use (see Odermatt et al. 2012 and references therein for a review).
- ❖ Algal blooms — in addition to chlorophyll-*a*, specific marker pigments (e.g., phycocyanin for cyanobacteria) or other unique spectral features, allow identification of potentially harmful algal blooms, as well as measures of their spatial extent, severity and duration. (Matthews et al. 2012; Stumpf et al. 2012; Binding et al. 2018; Clark et al. 2017; Urquhart et al. 2017).
- ❖ Submerged, emergent and floating aquatic vegetation (Gower et al. 2006; Hu 2009; Shuchman et al. 2013).
- ❖ Bottom substrate, bathymetry — may be retrievable in optically-shallow waters where bottom reflectance is significant (Lee et al. 2007c; Dekker et al. 2011; Vahtmäe and Kutser 2007).
- ❖ Suspended sediments — algorithms are available to retrieve total or mineral suspended particulate concentrations to study river plume dynamics, shoreline erosion, and bottom

re-suspension events (Stumpf and Pennock 1989; Doxaran et al. 2003; Dogliotti et al. 2015; Han et al. 2016).

- Coloured dissolved organic matter (CDOM) — represents the optically-active fraction of dissolved organic matter (DOM). CDOM can be retrieved from its exponential absorption signature, and has contributed to many studies of coastal and inland water DOM dynamics and biogeochemical cycles (Mannino et al. 2014). Where robust relationships between CDOM and dissolved organic carbon (DOC) can be demonstrated, DOC may also be retrieved, although that relationship has been shown to be spatially and temporally variable (Brezonik et al. 2015).
- Sea/lake surface temperature — although not derived from aquatic colour, it is included here as a well-established remote sensing capability using thermal infrared or passive microwave remote sensing (Reynolds et al. 2007).
- Surface oil slicks — typically detected using active microwave sensors like Synthetic Aperture Radar (SAR) but optical imagery offers some additional benefits such as discriminating surface oil slicks from algae (Brekke and Solberg 2005).

2.3.3 Additional desirable water quality parameters not directly measurable from space

- Trophic status — may be inferred if reasonably defined (see Section 2.3.2) from algal biomass and/or water clarity (Olmanson et al. 2008; Binding et al. 2011; Matthews et al. 2012).
- Primary productivity — can be estimated from satellite-derived chlorophyll-*a* or phytoplankton absorption (Behrenfeld and Falkowski 1997) by including models/assumptions for contributing factors such as algal depth distributions, light availability, temperature, and algal physiology variables (e.g., photosynthetic quantum yield). See Lee et al. (2015a) and Kahru (2017) for recent reviews.
- Algal toxins — most toxins are colourless and so are not directly measurable from aquatic colour remote sensing. Cyanobacteria toxicity may correlate regionally with phycocyanin (e.g., Hunter et al. 2010), or other phycobiliproteins, however not all cyanobacteria are toxic and toxins may persist in the water long after a bloom has collapsed. The relationship between pigments or cell densities and cyanotoxins is therefore highly variable and remains the challenge for satellite remote sensing of algal bloom toxicity (Stumpf et al. 2016).
- Nutrients — although nitrogen and phosphorus do not contribute directly to a waterbody's spectral signature they contribute to colour indirectly through their promotion of algal growth. While a strong statistical response of phytoplankton biomass to nutrient enrichment is evident on broad scales (Smith 2006), a proxy-based approach to mapping nutrients will vary regionally and temporally due to variations in physical processes, phytoplankton/zooplankton community composition, and nutrient stoichiometry (Li et al. 2010; Filstrup et al. 2014). Statistical relationships are often based on an increase in chlorophyll with nutrients, as long as nutrients are the limiting growth factor.

- Dissolved oxygen — not measurable directly using aquatic colour but remote sensing of chlorophyll-*a*, algal blooms and/or temperature (driving water column stability) may provide valuable information to further understand hypoxia events such as those observed in the Gulf of Mexico (Le et al. 2016) and Lake Erie (Zhou et al. 2015).
- Pollutants/metals/microbial contamination — not measurable directly with remote sensing but may be inferred indirectly through their association with particulate and/or dissolved organic matter in plumes or resuspension events.

2.4 Water Quality Retrieval Algorithms

The signal retrieved by a satellite sensor is confounded by large contributions from the intervening atmosphere and sun and sky glint, for which correction algorithms must first be applied. Rigorous atmospheric and air-water interface correction therefore forms a critical primary step in satellite image processing for most water quality applications. After removing the effects of the atmosphere to obtain a measure of the spectral water-leaving radiance or reflectance, extracting quantitative information on water quality parameters requires the application of appropriate algorithms. Retrieval algorithms take many forms, but are driven by expected variations in the spectral shape and/or magnitude of the water-leaving radiance signal in response to the water quality parameter of interest. Algorithms are often divided into empirical (data driven) or physics-based semi-analytical solutions. Empirical algorithms may have a bio-optical basis such as the blue-to-green ratio adopted for open ocean chlorophyll-*a* retrievals (most algae absorb blue light more strongly than green), or may use implicit approaches based on machine learning techniques (e.g., neural network approaches, support vector machines and hybrid active learning models). Unlike the open ocean, where optical properties and therefore retrieval algorithms can be reasonably defined by the effects of phytoplankton and their byproducts, algorithms for inland and coastal waters are multi-variate problems where the added optical influence of suspended minerals and dissolved organic matter must be considered. Semi-analytical algorithms are based on bio-geo-optical models which define the relationships between water-leaving radiance, inherent optical properties, and biogeochemical constituents.

Spectral inversion algorithms have often outperformed empirical approaches (IOCCG 2000; Dekker et al. 2011) but depend strongly on the initial parameterization as well as robust atmospheric correction, which remains a challenge for many coastal and inland waters. The choice of approach, or combination of approaches, depends largely on the level of optical complexity of the waters under consideration, the optically-active constituent concentration ranges, the spectral characteristics of the sensor to which they will be applied, the amount of information available regarding inherent optical properties, and computation time/resources. For a more in-depth discussion of specific algorithm approaches for water quality retrievals the reader is directed to Chapter 5 of this volume.

2.5 Platform and Resolution Considerations

Remote sensing platforms come with a diverse set of spatial, temporal and spectral resolutions which depend on the sensor specifications and satellite orbit. Spatial resolution determines the smallest feature an image can detect, defines the image pixel size in full resolution, and is determined by the sensor's field-of-view and satellite altitude. Temporal resolution, or revisit time, is the time between consecutive views of the exact same area of the Earth, although due to partial overlap between swaths, an object may be viewed more frequently. Spectral resolution defines the number and width of bands measured; typically the wavelength range for water quality applications extends across the visible and near-infrared domains of the electromagnetic spectrum, with sensors ranging from multi-spectral (measuring a small number of discrete wavelengths) to hyperspectral (measuring near continuously across the full spectrum). Historically, sensor and orbit capabilities have resulted in trade-offs between the spatial, temporal, and spectral resolutions available on satellite missions. For example, the Landsat series of satellites provide medium to high spatial resolution (~30-m) but coarse spectral resolution and revisit times of 16 days, while a sensor such as MODIS and the two Sentinel-3 sensors operate with a coarser ground spatial resolution of 1-km and 300 m respectively, enhanced spectral resolution, and with daily revisit. Such limitations are decreasing with advances in modern sensor technology but remote sensing applications still face trade-offs between different sensor capabilities. Table 6.4 in Chapter 6 summarises the existing and forthcoming satellite capabilities of value for water quality applications.

Alternate platforms such as aircraft or, more recently, drones provide additional solutions for targeted nearshore high resolution observations. Although frequently used for research or demonstration purposes, airborne remote sensing is often prohibitively expensive for operational use in water quality monitoring. For brevity, this chapter deals only with satellite platforms and their applications.

2.6 Advantages and Limitations of Remote Sensing for Water Quality Monitoring

With limited resources and logistical constraints on traditional monitoring programmes, remote sensing offers a cost-effective solution for large scale lake and coastal water quality monitoring. The growing sophistication of satellite missions, as well as advances in computing capabilities, and increasingly robust processing algorithms for optically-complex inland and coastal waters, have made operational satellite-based water quality monitoring a reality. The approach brings with it many advantages, and remaining challenges, which are summarized below.

Advantages

- ❖ Provides water quality observations over large areas of our oceans (including coral reefs), coastal, estuarine and inland waters including some large rivers, delivering synoptic views of dynamic water quality features simply not possible using ground based observations;

- Provides observations for remote locations often logistically difficult and expensive to reach using traditional monitoring approaches;
- Frequent revisit times provide observations adequate for time-series analysis and event monitoring;
- Increased commitment from space agencies to ensure data and product continuity allows for confidence in long-term time-series;
- Advancements in data delivery and processing allows for near-real-time observations, providing value in early warning systems;
- Variety of products — a large suite of water quality variables is available at a range of resolutions;
- Archived historical data allows for retrospective analysis up to several decades;
- Non-commercial imagery — freely available datasets as well as open-source processing software allow for low cost monitoring.

Limitations/challenges

- Imagery is atmospheric visibility limited — the effective revisit frequency is reduced by cloud-cover, fog, smoke and related effects over an area of interest;
- Potential spatial/temporal bias — in addition to the lack of spatial resolution for many rivers, streams and tributaries, cloud cover may result in nearshore, seasonal and latitudinal bias in data availability;
- Products directly measurable from remote sensing are limited to those with a discernible effect on VIS-NIR colour;
- Near surface water column only observations — as the remote sensing signal originates from the depths to which sun and sky light are reflected, water quality observations are representative of that water column layer only;
- Some algorithm/image processing challenges remain for optically-complex, nearshore, and optically-shallow waters (atmospheric correction, algorithm validity, atmospheric land adjacency effects), leading to greater product uncertainty under some circumstances;
- Satellite data, derived products, and processing software, are not always easily manipulated/interpreted by the non-specialist.

2.7 Case Studies

2.7.1 Inland water eutrophication and harmful algal blooms

Eutrophication and associated HNABs is perhaps the most pervasive problem affecting inland water quality. There is substantial evidence that the frequency and magnitude of HNABs in coastal and inland waters around the world have been increasing, attributed in large part to cultural eutrophication, and climate change (Hallegraeff 1993; Glibert et al. 2005; Heisler et al. 2008; Paerl and Huisman 2008). Blooms pose a serious threat to the integrity of freshwater systems and generate public health concerns because of their potential to produce potent toxins, leading to significant socio-economic impacts on ecosystem services. Finite resources for monitoring these events often results in fragmented long term datasets, impeding our ability to resolve spatial and temporal trends and develop robust management strategies.

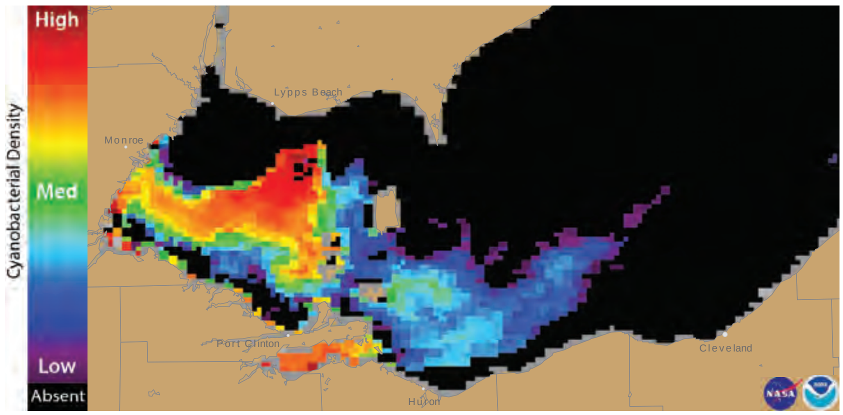

Figure 2.2 Cyanobacterial Index from NASA MODIS-Aqua data collected 17 September, 2017 at 13:31 EST. Grey indicates clouds or missing data. The estimated threshold for cyanobacteria detection is 20,000 cells ml^{-1}. From NOAA's Lake Erie HAB Bulletin.

Several studies have demonstrated the value or validity of remote sensing in the detection, monitoring, and short term forecasting of north American inland water algal blooms (Wynne et al. 2010; Stumpf et al. 2012; Urquhart et al. 2017; Binding et al. 2018). NOAA's Lake Erie HAB Bulletin (see Figure 2.2 and https://www.glerl.noaa.gov/res/HABs_and_Hypoxia/bulletin.html) is an operational remote-sensing based harmful algal bloom detection and forecasting system for Lake Erie adopting the Cyanobacteria Index (Wynne et al. 2008). Lake Erie, the shallowest of north America's Great Lakes, is prone to annual, often severe algal blooms typically dominated by the potentially toxic cyanobacterium *Microcystis*. Bi-national remediation efforts in the 1970's to reduce phosphorous loadings to the lake led to significant declines in phytoplankton biomass but since the early 2000's blooms have seen a resurgence. The bloom of 2011, the most extensive recorded, covered over 5000 km^2 (Stumpf et al. 2012) and cost an estimated US$71m in terms of impacts on property values, tourism/recreation and additional water treatment (Bingham et al. 2015).

Environment and Climate Change Canada uses remote sensing to report on algal bloom conditions in several of Canada's inland waters. Lake Winnipeg, for example, has experienced dramatic increases in nutrient loading from intensified agricultural practices and livestock production in the watershed. The result has been a marked shift in community composition towards the dominance of cyanobacteria, with extensive blooms on an annual basis. Remote sensing indices for algal bloom intensity, spatial extent, and duration (Figure 2.3) are reported using MERIS and Sentinel-3 OLCI derived chlorophyll (Binding et al. 2018). Prompt and synoptic detection of HNABs afforded by near-real-time delivery of these products is fundamental to effective mitigation of detrimental impacts on lake systems and services. Furthermore these lake-wide observations allow for more comprehensive studies of spatial and temporal trends, assessment of the efficacy of nutrient management practices, and further understanding processes driving bloom variability.

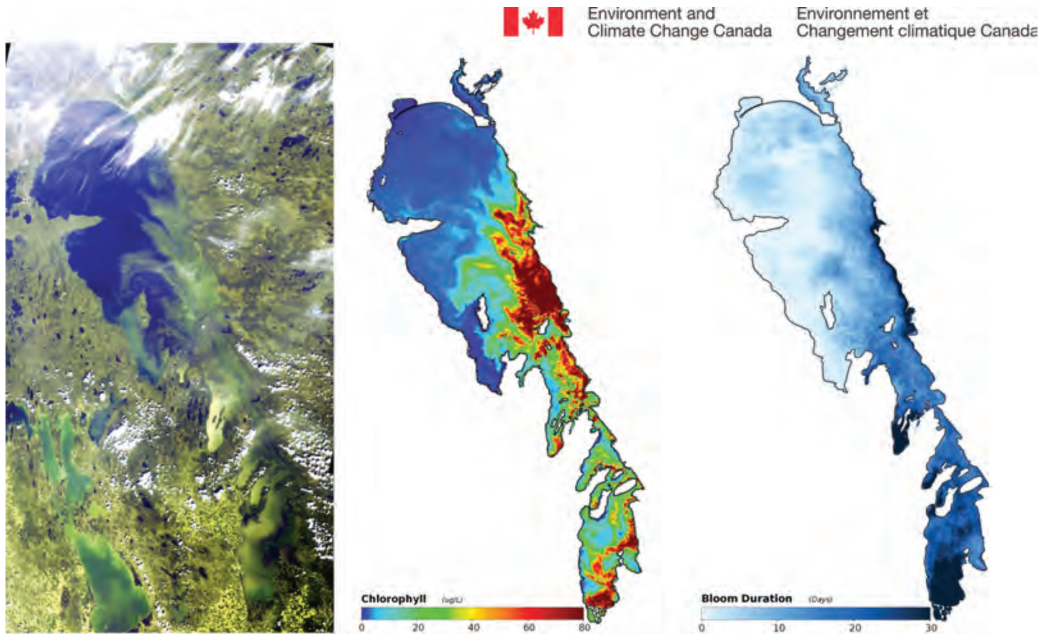

Figure 2.3 Examples of bloom detection and reporting in Lake Winnipeg. a) Sentinel-3 OLCI image of Lake Winnipeg captured on 12 August 2017 (credit: ESA/EUMETSAT), b) Chlorophyll-*a* concentration: lake average Chl 21.1 μg l^{-1}, peak Chl 180.9 μg l^{-1}, bloom intensity 42.8 μg l^{-1}, bloom extent 10,729 km^2 (44%), c) bloom duration: 10.4 days (avg.), 66 days (peak). Image credit: Environment and Climate Change Canada.

2.7.2 Phytoplankton phenology

The decadal-scale, internally-consistent, time series data acquired by both former and present ocean colour satellite sensors such as Envisat MERIS and Aqua-MODIS are an invaluable resource for studying the impacts of climate and land use change on large lakes and reservoirs. In particular, they offer the ability to observe changes in the concentration of chlorophyll-*a* at a spatial resolution of 0.25–0.5 km and a temporal resolution of 3 days or better. In turn, the high-frequency chlorophyll-*a* time series that can be produced from these sensors enable changes in the phenology of phytoplankton communities in lakes and reservoirs to be examined from space at spatial and temporal scales not possible using *in situ* data alone.

Phenology refers to the seasonal timing of life cycle events and, in the context of phytoplankton, includes features such as the start and end timing of blooms, the rate at which blooms grow and senesce, their duration, and the magnitude and timing of the seasonal chlorophyll maximum. There is significant scientific interest in phenology because it is widely accepted to be strongly coupled to climate. Indeed, the IPCC have suggested that phenology is the simplest method to track how the biosphere is responding to climate change (Rosenzweig et al. 2007) and there are numerous empirical studies evidencing temperature-driven changes in the timing of phytoplankton blooms in lakes (Vadadi-Fülöp and Hufnagel 2014; Thackeray et al. 2008).

Metrics of phenological change can be extracted in a relatively straightforward manner from satellite time series data and the use of satellite data for studying the phenology of phytoplankton blooms in the oceans is now well established (e.g., Kahru et al. 2011). More recently, comparable approaches have been used to examine changes in the phenology of phytoplankton communities in lakes in response to climate changes (Matthews 2014; Palmer et al. 2015a), see Figure 2.4). For example, Palmer et al. (2015a) were able to derive changes in the timing and duration of seasonal cyanobacterial blooms in Lake Balaton by analysing ten years of Envisat-MERIS data. The comparison of the satellite-derived estimates of bloom phenology showed very strong agreement with equivalent metrics established by applying the same analysis approaches to long-term *in situ* chlorophyll-*a* data.

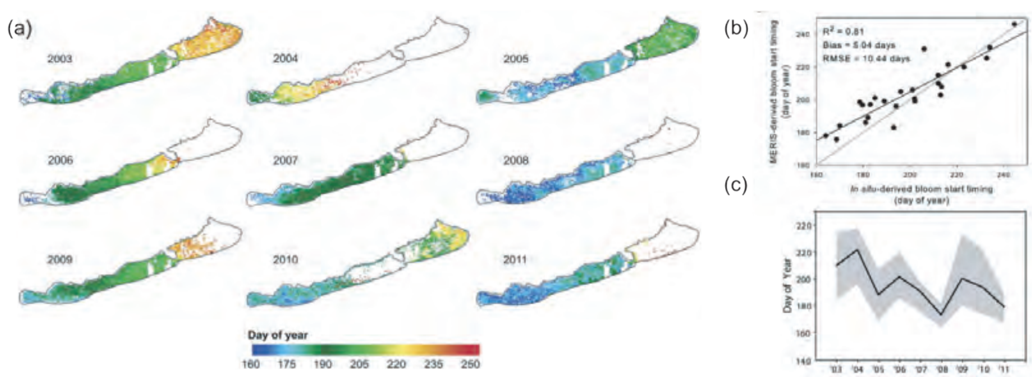

Figure 2.4 (a) Time-series images showing the change in the start time of the summer phytoplankton bloom in Lake Balaton, Hungary derived from ten years of Envisat-MERIS observations. (b) Comparison of bloom start times derived from Envisat-MERIS and *in situ* chlorophyll-*a* data. (c) Lake-scale decadal changes in the start time of the summer phytoplankton bloom in Lake Balaton from ten years of Envisat-MERIS observations. Figure adapted with permission from Palmer et al. (2015a).

The untimely end of the Envisat mission, allied to the now ageing Aqua-MODIS sensors, mean that future research on phytoplankton phenology from space will be reliant on the acquisition of new long-term datasets. This need is now being addressed through the recent launch of Sentinel-3A/B OLCI which, in conjunction with its scheduled replacements, will potentially provide a continuous time series of chlorophyll-*a* concentrations in large lakes and reservoirs globally every three days or better. In combination with improvements in the approaches used to extract phenological metrics from satellite data (e.g., Cole et al. 2012; Racault et al. 2014; Land et al. 2014), these data will be invaluable to future studies concerned with the effects of climate change on freshwater ecosystems.

2.7.3 Water clarity in the Great Lakes

Water clarity is an important indicator of water quality and ecosystem health, plays a central role in regulating pelagic and benthic primary productivity, and aesthetically has a direct impact on a waterbody's tourism and recreation value. As such, a measure of water clarity, as defined by the diffuse attenuation coefficient, turbidity, euphotic zone depth, or the Secchi disk depth (Z_{SD}), is often integral to inland and coastal water quality monitoring programmes. A variety of approaches have been used to derive water clarity from aquatic colour remote sensing. Diffuse attenuation coefficients in the open ocean have been typically estimated empirically from blue-to-green reflectance ratios (Mueller 2000) but this approach performs poorly in optically-complex waters where the optically-active constituents may not co-vary (Doron et al. 2007). Empirical algorithms based on a range of band combinations have been used successfully to map Secchi depths for inland waters (Chipman et al. 2004; Olmanson et al. 2008), while Lee et al. (2005, 2007b) and Doron et al. (2011) developed analytical models for estimating Secchi disk depth and euphotic depths appropriate to the band selections of most recent ocean colour sensors. More recently Lee et al. (2015b) and Lee et al. (2018) presented a new theoretical model for the interpretation of Z_{SD} and its relationship with the diffuse attenuation coefficient, K_d, or euphotic zone depth, Z_{eu}, providing significant advancement in the potential for global monitoring of water transparency using satellite remote sensing.

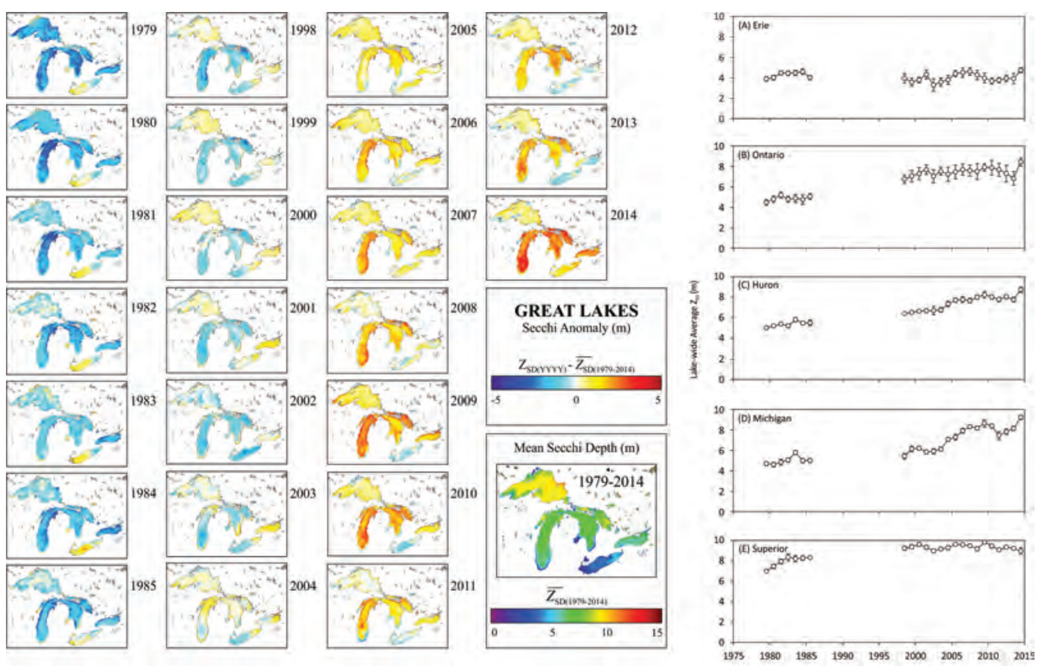

Figure 2.5 Satellite-derived Z_{SD} anomalies in the Great Lakes obtained from CZCS, SeaWiFS and MODIS data. Blue represents those areas below the long term mean Z_{SD}, red above the long term mean. The subplot shows the long term mean Z_{SD} from which the anomalies are calculated. The extracted annual lake-wide average Z_{SD} trends for each of the lakes are shown on the right-hand side. Adapted from Binding et al. (2015).

Water clarity in North America's Laurentian Great Lakes has undergone considerable change over the last several decades as a consequence of eutrophication, the introduction of the invasive zebra mussels, and nutrient management practices arising from the Great Lakes Water Quality Agreement (GLWQA). The Secchi depth is a simple but key integrative diagnostic of aquatic biogeochemical processes and has been used as a measure of water transparency in the Great Lakes for decades (IJC 1976). Nevertheless, sparse spatial coverage and the discontinuous nature of such ground-based monitoring have often precluded reliable conclusions regarding long-term basin-wide changes in Great Lakes' water clarity. An empirical relationship based on >1300 matchups of historical Secchi disk measures and R_{rs}~550 nm spanning three satellite missions provided a simple method for obtaining consistent synoptic observations of water clarity for these vast lakes (Binding et al. 2015). A multi-decadal analysis of spatial and temporal variations in water clarity documented remarkable and complex changes (Figure 2.5) across the Great Lakes, with dramatic increases in offshore Z_{SD}, regional decreases in nearshore Z_{SD}, and considerable variability in seasonal cycles from lake to lake. Spatial and temporal variations in Z_{SD} are in agreement with documented reductions in many of the Great Lake's bio-productivity, recent increases in bloom events on Lake Erie, degrading nearshore water quality, and changing biogeochemical processes influencing whiting events and sediment resuspension.

This chapter provided the theoretical basis for remote sensing of water quality, the current capabilities, its advantages and disadvantages over other monitoring methods and an understanding how satellite imagery is transformed into data products. Additionally, examples were given to demonstrate current applications. The use of remote sensing for water quality monitoring is a quickly evolving field and improvements in spatial, temporal and radiometric resolution will continue to increase the use of this monitoring tool. The following chapters will provide a closer look into a number of aspects of remote sensing as a monitoring system.

Chapter 3

Complementarity of *In situ* and Satellite Measurements

Steven Greb, Daniel Odermatt, Blake A. Schaeffer, Evangelos Spyrakos and Menghua Wang

This chapter provides an overview of water quality monitoring approaches. Various tools or options are available depending on the needs and objectives of the user. In addition, the technical advantages and disadvantages of the approaches including accuracies, limits of detection and representativeness are discussed in the context of stakeholder frameworks and institutional requirements. The objectives of monitoring may include water characterization for trends, problem identification, compliance, design of pollution and remediation programmes, and emergency response (Mahadevan et al. 2003). New and future methodologies including complimentary monitoring (e.g., *in situ* and satellite remote sensing) approaches are highlighted along with links to resources to assist in further pursuit of these strategies. Water quality monitoring efforts need to recognize the underlying temporal and spatial variability of relevant processes as summarized in Figure 3.1, and monitoring strategies need to be designed appropriately.

3.1 Discrete *In Situ* Measurements and Water Sample Analyses

3.1.1 Prevalent techniques and suitability

Historically, discrete *in situ* sampling was the only means available for water quality management authorities to assess the condition of coastal and inland waters. Today, most water quality monitoring programmes still rely on discrete *in situ* point samples. While these *in situ* measures provide valuable snapshots over time, they are not intended, nor designed to address water quality issues that require more synoptic spatial and temporal monitoring. The frequency at which point-based sampling programmes are carried out varies from daily (for drinking water) to weekly, monthly or seasonally for longer-term evaluation. Sampling schedules are often dependent on perceived threats and/or the intended uses for the water.

Advantages of *in situ* sampling include flexibility to measure a wide range of chemical, biological and physical parameters, including trace metals, organic and inorganic micro pollutants, nutrients, cyanobacteria, and optical properties. *In situ* monitoring provides an opportunity to collect environmental data that are not detectable by satellite, and can be important in terms of a more complete understanding of complex aquatic processes. The

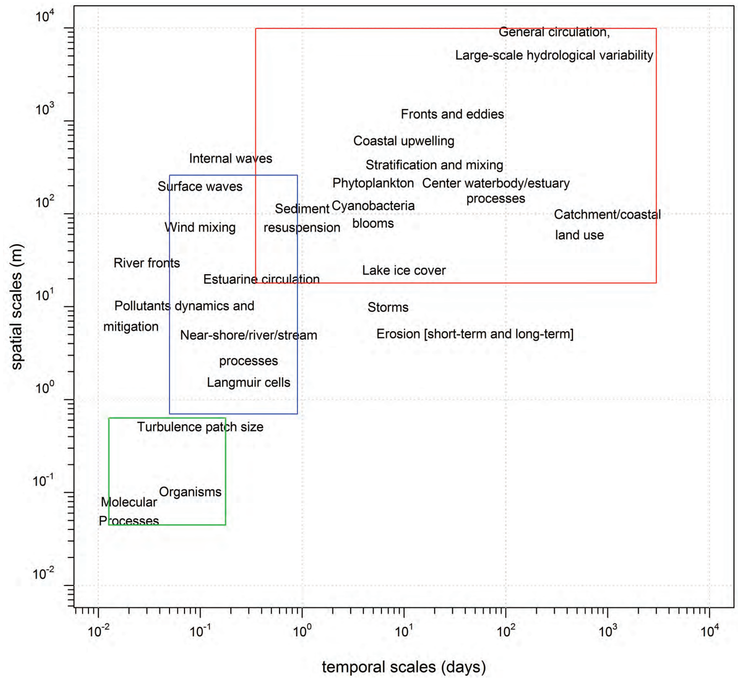

Figure 3.1 Spatial and temporal scales of processes related to water quality in inland and near-shore systems and their coverage by satellite sensors (red box) airborne data (blue box) and field-based efforts (green box).

measurements are usually highly replicable within a sample (space and time considerations such as depth profiles and time of day are investigator dependent). Disadvantages include logistics, weather dependencies, travel distances, collecting representative samples over large areas, consistency in methodologies, limited resources, and readily open access to data. For example, very few freshwater lakes with recreation activity and drinking water use are monitored regularly.

3.1.2 Examples of *in situ* databases

Most *in situ* data collected by local organizations is often difficult to obtain and use. Because of the inconsistencies in the way data are generally collected and disseminated, multiple groups have worked together to aggregate water quality data through web services.

The US Water Quality Portal (WQP) is a cooperative service sponsored by the United States Geological Survey (USGS), the Environmental Protection Agency (EPA), and the National Water Quality Monitoring Council (NWQMC). It serves data collected by over 400 state, federal, tribal, and local agencies. Their website (`http://www.waterqualitydata.us/`) currently provides almost 3 million water quality records from all 50 states (Read et al. 2017).

The United Nations Global Environment Monitoring System (GEMS) Water Programme is dedicated to providing environmental water quality data and information of the highest integrity, accessibility and interoperability. These data are used in water assessments and capacity-building initiatives around the world. The Water Data Centre (http://www.gemstat.org/), hosted at the European Environment Agency (EEA), provides a central access point to several web-services: interactive maps, data viewers, European datasets and indicators. These services are mostly based on reporting from countries as part of implementation of EU directives or via the European Environment Information and Observation Network (EIONET) framework (www.eea.europa.eu/themes/water/dc).

3.2 Continuous *In Situ* Measurements

3.2.1 Prevalent techniques and suitability

Significant technological developments in autonomous underwater vehicles (AUVs) and automated moorings in recent years have promoted a greater understanding of water quality variability, particularly at short time intervals. AUVs are submarine-like vehicles that follow a programmed course and employ sensors mounted in the nose to record pertinent water quality information such as temperature, dissolved oxygen, chlorophyll and bathymetry. An excellent review by Wynn et al. (2014) is presented in the context of oceanographic measurements. Applications in inland and coastal systems are currently also increasing (Jackson and Reneau 2014).

Automated moored buoys are platforms for continuous *in situ* systems that capture hourly, daily, diurnal, and sometimes extreme events. Examples of *in situ* measurements from permanently installed instrumentation include algal pigments, coloured (or chromophoric) dissolved organic matter (CDOM), nitrates and turbidity, as well as physico-chemical measurements including conductivity, salinity, dissolved oxygen and temperature. An excellent review of commercially available *in situ* sensors can be found in Zielinski et al. (2009). Obvious advantages are the ability to measure several physico-chemical and bio-optical variables simultaneously, at high frequency and continually at one location with high sensitivity. *In situ* sensors can store data, or transmit data in (near) real time using radio telemetry, mobile phone or wireless networks. The limitations of autonomous systems include limited number of parameters one can measure, surrogate measurements not reflecting true quantities, and equipment maintenance, vulnerability, power usage, fouling and high capital expense. Much like *in situ* collection, autonomous instruments do not address spatial representation.

3.2.2 Example: Great Lakes Observing System (GLOS)

The Great Lakes Observing System (GLOS, http://data.glos.us/portal/) provides automated water quality data through the GLOS Great Lakes Buoy Portal App (Figure 3.2). Tools allow users to view, search, and optionally download data providing users with near real-time weather, wave, and water quality conditions observed in the Great Lakes. The portal allows users to check weather and wave forecasts, and to view hazard information from the National Weather Service. Observations come from both privately- and publicly-owned buoys.

Figure 3.2 Great Lakes Buoy Portal App showing location of Great Lakes buoys (photo courtesy of the Great Lakes Observing System).

3.3 Remotely-Sensed Water Quality Products

Optical remote sensing of water quality makes use of various ground-based, air- and spaceborne platforms (see Chapter 2). Aircraft-mounted spectrometers have been used successfully for water quality monitoring. They have the advantage of providing large amounts of radiometric information, i.e., generally being hyperspectral, can be used in smaller water bodies such as rivers (Olmanson et al. 2013) and do not have the extent of atmospheric interferences that satellite remote sensing encounters. The disadvantage is the higher, sometimes prohibitive costs that need to be paid directly by the end-user (rather than public space agencies paying the costs of very expensive satellite systems).

Unmanned aerial vehicles (UAVs) are increasingly receiving interest in the water quality monitoring field. They may prove less expensive and more flexible to operate than manned aircraft, and also provide high spatial resolution. As UAV platform and sensor capabilities increase in the future, they may offer an alternate tool to resource managers for particular monitoring needs. A review of current aquatic applications of UAVs is given by Klemas (2015).

Polar orbiting satellites are currently the most suitable platforms for monitoring surface water quality dynamics. Remote sensing implicates a resolution trade-off. As far as polar orbiters are concerned, Landsat-8 or Sentinel-2 provide for a 30 to 10 m spatial resolution respectively, at the expense of a relatively long revisit time of 10–16 days and limited spectro-radiometric sampling. On the other hand, moderate resolution instruments (MODIS, MERIS, VIIRS, Sentinel-3 and SGLI, see Table 6.4, Chapter 6) have lower spatial resolution but improved spectral resolution required to detect absorption features, and a shorter revisit time of 2–3 days. Geostationary satellites such as GOCI and the proposed GEO-CAPE mission enable almost equivalent spatial and spectro-radiometric resolutions at revisit times as low as 1 hour, but for limited geographic areas (for example GOCI covers an area 2500 km by 2500 km around the Korean Peninsula).

The strength of remote sensing techniques lies in their ability to provide both spatial and temporal views of surface water quality parameters not typically possible from *in situ* measurements. Some satellite programmes such as Landsat have a legacy of historical imagery, which may be processed for retrospective analysis (e.g., long-term trends). Satellite aquatic colour imagery is generally available free of charge (apart from high resolution commercial satellites such as IKONOS, QuickBird, SPOT etc.) and is easily assessable. Various retrieval algorithms are available whose suitability depends on the selected sensor and the parameter of interest, as well as on the optical water type (see Chapter 2 for more details). A strong science programme supporting satellite remote sensing continues to develop robust algorithms (see Matthews 2011 and Odermatt et al. 2012 for recent reviews) and provide information and operational products for societal use. The main disadvantages of using remote sensing for monitoring include weather (cloud cover) and atmospheric conditions (smoke, haze and dust), which interfere with the optical signal. Inclement weather may also coincide with periods of critical monitoring, such as runoff events, when satellite monitoring will be ineffective. Another disadvantage is that only those parameters that are optically-active can be detected, others need to be inferred. Spatially, remote sensing only measures surface water quality conditions (no profiles) and smaller lakes, rivers and streams may be excluded because of sensor spatial limitations. Some satellites have long revisit periods, thereby decreasing the probability to monitor episodic events.

3.3.1 Example 1: Diversity II Project

Diversity II was an ESA sponsored project utilizing EO to support the Convention on Biological Diversity (Odermatt et al. 2008). The objectives of the “Inland Water Component” of the Diversity II Project were to provide status maps, associated change maps, status indicators and trend indicators aggregated at different administrative and biome levels for selected key parameters. These included availability of freshwater and quality of freshwater, reflected in water constituents such as chlorophyll-*a* and/or suspended matter concentration, as well as temperature. The products were provided on a global scale by producing results for at least 300 large perennial inland waters, and covering the time period from 2002 to 2012 (see http://www.diversity2.info/objectives/). Below are some example products from the Diversity II Project. The illustrations in Figure 3.3 show monthly-averaged chlorophyll-*a* in Lake Turkana in 2010. Highest concentrations occur in the north, where the Omo River contributes about 90% of the lake’s terrestrial inflow and accordingly large nutrient loads that become more and more scarce in the south of its endorheic basin. Increasing hydroelectric power production on the Omo River intensifies the salinization of the lake, whose surface level has recently dropped about half a meter each year.

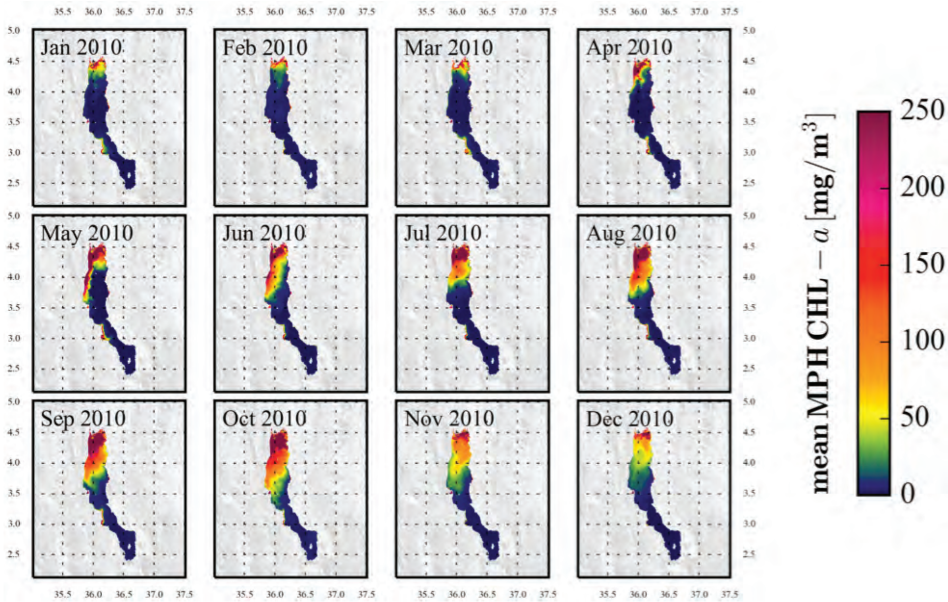

Figure 3.3 Monthly mean chlorophyll-*a* concentrations in endorheic Lake Turkana (Kenya) in 2010 from MERIS observations (Odermatt et al. 2018).

3.3.2 Example 2: CyanoLakes EO National Eutrophication Monitoring Programme

The Earth Observation National Eutrophication Monitoring Programme (EONEMP), developed by Cyanolakes (Pty) Ltd., integrates remotely-sensed estimates of cyanobacteria blooms and eutrophication (chlorophyll-*a*) into the national water management database of the Department of Water and Sanitation of the government of South Africa (see Figure 3.4). The information is being used for near-real time monitoring, and to assess historical changes in cyanobacteria blooms and eutrophication. This has dramatically increased South Africa‘s ability to both monitor and assess changes in cyanobacteria and eutrophication on a national scale (see `http://www.cyanolakes.com/`).

3.4 Considerations and Recommendations

All three approaches discussed in the previous sections have their merits and drawbacks. The monitoring objective will dictate which approach is most appropriate. Often a balance may be required with the general reciprocal relationship between spatial coverage and amount of information. Thus, *in situ* measurements evaluate processes at different time/space scales than satellite-based measurements. Zielinski et al. (2009) illustrated this relationship in the context of marine hazardous substances (see Figure 3.5).

Irrespective of the measurement approach, it is important to understand measurement uncertainties in the context of its use. Because of the rapid evolution of sensor technologies, the challenge is to provide systematic evaluations of these emerging technologies. Often researchers and managers rely on manufacturers’ specifications and do not fully understand

Figure 3.4 A view of the 102 South African water bodies included in the EONEMP public information services showing the health risk posed by cyanobacteria blooms towards recreational water users (`http://eonemp.cyanolakes.com`).

instrument performance in the context of field applications (Waldmann et al. 2010). It is critical to agree on calibration, quality control and quality assessment procedures because data are increasingly being made available to the larger end-user community beyond the initial project's intended use.

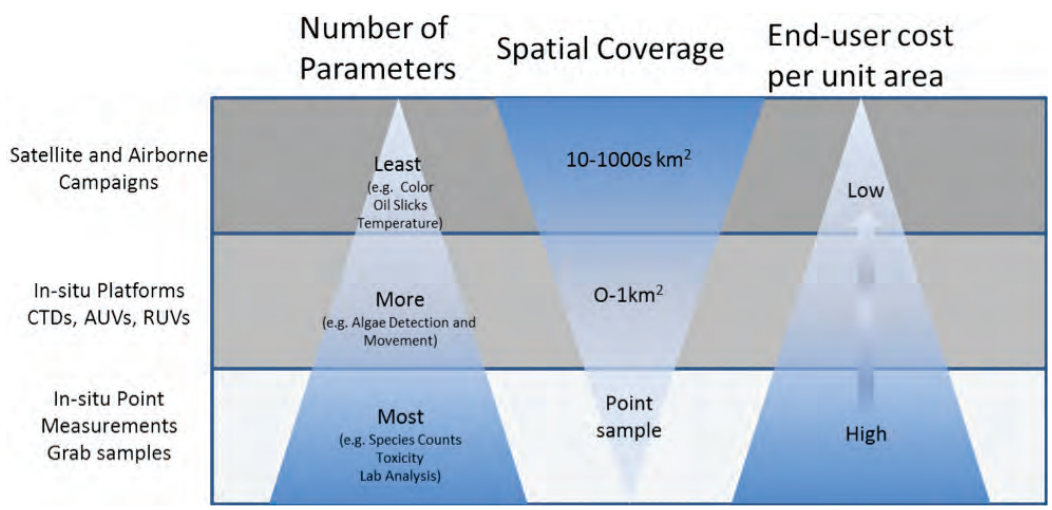

Figure 3.5 Comparison of the three generalized monitoring approaches. Adapted from Zielinski et al. (2009).

3.4.1 Satellite remote sensing accuracy

The accuracy of water quality constituent concentrations derived from remote sensing will vary depending on derived product, region of interest, and time of the year. Accuracy will also vary due to concentration of the substance, the matrix of other optically-active substances in the water, availability of appropriate satellite sensor wavebands, atmospheric corrections, and the accuracy and representativeness of the *in situ* data set (see below). Typical accuracy targets for chlorophyll-*a* are better than ±30% (IOCCG 2000) and inland and coastal waters are generally expected to have the same magnitude of accuracies. The additional value of satellite remote sensing is not always absolute accuracy of individual retrievals, but synoptic and frequent coverage of numerous water bodies, as well as changes (anomalies) from measurements (e.g., chlorophyll-*a* anomalies can be used for algae bloom indications).

Monitoring objectives concerned with trends, episodic events, and step changes will certainly benefit from satellite sensors. Even if satellite-derived data have greater uncertainties than *in situ* measurements, parameter concentration changes can nevertheless be detected if the product was derived with a consistent methodology (Stumpf et al. 2003; Hu et al. 2005). Uncertainties also need to be considered in the context of the area of interest. Algorithms developed for one water body may not provide the same degree of accuracy when applied to nearby water bodies, depending on inter-lake variability of optical properties. Zheng and DiGiacomo (2017) describe the sources of uncertainties in satellite-derived products. Though using a consistent algorithm can produce comparative errors between water bodies from different global regions, the estimated values tend to converge at higher concentrations, suggesting the possibility of a future universally-applied algorithm, particularly for turbidity and chlorophyll. Algorithms applied to operational efforts require peer-review and should be robust in covering the range of constituent concentrations with quantifiable errors. Space agencies such as NASA have documented maturity levels (https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels/) which describe their product's quality and accuracy.

3.4.2 Representativeness considerations

Ecological systems are dynamic and interact across a wide range of spatial, temporal, and organizational scales (Ostendorf 2011). Space and time considerations of system representativeness are important when considering the three monitoring approaches. For example, a discrete surface sample may represent a depth of 0 to 0.5 meters at a single point in a lake. Its representativeness will depend on environmental conditions such as light, wind, currents, degree of both vertical and horizontal mixing, and algal bloom patchiness. Patalas and Salki (1993) suggested an increase in the number of sampling locations is required with increased lake size to properly represent lake conditions. Conversely, remote sensing generally represents a greater unit of coverage (e.g., one pixel = 10 × 10 m, 30 × 30 m, 300 × 300 m to 1 × 1 km) and presents a better picture of the aggregated spatial distribution over a much greater areas (see Figure 3.6). Using MODIS satellite imagery, Ostendorf (2011) illustrated that a highly accurate, *in situ* transect in an Australian coastal area has potentially limited value despite extensive time and resources requirements, resulting in minimally improved understanding of the system variability.

Comparisons (match-ups) are often made between remotely-sensed parameters and *in situ* measurements. These exercises are sometimes erroneously termed "ground-truthing" because

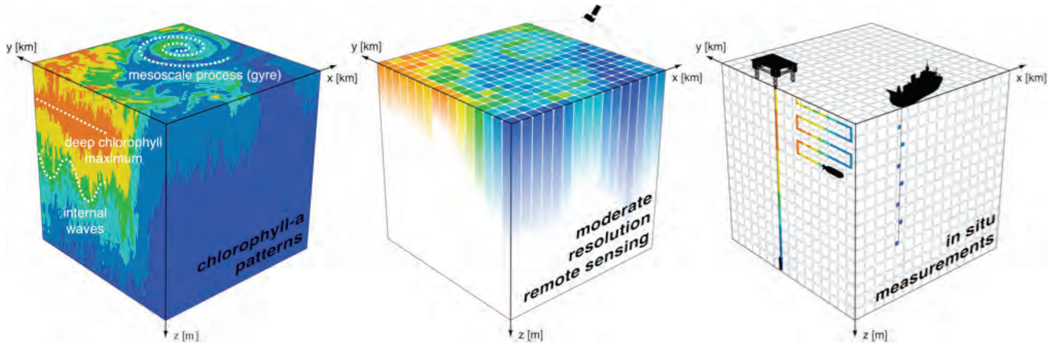

Figure 3.6 Schematic surface and near-surface spatial structures in ambient waters (left) and typical sampling patterns using remote sensing (centre) and *in situ* measurement platforms (right). Figure from Odermatt et al. (2018) available under Creative Commons license.

each of these approaches measure different spatial scales. For example, in a mesotrophic lake, a surface sample collected with a Kemmerer bottle might estimate chlorophyll-*a* concentrations in the top 1 m^2 surface area to a depth of 0.5 meters, resulting in a sample representation of 0.5 m^3. Satellite-derived chlorophyll-*a* concentrations are based on pixel size (e.g., 30 m for Landsat) and sensor penetration depth. The penetration depth is the depth a satellite "sees" into the water column and is dependent on the concentration of water constituents, and sensor wavelengths. A Landsat pixel represents an area of 900 m^2 and a volume of 900 m^3 if we assume a penetration depth of one meter.

The extent to which discrete and satellite samples correlate (match-up) depends on the underlying spatial variability (uniformity over a given pixel) and how well the point sample represents the greater average satellite coverage. In some cases the correlation between discrete transects and satellite observations is poor (see Galat and Verdin 1989). Kutser (2004) concludes that a single-point *in situ* measurement is inadequate for validation of satellite chlorophyll-*a* estimates, particularly during cyanobacterial blooms with surface scums. Other factors may influence the differences seen in match-up values, including sub-surface algal maxima, timing of sample collections, analysis methodologies and weather conditions. The use of continuous automated instrumentation and well-timed discrete samples, preferably within the shortest time between sample collection and the satellite overpass, will improve the correlation between satellite and *in situ* observations, particularly for highly dynamic events such as algal blooms and turbidity plumes.

The question is not which monitoring approach is better, but which combination of monitoring approaches is best suited for the intended objective. Temporally, *in situ* sampling (discrete or continuous) might be most appropriate for short-term temporal processes and remote sensing might be better suited for longer trends over time. Spatially, *in situ* sampling may be appropriate for small spatial areas such as estuarine tributaries, narrow lake reaches or near shore, and remote sensing for open waters and large waterbodies. The continued improvement in remote sensing capabilities has provided new opportunities to the end-user community.

In a comparison of archived MERIS imagery with historic long-term monitoring stations on Lake Geneva in Switzerland, Kiefer et al. (2015) were able to determine how well the long-term monitoring sites represented the lake chlorophyll-*a* concentrations on a seasonal and annual basis, as well as capture the variability. They found that the monitoring stations represented summer concentrations well, but missed both spring and fall temporal variability as well as spatial variability, particularly in the nearshore regions. They further provided guidance on future placement of *in situ* sites which would better capture lake chlorophyll variability.

3.4.3 Complementary role of remote sensing with *in situ* measurements

It is important to state that using satellite data does not obviate the need for *in situ* monitoring programmes, as both systems provide relevant information at different spatial and temporal scales. The power of utilizing remote sensing will not be a replacement of traditional sampling approaches, as both approaches play a complementary role. Use of either *in situ* or remotely-sensed data in isolation has reduced value as compared to the monitoring tools used together (Devlin et al. 2013).

Remote sensing has the ability to build on, or extrapolate between limited *in situ* measurements by expanding the spatial and temporal coverage to provide better characterization of the water body. Combining these two data sources in their study of chlorophyll-*a* variability in the Great Barrier Reef, Devlin et al. (2013) used remote sensing to extrapolate point data into a spatial framework to better determine the conditions under which chlorophyll-*a* concentrations became elevated. Kallio et al. (2003) used airborne remote sensing to present complete spatial chlorophyll-*a* coverage for two Finnish lakes. Comparing mean chlorophyll-*a* concentrations from the three routine lake stations with mean chlorophyll-*a* obtained from the remote-sensing product yielded a difference of 47%. Remotely-sensed chlorophyll-*a* products can be used to help target priority areas of interest for more intense sampling and identify future sampling stations that best represent lake conditions.

3.4.4 Complementary role of remote sensing with modelling

The complexity and dynamic nature of inland and coastal waters can be difficult to characterize. Robust models (catchment run-off, 3-D hydrodynamic and biogeochemical) are being increasingly used for water management, but current models may not resolve events because of data and time-step limitations on the timing and location of these events (e.g., storm-water runoff, algal blooms, coastal currents). New modelling methods are being advanced which merge satellite observations as input parameters in an effort to better understand underlying biogeochemical processes, and use their predictive powers to forecast future change. Modelling coastal and inland waters is complex because connections between environmental variation and ecological systems occur across multiple and interactive spatial, temporal and organizational scales (Devlin et al. 2013).

Modelling tools can simulate and predict transport of nutrients, pollutants and contaminants. Furthermore, modelling efforts can expand the temporal coverage of the remote-sensing products. For example, persistent cloud cover can hamper satellite remotely-sensed products and these gaps can be filled-in with modelling efforts. Remote-sensing data may be used for defining initial conditions, boundary conditions, model parameterisation, forcing and validation. Remotely-sensed data assimilation into biogeochemical models is commonly used to make mid-course simulation corrections and model parameterisation. A key issue in utilizing remotely-sensed data in modelling efforts is whether the data products represent the same quantities modelled. This can be due to depth of light penetration or imagery spatial scales vs. modelling grid.

3.4.5 Costs

It is difficult to do a comparative cost analysis of the three major monitoring approaches described above in Sections 3.2 to 3.4. Each approach has its strengths and weaknesses, and though cost is one factor, one must start with the monitoring objectives and determine whether each of the approaches will provide the necessary information. Clearly, costs of traditional *in situ* monitoring networks continue to rise. The implementation of the European water directive framework costs are estimated at 6–11 million Euros in the UK and Netherlands (Nocker et al. 2007) and 6–9 million Euros for Norway, Sweden and Finland (Halleraker et al. 2013).

Autonomous data sondes are becoming increasingly popular for monitoring constituents such as dissolved oxygen, temperature, conductivity, pH, turbidity, chlorophyll and cyano-pigments fluorescence and NO_3. Decreasing costs and increased memory allows enormous amounts of data to be collected in key locations. Though initial costs may be 5–10K for some of these devices, the cost per measurement (10's of thousands over a season) will be quite low. A good resource guide to current *in situ* monitoring equipment costs and new emerging technologies was compiled by the Chesapeake Conservancy's Conservation Innovation Center (http://www.chesapeakeconservancy.org/images/Low_Cost_Water_Quality_Monitoring_Needs_Assessment_small1.pdf).

Dekker and Hestir (2012) provide a cost-benefit analysis for setting up a prototype Earth observation monitoring system for Australia utilizing either Landsat or MODIS/MERIS satellites. Their analysis provides both the initial parameterization of service and the operational aspects, and builds upon current research activities and infrastructure. For other countries or regional programmes, the situation may be different. Campbell (2013) points out that it is probably not possible to provide a generic cost assessment of remote sensing given each situation has variable factors, e.g., expediency of collecting a point sample vs. need for spatial characterization. Bukata (2005) suggests a perspective of "cost per monitored area" (i.e., cost per variable per square area). For example, if only one chlorophyll sample/year was required on a 5000 hectare (ha) lake, then the costs for remote sensing (infrastructure and FTE time) is probably unreasonable. On the other hand, if water quality measurements were required for every 10 ha of the 5000 ha lake, then remote sensing would be more attractive. In Wisconsin, where water clarity for 8000 lakes is determined annually from Landsat (http://dnr.wi.gov/lakes/clmn/remotesensing/), image processing labor costs run approximately $1.50 per lake (not including computer hardware and software costs). It would cost far more to use a traditional approach involving staff time, boats, travel costs, etc. to meet those same deliverables. In conclusion, cost considerations, though important, must be taken in the context of the monitoring objective where the informational needs define the monitoring requirements.

Questions the End User Should Consider

Monitoring requirements

- ❖ Can I use satellite remote sensing information to bolster my field monitoring data and what are some key limitations/restrictions of using satellite remote sensing?
- ❖ What parameters can satellite remote sensing monitor?
- ❖ What are my monitoring needs in terms of temporal and spatial requirements?
- ❖ How can satellite remote sensing help me with water quality standards development, regulatory needs or long-term trends?
- ❖ What are the published accuracies of satellite remote sensing parameters of interest, and are they applicable to my water bodies?

Satellite Sensors

- ❖ How can I determine which satellite(s) to use for my waterbody specific project?
- ❖ Can I use information from multiple satellites?
- ❖ How long will the current satellite remain operational and what happens if my satellite is decommissioned in the future?
- ❖ Which satellites are best suited to my waterbody e.g., lakes, rivers, estuaries, offshore waters, and are there certain waterbody types where satellite remote sensing is difficult or not yet feasible to apply?
- ❖ What is satellite product or variable validation and why is this step important?

Remote Sensing Resources

- ❖ Are satellite-derived water quality products readily available from government agencies or other reputable sources, and is the data easy to download and work with?
- ❖ If not available and I want to produce these water quality products, what technical expertise and software do I need?
- ❖ What are some key resources that can give me more information on satellite remote sensing?
- ❖ What are some examples where remote sensing has been used successfully for assisting water quality monitoring programmes?

Validation questions

- ❖ How representative is the dynamic range of the satellite validation results?
- ❖ How spatially and temporally representative are the satellite results?
- ❖ Do the satellite results hold under different conditions such as seasons, or narrow vs. centralized locations?

3.5 Resources

3.5.1 Monitoring strategies

The U.S. EPA Watershed Academy training modules found at `http://www.epa.gov/watertrain` provide self-paced training modules and webcasts from national experts about a range of watershed management topics. The technical report on Planning of Water Quality Monitoring Systems was developed by the World Meteorological Organization (WMO) jointly with UNEP GEMS/Water (WMO 2013) is an effort to provide basic know-how and the materials needed to plan, establish and operate water-quality monitoring systems on national levels, but also with a view to improving access to water-quality data and information in transboundary basins and globally.

The U.S. National Water Quality Monitoring Council (NWQMC, https://acwi.gov/monitoring/) provides numerous resources on all aspects of water quality monitoring. The NWQMC was created in 1997 as a vehicle for bringing together diverse expertise needed to develop collaborative, comparable, and cost-effective approaches for monitoring and assessing the U.S. water quality.

The European funded Copernicus Marine Environment Monitoring Service (http://marine.copernicus.eu/) was designed to respond to issues emerging in the environmental, business and scientific sectors. Using information from both satellite and *in situ* observations, it provides state-of-the-art analyses and forecasts daily, which offer an unprecedented capability to observe, understand and anticipate marine environment events. The Copernicus Global Land Service (http://land.copernicus.eu/global/themes/water) reliably provides a set of biophysical variables which describe the state and evolution of vegetation, the energy budget, the water cycle and the cryosphere over the land surface at a global scale. Currently, surface water area and elevation are provided. In the near future, the dataset will include surface water temperature, reflectance, turbidity and trophic status for over 1000 of the largest water bodies.

The U.S. Great Lakes data are accessible through the GLOS web-based data portal and specialized decision support tools are available (http://data.glos.us/portal/, see also Section 3.2.2). The Data Portal provides browsing access to near-real time data for satellite observations as well as numerous *in situ* observations and model forecasts.

3.5.2 Access to satellite imagery and processing software

Several repositories offer historic and current satellite imagery:

- SeaDAS (https://seadas.gsfc.nasa.gov/) is a comprehensive software package for processing, display, analysis, and quality control of ocean colour data. While the primary focus of SeaDAS is ocean colour data, it is applicable to many satellite-based Earth science data analyses. Originally developed to support the SeaWiFS mission, it now supports most U.S. and international ocean colour missions. Tutorials are offered on line.
- NASA's Ocean Biology Processing Group (OBPG, https://oceancolor.gsfc.nasa.gov/data/overview) serves as a Distributed Active Archive Center (OB.DAAC), responsible for archiving satellite ocean biology data produced or collected under NASA's Earth Observing System Data and Information System (EOSDIS). Their holdings include a mixture of historical and current missions, as well as data from both NASA and partner space organizations.
- The Ocean Color Viewer (OCView: https://www.star.nesdis.noaa.gov/socd/mecb/color/ocview/ocview.html) is an online resource from the NOAA Ocean Color Team providing an interactive view of the global satellite ocean colour (water quality) product and true colour imagery with additional data layers and functionality. Satellite data are primarily from VIIRS on SNPP

and NOAA-20, but also include ocean colour data from OLCI on Sentinel-3 and regional geostationary GOCI (South Korea). VIIRS ocean colour (water quality) data can be freely downloaded from NOAA CoastWatch website at: https://coastwatch.noaa.gov/.

- ❖ Global Visualization Viewer (GloVis, https://glovis.usgs.gov/) is operated by the U.S. Geological Survey and provides a free service to view, order, and/or download remotely-sensed data. Their archive contains both Landsat and Sentinel-2 imagery.
- ❖ Copernicus Open Access Hub (https://scihub.copernicus.eu) is operated by the European Space Agency and the European Commission. It provides complete, free and open access to global Sentinel-1, Sentinel-2 and Sentinel-3 user products, starting from the In-Orbit Commissioning Review (IOCR).
- ❖ Sentinel Application Platform (SNAP: http://step.esa.int/main/toolboxes/snap/) is a collection of executable tools and application programming interfaces which have been developed to facilitate the utilisation, viewing and processing of a variety of remotely-sensed data. The functionality of SNAP is accessed through the Sentinel Toolbox. The purpose of the Sentinel Toolbox is not to duplicate existing commercial packages, but to complement them with functions dedicated to the handling of data products from Earth observing satellites.

In addition, there are a number of private consultants that provide geo-spatial services that specialize in aquatic resources. They provide information for commercial as well as governmental uses. Examples of these services include:

- ❖ EOMAP (http://www.eomap.com/)
- ❖ Brockmann Consult (https://web.brockmann-consult.de/)
- ❖ CyanoLakes (Pty.) Ltd. (http://www.cyanolakes.com/)

3.5.3 Training

The NASA ARSET programme (https://arset.gsfc.nasa.gov/) offers satellite remote sensing training that builds the skills to integrate NASA Earth science data into an agency's decision-making activities. Various modules are offered related to water quality. These modules generally require no, or minimal remote sensing training.

The International Ocean Colour Coordinating Group (IOCCG) also provides links to a wealth of information and resources on all aspects of satellite remote sensing, including advanced training opportunities (see http://ioccg.org/what-we-do/training-and-education/).

Chapter 4

Linkages Between Data Providers and End Users

Richard P. Stumpf, Carsten Brockmann, Blake A. Schaeffer and Arnold Dekker

4.1 Context

Multiple stakeholders and user requirements for products derived from remote sensing (Chapter 1) lead to a number of criteria involved in providing those products. These criteria cover several broad categories: delivery, quality, temporal context, and timeliness. At the highest level is the nature of the data delivery; this covers identifying appropriate products, tools, and training to support applications for managers. It is tempting for remote sensing scientists to process products for delivery to a web page, with the assumption that the availability of the products will help solve managers' concern. However, if data delivery issues such as format, training, and access are not properly addressed, the data will not be used. The key concern is data quality and consistency. Managers need to have an evaluation of data quality, and information on data consistency and potential failures. They must have confidence in the data and be able to identify errors or failures. In return, remote sensing scientists require data sets from the user community to support validation. Also of concern is the timeliness characteristics of the data; does the application require retrospective data or current data, and if the latter, is the data required in real-time or is a delay of a season or more acceptable? These four areas of concern — delivery, quality, temporal context, and timeliness, shape the linkages between data providers and end users.

4.2 Data Related Information Delivery

Data related information delivery captures a range of complexities, including access methodology, data format, metadata requirements, analysis and analysis tools, and training. The fundamental challenge with data delivery is that none of these issues can be correctly identified without direct interaction with the end users. This interaction must identify users' capabilities, knowledge, and resource commitment. End users need to extract the maximum amount of information for their requirements with the minimum effort in processing image data.

New advances in computation discussed in Chapter 8 offer substantial changes in data delivery. Cloud storage and access, cloud computing, smartphones and computer applications ("apps") offer capabilities that have not been previously considered. They also have the potential to address the need for multiple delivery mechanisms and data formats.

4.2.1 Data formats

Typically products that require advanced remote sensing analysis tools, such as NASA's SeaDAS (Sea Data Analysis System) will be beyond the scope of a resource manager. Products that are directly compatible with geographic information systems (GIS) will have the greatest value for most managers and applications. For water quality products, GIS compatibility will depend on the user requirement. Recognition of these distinctions by the data provider will lead to the greatest uptake of the product.

For map products, GIS compatibility should be maintained. Graphics files, such as GIF, PNG, and JPG, are common, and are certainly useful as a screening tool for identifying cloud-free images or seeing features that need only qualitative visual assessment. They are, however, the least useful to a user, as they do not store geographic information internally (geography must be stored in a separate "world" file) and are not designed to preserve data values. For small lakes this is not necessarily a problem; if users can readily identify the lake, they may use colour to qualitatively assess the pattern. For larger or unfamiliar water bodies, or for habitats, the user has to guess locations and values from these products. GIS compatible formats are thus critical. GIS-based image formats, such as geoTIFF, provide a compromise, allowing construction of consistent image display and addressing the geographic and data value needs.

Several data format options allow at least the extraction of latitude and longitude (Table 4.1). Websites can be constructed to allow extraction of latitude and longitude from pictures with no knowledge of a computer programme (NASA WorldView; https://earthdata.nasa.gov/labs/worldview/). More advanced options exist within programmes. For the general user, the standard PDF Acrobat Reader supports extraction of spatial information, so geoPDFs can provide a simple, usable information set (Figure 4.1, Florida geoPDF, products available at https://tidesandcurrents.noaa.gov/hab/gomx.html). Vector data values can also be imbedded in the PDF, so more information can be extracted. Online mapping tools, such as GoogleMaps or GoogleEarth, allow similar extraction of some geographic and vector (or graphical) information. At the next level, GeoTIFF files provide pictorial information as well as being geographic data files. They can maintain both data values and the colour information in "8-bit" (256 value) or 24-bit (true colour) files. TIFF has "tags" that can provide information on the file content. This provides a dual use — an immediate view of the information, while allowing data extraction in a GIS programme. Data analysis formats such as HDF and netCDF offer detailed metadata, but are not designed for pictorial representation, and do not currently interact well with GIS software. These formats are more suitable as the background formats for data processing and extraction tools.

Habitat mapping requires GIS formats, as most questions revolve around the relationship between the habitat and other land use patterns, or spatial changes in habitat type. Water quality applications have a more variable requirement. Monitoring of algal blooms or sediment plumes in large lakes or bays may need the image information to capture the spatial patterns.

In small water bodies, data extraction may become more useful. A manager addressing a specific water body may want to obtain temporal patterns: is the bloom increasing over a

Table 4.1 File formats and applicability to remote sensing applications

Product	Pictorial	Geographic	Data
GIF, PNG, JPG	Yes	Only with separate "world" file	No
PDF	Yes	Yes as geoPDF	Vector
geoTIFF	Yes (as 8-bit or 24-bit)	Yes	Raster
Data files (HDF, netCDF, etc.)	Not at present	Yes	Raster and vector

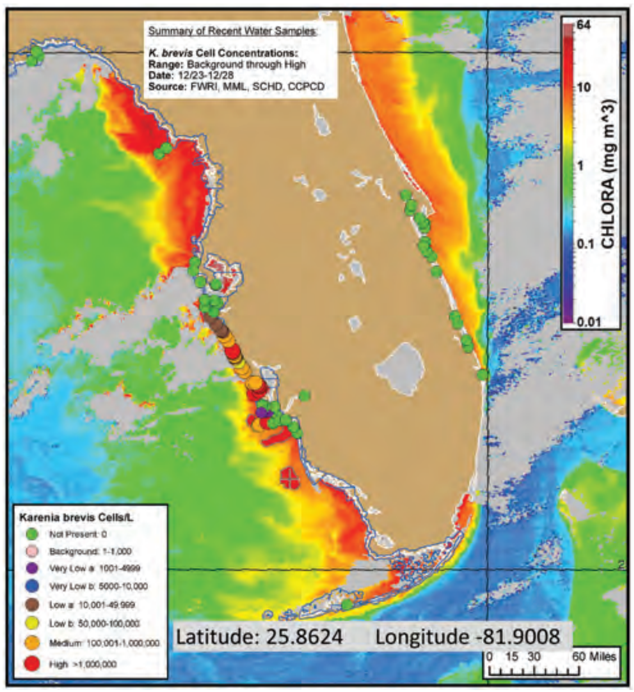

Figure 4.1 Image of a GeoPDF of Florida from the NOAA Florida harmful algal bloom bulletin. Image was taken by MODIS on 31 Dec 2017 (from Bulletin 2018-001 at `https://tidesandcurrents.noaa.gov/hab/gomx.html`.)

specific time period, or has the turbidity spiked? In this case data extraction tools would be potentially more useful. Metadata for files will need to capture the key points: what the values mean (whether scaled integers or real numbers), units, algorithms, applied masks or flags, as well as information on quality control.

4.2.2 Data extraction and analysis tools

Data extraction tools will develop rapidly over the next few years. Among the options for most managers are ArcGIS-based, open access GIS, smartphone app-based, and Web-based tools. Open access GIS software has a long history, starting in 1982 with the Geographic Resources

Analysis Support System (GRASS, https://grass.osgeo.org/) and the recent development of QGIS (http://www.qgis.org/en/site/). These two packages are also establishing compatibility to take advantage of their complementary strengths. On the commercial side, ArcGIS is the *de facto* standard, as it is widely used in the management community. GIS data, of course, would allow a GIS lab in the management office to extract the time series of interest, and adjust the methods and results. The incorporation of Python as a scripting tool enhances this option when the tools are written in Python. Web-based options exist, where data can be extracted using a website. One of the best examples at present is NASA's Giovanni site (https://giovanni.gsfc.nasa.gov/giovanni/). It requires only enough knowledge to choose a product (although only 4-km or 9-km resolution), and it can deliver data from a rectangle to a graphic, and to an exportable form compatible with a spreadsheet. Some websites can automatically create time series from fixed locations. With the rise of cloud storage and computing, web-based options for user selection will become more frequent and flexible. The development of Smartphone apps may promote the use of satellite data, encouraging more users and potentially new ideas in distribution and display. Figure 4.2, shows an example of the U.S. Environmental Protection Agency (EPA) Cyanobacteria Assessment Network (CyAN) app (source code located at https://github.com/USEPA/EPA-Cyano).

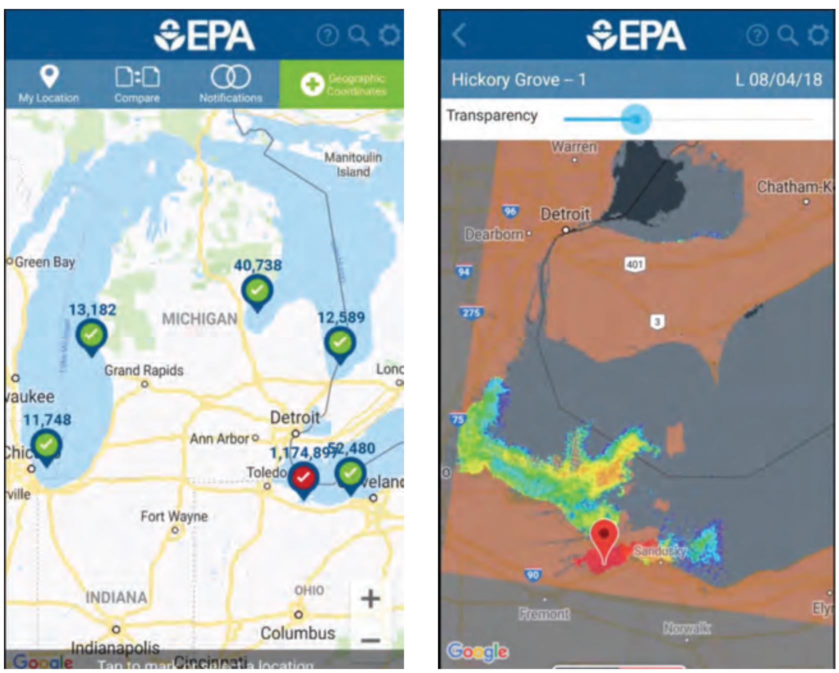

Figure 4.2 Example of the ability to drop pin locations in water bodies of interest. The pin extracts satellite-derived data from the specific lat/long coordinates. The CyAN application can also display GeoTIFF files of satellite-derived products (Mattas-Curry et al. 2015).

4.3 Training

Training of end users will involve understanding the options for Earth observation data acquisition and data extraction, and also understanding the data quality and data limitations. Training is not a substitute for robust algorithms and proper quality control. This may seem obvious, but it is not. Providing a standard ocean chlorophyll-*a* algorithm to estuary managers, then "training" the managers to ignore the "high chlorophyll" (i.e., when the water is optically shallow, or turbid, or high in CDOM), will not lead to use of the data product, and is a waste of time for both the user and the product distributer/producer. Training strategies are rarely presented in the literature, and most scientists have little experience in training managers. The data producers/product distributers may generate the product themselves, or modify a standard product created by an agency like NASA or ESA. They often start from scratch with little knowledge of what has been learned about the user needs by other data producers.

The training needs to cover quality control, accuracy, and uncertainties. Also, as no remote sensing model is 100% reliable, managers need to know what to look for in order to exclude the small percentage of suspect data. Training may also lead to interesting feedback. A producer may automatically disregard image portions that are suspect, while a user will assume that they are valid. Noting this discrepancy in quality can lead to review and improvement of the algorithms. On the other hand, accuracy requirements can differ between scientists and managers. A state or provincial resource manager may want the relative water clarity for their lakes, while a scientist developing an ecological model requires accurate light attenuation (IOCS 2015). It is recommended that Earth observation-based information products also contain associated images of data accuracy assessment.

4.4 Quality Control

Quality control (QC) is inconsistent across remote sensing applications. Habitat mapping has a well-established procedure for skill assessment going back decades (Congalton and Green 1999; Foody 2002). This includes user and producer errors across habitat classes and eco-regions, and methods for change evaluation.

QC strategies for water quality are much less robust. The emphasis tends to be on algorithm accuracy, following the point-based matchup methods used for the global chlorophyll algorithm, while reproducibility, robustness and image accuracy are not frequently considered. Algorithm accuracy (Table 4.2) has examples of parameters that should be addressed. Simple regression metrics do not address algorithm robustness. Spatial and temporal patchiness (Kutser 2009) introduce artifacts that confound data misfit with data error (Lynch et al. 2009). For some topics, such as bloom detection, type 1 (false positive) and type 2 (false negative) errors are of particular concern to managers (Tomlinson et al. 2004) and classification metrics are particularly important. For example, classification is subject to auto-correlation error (Congalton and Green 1999) where pixels that are adjacent in time or space will classify the same, correctly or incorrectly. The auto-correlation issue forces a need for spatially- and temporally-discrete sampling. For continuous quantities, such as chlorophyll or IOPs, water

Table 4.2 Quality control requirements

Image quality control	**Parameter quality control**
Consistency within the image (no false contours)	Accuracy over the data range
Robustness (consistency between images having different atmosphere, look angles etc.)	Reproducibility under varying water quality conditions
Invalid data failure rate	Algorithm failure rate
Consistent masking/flagging of invalid data	Impact of flags on accuracy assessment

type errors may occur, the algorithm may perform well in one water type, and poorly in another (Moore et al. 2014), or the algorithm may consistently underestimate in one regime, and overestimate in another.

4.5 Validation Data

Validation data sets may originate from many sources. For habitat mapping projects, the producer depends on data collected through programmes run by the user community, such as regional resource management agencies, and in some cases, users may enhance community run programmes if they perceive the remote sensing products to be of value. Major challenges in obtaining validation datasets are access, inconsistent formatting, and variable methods. These problems can be solved for programmes that are coupled with remote sensing (Table 4.3), but are harder to solve for datasets collected for other purposes.

The remote sensing data producer faces some significant challenges in using existing data collection programmes. The data collected in a standardized programme may not be optimal for remote sensing validation. One programme may systematically measure chlorophyll-*a* using a laboratory fluorometer, uncorrected for phaeopigments, another may use HLPC. One programme may use cell counts for HABs, another will use bio-volume. These variations imply that a single validation strategy will not work. Classification metrics may be necessary, and relative (rather than absolute) concentrations may become part of the validation.

Using HABs as an example, different validation concepts are evident (Table 4.3). A coupled programme assures that the field data is available, usable, and directly compatible with the remote sensing data. The next best option is drawing on a systematic measurement programme. The data set is self-consistent and the management community has established format and access protocols. This is most effective in water quality programmes, however, HAB monitoring in the Gulf of Mexico also fits this description (Stumpf et al. 2003); the states all used cell count concentrations from standard microscopy. Intensive programmes such as the U.S. National Lake Assessment have the consistency and access of other systematic programmes, however, they are focused in time, and are not repeated each year.

Ad hoc programmes i.e., those that are conducted in response to an event or as part of an independent research project, may provide key validation data, but they have significant challenges. Methods may differ, quality control may be lacking, and even data organization

Table 4.3 Example programmes that provide validation data sets

Validation programme	Examples	Typical parameters	Issues
Integrated satellite and field	Finland, Norway, Lake Erie	Cell counts, HAB pigments	Establishing the programme
Systematic national and regional field collection	EU Water Directive, GBRMPA, U.S. EPA Estuary programmes (Chesapeake Bay, San Francisco Bay, Tampa Bay)	Chlorophyll, turbidity, phytoplankton taxonomy	Limited areas
National intensive programmes	U.S. National Lake Assessment	Chlorophyll, nutrients, oxygen, taxonomy, etc.	Limited time, parameter
Routine local programmes	States, municipalities, parks	HAB cell counts, chlorophyll, turbidity	Format, parameters
Ad hoc: research, event response	Universities, various governments	Various	Format, parameters, access

may be inconsistent. For the organization producing the remotely-sensed product, the key challenge is to convince a user organization that is collecting field data to address these issues. If the product is useful to the user, one effective way to solve the problem is to fund the field data provider to address the data deficiencies. If the product is demonstrated to have real value to users, they may modify or augment their field programme to support validation data sets.

Two established data sets widely used include the Bio-optical Archive and Storage System (SeaBASS), a publicly shared archive of *in situ* oceanographic and atmospheric data maintained by the NASA OBPG (https://seabass.gsfc.nasa.gov/) and LIMNADES, a freshwater focussed repository for inherent and apparent optical property datasets and associated water constituent measurements as well as *in situ* water constituent measurements for satellite validation (http://www.globolakes.ac.uk/limnades.html).

4.6 Timeliness

For users that need to respond to specific WQ events, products must be delivered in a timely and useful way. For example, health agencies need to know whether potentially toxic blooms are present, water suppliers need to deal with phytoplankton biomass and toxicity, environmental agencies need to anticipate impacts on aquatic life and wildlife, clean-ups of fish kills, and public reports of unusual water conditions. Harmful algal blooms are an obvious application of real-time monitoring, and several examples exist (Florida - Stumpf et al. 2003; Lake Erie - Wynne et al. 2013b; the Finnish Baltic - Hansson and Hakansson 2007; Ireland, Maguire et al. 2016).

4.6.1 Data latency

Data latency, the time delay from satellite acquisition to delivery to the user, depends on several processes: data transfer from satellite, speed of the ground processing system, delivery to data producer, production time (which may include integrating other inputs), and finally product review. In principle, a product from a morning satellite can be delivered to users before the close of the business day. In most cases, products are available the next day, which will meet HAB public health requirements. If manual review is needed, the delay may increase. Clouds are a significant confounding impact for all optical and thermal sensors. Data compositing or other modelling may be required to address data loss due to cloud cover. The objective for many remote-sensing products is same day latency, but in reality many days may pass before usable products are available.

For habitat mapping, the timeliness requirement can range from days, in the case of habitat damage, to weeks for mapping projects. Products that take weeks to produce (such as habitat maps) will need continued algorithm development to reduce labor and increase timeliness. Algorithm development will also help in merging data from multiple sensors such as Landsat OLI and Sentinel-2 MSI in order to achieve an acceptable production latency for cloud-free imagery.

4.6.2 Real-time monitoring and response

Public health and environmental emergencies need timely products. Monitoring and response place a substantial burden on the data producers. The weather forecast community refers to models as “model guidance”, not as forecasts. The forecasts are generated from the combination of models, data, and analysis. If the models are distributed as the product, the end user has the job of creating a forecast. A similar concept is needed for satellite data. When supporting a response, the satellite data set is essentially a model, leaving the question of how the forecast (hazard) is determined. Automatic distribution of satellite data is the equivalent to distributing a weather model. The user has been provided the satellite guidance, but not the forecast. This can be appropriate, but requires the user to become an expert at interpreting the satellite data, understanding product idiosyncrasies, and generating the appropriate forecast. There are alternatives. Using the weather analogy, the U.S. National Weather Service produces a National Digital Forecast Database (NDFD), where the actual forecasts (made by weather forecasts) are distributed in a compatible format that is readable as a model or dataset. In the realm of satellite data, the Florida HAB bulletin (Stumpf et al. 2003) uses analysts to incorporate previous knowledge to identify features in the satellite image that are likely HABs. The Lake Erie Bulletin (Wynne et al. 2013b) has imagery where the stray and invalid pixel values have been edited out, both digitally and manually (the latter with standard protocols). With such products, false positives or false negatives are not repeated endlessly when the algorithm systematically fails, and random failures do not translate into products when anomalous conditions occur (such as sediment resuspension events). Similar strategies can be developed by coupling satellite data with hydrodynamic or ecological models (Wynne et al. 2013b; Baird et al. 2016; Maguire et al. 2016). The value of the satellite data increases as a result of the additional analysis.

4.6.3 Current assessment

Current assessment involves identifying the relative health of water bodies or habitats at the present time. Assessment and monitoring (Section 4.5) can cover a continuum, and repeating assessments over multiple years leads to retrospective analysis. Assessment provides the status of the system, while monitoring would typically support an immediate management response. The quality control for assessment is more stringent than real-time applications. Assessments have been applied with a variety of satellite sensors and require algorithms that are valid across water bodies for the variable of interest. Landsat has been used to examine the "10,000" lakes in Minnesota every few years (Olmanson et al. 2008) as well as the Great Barrier Reef (Roelfsema et al. 2006). Habitat studies, such as seagrass extent or coral health, are a typical example of current assessments.

4.6.4 Retrospective assessment

Retrospective assessment involves evaluation of trends in water quality and whether water bodies have changed. These have particular value in developing scenarios that might support forecasts or allow development of management strategies. Examples include studies of cyanobacteria blooms in the Baltic (Kahru and Elmgren 2014) and in Lake Erie (Stumpf et al. 2012) where evaluation of the inter-annual variability allowed determination of the role of nutrient loading. The study by Stumpf et al. (2012) helped inform the development of nutrient target loads by the U.S. and Canada through the Great Lakes Water Quality Agreement. Retrospective studies also capture the phenology of blooms (e.g., in Hungary, Palmer et al. 2015a), and patterns between lakes (e.g., in South Africa, Matthews 2014) and the frequency of events that pose a risk for various uses, such as the potential risk of toxic cyanobacteria to drinking water suppliers (e.g., Lake Erie, Wynne and Stumpf 2015). They can also identify when conditions changed prior to development of monitoring programmes. For example, researchers in the late 1980s discovered dying seagrass in Florida Bay which appeared to lead to an increase in turbidity. A retrospective analysis using remote sensing determined the scale of seagrass loss and timing of turbidity development before a field monitoring programme was implemented (Stumpf et al. 1999).

Retrospective assessments are particularly challenging with regard to the difficulty of evaluating the data products. The monitoring programmes that support algorithm development typically post-date the available satellite data (especially with Landsat). As a result, the quality control requirements (Section 4.4) should become both rigorous and flexible for these studies, which appears to be an oxymoron. The rigor is in assessing the robustness of the algorithm under potentially variable conditions that may have occurred. The flexibility is in the types of observations used to provide confidence in the retrospective conditions. For example, if turbidity changed, a chlorophyll algorithm that may be valid in clear water may perform poorly during periods of turbid water. The algorithm must be evaluated over the range of turbidity and chlorophyll conditions observed over the time frame of interest, which will increase the rigor of quality control. For flexibility, qualitative validation methods become necessary. In the Florida Bay case mentioned above, seagrass researchers reported a rapid die-off of seagrass in a narrow time frame (i.e., late 1989). Stumpf et al. (1999) evaluated the satellite data and confirmed that it identified a change in the appropriate area during this narrow period. Dekker et al. (2005), Schroeder et al. (2012) and Devlin et al. (2012) demonstrated the value of satellite data in identifying the influence of river plumes on the Great Barrier Reef.

4.7 Future Collaborative Efforts

Schaeffer et al. (2013b) observed that an open and effective dialogue is needed between scientists, policy makers, environmental managers, and stakeholders at national, state, and local levels. This is a recurring challenge — the same issues were identified by Specter (1990) regarding training and understanding. Managers and scientists do not necessarily travel in the same circles or even address the same issues. Fortunately, many global routine management applications use satellite data products. Each of these has developed skills and knowledge that can help advance the application of satellite data in other areas. The insights and understanding developed through collaboration between data providers and managers needs to be shared.

Frequently, the remote sensing community works with managers or researchers who are extremely knowledgeable about remote sensing. However, the key user communities should not be required to have a deep understanding of remote sensing. Knowledge of a satellite product should be comparable to their understanding of a chlorophyll measurement, but not to the same level as being able to manage the nuances of HPLC, or atmospheric correction. Training programmes for managers are becoming more common. One example, NASA's Applied Remote Sensing Training (ARSET) programme, introduces managers to satellite products through Webinars with global access. After 22+ years the same issues identified by Specter (1990) regarding training and understanding still stand today.

4.8 Recommendations to Reach Users

Data delivery implies educating and informing end users so they can educate and inform the product scientists. Local efforts exist now, but international strategies are necessary. Some specific strategies include the following:

1. Assessments within existing monitoring systems should be used to identify algorithm strengths and deficiencies, and gaps in remote sensing. International programmes, such as GEO, AquaWatch and Blue Planet as well as the European Union Directives, need to make it easier to share this information. Algorithm evaluation should occur in the application setting, with confirmation that the algorithm is addressing the user requirements. In turn, research programmes need to be informed of deficiencies, so that improvements can target the application weaknesses.
2. International programmes and journal editors need to promote transfer and comparison

of algorithms between regions in order to evaluate the robustness of methods; the results will identify strengths, improve quality control, transfer knowledge and identify gaps that can inform future research. Consistent metrics that are appropriate for science and applications need to be identified, and authors and reviewers should be encouraged to use these.

3. International programmes should be encouraged to organize workshops to help share successes and "lessons learned" between different communities in sharing data with users. These programmes need to seek out successful projects and provide resources to develop them, specifically courses and training materials, and not just workshops.
4. A common resource should be developed on strategies for supporting end users and WQ managers; journal editors should be encouraged to help promote this exchange, which may involve special issues of journals on management applications, with managers as key participants in the papers, or management sections (e.g., journals such as Science or Nature have sections that address different audiences).

Chapter 5

Understanding the Satellite Signal from Inland and Coastal Waters

Mark William Matthews, Stewart Bernard, Lisl Robertson Lain, Derek Griffith, Daniel Odermatt and Tiit Kutser

5.1 Introduction

The third report in the IOCCG series (IOCCG 2000) addresses remote sensing in coastal and other optically-complex waters. In this report, an introduction is presented on the colour of case 2 waters, defined as those waters where the water-leaving signal is significantly affected by constituents other than phytoplankton, namely tripton, composed of detritus and minerals, and coloured dissolved organic matter (CDOM) consisting of humic and fulvic acids (the reader is referred to Chapter 2 in IOCCG 2000 for further details).

General challenges for optically-complex waters are extensively addressed in IOCCG (2000). More recently, however, a significant body of literature has developed related to remote sensing of spatially-constrained inland waters, which sets apart particular challenges that do not equally apply for coastal waters. In addition, the development of new sensors and concomitant algorithms and approaches means that significant advances have been made since 2000.

Understanding the signal measured at the top of the atmosphere (TOA) by a satellite in space begins with radiative transfer in water and the atmosphere. As described in Chapter 2 of this report, the signal leaving the water arises from several sources including the water itself, the water constituents (namely phytoplankton, tripton and CDOM), benthic or submerged vegetation (if present), and the bottom substrate (if optically shallow). Note: tripton is equivalent to non-algal articles (NAP) and represents particulate matter minus the extracted pigments. The signal from the atmosphere is affected by atmospheric gases (e.g., O_2, H_2O) and aerosols (e.g., dust and smoke particles). In addition, the atmospheric signal may contain stray light scattered into the instrument field-of-view from adjacent land (called the adjacency effect which depends on the target size and the optical properties of the surrounding vegetation or soil), cloud (if present) and light reflected from the water surface (sun glint or specular reflectance, if present).

The unique challenges faced in inland water bodies results from processes occurring both in the water and in the atmosphere. This may include extreme ranges in the concentrations of independently varying water constituents; the presence of blooms of cyanobacteria driven by nutrient concentrations that are extremely high when compared with coastal and open ocean waters; bottom signals in shallow water and benthic, submerged or floating vegetation; unpredictable and extreme concentrations of atmospheric aerosols resulting from, e.g., urban pollution and fires; high levels of stray light from adjacent land and vegetation; highly variable optical properties of inorganic matter dependent on the surrounding geological formations and landscape, e.g., sediment features. In combination, these present a substantial challenge for obtaining quantitative estimates of biogeochemical variables in inland waters, and demand methods which account for some of these challenges simultaneously. The following section discusses the variability and ranges of the water-leaving and atmospheric signals typically encountered over inland waters, as measured by satellites in space at top-of-atmosphere.

5.1.1 The water-leaving signal

The constituents in optically-complex waters are generally summarized as belonging to phytoplankton, tripton and CDOM. However, characterising the water-leaving signal requires an understanding of the considerable optical complexity within these groups, and having a quantitative ability to assess their cumulative effects on the underwater light field. Figure 5.1 provides a quantitative illustration of the complexity and variability of the remote sensing reflectance routinely observed in inland waters, arising from the optical complexity and range of concentrations of in-water components, which are discussed below.

The phytoplankton component consists of groups with highly variable optical properties from eukaryotes (algae) to prokaryotes (cyanobacteria). This variability results from differences in pigmentation, spectral fluorescence emission, population particle size distribution, and intra-cellular structural features. For example, cyanobacteria have significantly different optical properties than algae, caused by significant scattering from internal gas vacuoles (Matthews and Bernard 2015), a lack of characteristic chlorophyll-*a* fluorescence emission (Seppälä et al. 2007), and phycobilipigments which alter their spectral absorption. Added to this complexity arising from optical features is the very large range of productive biomass that occurs in inland waters. Chlorophyll-*a* concentration routinely varies over five orders of magnitude from 0.1 to 1 000 mg m^{-3}, from alpine lakes to subtropical reservoirs. The large concentration range, and optical variability for which chlorophyll–*a* algorithms are expected to perform, presents a substantially different set of challenges for inland remote sensing in comparison to the oceanic environment.

The tripton component composed of detritus and minerals also varies significantly in optical characteristics and concentration ranges. Detritus material composed of dead phytoplankton cells and decaying organic matter is often stirred into the water column in very high concentrations in shallow eutrophic lakes (e.g., Lake Ijsselmeer in the Netherlands, or Zeekoevlei in South Africa). This significantly reduces the availability of light in the blue spectral region due to the exponential increase in absorption due to detrital matter. Mineral particle composition depends on the surrounding geology, and variability in the particle shape and size results in very wide ranging absorption and scattering properties (e.g., Stramski

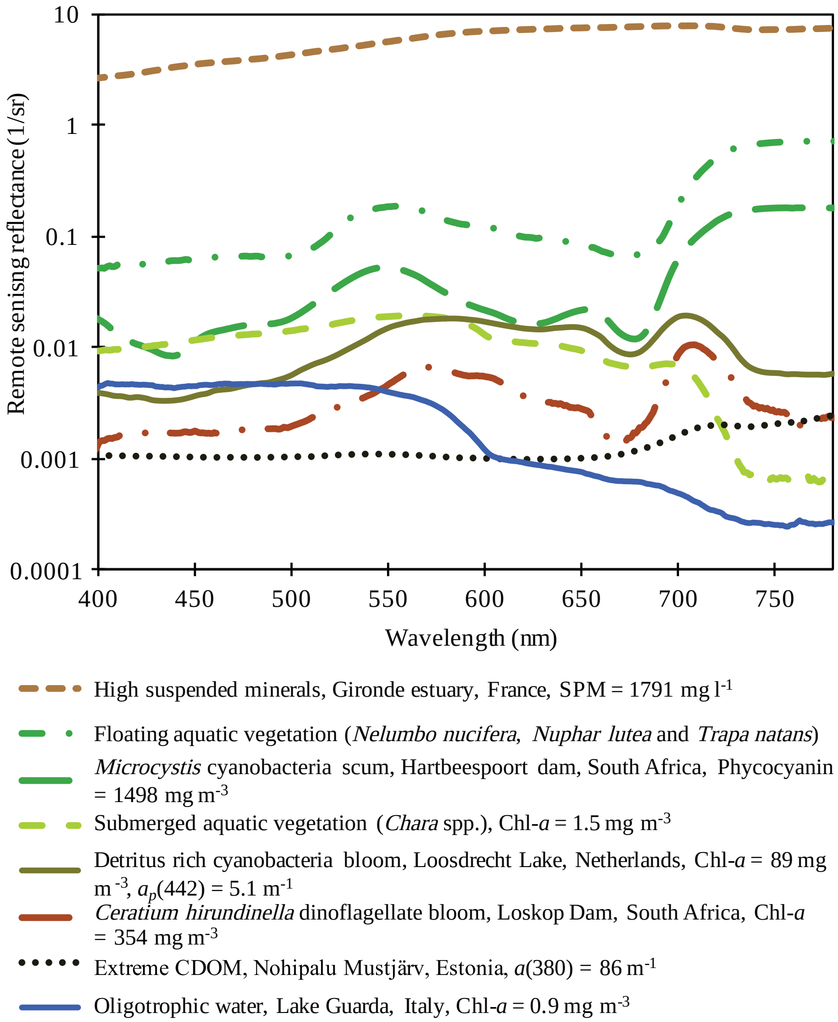

Figure 5.1 Examples of measured remote sensing reflectance illustrating variability in reflectance values often encountered in inland and near-coastal waters over five orders of magnitude. Note y-axis is log-scale. Legend provides information on reflectance target and water constituent concentrations. Data provided by David Doxaran, Claudia Giardino, Erin Hestir, Tiit Kutser, Mark Matthews and Stefan Simis. Figure credit Mark Matthews.

et al. 2007). Suspended clay particles (usually measured as total suspended matter, TSM) may exhibit high concentration ranges greater than 2000 g m^{-3} (Doxaran et al. 2006). The result is bright water-leaving signals, including for wavelengths greater than 700 nm. Such high concentrations cause significant interference with conventional retrieval algorithms for chlorophyll-*a* based on reflectance ratios or fluorescence (e.g., Mckee et al. 2007; Kobayashi et al. 2011), as well as atmospheric correction procedures.

High concentrations of humic and fulvic acids (CDOM) leached from surrounding vegetation and soils significantly reduces the light availability in the blue spectral region in boreal and brackish waters. This is in addition to detrital CDOM produced by the phytoplankton themselves. Dark waters have absorption values that may exceed 10 m^{-1} at 440 nm (Kutser et al. 2016), with typical values for inland water between 1 and 2 m^{-1} at 440 nm (Kirk 1994). In such cases, the water-leaving signal may be so small as to make detection at TOA very challenging or even infeasible, taking into account the signal-to-noise ratios of current satellite instruments.

The frequent presence of submerged aquatic vegetation (SAV), emergent, or floating aquatic vegetation (FAV) may add to the signal in inland waters, particularly in shallow marginal systems. FAVs negate the influence of absorption and scattering by water resulting in spectra resembling land or vegetation. Various types of SAV cause significant alterations in the shape and magnitude of the water-leaving spectra, such that these might be discriminated from other vegetation types (Hestir et al. 2008).

Such composition, concentration ranges and variability in water constituents described above are absent in ocean colour applications further than a few kilometers from the coastline. This demands improved approaches using instruments that are capable of measuring the variability of the water-leaving signal accurately across five orders of radiance magnitude (see CEOS 2018).

The expected range of water-leaving signals resulting from the three primary determinants of that signal (variable phytoplankton types/concentrations, CDOM absorption and non-algal particle concentrations) were modelled using a radiative transfer model. This provides a preliminary assessment of the range of variability in remote sensing reflectance typically encountered in natural inland waters. The model uses three phytoplankton types commonly occurring in inland waters: dinoflagellates, cryptophytes and vaculoate cyanobacteria (Evers-King et al. 2014; Robertson Lain et al. 2014; Matthews and Bernard 2015) at chlorophyll-*a* concentrations between 0.1 to 2.5 mg m^{-3}, and 20 to 60 mg m^{-3}. For each chlorophyll-*a* concentration, the reflectance was modeled for low/high CDOM absorption, and low/high non-algal particle (NAP) concentrations scenarios. Figure 5.2 shows the R_{rs} and Figure 5.3 shows the corresponding frequency plots for the 1st and 2nd derivatives to highlight the significant peaks, troughs and inflection points in the R_{rs}.

It is apparent from Figures 5.2 and 5.3 that by accounting for variability only due to three phytoplankton types and two CDOM and NAP ranges, large complexity is introduced in the water-leaving signal, evidenced by significant changes in the shape and magnitude of R_{rs}. For the high biomass range, the red peak near 700 nm becomes an important peak feature, highlighting the value of red wavelengths for high biomass scenarios.

5.1.2 The atmospheric signal

The atmosphere typically contributes around 90% of the signal at TOA over a clear ocean. Thus the signal from the water is challengingly small in comparison to the atmosphere. In inland waters, the water-leaving signal may be substantially larger (in the case of high concentrations of phytoplankton or suspended matter) or smaller (in the case of high CDOM) than that observed in the open ocean. This makes correcting for the atmosphere in a consistent manner in inland waters substantially more challenging, potentially requiring the use of

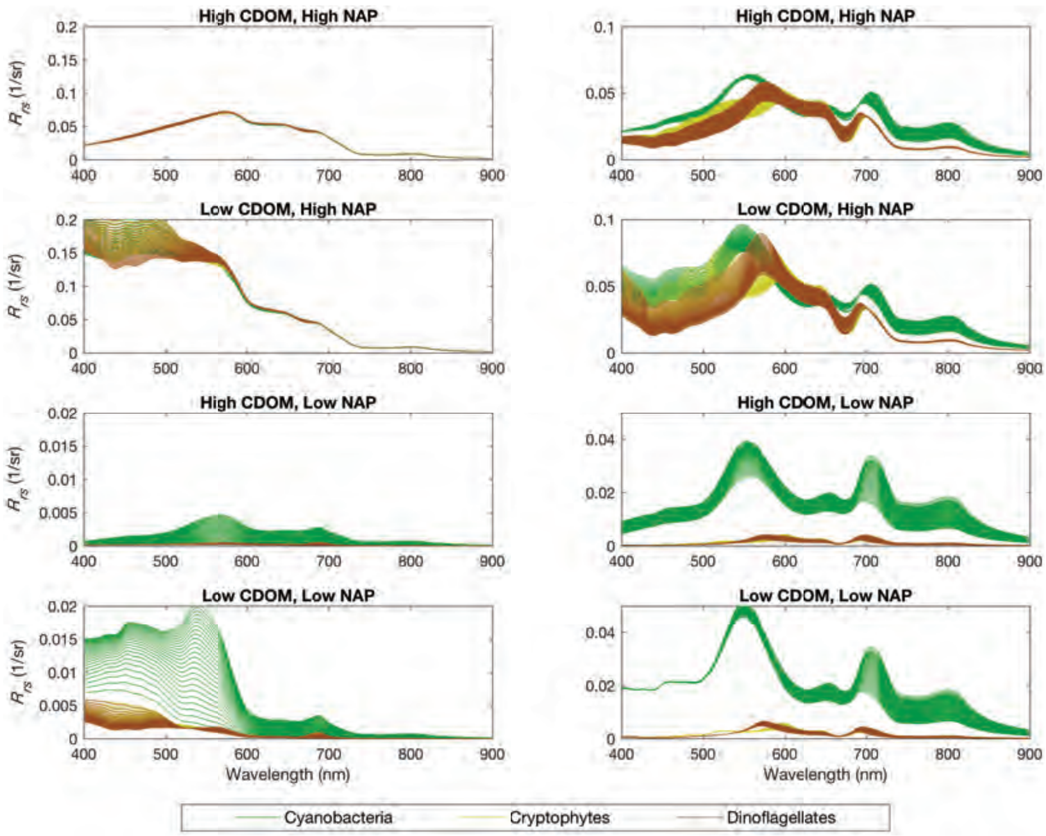

Figure 5.2 Modelled remote sensing reflectance for three phytoplankton groups (dinoflagellate, cryptophyte, cyanobacteria) for two Chl-*a* biomass ranges and combinations of low (0.02 m^{-1}) and high (2.0 m^{-1}) combined detrital and CDOM absorption, and low (5×10^{-4} m^{-1}) and high (0.5 m^{-1}) non-algal particle (NAP) scattering scenarios. Left panel: low Chl-*a* concentration range 0.1 to 2.5 mg m^{-3}. Right panel: high Chl-*a* concentration range 20 to 60 mg m^{-3}. The spectra were modelled at 2 nm resolution using Ecolight (Sequoia Scientific). Note differences in y-axis scale. Figure credit: Lisl Robertson Lain.

different atmospheric correction schemes dependent on conditions. The main challenges for atmospheric correction over small to intermediate inland targets arise from contamination by atmospheric aerosols and stray light, as discussed below and illustrated in Figure 5.4.

Concentrations of aerosols over land are often more extreme than over the ocean, resulting from smoke and dust particles from industrial, agricultural and urban activities. This may lead to a substantially higher contribution by aerosol scattering to the total signal at TOA and significant dampening of the available signal (Figure 5.4). This has the effect of reducing the relative signal from water, especially over oligotrophic waters (Figure 5.4C). Typical methods used to retrieve aerosol optical thickness using estimates from NIR satellite reflectance measurements are often invalid due to non-negligible water-leaving reflectance from high concentrations of in-water scattering constituents. Correcting for the atmosphere in such cases usually requires detailed atmospheric profiles and/or simultaneous aerosol optical thickness measurements from AERONET stations, not conventionally available for most targets. Therefore, alternative

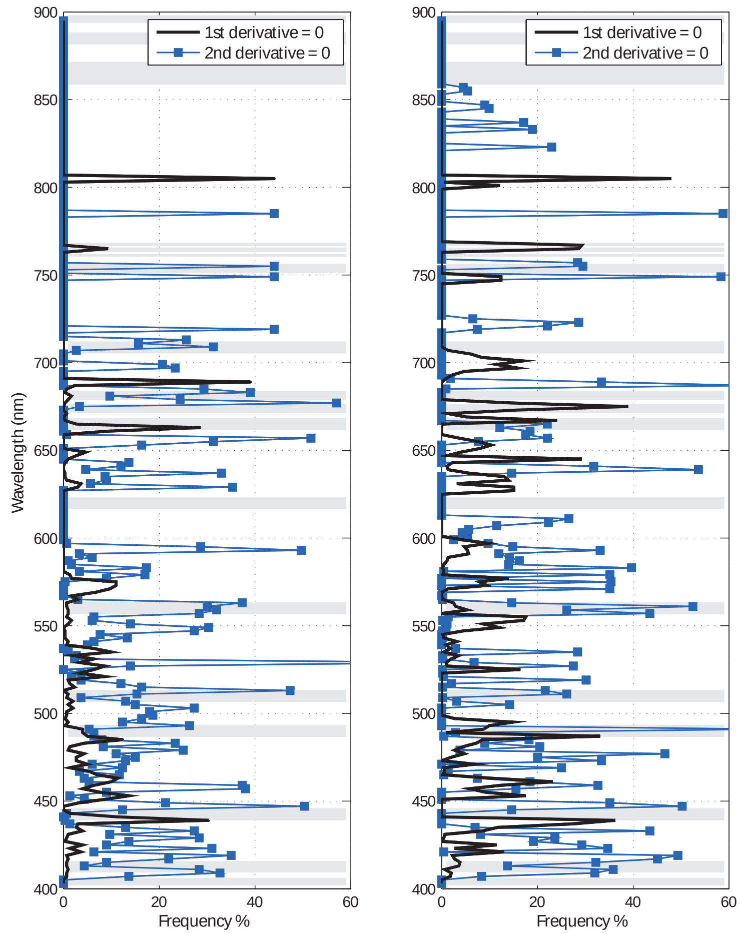

Figure 5.3 Corresponding frequency plots for R_{rs} in Figure 5.2 for the 1st (peaks or troughs) and 2nd derivatives (inflection points). Gray shading shows position of OLCI wavebands. Left: low Chl-*a* concentration range 0.1 to 2.5 mg m^{-3}. Right: high Chl-*a* concentration range 20 to 60 mg m^{-3}. Figure credit: List Robertson Lain

methods are required to obtain aerosol estimates over inland waters.

The adjacency effect causes enlarged reflectance mainly noticeable at NIR wavelengths, and is particularly severe for small dark water bodies surrounded by dense vegetation (Figure 5.4) or bright sands. The adjacency effect may be significant up to 30 km from the shoreline, depending on the surrounding vegetation and shape of the target (Santer and Schmechtig 2000). The effect complicates the estimation of aerosol properties from NIR reflectance. The adjacency effect over a clear alpine lake may contribute more than 30% of the signal at TOA (Odermatt et al. 2008). This makes oligotrophic and organic matter-rich water bodies the most challenging targets from a quantitative perspective, due to the small water-leaving signal with a relatively low dynamic range but high stray light contamination. Various approaches to correct for the adjacency effect have been proposed (e.g., Santer and Zagolski 2008; Kiselev et al. 2014; Sterckx et al. 2014). In most cases, the implementation of a correction for the

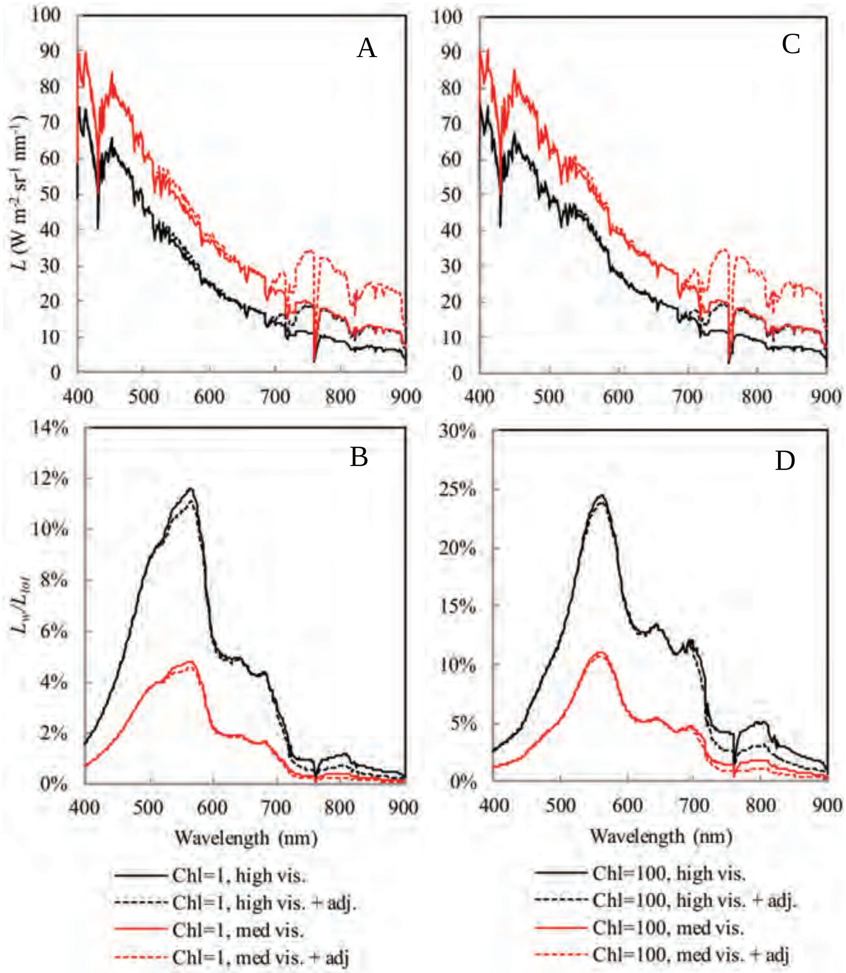

Figure 5.4 Effect of atmospheric turbidity and the adjacency effect on the signal measured at TOA by a satellite sensor. The figure shows two scenarios for atmospheric visibility (high and medium), two scenarios for phytoplankton biomass (low = 1 mg m^{-3}, high = 100 mg m^{-3}), and the effect of adding a moderate adjacency effect for a small inland water target. The upper panel shows top-of-atmosphere radiance, the lower panel shows the contribution of water leaving radiance to TOA radiance (L_w/L_{tot}). TOA radiances were modelled using MODTRAN and water leaving reflectance was generated with Ecolight at 1-nm resolution. Note differences in scale on y-axis. Simulations: Mark Matthews (Ecolight) and Derek Griffiths (MODTRAN). Figure credit: Mark Matthews.

adjacency effect is required to derive accurate water-leaving reflectance estimates over inland waters; however, the performance of correction methods needs careful assessment, especially when used operationally.

Due to the commonly large concentration of phytoplankton or mineral particles in inland waters, the contribution to the signal at TOA from water may be substantially higher than 10%. For these “bright” waters the relative signal from the water may be comparable to that of the atmosphere (Figure 5.4). This provides an opportunity to take advantage of the resulting increase in SNR at TOA. It also means that various approaches using TOA data are feasible, reducing the need for an atmospheric correction for the full aerosol component (see Figure 5.5).

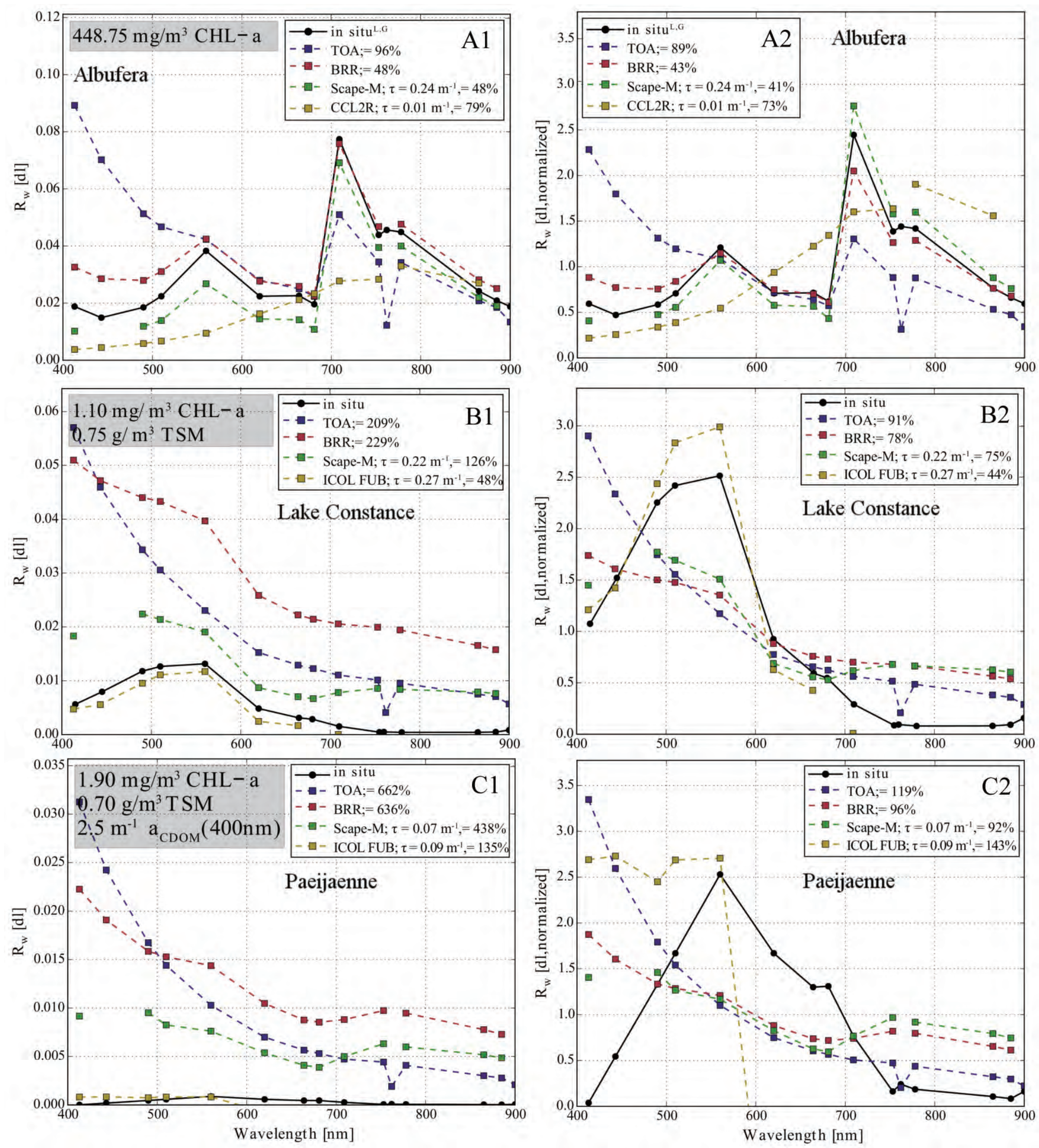

Figure 5.5 Comparison between remote sensing reflectance measured *in situ* and a variety of corresponding MERIS reflectance types, which include TOA reflectance, bottom-of-Rayleigh reflectance (BRR), and remote sensing reflectance derived using $SCAPE_M$ (spatial interpolation of aerosols) and a coupled water-atmosphere Neural Network (CoastColour). Left hand panels show reflectance, right hand panels show reflectance normalised to the integral to indicate retrieval of the spectral shape. Three diverse water cases are shown. Top: High biomass Albufera. Middle: Oligotrophic waters of Lake Constance. Bottom: Dark CDOM rich waters of Päijänne (called Paeijaenne). Data provided by: Antonio Ruiz-Verdù, Thomas Heege (EOMAP GmbH & Co.KG), Sampsa Koponen, Kari Kallio, Timo Pyhä lahti. Figure credit: Daniel Odermatt.

5.2 Deriving Water Quality Products from Satellites: Algorithms and Issues

Given the complexity present in the water and atmosphere briefly discussed above, pragmatic approaches are required with respect to quantitative retrievals of water quality parameters suitable for general application in inland waters. In the absence of a comprehensive knowledge of water and atmospheric constituent optical properties, the requirements remain unmet to satisfy a fully reductionist bio-optical modelling approach leading to quantitative water quality estimates. Here we discuss applications of recent algorithms suitable for use with both intermediate TOA and atmospherically corrected bottom-of-atmosphere reflectance products over inland waters. Candidate atmospheric corrections applicable in various scenarios are discussed. Algorithms and approaches are illustrated for the typical parameters of interest in inland waters namely chlorophyll-a , cyanobacteria, FAV, CDOM, Secchi disk depth and water transparency (K_d), and total suspended matter.

5.2.1 Algorithm types: partial atmospheric correction

A growing number of publications present approaches which utilise partial atmospheric correction and resulting intermediate reflectance products to obtain various quantitative and diagnostic products for inland waters (Hu et al. 2010; Matthews et al. 2012; Wynne et al. 2013a). These approaches often take advantage of the relatively higher signal at TOA caused by high constituent concentrations or bright surface features. By correcting for the more predictable and stable Rayleigh (non-aerosol) component of gaseous absorption and scattering, the reflectance at bottom-of-Rayleigh (BRR) can serve as a useful intermediate product. Partial atmospheric corrections are most often used in combination with empirical band ratios and peak height (derivative) subtraction methods to effectively normalize for aerosol effects. As illustrated in Figure 5.5A, TOA and BRR data types preserve both the magnitude and shape of R_{rs} in the case of high biomass blooms, especially for red wavelengths. Thus the need to correct for aerosols in the case of bright waters is negligible when implementing empirical-type algorithms. Indeed, in these cases application of unsupervised atmospheric corrections to retrieve R_{rs} often leads to warping of spectral shapes and errors due to out-of-range concentrations associated with underlying bio-optical models. This is especially true for coupled water-atmosphere models, such as the Coast Colour Level 2 Reflectance (CCL2R) Neural Network. If desired, improved R_{rs} estimates are provided through spatial interpolation methods such as SCAPE-M (Guanter et al. 2010) for bright waters.

In the case of oligotrophic and dark waters, partial atmospheric correction, as expected, does not often reproduce the shape or magnitude of R_{rs} adequately (Figure 5.5B,C). The high values for BRR are the result of correcting for absorption by atmospheric gases. Nevertheless, some studies demonstrate the value of partial atmospheric correction for simple trophic status estimation even in oligotrophic waters (e.g., Matthews and Odermatt 2015), when the requirements for inland waters are focused on gross measures of water quality (such as trophic status) rather than specified bio-optical or biogeochemical parameters.

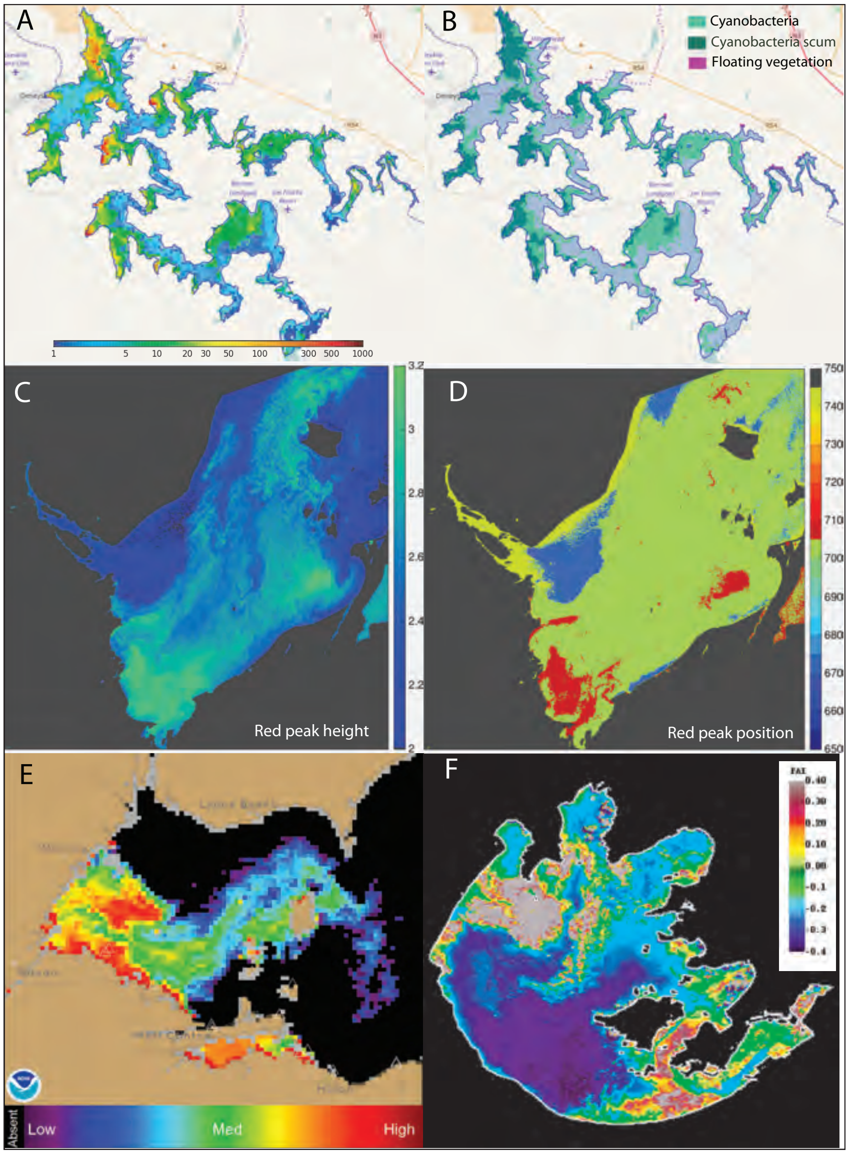

Figure 5.6 Various approaches making use of partial (Rayleigh) atmospherically corrected data for the detection of Chl-*a* fluorescence (A, C, D, E); cyanobacteria spectral features (B, E); red-edge bloom features (A, C, D); and floating algae and vegetation (B, F). A, B) Vaal Dam, South Africa, 2 April 2017, OLCI, MPH algorithm, Mark Matthews. C, D) Lake Erie, USA, 3 September 2011, HICO, adaptive reflectance peak height (ARPH), Nick Tufillaro. E) Lake Erie, USA, 3 August 2014, MODIS, cyanobacterial chlorophyll index (CI), R. Stumpf. F) Lake Taihu, East China, 3 October 2009, MODIS, floating algal index (FAI), Chuanmin Hu.

Various product types which may be derived from TOA data types are shown in Figure 5.6. Chlorophyll-*a* fluorescence and absorption features are clearly discernable enabling quantitative Chl-*a* estimates using an algorithm like fluorescence line height (FLH) (Gower et al. 1999) and maximum peak height (MPH) (Matthews et al. 2012) with MODIS or MERIS/OLCI data. The spectral features associated with cyanobacteria are also preserved at TOA, enabling discrimination of cyanobacteria using feature detection algorithms such as the cyanobacteria index (CI) (Lunetta et al. 2015) and MPH. Red-edge features in bands near 700 nm associated with algal blooms enable quantitative chlorophyll-*a* estimates to be obtained using indices such as the maximum chlorophyll index (MCI) (Palmer et al. 2014), MPH, and adaptive reflectance peak height (ARPH) (Ryan et al. 2014) algorithms from MERIS or hyperspectral type sensors, e.g., HICO, with suitable red-edge bands (Mishra et al. 2014). Detection of FAV can also be performed from TOA using indices such as the floating algal index (FAI, MODIS) (Hu et al. 2010) or MPH (MERIS and OLCI).

The TOA or partial atmospheric correction approach can therefore be useful and relatively simple to implement for monitoring phenomena such as eutrophication (chlorophyll-*a*), cyanobacteria blooms and aquatic vegetation in inland waters. However, as discussed in the next section, it is less well-suited to applications requiring blue wavelengths or the full visible water-leaving reflectance spectra required for CDOM determination or analytical reflectance inversion algorithms.

5.2.2 Algorithm types: full atmospheric correction

Given the challenges with aerosol retrieval over inland waters, further correcting the TOA signal for the aerosol component may lead to large uncertainties in the water-leaving reflectance product. From a signal perspective, it is likely only necessary to correct for the aerosol component in scenarios where the water-leaving reflectance constitutes less than ~10% of the signal at TOA, typical of ocean reflectance. However, estimates of R_{rs} can be obtained using radiative transfer codes such as 6S (Giardino et al. 2014) or by interpolating aerosol estimates made over land (e.g., SCAPE-M, Guanter et al. 2010) even for bright targets (Figure 5.5A).

Methods to derive R_{rs} include coupled water-atmosphere models that allow for non-negligible NIR reflectance. However, these models are usually unable to account for the extreme range of constituent concentrations and variability of the IOPs of inland waters. In oligotrophic waters, coupled neural network approaches more adequately reproduce spectral shapes and magnitudes (Figure 5.5C). In strongly absorbing waters with very small water-leaving signal, these approaches may also be more useful due to the flexibility of IOP variability afforded the atmospheric correction (Figure 5.5C).

In the case of R_{rs} derived over bright waters, and simultaneously accurately correcting for the adjacency effect from surrounding land, large uncertainties are likely to be present in the result. In reality, only a three dimensional radiative transfer correction accounting for a full atmospheric profile of aerosols and surrounding land terrain will likely yield systematically accurate R_{rs} estimates for small inland water bodies. As this is currently not routinely implemented for any satellite data sources, this remains a challenge for future missions.

Notwithstanding the above challenges, and assuming an atmospheric correction provides satisfactory results, using R_{rs} can yield significant benefits. Numerous methods exist using R_{rs} to provide a suite of physical and biogeochemical products, from algorithmic derivation based on the IOPs, to neural networks and advanced bio-optical radiative transfer inversions. One

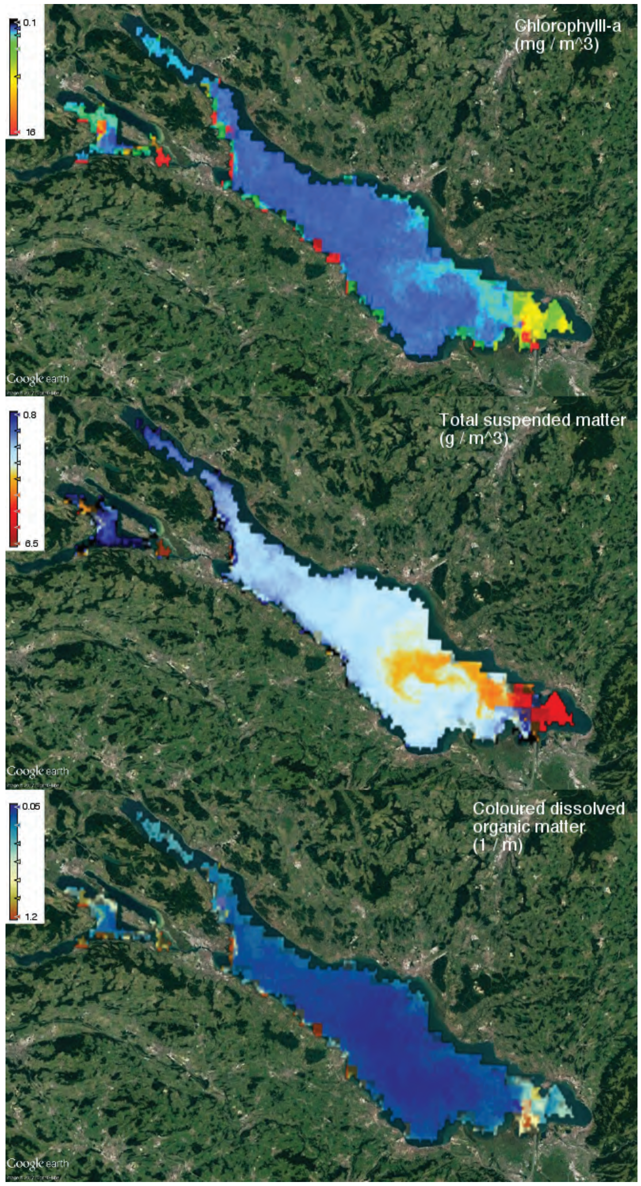

Figure 5.7 Three products derived using the FUB-WeW Water Processor (neural network approach) for Lake Constance from MERIS, on 4 July 2011. Credit: Google Earth, Landsat, Copernicus, ESA. Figure: Mark Matthews.

such example of an available algorithm is the Free University of Berlin (FUB) Water processor (FUB-WeW) algorithm (Schroeder et al. 2007) which provides a variety of physical and biological estimates (Figure 5.7). Nevertheless, the challenges from optical variability remain, and in order to obtain accurate quantitative estimates from inversion methods, the optical characteristics of the water in question should be accurately known. However, these complex models are, for the moment, incapable of adequately characterizing all scenarios encountered in inland waters. It may be necessary to use water-type classification (e.g., Moore et al. 2014) in combination with algorithms targeted at specific water or IOP types, or to use inversion algorithms that are capable of dealing with multiple water body optical characteristics, e.g., the adaptive linear matrix inversion method by Brando et al. (2012) implemented in abbreviated form in SeaDAS as the GIOP method.

5.3 Outlook

Significant progress has been made to address the challenges of optical complexity encountered in inland waters, and more knowledge of the IOPs and range and variability of water types are being obtained. This should lead to greater quantitative accuracy from algorithms, especially when used in combination with water type classifications. Whilst methods which use spectral shape and magnitudes applied to partially atmospherically corrected data provide useful information, adequately correcting the signal for atmospheric contamination remains the greatest challenge in inland waters. It remains to be seen whether recently developed methods can be used to provide an accurate and consistent reflectance product for inland waters for general applications of inversion algorithms.

Whilst low signal-to-noise ratios, and impractical band combinations have limited the use of historical high spatial resolution sensors, the current high spatial resolution sensors such as Sentinel-2 MSI and Landsat ALI are likely to yield significantly improved products (e.g., Toming et al. 2016). Hyperspectral sensors have the challenge of obtaining adequate radiometric sensitivity and calibration to meet the highly quantitative demands of dark water targets. The gains from hyperspectral imagery will see the addition of various improved phytoplankton type detection methods, provided the aforementioned challenges are adequately addressed. The Sentinel-3 OLCI series of satellites will continue to be the go-to product for large (in excess of 1×1 km) inland waters given its frequent global coverage, highly quantitative radiometry, sufficient spatial resolution and data availability, and growing suite of algorithm products.

Chapter 6

Sensors

Arnold Dekker, Erin Hestir, Menghua Wang, Mark Matthews and Evangelos Spyrakos

6.1 Introduction

Earth observing satellites play an important role in providing information for monitoring and assessing the water cycle and inland water resources (Lawford 2014). Satellite-based systematic, global coverage also addresses problems of data continuity, particularly in trans-boundary basins where complete, consolidated, and consistent information may be difficult to obtain (Tyler et al. 2016). Due to the lack of operational satellite sensors designed for inland water quality measurements, current applications are limited to using ocean colour sensors that lack sufficient resolution for water bodies smaller than 1×1 km^2, or high spatial resolution land sensors that lack sufficient spectral and radiometric resolution. The GEOSS Water strategy (Lawford 2014) recommended i) a global-scale coordinated effort to advance the future use of satellite remote sensing for water quality applications, and ii) the Committee on Earth Observation Satellites (CEOS) assess the benefits and technological challenges of a hyperspectral satellite mission focused on water quality. CEOS, in interaction with the GEO AquaWatch community, responded by assessing the feasibility of an aquatic ecosystem (non-oceanic) Earth observing system (CEOS 2018). Mouw et al. (2015) presented a generic overview of requirements for inland and coastal Earth observing systems. (Hestir et al. 2015) provided more specific rationale for hyperspectral sensing of inland waters. The CEOS (2018) feasibility study updated these recommendations and went a step further by providing quantitative sensor specifications. This chapter refers to the CEOS feasibility study, and reviews the following:

- Optically-active water quality variables/constituents (OACs) relevant to end-users that can be measured from space;
- Specific inherent optical properties (SIOPs) that determine the effect of varying concentrations of OACs on the spectrum;
- Spectral band requirements for OACs and for atmospheric correction;
- Spatial requirements (by examining global size class distribution of lakes and rivers);
- Radiometric accuracy and sensitivity requirements;
- Trade-off required between spectral, spatial, radiometric and temporal resolution.

The second half of the chapter assesses the application potential of existing and planned spaceborne sensors (where the specifications are already set) and recommendations for desired specifications of future sensors are also presented.

The accuracy of water quality constituent concentrations derived from remote sensing will vary depending on the region of interest, the type of water use, and the time of year (see Section 3.4.1). Accuracy will also vary due to concentration of the substance, the matrix of other optically-active substances in the water, availability of appropriate spectral bands, sensor radiometric sensitivity, calibration, atmospheric corrections, the amount of irradiance (latitude and season dependent) and the accuracy and representativeness (see below) of the *in situ* data set. Typical accuracy targets for most ocean colour products are better than ±30% of the variable concentration (e.g., chlorophyll-a , IOCCG 2000), and inland and coastal water products are generally expected to have the same magnitude of accuracies. These accuracy requirements are addressed in the context of existing satellite sensors and possible new, dedicated inland and near–coastal water sensors.

The bulk optical properties of natural waters can be divided into *inherent* and *apparent* optical properties (IOPs and AOPs, respectively). IOPs include light absorption, scattering, and beam attenuation extinction coefficients (a, b, and c, respectively). For remote sensing purposes the backscattering coefficient, b_b, is relevant as it specifies the amount of light backscattered (via the water column, the air-water interface, and the atmosphere) to the remote sensor. By definition, IOPs depend only upon the medium, i.e., pure water and its dissolved and suspended components. The geometry or magnitude of the incident light field does not influence the IOPs. Concentration-specific IOPs (SIOPs) are calculated by dividing the absorption or backscattering by the unit concentration of an OAC. SIOPs are used to simulate spectral reflectances (or normalised water-leaving radiances) of water bodies with any range of optically active constituents. Figure 6.1 shows an example of SIOPs used in the CEOS (2018) study for reflectance and radiance simulations.

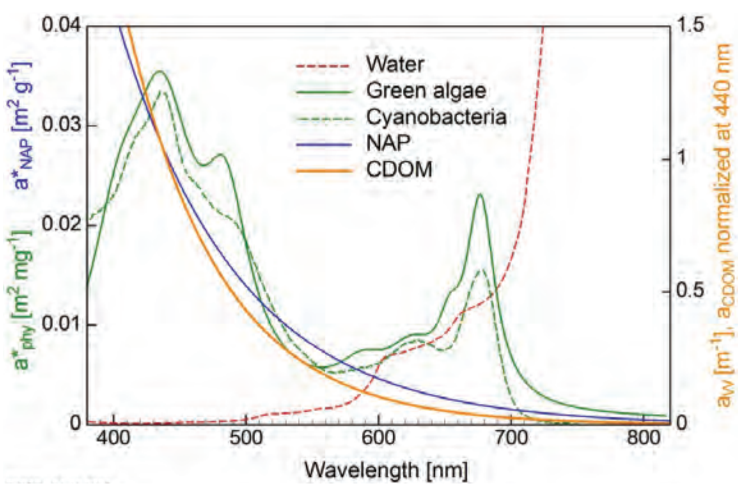

Figure 6.1 Specific absorption coefficients used for the simulations (CEOS 2018).

AOPs depend on both the IOPs and the solar-sensor geometry and magnitude of the incident light field. AOPs include irradiance reflectance, R (upwelling irradiance E_u, divided by the downwelling irradiance E_d), remote sensing reflectance, R_{rs} (upwelling radiance just above the water surface, L_u, divided by E_d), and the coefficients of vertical light attenuation (K-functions).

6.2 Spaceborne Sensor Requirements

Several of the mission requirements for future inland and near-coastal water quality sensors are similar to those of coastal ocean colour sensors, documented in IOCCG Report 13 (IOCCG 2012). This chapter discusses additional mission requirements for inland and near-coastal water quality observations, namely:

- ❖ Additional spectral band requirements to address increased variety, range and composition of optically-active substances and their relative contributions to the measured signal, as well as coping with optically-shallow waters.
- ❖ Differences in spatial scales (smaller water bodies with high spatial complexity of inland-water boundaries).
- ❖ Atmospheric and air-water interface correction, including land adjacency effect, altitude of water bodies (minus 400 m for the Dead Sea to ~5800 m for mountain lakes), effects of highly turbid waters, strongly absorbing aerosols, etc.

6.2.1 Spectral band requirements for estimating water variables

The spectral reflectance of inland and near-coastal waters is caused by the OACs interacting with the incoming light via their SIOPs creating the IOPs and AOPs. Spyrakos et al. (2017) give an excellent overview of a significant range of inland water body reflectance spectra. Three approaches are necessary to determine spectral band requirements for estimating water quality variables from remote sensing:

- ❖ Use of measured and simulated spectral data to identify spectral activity ranges of optically-active substances in inland and near-coastal waters;
- ❖ Derivative analysis of measured and simulated spectra to help identify the peaks and troughs, shoulders and inflexion points in spectra (See Figure 5.3);
- ❖ Recommendations from the literature.

Each method has its strengths and weaknesses — combining all these methods will give the most comprehensive result.

6.2.1.1 Spectral absorption features of phytoplankton and cyanobacteria

The main *in vivo* spectral absorption features in all phytoplankton and cyanobacteria are centred around 438 and at 676 nm, reflecting the blue and red chlorophyll-*a* maxima respectively (see Figure 6.1). Other light harvesting pigments can provide useful information on phytoplankton species composition or functional types (see Figure 5.2) and many phytoplankton pigments have significant spectral activity in the 470 – 490 nm region with many overlapping absorption features (e.g., beta-carotenes). Similarly, various forms of chlorophyll (*a, b* and *c*) are active in the blue as well as orange to red region of the spectrum. In general, absorption spectra of algal pigments have an increasing Gaussian shape with increasing pigment concentration. Chlorophyll-*a* also exhibits a chlorophyll fluorescence peak at 683 nm *in vivo* (see Figure 5.6).

Cyanobacteria have specific light harvesting pigments, the most optically active of which are cyanophycoerythrin (CPE) and cyanophycocyanin (CPC) (visible in the cyanobacterium spectrum in Figure 6.1) that have *in vivo* absorption features at 565 and 615–624 nm, respectively, with the CPC peak being the most ubiquitous. An increased state of eutrophication of a water body is often accompanied by cyanobacterial blooms, so these pigments are highly relevant as a diagnostic water quality measure. Global inland water EO systems therefore require these spectral bands. Two algorithmic approaches can be used to detect these pigment absorption features:

- ❖ Algorithms with 1 to 4 spectral bands can be used to quantify pigment absorption or fluorescence features, such as the robust 3-band algorithm which uses two bands on either side of the absorption/fluorescence feature plus a band across from the absorption/fluorescence maximum. An estimate of absorption/fluorescence can be calculated from a baseline of these two bands and adding/subtracting the absorption/fluorescence feature. This leads to a spectral band requirement located at: 418–438–458 nm and 647–667–697 nm for the Chl-*a* blue and red absorption features; 545–565–585 nm and 604–624-644 nm for CPE and CPC respectively, and 680–683–686 nm for the chlorophyll fluorescence feature (a much narrower feature that must avoid the Chl-*a* red absorption maximum). The spectral bands must be centred on the pigment absorption or fluorescence features, but the requirements for the ancillary bands are much less stringent. They should be close to the absorption/fluorescence feature, but not too close. As explained in Section 6.2.1.4, spectral peaks and troughs may shift as a function of increasing concentrations of OACs so caution should be exercised when using fixed band combinations.
- ❖ Physics-based inversion approaches calculate, over a range of spectral bands, the contribution of all the OACs to each spectral band reflectance via their contribution to the IOPs(λ), making use of the SIOPs. These inversion approaches need a measurable effect of each OAC on the reflectance. Ancillary bands are not necessarily required for physics-based inversion algorithms — it is sufficient to have spectral bands that measure the absorption or fluorescence feature as long as some spectral bands are available that estimate the spectral backscattering.

6.2.1.2 Spectral bands for CDOM and NAP

Coloured dissolved organic matter (CDOM) does not scatter light in a measurable way and exhibits a smooth declining absorption from blue to red wavelengths (see Figure 6.1), so does not have a specific spectral band location for estimation by remote sensing. It is advisable to have 2 or 3 spectral bands outside of the pigment absorption and fluorescence bands to estimate CDOM, preferably in the blue to green regions. This requirement is less stringent for physics-based inversion methods as the various contributions of optically-active constituents are calculated for each spectral band through the SIOPs and IOPs.

The same line of reasoning can be used for the NAPs (see Figure 6.1), which are composed of the algal biomass (minus the extracted pigments), dead organic material and mineral particles (NAP + algal pigments = TSM or TSS), and which absorb as well as scatter light. The dead organic matter absorption usually imposes a yellow to brown colour (exponentially declining absorption with increasing wavelength) whereas mineral particles vary in colour from white/grey to yellow to orange (iron oxide) to black (e.g., volcanic silt). NAP scatters light significantly, varying from a strongly declining spectral scattering with increasing wavelength for very small particles, to spectrally neutral (grey or white) scattering for large particles. From a spectral-band point of view, it is advisable to have two or three spectral bands outside of the pigment absorption and fluorescence bands to estimate NAP, preferably across the blue to NIR regions. The optimal locations for assessing NAP are in the green (algal pigments absorb little in the green) and in the NIR (only pure water absorbs strongly in the NIR).

6.2.1.3 Simulations to estimate spectral band characteristics

A substantial set of simulations were performed in the CEOS (2018) report to estimate the best spectral band settings for a multi-spectral sensor and an imaging spectrometer for aquatic ecosystems. A summary of the inland-water relevant inputs, simulations and the main findings are presented in this chapter. Readers are referred to CEOS (2018) for a comprehensive discussion on this subject. The simulations assume a Gaussian shaped spectral response for each band with a full width at half maximum (FWHM) of 5 nm. The SIOPs are chosen as follows (CEOS 2018):

- a^*_{phy}: two specific absorption spectra of green algae were used, i.e., from the WASI database (Gege 2014), and from cyanobacteria (GLaSS 2015) — see Figure 6.1.
- a^*_{CDOM} is approximated by an exponential equation with slope sCDOM = 0.014 nm^{-1} (Figure 6.1).
- a^*_{NAP} is approximated by an exponential equation with slope sNAP = 0.011 nm^{-1} (D'Sa and del Castillo 2006; also average of GLaSS 2015 data) and specific absorption coefficient of 0.027 m^2 g^{-1} at 440 nm (Babin et al. 2003) — see Figure 6.1.
- $b^*_{b,\mathrm{phy}}$: specific backscattering coefficients from Lake Garda for green algae from normal clear water and for water with the cyanobacteria *Anabaena* sp. (Figure 6.2).
- $b^*_{b,\mathrm{NAP}}(555)$ = 0.011 m^2 g^{-1} and n = 0.75 (result from GLaSS 2015).

With this input data on SIOPs and using concentration ranges: TSM 0.5 to 5 mg l^{-1}; $a_{\mathrm{CDOM}}(440)$ 1 to 10 m^{-1}; chlorophyll-a 1 to 100 μg l^{-1} the resultant R_{rs} spectra in Figure 6.3 can be generated. Many more simulations were performed in CEOS (2018), the results of which are summarized in this Chapter. The simulations in Figure 6.3 fit as a subset of the field-measured spectra (Figure 6.4), which show significant variation. Many of the high reflecting spectra in Figure 6.4 are from rich suspended matter waters with little influence from phytoplankton pigment absorption. Measured R_{rs} spectra of, for example, many eutrophic Chinese lakes closely resemble several of the spectra shown in Figure 6.3 (Sun et al. 2015).

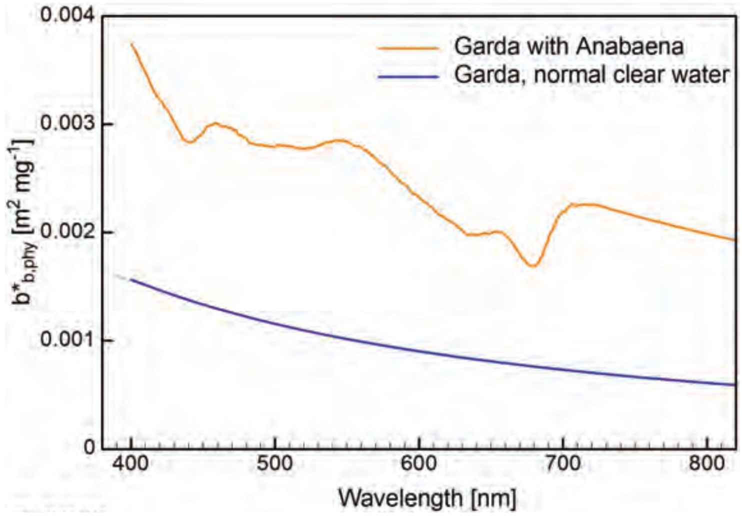

Figure 6.2 Specific backscattering coefficients of phytoplankton in Lake Garda used for the simulations (CEOS 2018). Blue line — green algae from normal clear water; orange line — water with the cyanobacteria *Anabaena* sp. (both spectra provided by C. Giardino, personal communication).

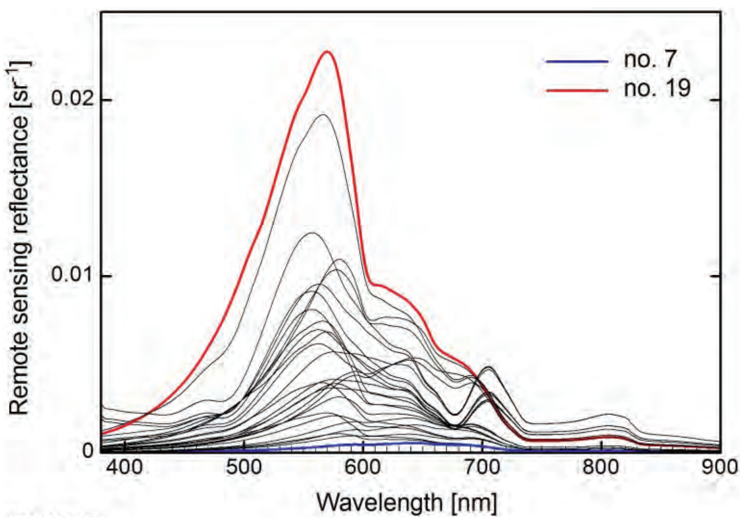

Figure 6.3 Simulated remote sensing reflectance spectra: No. 7 represents the darkest spectrum, no. 19 the brightest (CEOS 2018). Note Y-scale difference with Figure 6.4.

6.2.1.4 Assessing spectral band locations using derivative analysis

Derivative analysis of simulated and measured hyperspectral data has been used to suggest the optimal location of spectral bands for remote sensing of a specific environment (e.g., Lee et al. 2007a; CEOS 2018). The first derivative identifies the location of the spectral peaks and troughs, the second derivative identifies shoulders in the original spectra. Shoulders may be indicative of spectral absorption features that are not able to produce a spectral reflectance peak or trough. The use of spectral derivatives should be considered a supportive tool rather than an

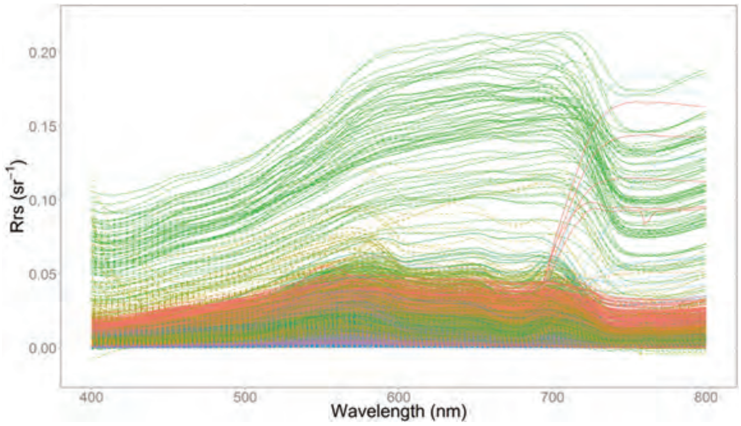

Figure 6.4 Measured remote sensing reflectance spectra from the Limnades database (Spyrakos et al. 2017). Note Y-scale difference with Figure 6.3. Colours denote different sources of data.

explanatory tool, especially when looking at large sets of spectra and using the frequency of the 1st and 2nd derivative outcomes. Spectral peaks and troughs may also shift as a function of increasing concentrations of OACs. For example, with increasing chlorophyll-a absorption centred at 676 nm (with a widening Gaussian shape) a characteristic reflectance peak (caused by low combined OAC and pure water absorption) at ~690 nm can shift up to ~720 nm (CEOS 2018). This feature will disappear in a frequency diagram of 1st and 2nd derivatives. Thus the highest frequencies 1st and 2nd derivative spectral analysis are useful for identifying regularly occurring fixed spectral features, but not for spectral features that change wavelength due to increases in concentration. One such fixed spectral feature to be considered is the shape of the pure water absorption (see Figure 6.1) as it contains multiple absorption features (troughs and shoulders) related to the harmonics of pure water absorption.

6.2.1.5 Optimal spectral resolution

Spectral reflectance simulations in the CEOS (2018) study were performed over the following ranges of OACs: Chl-a : 0.5 – 1000 μg l^{-1}; TSM: 0.2 – 300 mg l^{-1} and CDOM 0.04 – 10 m^{-1}. Rather than only looking at 1st and 2nd derivatives, a more sophisticated approach was taken to also estimate the shift in wavelength with increasing concentration as well as taking the noise equivalent reflectance into account. To obtain a sensor recommendation for spectral resolution, the resolutions were averaged for all water types and ranges. The result is shown in Figure 6.5 for optically-deep water simulations.

Optimal spectral resolution for water scenarios range from 2 to 12 nm with an average of ~5 nm from 380 to 737 nm, and ~15 nm above 737 nm (Figure 6.5). The green line in Figure 6.5 is a fair compromise for all considered water types and wavelengths. Thus, the recommended spectral resolution of a hyperspectral sensor, based on these simulations, is 5 nm from 380 to 737 nm, and 15 nm from 737 to 900 nm. If radiometric sensitivity considerations are also taken into account (increasing the SNR), the preferred spectral resolution is ~8 nm from 380

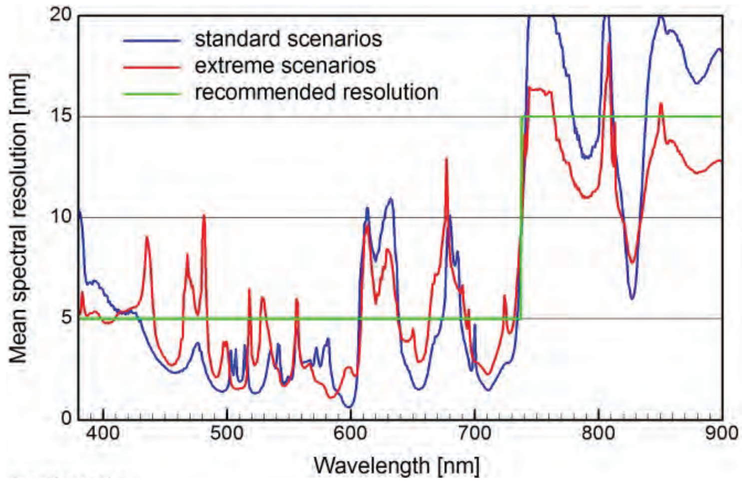

Figure 6.5 Averages of optimal spectral resolutions for a large range inland and coastal waters. Figure from CEOS (2018).

to 737 nm (CEOS 2018).

A different approach by Lee et al. (2014) for ocean and coastal waters, further augmented to turbid eutrophic waters by Sun et al. (2015), indicates that most measured spectra can be reconstructed using 15 spectral bands (5 – 10 nm width) such as those from the MERIS sensor. For turbid eutrophic lake waters, additional finer spectral bands near 550 nm, 620 nm and around 700 nm are required for accurate reconstruction of the measured spectra. These results, using an alternative approach, are in reasonable agreement with the simulation results in CEOS (2018) and in Table 6.1 (see below).

A set of multispectral bands can be determined (Table 6.1) making use of all of the above mentioned approaches; measured and simulated spectra, derivative analysis, and literature recommendations. The Table does not include bands for monitoring terrestrial surfaces, emerged vegetation, or for correcting environmental influences (e.g., atmosphere, reflections at the water surface, cloud shadows, see Table 6.2). The bands in Table 6.1 are suitable for assessing OACs, benthic composition, shallow water bathymetry, AOPs, IOPs and SIOPs. However, it is recommended that NIR and SWIR bands sensitive to terrestrial plant features (between 1500 – 1700 nm and 2100 – 2400 nm) be added to separate plants floating at, or just below, the surface from water column chlorophyll, and to aid in the interpretation of water quality retrievals (Hestir et al. 2012; CEOS 2018). Reference bands have been included for the 3-band pigment absorption line height approaches. Physics-based spectral inversion methods do not specifically need these pigment reference bands but do require spectral bands where the pigments absorption effects are measurable.

Inland and coastal waters require more spectral bands at a higher spectral resolution due to their optical complexity compared to oceans where algal pigments, biomass and breakdown products are largely responsible for determining the colour. In most inland and coastal waters, the optically active constituents can both co-vary and vary independently, sometimes in the same water body (Ampe et al. 2014). In inland lakes it is possible to have high CDOM, NAP

Table 6.1 Recommended minimum set of spectral bands for extracting information from remote sensing reflectance spectra of optically deep and shallow waters. Source CEOS (2018). See Table 6.2 for NAP relevant bands beyond the O_2 absorption feature at 761 nm. Refer to Appendix for acronyms.

Centre [nm]	**FWHM [nm]**	**Water quality and benthic characterisation related application**
±380	15	CDOM (Mannino et al. 2014), NAP, phytoplankton functional types, PFT (Wolanin et al. 2016), mycosporin-like amino acids (Dupouy et al. 2008)
±412	5 to 8	CDOM (Mannino et al. 2014), PFT (Wolanin et al. 2016)
± 425	5 to 8	CDOM, blue Chl-*a* absorption reference band, NAP, PFT (Wolanin et al. 2016)
±440	5 to 8	CDOM (Mannino et al. 2014), blue Chl-*a* absorption maximum, PFT (Wolanin et al. 2016)
467	5 to 8	Band required to separate *Phaeocystis* from diatoms (Astoreca et al. 2009), blue Chl-*a* absorption reference band, accessory pigments
±475	5 to 8	Accessory pigments, blue Chl-*a* absorption reference band, PFT (Wolanin et al. 2016), NAP
±490	5 to 8	Blue Chl band-ratio algorithm, PFT (Wolanin et al. 2016), accessory pigments
±510	5 to 8	Blue Chl band-ratio algorithm, NAP
±532	5 to 8	PFT and carotenoids (Wolanin et al. 2016), NAP
±542	5 to 8	NAP
555	5 to 8	NAP (low algal pigment absorption), CPC reference band, PFT (Wolanin et al. 2016)
565	5 to 8	CPE *in vivo* absorption maximum and possibly fluorescence (Dierssen et al. 2015)
±583	5 to 8	CPE and CPC reference band; chlorophyll-*a*, *b* and -*c* (Johnsen et al. 1994), CPE fluorescence (Dierssen et al. 2015)
±594	5 to 8	PFT (Wolanin et al. 2016)
±615	5 to 8	CPC *in vivo* absorption maximum (Hunter et al. 2010, avoiding chlorophyll-*c*)
624	5 to 8	CPC *in vivo* absorption maximum (Dekker 1993; Simis et al. 2007), suspended sediment, PFT (Wolanin et al. 2016), Chlorophyll-*c* (Johnsen et al. 1994)
631	5 to 8	PFT (Wolanin et al. 2016)
±640	5 to 8	NAP, CPC reference band
649	5 to 8	Chl-*b in vivo* absorption maximum (Johnsen et al. 1994)
665	5 to 8	FLH baseline (Gower et al. 1999; Gilerson et al. 2008)
676	5 to 8	Red Chl-*a in vivo* absorption maximum (Johnsen et al. 1994)
683	5	Chlorophyll fluorescence (FLH) band (Gower et al. 1999; Gilerson et al. 2008)
±700	5 to 8	HABs detection, NAP in highly turbid water, reference band for 2 or 3 band Chl-*a* algorithms
±710	5 to 8	FLH baseline (Gower et al. 2006), HABs detection, NAP in highly turbid water, reference band for 2 or 3 band Chl-*a* algorithms
±748	15	NAP in highly turbid water (Ruddick et al. 2006), FLH baseline band (Gilerson et al. 2008)
± 775	15	NAP in highly turbid water (Ruddick et al. 2006)

Table 6.2 Recommended spectral bands for atmospheric correction and NAP concentration estimation (shade bands are included in Table 6.1). Source CEOS (2018).

Centre [nm]	FWHM [nm]	Atmospheric characterisation and air-water interface effect removal bands
±360	8	To constrain the SWIR-based aerosol model over turbid waters
±368	8	To constrain the SWIR-based aerosol model over turbid waters
±412	8	NO_2
±520	8	Aerosol retrieval
±575	8	Chappuis band for O_3 absorption (Gorshelev et al. 2014)
±605	8	Chappuis band for O_3 absorption (Gorshelev et al. 2014)
±620	8	Aerosol retrieval
±709	8	Aerosol retrieval
±740	8	Sun glint removal
±761	3	Sun glint removal
±775	16	Aerosol retrieval; water vapour reference band
±820	16	Water vapour absorption
±865	16	Aerosol retrieval, water vapour reference band, sun glint removal (Dogliotti et al. 2015)
±940	16	Water vapour absorption
±1020	16	Water vapour reference band
±1050	16	Water vapour reference band
±1130	16	Water vapour absorption
±1135	16	Water vapour reference band
±1380	16	Cirrus clouds

and chlorophyll-*a* concentrations resulting in spectral reflectance features being changed to longer wavelengths. Another example is high latitude boreal lakes with high CDOM absorption values, whilst the water management issue is estimating chlorophyll-*a* concentrations to detect eutrophication. The high CDOM absorption prevents use of the blue wavelengths for detecting the blue Chl-*a* absorption peak (at 438 nm) requiring detection of the red Chl-*a* 676 nm maximum in a low reflecting water body. Optimizing band positions is thus highly dependent on the inland water quality conditions, which can vary widely across geographic regions and seasons (Kutser et al. 2016). For this reason, an optimal, inland water-quality sensor should ideally have many narrow spectral bands, eliminating the need for *a priori* selection of band positions.

In the case of optically-shallow inland, coastal and coral waters where it is also desirable to map the benthos and bathymetry, the spectral features of the benthos need to be mapped. The spectral reflectance features vary across microphytobenthos, seagrasses, macro-algae, corals, sponges, coralline encrusting algae, sand, silt and mud etc. Therefore, an imaging spectrometer with spectral bands of between 5 (optimal from a spectral feature point of view) and 8 nm (optimal from SNR and spectral feature point of view) would be best (CEOS 2018).

6.2.1.6 Spectral bands for atmospheric correction

A key pre-processing procedure in remote sensing of coastal and inland waters is atmospheric and air-water interface effects correction, to derive the normalized water-leaving radiance, nL_w (or R_{rs}) as discussed in Chapter 5. All other water optical, biological, and biogeochemical properties are derived from these nL_w or R_{rs} spectra. Since nL_w usually contributes <10% to the top of the atmosphere (TOA) radiance in the visible wavelengths, data quality over inland waters is highly sensitive to the performance of the satellite on-orbit calibrations. For open oceans (or large clear inland lakes) ocean colour products can be produced routinely using the near-infrared (NIR)-based atmospheric correction (IOCCG 2010). However, over turbid coastal and inland waters, atmospheric correction using the shortwave infrared (SWIR)-based and NIR-SWIR combined approaches are better suited (Wang and Shi 2007). Thus, for remote sensing of coastal and inland waters, both the NIR and SWIR bands are necessary, located at about ~745 and ~865 nm for NIR, and ~1240, 1600 to 1640, and ~2130 or 2257 nm for the SWIR bands. To meet the requirement for atmospheric correction over coastal and inland waters, Wang and Shi (2012) demonstrated that the required SNR values for the NIR bands are ~600, while for the SWIR 1240, 1640, and 2130 nm bands they are ~250, ~200, and ~100, respectively.

Although the addition of SWIR bands to a satellite sensor does drive up the weight and energy requirements, the benefits for deriving water quality products accurately are significant particularly over turbid coastal and inland waters. Significant cost reduction is possible by limiting the sensor detectors to Si based detectors that can work between 380 and 1000 nm. However, new technology and development may further encourage cheaper and better sensors in the SWIR bands. A dedicated inland and near coastal water quality Earth observing system could also be limited to the ~360 to 1000 nm range whilst flying in tandem with other sensors that can provide the SWIR capability, such as dedicated ocean colour or atmospheric Earth observing sensors. This would be a cost-effective solution.

A specific atmospheric correction issue is the adjacency effect (see Section 5.1.2. and Figure 5.4). The adjacency effect occurs when photons reflected from a bright target next to the water body are scattered in the atmosphere on their way to the satellite sensor and appear to be coming from the water body, thereby providing (seemingly) higher water reflectance values. This effect occurs more with increased aerosol loading, and decreases as the pixels are further away from the shoreline towards the centre of the water body. Unfortunately, in many water bodies, the shorelines are shallow and prone to resuspension of sediment also causing increased reflectance. Separating these two signals is not easy. Being able to access several spectral bands in the NIR does help, as land vegetation can reflect highly, causing NIR adjacency effects.

6.2.2 Spatial resolution requirements

One of the limitations in adapting ocean colour data to inland and coastal applications is the spatial resolution of the sensor's pixels relative to the size of the water body, and the spatial complexity of the land-water boundary. Because of the need for higher spatial resolution, researchers frequently appropriate land-imaging missions (e.g., Landsat, WorldView-2 and -3, MSI-Sentinel-2, etc.) for inland and near-coastal water quality applications. This comes with significant trade-offs, however, because most land-imaging missions do not meet the spectral or radiometric resolution requirements. As a general rule, to obtain one valid pixel over a small water body (small in relation to pixel size) one requires 3×3 or 4×4 pixels that fit within the water body boundaries.

The global abundance and size distribution of lakes have been reported by Verpoorter et al. (2014) using analyses based on Landsat imagery. The authors quantified the number and surface area of the world's lakes larger than 0.002 km^2 (2000 m^2). Andreadis et al. (2013) reported estimates of global river width, depth and discharge using a combination of Landsat image analysis and hydrologic modelling. Using both these datasets the total number of lakes (larger than 0.002 km^2) and rivers globally resolvable by different sensor spatial resolutions can be estimated. The vast majority of lakes occur in size classes less than 1 km^2, and these smaller lakes and reservoirs are often essential for the local population and environment. While there are fewer lakes in size classes >1 km^2, they contribute towards a large portion of the total surface area covered by lakes. In theory, the majority of the world's surface lake area (~60%) can be resolved with a sensor ground sampling distance (GSD) of ~333 m. This is the equivalent of a sensor with MERIS/OLCI-type resolution. If smaller lake classes are considered, nearly 80% of the global lake surface area can be viewed with a sensor with a GSD of 105 m, whereas 100% of the global lakes with an area of 0.002 km^2 or larger can be resolved with 15 m spatial resolution (e.g., Sentinel-2 type sensor resolution of 10, 20 and 60 m bands) and 90% with a Landsat resolution sensor (30 m).

The ability to resolve rivers from space requires much higher GSD than lakes. The vast majority of global river reaches are less than 10 m wide, requiring a sensor resolution of ~3 m. Less than 1% of total river reaches are resolvable at the MERIS/OLCI sensor type resolution or with VIIRS imagery band spatial resolution, and only 12% of all river reaches are resolvable using Landsat sensor type resolution. Encouragingly, more than one quarter of global river reaches are wide enough to be resolved e.g., using Sentinel-2 type sensors (<17 m GSD).

Due to shoreline complexity of water bodies and cloud cover, the actual number and area of lakes and river widths resolvable in each size class will likely be less than the estimates provided. For example, Sayers et al. (2015) determined that approximately 80,000 lakes were resolvable globally in the 2011 growing season using MERIS, and only 58,000 lakes resolvable using MODIS. Similarly, using an analysis of polygons, Hestir et al. (2015) determined that MERIS/OLCI resolution is capable of observing more than 50% of the area of inland waters in Europe. By comparison, MERIS can observe only a few percent of Australia's water bodies, where a 30-m resolution sensor resolves less than 50% of the area due to differences in topography and water body geometry. This demonstrates that spatial resolution requirements may differ substantially based on geography.

Based on these calculations, the minimum spatial resolution requirement for inland water bodies can be categorized into two bins. A GSD of 300 m is satisfactory to observe the majority of the world's lake surface areas, representing only a small fraction of the number of lakes on the planet. A sensor with a minimum GSD of 15–17 m would enable observations for nearly a quarter of global river reaches and between 90 and 100% of global lakes 0.002 km^2 or larger. The Sentinel-3 series of OLCI sensors have 22 spectral bands, high SNR and a GSD of 300 m, thus should cater for the requirements for large lakes adequately. The focus for new sensors should be around 5 to 8 nm spectral resolution and a GSD of about 17 m, between ~30 m (CEOS 2018) and ~60 m (Hestir et al. 2015) to achieve reasonable coverage and provide continuity in the current Landsat-Sentinel-2 class of sensors.

6.2.3 Radiometric requirements

Radiometric resolution determines the lowest interval of radiance or reflectance that the sensor can reliably detect and discriminate per spectral band. As the spectral and spatial resolution increase, the useful signal relative to noise in the data decreases (as less photons are captured). This trade-off in spectral, spatial, and radiometric resolution is countered by improvements in instrument design and technology. Radiometric accuracy through absolute radiometric calibration is required to convert sensor digital read out to radiance in physical units.

6.2.3.1 Radiometric sensitivity requirements

Radiometric sensitivity affects both the accuracy of atmospheric correction performed on sensor radiance measurements as well as the subsequent retrieval of IOPs, OACs and physical water measures (Qi et al. 2017). A poor signal-to-noise ratio (SNR) can contribute up to one quarter of the OAC retrieval error (Salama and Stein 2009). OAC retrieval accuracy is strongly related to being able to separate the desired radiance signal from the overall noise in a pixel or image (Wettle et al. 2004). Three parameters can be used to describe the required or measured sensitivity of an Earth observing sensor (Wettle et al. 2004): the noise equivalent reflectance difference (NEdR), the noise equivalent radiance difference (NEdL), and the SNR. While the NEdR is more easily simulated or inverted using bio-optical forward and inverse models, it can vary with illumination conditions. NEdL, on the other hand, is an absolute measure of the radiance level that a sensor needs to discriminate, remaining constant under all illumination conditions, and is thus the most relevant for sensor design. The SNR is often used to compare or specify optical sensors. Muller-Karger et al. (2018) recommend a SNR of 800 in the visible region for coastal waters.

The effect of radiometric sensitivity on retrieval accuracy varies based on the concentration of the optically-active constituent in the environment, as well as on the total amount of backscattered light. Typically, the higher the concentration for scattering constituents, the higher the relative accuracy of retrieval for a given sensitivity as more radiance is available, although at very high scattering constituent concentrations multiple scattering effects will reduce this relative accuracy. Simulation results in the CEOS (2018) study indicate that a NEdL should lie in the range 0.005 mW m^{-2} sr^{-1} nm^{-1} (optimal) and 0.010 mW m^{-2} sr^{-1} nm^{-1} (as a minimum) to be able to detect relevant changes in, for example, Chl-*a* concentration globally (including high latitudes). A study by Hoogenboom et al. (1998) for detecting a change of 2 μg l^{-1} Chl-*a* (with TSM of 20 mg l^{-1}) at a level of 20 μg l^{-1} Chl-*a* in the mid latitude North Sea estimated a required NEdL of 0.2 mW m^{-2} sr^{-1} nm^{-1} (due to the higher reflectance caused by the TSM). A dedicated Earth observing sensor for inland waters also needs to have at least a maximum radiometric range for monitoring highly reflecting turbid waters (such as heavy mineral loads or dense algal scums) and shallow waters with bright sand of up to 400 mW m^{-2} sr^{-1} nm^{-1} in the blue and 200 mW m^{-2} sr^{-1} nm^{-1} in the red.

Retrieval accuracies can be improved by making radiometric enhancements that increase the number of photons measured at each pixel through modifying hardware, data acquisition strategies, or through image processing techniques by 1) increasing the F-number (aperture) of the camera lens; 2) increasing the detector pixel size; 3) increasing integration time (possible from geostationary without consequences for pixel size or shape but not from polar orbit, as the overpass speed needs to remain constant); 4) make use of dwelling, i.e., focus the sensor on one target whilst the spacecraft passes over (causing variable look angles during acquisition).

Using simulations, Moses et al. (2015) found that a 12 times increase in pixel photons resulted in a SNR increase of four times through the VIS and up to 10–12 times higher in NIR (due to significant dark noise and read noise improvements). Another way to increase SNR is to average across multiple pixels (often 3×3, 5×5, etc.), which also results in an increase in product retrieval accuracy (e.g., Brando and Dekker 2003; Giardino et al. 2007; Vanhellemont and Ruddick 2014; Moses et al. 2015). Unfortunately, the end result of this spatial binning is an effective decrease in spatial resolution (Hestir et al. 2015). Given that a GSD of 17 to ~33 m (CEOS 2018) or 60 m (Hestir et al. 2015) and a spectral band width of between 5 and 8 nm has been recommended, the requirement for SNR is 800 for coastal waters (Muller-Karger et al. 2018), or for inland waters as high as technologically feasible (within funding constraints) given the priority requirements of spatial and spectral resolution.

6.2.3.2 Radiometric accuracy requirements

Both IOCCG (2010) and IOCCG (2012) set a goal of 0.5% accuracy for TOA radiance at 443 nm. This is necessary to achieve a water-leaving radiance accuracy of 5% (at 443 nm) and a chlorophyll-*a* product accuracy of 30%. Dekker et al. (2001) evaluated these requirements for inland chlorophyll-*a* product accuracy across a range of oligotrophic to hypertrophic water bodies and recommended similar accuracy goals for green and NIR bands rather than just the blue bands of the IOCCG reports due to the spectral properties of inland waters (see spectral resolution requirements above). In inland waters the combined absorption of phytoplankton pigments, CDOM and NAP may cause very low R_{rs} in the 400 to 480 nm region, making green-red and even NIR wavelengths essential to water OAC retrieval. Thus, a goal for inland sensors is 0.5% for the TOA radiance uncertainty at all visible bands after vicarious calibration (see IOCCG 2012 for details).

6.2.4 Temporal requirements

Temporal (or revisit) requirements vary significantly per application. A useful discrimination is between lentic (standing) and lotic (flowing, e.g., rivers) water bodies. Table 6.3 summarises phenomena and the timescales at which they occur, as well as end-user or management required frequencies (applied to boat-based *in situ* sampling, autonomous *in situ* instrumentation, as well

Table 6.3 Observational frequency required to resolve phenomena occurring on various time scales (see Figure 3.1).

Phenomenon	Time-scale of phenomenon variability	Frequency to resolve changes from an end-user perspective
Algal diurnal migration and cycle	hourly	morning and afternoon
Early warning as well as development and movement of a (potentially harmful) algal bloom	hourly to daily	daily
Phytoplankton community composition	sub-weekly	weekly
Suspended sediment, CDOM, Secchi disk transparency, visibility, K_d, turbidity	lotic: hourly, lentic: daily	weekly (many water management authorities can only measure a few water bodies monthly)
Wetland phenologic change	monthly	quarterly
Aquatic invasive species response to management	monthly	quarterly
Seasonal responses in biomass	monthly	weekly

as Earth observation measurements from bridges, platforms, drones, UAVs, aircraft, balloons and satellites). Temporal requirements also vary with the availability of *in situ* measurements: where there are no *in situ* measurements (due to remoteness, lack of infrastructure or state of nation development) even one water quality image per year will be valuable, especially if retrospective analysis is possible (e.g., analysing the Landsat 30 m spatial-resolution archive back to 1984). Alternatively, if a sophisticated water sampling and monitoring programme is already in place, the requirement for temporal resolution from Earth observations significantly increases.

On average, only one to two thirds of images taken over specific areas are suitable for further analysis due to adverse weather and air-water interface conditions. Many images are rejected because they are affected by atmospheric conditions (mist, fog, haze, dust or clouds), low sun-angle effects due to season or latitude, and sun/sky glint effects at the water surface (due to sensor-sun-wave geometry). Solutions for avoiding sun glint effects are to tilt the sensor away from the sun in combination with the timing of the overpass. Solutions for increasing temporal sampling include:

- Making use of constellations of polar orbiting sensors, e.g., MODIS-Terra and Aqua sensors, VIIRS on SNPP and later on the JPSS series, and the Sentinel series (e.g., Sentinel-2 and -3), or RapidEye sensors of which five are in orbit, to even larger constellations;
- Consider additional orbits, e.g., around the equator, or equator to mid latitudes, to enhance the likelihood of capturing cloud-free pixels in the tropics;
- Making use of geostationary sensors as they can measure part of a semi-globe once every 10 minutes (e.g., Himawari-8 and -9).

Most water quality managers or other end-users require as high a temporal resolution as possible. One of the consequences of high temporal resolution, however, is a much higher data rate which needs to be processed to a final end product (often terabytes of data per day). There are also costs associated with designing, building, launching and operating multiple satellite sensors. Polar orbiting satellites are less costly to launch than geostationary satellites, but geostationary satellites need less fuel to stay in orbit (no atmospheric drag).

6.2.5 Requirements trade-offs and solutions

Trade-offs are required between available funding and maximum end-user requirements for satellite sensors, data processing systems and associated *in situ* measurement infrastructure. Only a limited amount of photons (limited by spectral, radiometric and spatial resolution) can be measured from space, noting that polar orbiting satellites pass over at a velocity approaching 30,000 km per hour at altitudes between 450 to 800 km. One orbit of the Earth generally takes about 90 to 100 minutes depending on the altitude. Geostationary satellites, on the other hand, have a longer sensor–Earth distance (~36,000 km) allowing higher integration times as the sensor remains fixed at the same location over the Earth (geostationary satellites match the Earth's equatorial velocity exactly).

From the discussion on spectral resolution, spectral bands of 5 to 8 nm are required for most OACs (with 3 to 5 nm for chlorophyll fluorescence), whereas 15 nm wide bands or even wider are sufficient for the OACs that show a more gradual (often exponential) relationship with increasing wavelength. The spatial analysis results indicate that a GSD of ~15 to 17 m will sample 90 – 100% of global lakes >0.002 km^2 and 24% of rivers, while a GSD of ~30 to 33 m will sample 90% of lakes plus 12% of river reaches. A GSD of ~3 m would also sample 80% of river reaches.

A global water quality mapping system should therefore have 5 to 8 nm spectral bands, preferably from ~340 nm to 720 nm, with a few broader (~15 nm) atmospheric correction bands in the NIR and SWIR wavelengths. A GSD of 33 m seems to be a threshold for a global mapping mission, but higher spatial GSD resolution will include more water bodies (especially rivers) and will make the satellite sensor more relevant.

6.3 Recommended Specifications for Future Sensors

Specifications of existing and near future sensors are examined next, assessing the suitability for inland water body remote sensing. Table 6.4 presents an assessment of sensor suitability for detecting OACs as well as physical light-based measurements (e.g., K_d, Secchi disk transparency and turbidity). The table does not attempt to determine optimal spatial resolution as any particular end-user will have different spatial resolution requirements based on the size and shape of the water body being assessed. It is clear from the table that more spectral bands lead to more variables being discriminated. The planned experimental space-based imaging spectrometers are most relevant for all inland and near-coastal water applications.

Table 6.4: Historical, existing and near-future satellite sensor systems of relevance for inland and near-coastal water quality (revised and updated after Dekker and Hestir 2012). 🔵 = highly suitable; ⚪ = suitable; 🟠 = potential; 🔴 = not suitable. Data cost = raw data cost per km^2 ($USD), free = publicly available, free (?) = available upon request for research, CHL = Chlorophyll, CYP = cyanobacterial pigments, TSM = total suspended matter, CDOM = coloured dissolved organic matter, Kd = light attenuation coefficient, Turb = turbidity/Secchi depth, Emerg. = emergent, Float = floating leaved, Subm. = submersed and S = surface bloom.

Sensor Type	Sensor	Resolution (Pixel size)	Spec. Bands	Revisit Frequency	Data Cost	Launch Date	Water Quality Variables						Macrophytes		
							CHL	CYP	TSM	CDOM	Kd	Turb	Emerg.	Float	Subm.
ocean-coastal resolution	MERIS	1.2 km/ 300 m	15	2 days	free	Mar-02 to May-12	🔵	🔵	🔵	🔵	🔵	🔵	🟠	🟠	🟠
mid-spatial resolution	LANDSAT 1–7	30 m	4	16 days	free	Jul-72, multiple	🟠	🟠 S	⚪	🟠	⚪	⚪	⚪	⚪	🟠
Hyperspectral	Hyperion	30 m	60	60	free	2000 to 2017	⚪	⚪	⚪	⚪	⚪	⚪	🟠	🟠	🟠
Hyperspectral	HICO	90 m	100	orbit 51°N, 51°S, 3 to 5 d cadence	free	2009 to 2014	🔵	🔵	🔵	🔵	🔵	🔵	🟠	🟠	🟠
ocean-coastal	MODIS-A and T	1 km	9	daily	free	Dec-99	🔵	⚪	🔵	🔵	🔵	🔵	🔴	🔴	🔴
	MODIS-A and T	500 m	2	daily	free	Dec-99	🟠	🔴	⚪	🟠	🟠	🟠	🔴	🟠	🟠
	MODIS-A and T	250 m	2	daily	free	Dec-99	🟠	🔴	⚪	🔴	🟠	🟠	🔴	🟠	🟠
	OCM-2	300 m	8	2–3 days	free	Sep-09	🔵	🔵	🔵	🔵	🔵	🔵	🟠	🟠	🟠
	Suomi-VIIRS	750 m	10	daily	free	Oct-11	🔵	⚪ S	🔵	🔵	🔵	🔵	🔴	🔴	🔴
	Suomi-VIIRS	375 m	3	daily	free	Oct-11	🟠	🔴	⚪	🔴	🟠	🟠	🔴	🟠	🟠
geostationary	SEVIRI on MSG	1 km	2	96 per 24 h	free	2002	🔴	🔴	⚪	🔴	🔴	🟠	🔴	🔴	🔴
	GOCI	500 m	8	half-hourly	free	2010	🔵	🟠	🔵	🔵	🔵	🔵	🟠	🟠	🟠
	Himawari-8&9, GOES-R	500 m - 2 km	4	10 min	free	2014	🟠	🔴	🔵	🟠	🟠	⚪	🔴	🔴	🔴
mid-spatial resolution	LANDSAT-8	30 m	5	16 days	free	Sep-13	🟠	⚪ S	⚪	🟠	⚪	⚪	🟠	🟠	🟠
mid-to-high spatial res.	MSI	10 m to 60 m bands	10	10 d (5 days with two S-2's)	free	Jun-15	⚪	⚪ S	⚪	⚪	⚪	⚪	⚪	⚪	⚪

Continued on next page

Table 6.4 – *Continued from previous page*

Sensor Type	Sensor	Resolution (Pixel size)	Spec. Bands	Revisit Frequency	Data Cost	Launch Date	Water Quality Variables						Macrophytes		
							CHL	CYP	TSM	CDOM	Kd	Turb	Emerg.	Float	Subm.
high spatial resolution	QuickBird, SPOT6, GeoEYE	2 – 4 m	3 – 4	programmable 60 d to 2–3 d	5–15	1999 onwards		S							
	RapidEye	6.5 m	5	daily	1.5	Aug-08		S							
	WorldView-2	2 m spectral, 0.5 m B&W	8	programmable 60 d to 1 d	30	Oct-09									
	WorldView-3	1.2 m spectral, 0.5 m B&W	8	programmable 60 d to 1 d	30	2014									
ocean-coastal	OLCI	300 m	21	daily (2 sats.)	free	2016									
ocean-coastal	SGLI-2	250 m	9	2 – 4 d	free	2017		S							
	JPSS-1, JPSS-2, etc.	750 m	10	daily	free	2017, 2022		S							
	JPSS-1, JPSS-2, etc.	375 m	3	daily	free	2017, 2022									
	OCM-3	300 m	15	2–3 d	free	2017									
hyperspectral	EnMap	30 m	90	programmable (once/4 d)	free (?)	2019									
	DESIS	30 m	235	orbit 51°N, 51°S, 3 to 5 d cadence	free (?)	2018									
	HISUI-hyper	30 m	60	orbit 51°N, 51°S, 3 to 5 d cadence	free (?)	2018									
	PRISMA	20 m spectral, 2.5 m B&W	60	25 d/ pointing 7d	free (?)	2018									
	HySpIRI*	30	60	16	free	2022									

* *The 2017 US Decadal Survey recommended several designated target observables, including surface biology and geology (SBG). SBG has candidate measurement approaches that are similar to the HyspIRI mission concept that NASA was developing over the past decade, including inland and near-coastal aquatic ecosystems.*

Requirements for an "ideal" inland and near-coastal water quality sensor (with realistic physics and instrument constraints) would include an imaging spectrometer with 5 to 8 nm wide spectral bands from ~340 to 720 nm, 15 nm wide bands from 725 nm to 1000 nm, and the addition of at least three NIR/SWIR bands (around 1240, 1640, and 2130 nm) for atmospheric correction and vegetation chlorophyll separation. The SNR should be 800 in the visible (for coastal waters see Muller-Karger et al. 2018), or alternatively, for inland waters high as technologically feasible (within funding constraints) given the driving requirements of spatial and spectral resolution. These requirements build on the generic inland and coastal water recommendations of Mouw et al. (2015) and are slightly higher than those recommended for inland waters (Hestir et al. 2015) due to the incorporation of the CEOS (2018) simulation results. The spatial resolution would need to be as high as feasible, but at a minimum ~33 m GSD (CEOS 2018) or at a minimum ~60 m (Hestir et al. 2015), with an optimal GSD being ~17 m if at least 25% of river reaches are to be detected.

Simulation results in the CEOS (2018) study indicate that a NEdL should lie in the range 0.005 mW m^{-2} sr^{-1} nm^{-1} (optimal) and 0.010 mW m^{-2} sr^{-1} nm^{-1} (as a minimum) to be able to detect relevant changes in, for example, Chl-*a* concentration globally (including high latitudes). These requirements can be relaxed (if needed due to sensor and budget constraints) with the realisation that detection sensitivity for optically-active constituents (Chl-*a* , CPC and CPE, NAP and CDOM) and transparency measures (Secchi disk transparency, turbidity and K_d) will be reduced.

The revisit frequency should be as high as is affordable (either large swath width or multiple sensors from low Earth orbit or from geostationary orbit). The Sentinel-2 frequency (a global image every 5 days with two Sentinel-2 sensors) is suited for most water quality assessments except for those features that occur at hourly or daily time frequencies. These higher frequency observations may become possible using geostationary sensors, or equatorial orbit sensors. Sensors should preferably never get saturated (i.e., over cloud, white sand, land, etc.). In addition, sun glint should be avoided wherever possible, preferably through overpass timing and pointing the sensor away from the sun.

Two of the most relevant Earth observing sensors for coastal and inland waters (particularly for small area inland lakes) that are publicly available, well–documented and published, and which provide long term coverage, are the Landsat and Sentinel-2 missions. Both are, however, designed for land applications. Traditional global satellite ocean colour sensors such as MODIS, MERIS, VIIRS, and OLCI are also useful for water quality monitoring over coastal and relatively large inland waters. As new versions for Landsat and Sentinel-2 are foreseen, a cost effective manner to enhance these sensors and make them more useful for inland and near-coastal water remote sensing would be to add a few spectral bands and increase the spatial resolution where possible. For example, if all the bands on Sentinel-2 were 10 m spatial resolution, that would be a significant benefit for inland water remote sensing. For Sentinel-2 and Landsat some extra spectral bands (8 to 10 nm wide), such as at the red chlorophyll-*a* and cyanophycocyanin-suitable wavelengths (centered at 615 to 624 and 672 to 680 nm) would significantly enhance their suitability as global missions for inland water quality. For new multi- or hyperspectral ocean colour sensors, an increase in spatial resolution would significantly enhance their usefulness over inland and near-coastal water bodies.

Chapter 7

Ground Segment and User Segment

Steve Groom, Carsten Brockmann and Stefan Simis

7.1 Introduction

Next to the challenging task of building and launching satellites, the success of an Earth observation (EO) mission relies on being able to operate the satellite from the ground and ensure that the data gathered are of good quality and made available readily to users. Furthermore, for the data to be exploited by scientific, management and commercial end-users, a suitable processing chain is needed to generate variables of interest, such as chlorophyll-*a* or suspended particulate matter concentration for water quality monitoring. These may be produced and delivered in near-real time for operational monitoring applications, like harmful algal blooms, or as long time-series of archived data, to look at natural variability, and trends if the time-series is of sufficient duration. These activities are termed the ground segment (GS) and may be split into activities undertaken by the space agency that operates the sensor and delivers "upstream" data (the mission or satellite ground segment) and a "downstream" service that takes "upstream" data and produces services and products for the end-users (the user ground segment). This chapter briefly describes the mission ground segment and then focusses on the user ground segment. A number of issues such as data dissemination are common to both types of GS.

7.2 Mission or Satellite Ground Segment

7.2.1 Overview

The satellite ground segment typically comprises a flight operations and control centre with an antenna to send commands to the satellite, together with at least one ground station to receive data stored on-board the spacecraft as they are 'downlinked' from the satellite as it passes overhead. This may be complemented by direct-broadcast stations that typically only receive data recorded whilst the satellite is within line-of-sight. Direct broadcast can provide rapid access to regional data (i.e., the geographical coverage of the station) but typically requires a separate processing chain to that operated by the satellite agency. Facilities for data processing, storage and distribution are also needed. Last, but not least, the quality of the data and the performance of the satellite sensor has to be monitored continuously. For water quality applications based on visible radiometry, top of atmospheric (TOA) radiance data calibration is crucial, since the water signal is usually only a small percentage of the TOA signal.

Calibration of ocean colour satellites has to be carried out routinely, with regular re-assessments to guarantee the overall performance of the mission. Calibration is achieved by a combination of approaches including pre-launch characterisation and in-orbit calibration that may involve viewing internal lamps, the sun or moon, as reference sources of radiance. For ocean colour remote sensing, however, these approaches have been found insufficient to deliver radiances of the quality needed to retrieve water quality parameters. Hence, so-called system vicarious calibration (SVC) is undertaken which compares the expected TOA signal as detected by the sensor with a simulated system of in-water (measured) radiance together with an atmospheric model (e.g., Zibordi et al. 2015). Since this is a complete system calibration, it needs to be performed separately with different atmospheric correction models; hence, SVC is undertaken as part of the mission GS or the user GS. NASA undertake SVC on ocean colour sensors using the MOBY system located off Hawaii in clear oceanic case 1 waters. The French "BOUSSOLE" buoy located in the Ligurian Sea (western Mediterranean), is also used to calibrate ocean colour satellite observations and to validation the products. SVC is also performed in the ESA Ocean Colour CCI project on SeaWiFS, MODIS, MERIS, VIIRS and OLCI data using a variety of atmospheric corrections and includes approaches improved for use in case 2 waters. It should be recognised, however, that the use of novel atmospheric corrections for inland waters would require an SVC to be performed over representative reference sites; the use of MOBY alone may be problematic if the atmospheric correction uses concepts unique to enclosed water bodies like lakes, or are optimized for continental aerosols.

7.2.2 Mission ground segments

It should be noted that no single agency operates a mission ground segment that is dedicated to coastal or inland water quality (yet). An end-to-end demonstration of a user ground segment was established in support of the GEO 2012–2015 work plan within the ChloroGIN environment (see Subsection 7.3.1), and the new European Copernicus Global Land project uses the "Calimnos" processor to produce operational water-quality data: these are discussed in Section 7.3.

7.2.2.1 NASA/GSFC

The NASA GSFC Ocean Biology Processing Group (OBPG, https://oceancolor.gsfc.nasa.gov/) produce ocean colour data from NASA sensors such as SeaWiFS, MODIS and CZCS as well as third-party missions including ESA MERIS (both reduced and full resolution), NOAA VIIRS, and HICO, particularly relevant as a hyperspectral demonstrator for coastal and inland waters. Data are provided at Level-1 (reconstructed, unprocessed instrument data at full resolution, time-referenced and annotated with ancillary information) and Level-2 (derived geophysical variables processed using the "l2gen" atmospheric correction with standard products). These data can provide the starting point to a user ground segment: for example, users interested in standard Chl-a algorithms can use the L2 data and re-map to areas of interest. Alternatively, L2 R_{rs} data can be used with specific regional algorithms to produce user-specific products. Level-3 data (derived geophysical variables that have been aggregated/projected onto a well-defined spatial grid over a well-defined time period) are also provided at daily, weekly, monthly, seasonal and annual resolutions, 4 or 9-km (depending on sensor) with a variety of algorithms as "standard", "evaluation" and "test" products. Individual images can be downloaded as PNG or NetCDF files and subsets can be ordered. These L2 and L3 products are focussed on marine applications and no inland water specific products are produced.

7.2.2.2 ESA/Sentinel-2 and 3 collaborative ground station

ESA Sentinel data are freely available for academic or commercial use and a number of different access points are envisaged including rolling archives, national collaborative ground segments and multicast using EUMETCast (see below). European Copernicus services provide products derived directly from the agency ground segments. For inland waters, as noted below, this is the responsibility of Copernicus Global Land. For inland and coastal water quality applications the two key instruments are Sentinel-2 MSI and Sentinel-3 OLCI: each has a different ground segment structure. For Sentinel-3, L1 and L2 data are produced by EUMETSAT and distributed by GEONETCast as well as via FTP. The Copernicus Marine Environment Monitoring Service (CMEMS) led by Mercator Ocean has an Ocean Colour Thematic Assembly Centre (OCTAC) that will obtain Sentinel-3 data from EUMETSAT and produce regional products based on regional algorithms (e.g., for the Mediterranean, Volpe et al. 2007) as well as regional and global L3 mapped products, in both near-real time and through reprocessing.

The situation with Sentinel-2 MSI is less clear. The sensor is designed primarily for land applications but has water quality observation capability, at least for turbid waters (Sentinel-2 MSI data is collected for all land surfaces as well as coasts up to 30 km offshore and coral reefs). There is no formal ground segment currently planned, but efforts are in place for user GS to provide products, and the Copernicus Global Land Service is developing higher resolution products based on Sentinel-2. MSI data are disseminated at Level-1C (mapped to UTM tiles) and Level-2 (for land applications) and will thus require dedicated downstream processing for water quality. The Sentinel Application Platform (SNAP, http://step.esa.int/main/toolboxes/snap/) is an open source common architecture for ESA Toolboxes designed for Sentinel-2 processing and analysis.

7.2.2.3 NOAA STAR and CoastWatch

The NOAA NESDIS Center for Satellite Applications and Research (STAR) undertakes processing of ocean colour data from MODIS and VIIRS from Level-0 up to Level-3 products (see http://www.star.nesdis.noaa.gov/sod/mecb/color/) whilst mapped data for standard user regions of interest are available from NOAA CoastWatch that links through to different regional nodes.

7.2.3 Data distribution mechanisms

In general, the easier it is to access data, the more those data are used for applications and publications. This applies to all levels of users from experts (or operators of user ground segments) easily gaining access to data via file transfer protocol (FTP), to end-users who may want an Excel spreadsheet of numbers showing variability with a location or with time. There are a number of dissemination systems that can be described here ranging from traditional FTP, tape or web download to more complex and novel web-based services using Open Geospatial Consortium (OGC) standards or otherwise, and multi-cast through such approaches e.g., GEONETCast.

7.2.3.1 FTP, tape and web downloads

Data access by file transfer protocol and tape is well established in the community and is not described further herein. Web download is also well established and probably represents the most popular way of obtaining water quality data such as through the NASA Ocean Color web site (https://oceancolor.gsfc.nasa.gov/) or the ESA Ocean Colour Climate Change Initiative (OC-CCI) site (www.oceancolour.org).

7.2.3.2 GEONETCast near real time dissemination system (GEO)

GEONETCast is a distribution system based on Digital Video Broadcast technology with multi-casting environmental data via commercial satellites. It is particularly valuable for institutes or universities with poor internet access due to their location, such as marine institutes located at the coast, or due to limited national infrastructure. For Africa, a number of projects have attempted to build capacity amongst marine institutes. The European Commission funded the DevCoCast and EAMNet projects which installed low-cost GEONETCast receivers at approximately eight sites across the continent, including one focussed on inland waters on Lake Victoria. The low-cost systems had mixed success, not least due to the exposed locations at the coast. As a legacy of the EAMNet project, water quality data at 1-km resolution for user regions of interest covering the entire coast of Africa are produced by the Plymouth Marine Laboratory (PML) and University of Cape Town (UCT) and transmitted via GEONETCast. The on-going Monitoring of Environment and Security in Africa programme (MESA: http://moi.govmu.org/mesa/ completed in 2017) has installed further reception capacity based around Regional Implementation Centres including two involved in Marine and Coastal Management operated by the Mauritius Institute for Oceanography (in the Indian Ocean) and the University of Ghana (western Africa). GEONETCast data provision is expected to be maintained in the "GMES and Africa" project which is superceding MESA.

7.2.3.3 Web-based analysis systems

For exploitation of water quality data by non-specialist end-users it is important to provide easy-to-use tools, ideally web-based, that support simple analysis of datasets provided by the ground segments. This ensures that EO data have an impact beyond specialist academic communities. A variety are available ranging from simple tools to analysis systems.

7.2.3.3.1 OGC-based systems

The Open Geospatial Consortium (OGC) specifies standards for accessing data by the web. There are a number of standards including Web Mapping Service (WMS) whereby images (such as GIF) are provided, Web Coverage Service (WCS) which serves arrays of data, and Web Feature Service (WFS) that specifies point or other vector data such as ship-tracks or region of interest boundaries. In principle, web-based portals using these standards can communicate with other data portals and request and visualise data. Many of the portals have built-in analysis capabilities allowing time-series analyses. These offer great potential for the future exploitation of EO data since delivery is only required of the results of the analysis, not the full data-set which may comprise many gigabytes or terabytes of data.

An example of a web-vis system is the GloboLakes portal that was originally developed in the EC FP7 OpEc project (see Figure 7.1). This system allows selection of regions of interest (either square or arbitrary polygons) then produces simple time series, Hovmöller plots, or time animations of these data. Figure 7.1 shows an extracted time series of Chl-*a* from the NERC GloboLakes data set. The portal also provides data analysis in user-specified regions of interest defined by shapefiles, additional analyses such as scatterplots between two variables, and data extraction in time and space, such as along a ship track.

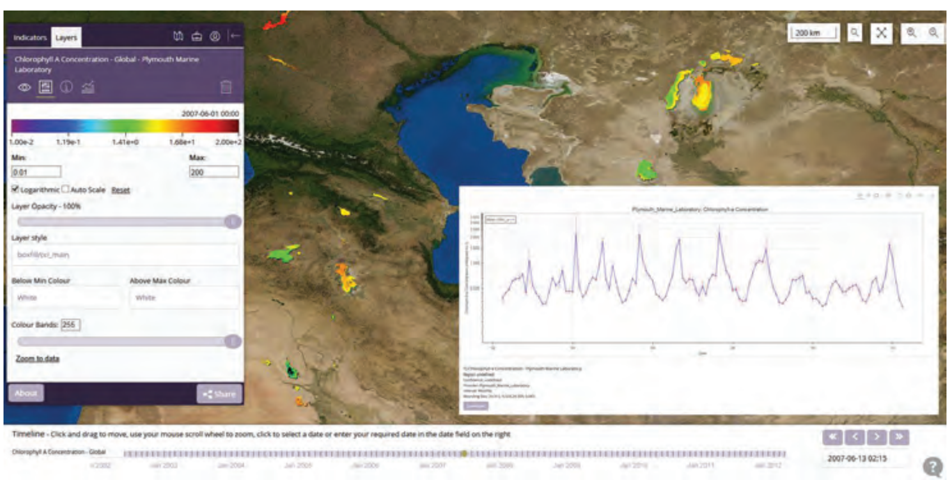

Figure 7.1 Example OGC based web-vis analysis system (https://globolakes.eofrom.space/) showing the Aral Sea and lakes in the Caucuses; inset time series of monthly Chl-*a* for a box in Lake Tanganyika, Africa.

7.2.3.3.2 User portals

There are a number of end-user portals available that provide access to information derived from *in situ* and EO data. These will become increasingly important since information is more relevant to most users than the original data. An example is the South African EO National Eutrophication Monitoring Programme (EONEMP) that is funded by the South African Water Research Commission and developed by CyanoLakes Pty (`http://www.cyanolakes.com/eonemp_1/`). The portal provides data from satellites (see Figure 7.2a) but also gives a status flag in terms of a Health Risk for each water body (Figure 7.2b).

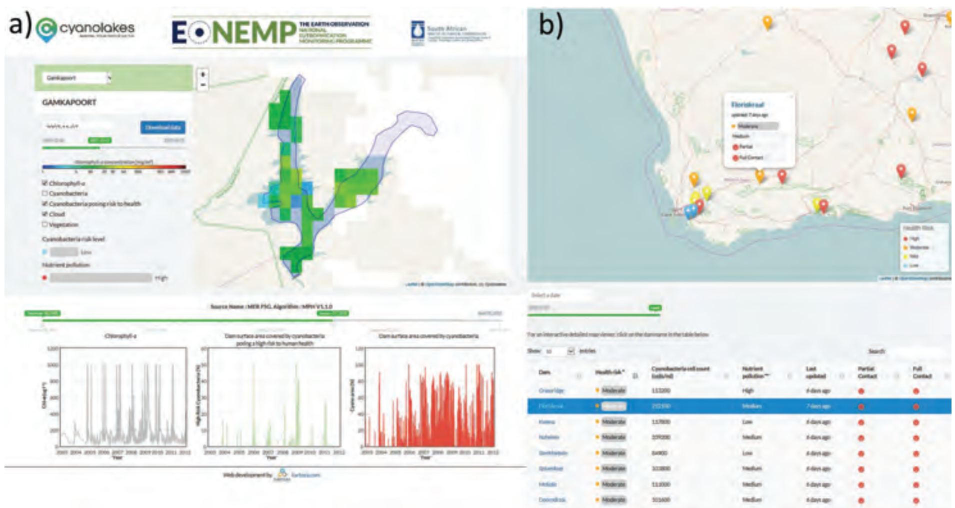

Figure 7.2 Screenshots of the South African EONEMP portal.

7.3 User Ground Segments

This section gives a brief description of a user ground segment to produce operational water quality observations from satellite data, essentially combining a number of steps described earlier in this report, including water-quality algorithms (Chapter 5) and data delivery (earlier in this chapter).

7.3.1 ChloroGIN-Lakes: an end-to-end demonstrator

In support of the Task Sheet for the "GEO 2012–2015 Work Plan: Global Inland and Near-Coastal Water Quality Information System" an end-to-end demonstrator was established at the start of 2012 based on ESA MERIS full resolution data. Due to the demise of Envisat in April 2012, the demonstrator only functioned briefly, but it served its purpose to give an overview of how a complete system can be produced based on a combination of agency and user ground segments. ChloroGIN-lakes started with L1 and L2 MERIS FR data obtained by Plymouth Marine Laboratory in near-real time from the ESA rolling archive via FTP. The data products comprised the standard ocean algal_1 and algal_2 Chl-*a*, yellow substance (CDOM + detritus) and SPM: it was accepted that these were not optimised for inland water bodies but the aim of the exercise was to show that an end-to-end demonstrator was possible. The Level-1 data were obtained and processed to Level-2 through SeaDAS, showing that local processing with potentially lake-specific algorithms was possible.

The data were then mapped to individual regions of interest using the same system as used at PML for UK and international projects such as Copernicus Marine Environment Monitoring Service (CMEMS). Each region was stored in a database and data were automatically processed when covering all or part of the region of interest. Finally, the images were made accessible via the standard ChloroGIN portal where users can "click" on an area of interest, select a date and then view individual scenes using the regional data producers' web site (in this case the PML MultiView web viewer).

Subsequent to the failure of Envisat, data from MODIS were processed at 500-m for various lakes. The quality of this MODIS data in terms of spatial resolution and number of bands was inferior to MERIS, but nevertheless demonstrated the feasibility of this system.

7.3.2 Calimnos: a dedicated approach to inland water quality data production

Calimnos is an inland water-quality data production framework based on the ESA Diversity II processing chain, developed by Brockmann Consult, together with updates from Plymouth Marine Laboratory and the University of Stirling, developed in the context of the UK GloboLakes project. Initially it was designed to process archived ESA Envisat MERIS data, but is also producing near-real time and archived products from Sentinel-3 OLCI and Sentinel-2 MSI data.

The system was selected for operational production of water quality data in the Copernicus Global Land project for an initial period of 2016–2019. The products comprise 10-day composites (decades) of trophic status, suspended particulate matter and reflectance both from archived data and in "near-real time". The Copernicus Global Land instance (see Figure 7.3) applies the HYGEOS Polymer atmospheric correction (Steinmetz et al. 2011) and in-water retrieval algorithms/processors to generate a range of products that can then be aggregated. Notably, the algorithms that are applied to atmospherically-corrected data are calibrated against a global set of *in situ* validation data representing a wide range of optical properties. Thus, regions where *in situ* validation data are scarce benefit from validation activities carried out for optically-similar water bodies elsewhere.

7.4 Summary

The success of an Earth observing satellite mission is critically dependent upon the ground segment activities undertaken by the space agency and, if separate, an operational data production centre. Mission ground segments exist for oceans and some coastal regions but to date there has been no dedicated inland and near-coastal ground segment. In projects such as ESA's Diversity II and the UK GloboLakes, methods have been developed to process EO data from large numbers of lakes worldwide using a variety of algorithms and so produce a user-ground segment. With the advent, notably, of the European Sentinel missions including Sentinel-2 and -3 along with the archive of MERIS, it is now becoming possible to contemplate an operational inland and near-coastal water quality ground segment. In Europe, the Copernicus

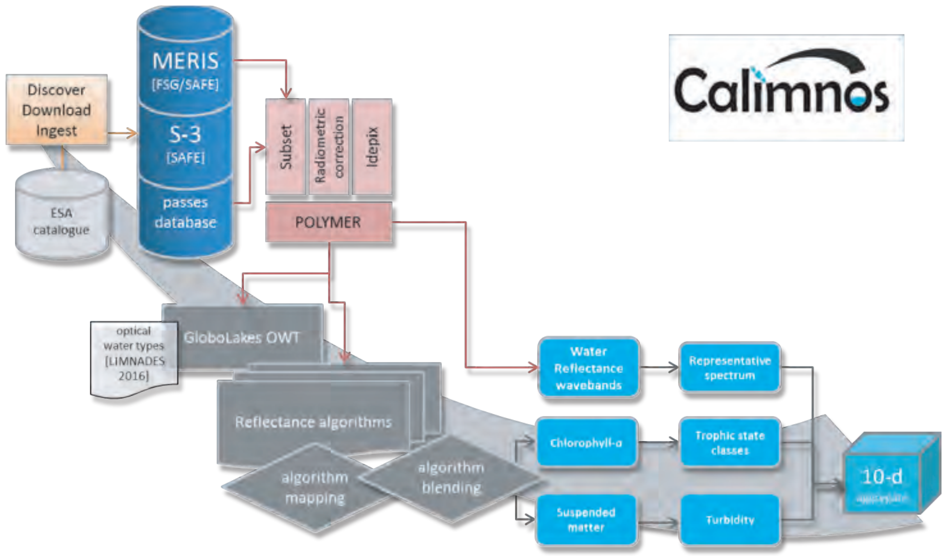

Figure 7.3 Data flow from satellite data through to final products in the Copernicus Global Land project using the Calimnos processing chain (version 1.2, December 2017). S-3 = Sentinel-3 OLCI, OWT = optical water type classifier. Figure courtesy of Stefan Simis, Plymouth Marine Laboratory, UK.

Global Land project is producing a global operational service for inland water quality products. Another example of an operational water quality service being developed is the UNESCO-IHP IIWQ World Water Quality Portal designed by EOMAP (https://www.eomap.com/portfolio_projects/unesco-ihp-iiwq-portal/).

Chapter 8

Moving Forward

Carsten Brockmann, Steve Groom and Blake Schaeffer

With the availability and advent of new missions providing Earth observation (EO) data at high to very high spatial resolution over a large swath (e.g., Sentinel-2 multi-spectral instrument) or in hyperspectral mode (e.g., EnMap, Germany's hyperspectral Earth observation satellite, the Italian PRISMA mission, the Japanese HISUI on ISS and DLR's DESIS also on ISS), the amount of data will increase by an order of magnitude. This expanding operational capability of global monitoring from space, combined with data from long-term EO archives (e.g., Landsat, ERS, Envisat), *in situ* networks and models, will provide users with unprecedented insight into how our oceans, coasts and inland waters interact with the atmosphere, land and ice, and are influenced by anthropogenic stimuli. While the availability of the growing volume of environmental data from space represents a unique opportunity for science and applications, it also poses a major challenge to achieve its full potential in terms of data exploitation. The emergence of large volumes of data (petabytes per year) raises new issues in terms of access, discovery, exploitation, and visualization (Hey et al. 2009). Interoperability will be necessary to address the growing diversity and complexity of data, and users will have to address different coding languages, file structures, semantics, and formats. Evolution in information technologies and the consequent shifts in user behaviour provide new opportunities to facilitate EO data exploitation. Examples of such new concepts can be found in the ESA Thematic Exploitation Platform (Bitto et al. 2014), the U.S. Virtual Laboratory, Australia Data Cube (http://www.ga.gov.au/dea) implemented in Digital Earth Australia which is open source and now being replicated in over 16 countries, Biodiversity & Climate Change Virtual Laboratory (BCCVL, http://www.bccvl.org.au/), and the international Geohazards Supersite (http://www.helix-nebula.eu/usecases/esa-ssep-use-case).

This chapter will discuss the challenges and opportunities of democratizing access to large EO data sets in combination with *in situ* measures and models. The concept is to provide a non-linear decision tree user platform to provide data and tools, instead of a pre-defined and linear processing format. Here, we provide examples of existing and planned platforms and virtual laboratories.

8.1 "Big Data" From Space — Historic Archives and Future Data Volumes

Space-borne EO has provided data since the early 1970's with the MSS sensor on Landsat-1 for systematic observations of the Earth's surface, including coastal and inland waters, in four spectral bands. However, on-board data storage and data transmission capabilities were very limited. A significant increase in data volume per acquired scene took place with the Thematic Mapper on Landsat-4 in 1982, shortly followed by Landsat-5 in 1984, which provided more spectral bands, and higher spatial resolution. The 160 MB per scene required three 9 inch tapes and dedicated computer hardware to process them. Today such data volumes are considered small; however, due to the 25 years of Landsat-5 operations, the total volume of all products available at the United States Geological Survey (USGS) is over 3.6 million scenes corresponding to 576 TB (status 2008, http://earthobservatory.nasa.gov/Features/LandsatBigData/) with a further 450 TB added recently from scenes acquired by the ground-based space-tracking stations for the European Space Agency at Kiruna, Sweden.

With every new generation of satellite missions the data volumes increase significantly. ESA's first series of EO satellites, ERS, produced about 100 TB during their 10-year mission life time. This corresponds to the amount of data produced by the subsequent ENVISAT mission in just one year. The ENVISAT archive now amounts to 1.2 PB, not counting derived products.

The Sentinel-1-2-3A satellites will provide a data stream of 500 MB per second (Bargellini 2013) equal to 43 TB per day which needs to be processed and stored under stewardship. The resulting core user products are estimated as 4 TB per day (Potin 2014). It should be noted that ESA will operate two satellites (A and B series) in parallel for most of the time, which will double the data volumes. Figure 8.1 shows the exponential increase of satellite data, just for the data available from the European Space Agency. A rough rule of thumb is that the data produced by one satellite mission during a typical 10-year lifetime is produced by the next generation within one year. It is also important to differentiate between the data acquired by a mission and the data required for an application or decision, which is only a portion of the complete data archive.

8.2 Paradigm Shift — Services for EO Data

The increase of data volumes described above is challenging for data processing, but even more so for accessing the data. Bandwidth and data transfer costs are inhibiting systematic near real-time processing at a global scale. This can also affect inland water processing if data selection and spatial sub-setting are not properly supported. In recent years, there has been a paradigm shift from downloading and processing data locally, to moving the processing software at the data source. Although there is a wide agreement on this change, it is an ongoing process and most users still download data and process in the traditional way. This may be attributed to the fact that specialized systems i.e., hardware and software with cost implications, are required to support the new way of processing EO data close to the data

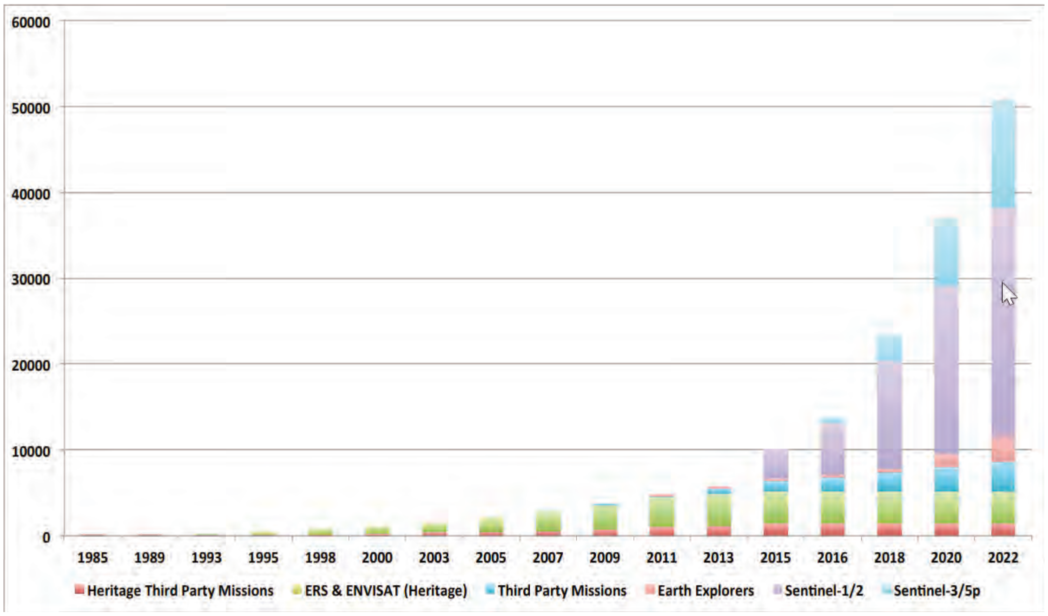

Figure 8.1 Archived data, European Space Agency, in terabytes.

source.

8.2.1 Service models

The trend toward large datasets and the need for appropriate computing resources is not specific to EO but is also observed in many data driven applications. Instead of hosting one's own technical infrastructure, developing in-house software and maintaining internal expertise, three different service models have emerged to deal with big data sets more efficiently and cost effectively.

8.2.1.1 Infrastructure as a Service (IaaS)

Infrastructure as a Service (IaaS) is a form of cloud computing that provides virtualized computing resources over the internet. In an IaaS model, a cloud provider hosts the infrastructure components traditionally present in an on-premises data center, including servers, storage and networking hardware, as well as the virtualization or hypervisor layer. The IaaS provider also supplies a range of services to accompany those infrastructure components. In the case of EO this includes access to the satellite data, processing, security, core load balancing and clustering, as well as storage resiliency, such as backup, replication and recovery. Research scientists can use IaaS to configure their own processing application. They can access resources and services through a wide area network, such as the internet, and can use the cloud provider's services to install the remaining elements of an application stack. Any IaaS model requires the participation of a provider, typically a third-party organization. Examples of

IaaS providers include Amazon Web Services, Microsoft Azure, or Google Cloud Platform. Organizations choose IaaS because it is often easier, faster and more cost-efficient to operate a workload without having to buy, manage and support the underlying infrastructure. With IaaS, a business can simply rent or lease the infrastructure from another business.

8.2.1.2 Platform as a Service (PaaS)

Platform as a Service (PaaS) is a cloud computing model in which a third-party provider delivers hardware and software tools — usually those needed for application development — to users over the internet. A PaaS provider hosts the hardware and software on its own infrastructure. This is currently the most popular model where EO data and EO processing software are offered on a dedicated hardware infrastructure. Google Earth Engine, the ESA EO Open Cloud, the Digital Earth Australia DataCube, or the Thematic Exploitation platforms are examples for PaaS.

PaaS combines the advantages of IaaS and SaaS (see below) into a single package. It requires less initial investment and less risk, has fast and adaptable software support and generally greater availability and security of data. Disadvantages include increased pricing at larger scales, lack of operational features, and reduced control.

8.2.1.3 Software as a Service (SaaS)

Software as a Service (SaaS) is a software distribution model in which a third-party provider hosts applications which users can download over the Internet to their local machines for data processing and analysis. This is the traditional way of accessing software and processing satellite data. In the case of EO, software such as NASA's SeaWiFS Data Analysis System (SeaDAS) or ESA's Sentinel Application Platform (SNAP) are used.

The advantages of SaaS include relative costs, with software generally sold as a subscription fee (versus software license), scalable and flexible, available anywhere, less hardware is required because the software is hosted remotely, and no software and hardware maintenance responsibilities. Disadvantages include security concerns of the cloud-based system and performance and speed issues running programmes over internet connections.

8.2.2 Supporting tools

Regardless of the service model described above, software support tools and devices greatly lessen the time requirement and level of effort in working with large EO datasets.

8.2.2.1 Exploratory tools

Applications such as warnings of algal blooms or identification of algal scums do not require systematic processing of each available product but rather identifying a certain subset of products relevant for the question to be answered. This can be achieved by means of content-based image retrieval (CBIR) using a pre-processing step of data mining and "feature extraction" (Fomferra et al. 2013) to identify suitable image features. An active learning component can also be used to improve the retrieval performance. Another option is to use a content-based time series retrieval (CBTR) which reuses the basic CBIR system and applies it to stacks of co-located data. Feature attributes, such as "plankton bloom" or "scum" are then added to the catalogue of EO data and these meta data can then be used to restrict processing to the classified subset.

8.2.2.2 Analysis ready data ("Data Cube")

Data cubes are analogous to data rods used in hydrology and meteorology to improve access and remove barriers between how data is archived and accessed (Teng et al. 2016; National Academies of Sciences and Medicine 2016). Earth observations are usually produced and treated as 3-dimensional singular data cubes, i.e., for each latitude/longitude point in space, and each overpass, an observation is available. The challenge is to take advantage of the numerous different EO streams and to explore them simultaneously. The basic concept of a data cube is to concatenate data streams such that a 4-dimensional data cube is available in latitude and longitude space, time, and satellite-derived parameter grid. For example, a data cube for a lake will include the latitude and longitude coordinates, temporal images, and satellite derived Chl, TSM and turbidity parameters. The advantage of such a data cube are listed below:

- Multi-parameter time series can be obtained for each latitude/longitude pair by investigating a single geographic location. These time series can be examined using established methods of multivariate time series analysis, and afterwards the results can be merged onto a global grid again.
- Assessing a single time stamp results in synoptic geospatial maps, whose properties can be investigated with geostatistical methods.
- Univariate spatiotemporal analyses can be performed on single parameters extracted from the data cube.
- Multivariate spatiotemporal analyses can be developed by utilizing the 4D data cube.

8.3 Examples

8.3.1 Mobile technology

The tools and devices available for end users to interact with (cloud) processing systems, and to visualise results, have improved significantly over recent years and continue to get better. This also applies to water quality information, not only for working with the EO based information but also for collection of reference *in situ* data.

As of 2014, 96.3% of people in the world had some form of mobile cellular subscription (Bank 2016). In 2015, 47% of the population had mobile technology with internet connectivity, which is quickly growing, with third-generation network (3G) coverage available to 69% of the world (Bureau 2015). Nearly ubiquitous global access to mobile technology provides new opportunities for both citizen scientists collecting data (Dickson et al. 2012; Newman et al.

2012) and as a new platform for environmental data dissemination to stakeholders (Jonoski et al. 2013; Mattas-Curry et al. 2015). Interactive web service portals using Open Geospatial Consortium formats, combined with advances in cloud-based infrastructure will allow for coordinated data sharing through online applications (Mouw et al. 2015). Some examples worth mentioning:

- **Citclops**, further developed into EyeOnWater (http://www.eyeonwater.org/), is a mobile app that compares a user-taken smartphone photo of the water body of interest to the Forel-Ule 21 colour-scale displayed on the screen of the smartphone (http://www.citclops.eu/home). The colour is used as an indicator of water quality conditions and the observation data is cataloged and displayed on the Citclops and EyeOnWater websites. Soon this information will be merged with satellite-derived water quality information.
- **HydroColor** (http://misclab.umeoce.maine.edu/research/HydroColor.php) is a water quality app that uses an iPhone camera to estimate the reflectance of natural water bodies. Using the camera's three visible bands (RGB), HydroColor can estimate water turbidity (0-80 NTU), concentration of suspended particulate matter (SPM, g m^{-3}) and the backscattering coefficient in the red (m^{-1}).
- **Secchi App** is part of the Secchi Disk study (http://www.secchidisk.org/) on global phytoplankton in the ocean and coastal areas. The phone app does not take measurements directly but is used to geo-locate and record Secchi disk measurements, which are subsequently transmitted to a data repository. Seafarers et al. (2017) compared the initial four years of data collected by this app with satellite estimated chlorophyll and Secchi depth values. Their results demonstrate the app's usefulness and the ability to assess future climate-induced changes in phytoplankton populations.
- **BloomWatch** is part of CitSci.org, a crowd-sourcing website designed to promote collaborative efforts between citizens and scientists to address local, regional, and global issues. The BloomWatch app (https://cyanos.org/) documents the location and frequency of potentially harmful algal blooms. The user is prompted through a series of screens to provide site information and photos.
- **CyAN mobile app** (Schaeffer et al. 2018) is currently used by United States environmental departments and some U.S. federal agencies, and was developed as part of the Cyanobacteria Assessment Network project (https://www.epa.gov/cyanoproject). The app provides satellite-derived measures of cyanobacterial biomass from the Copernicus Sentinel-3 mission's Ocean and Land Colour Instrument (OLCI) in near real-time to make initial water quality assessments and quickly alert managers to potential problems and emerging threats related to cyanobacteria. This app provides water quality managers with a user-friendly platform that reduces the complexities associated with accessing satellite data to allow fast, efficient, initial assessments across large lakes.
- **CyanoTRACKER app** developed at the University of Georgia, USA (http://www.cyanotracker.uga.edu/) encourages the community to provide observations on lake water quality by sending trustworthy information via online social media platforms for an early detection and rapid response system for harmful cyanobacterial blooms.

8.3.2 Copernicus Data and Information Access Services (DIAS)

Copernicus is a flagship space programme of the European Union, comprising a space segment with the Sentinel series of satellites, and a set of thematic services providing products relevant for environmental monitoring and assessment. As part of the Copernicus programme, the European Commission (EC) has launched an initiative to develop Copernicus Data and Information Access Services (DIAS) that facilitate access to Copernicus data and information from the Copernicus services. By providing data and information access alongside processing resources, tools and other relevant data, this initiative is expected to boost user uptake, stimulate innovation and create new business models based on Earth observation data and information. More information can be found at: http://copernicus.eu/news/upcoming-copernicus-data-and-information-access-services-dias

8.3.3 Australian Geoscience Data Cube

The effort and cost required to convert satellite EO data into meaningful geophysical variables has prevented the systematic analysis of all available observations. In 2014, too overcome these problems, Geoscience Australia, CSIRO and the NCI established the Australian Geoscience Data Cube (https://www.opendatacube.org/) and www.ga.gov.au/dea), building on earlier work of Geoscience Australia and expanding it to include additional EO and other gridded data collections (e.g., MODIS Digital Elevation Model) to expand the range of integrated data analysis capabilities that were available. An integrated high performance computing and data environment is used to rapidly process, restructure and analyse the Australian Landsat data archive. In this approach, the EO data are assigned to a common grid framework that spans the full geospatial and temporal extent of the observations — the EO Data Cube. This approach is pixel-based and incorporates geometric and spectral calibration and quality assurance of each Earth surface reflectance measurement. The utility of the approach has been demonstrated with rapid time series mapping of surface water as well as an intertidal Digital Elevation Model across the entire Australian continent using 27 years of continuous, 25-m resolution observations. The preliminary analysis of the Landsat archive (approximately 1 PB of data) has proven how the EO Data Cube can effectively liberate high-resolution EO data from their complex sensor-specific data structures, and revolutionise the ability to measure environmental change. This DataCube concept is now being realized in 16 other countries as well. For example, the National Science Foundation has funded Earth Cube for geosciences and space systems (https://earthcube.org/info/about). Furthermore, an inland and coastal water quality and shallow water bathymetry service is envisaged for 2019.

8.3.4 ESA Thematic Exploitation Platform

ESA's Thematic Exploitation Platform (TEP) concept aims to provide a working environment where users can access algorithms and data remotely, providing them with computing resources and tools that they might not otherwise have, and avoiding the need to download and store large volumes of data. This new way of working will encourage wider exploitation of EO data.

Google Earth Engine uses similar motivation with an objective of bringing science to the data for wider exploitation of EO information.

8.3.5 Climate, Environment and Monitoring from Space (CEMS)

The CEMS facility, located at Harwell, UK, comprises academic and commercial components with the aim of transferring academic applications to the private sector; the latter under the auspices of the UK Satellite Applications Catapult (SAC). The physical infrastructure consists of a parallel-NFS data cluster and computer nodes, which currently has 4,000 cores for data processing, 17 PB of high-performance disk storage and is accompanied by tape libraries. The facility provides services to the UK and European climate and Earth system science communities to support data analysis and processing, storage, batch computing, hosted computing and cloud computing. Users can provide a pre-configured Virtual Machine based on CEMS-provided templates and run this in parallel on the CEMS infrastructure, benefitting from the high-speed storage and extensible computing resources.

8.4 Considering Service Components

A service system should have access to all the data that the user may wish to access, for example the inland water community may want archived MERIS full resolution, Landsat, MODIS, SeaWiFS and Sentinel-3 or Sentinel-2 data. There should be sufficient processing capacity to deal with large quantities of data within a reasonable amount of time, with quality control code checks to ensure that users do not inadvertently consume CPU time unnecessarily. Data processing modules should be optimized for the required regions of interest as well as atmospheric corrections, algorithm and approaches, and models. A range of tools should be available to view, analyze and further process datasets based on user requirements. Download options should be available to obtain final results for further analysis and documentation. Appropriate archiving of results will be beneficial. Many of the IaaS providers mentioned in Section 8.2.1.1 are already moving toward, and demonstrate, these capabilities. Finally, the future development of data products and visualization tools need to follow the tenets of the Agile development process with continual and iterative communication with the water quality end-user community.

Chapter 9

Conclusions and Recommendations

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The quality of water is a critical issue for the world's population as conflicts in water usage coupled with environmental change impact freshwater and coastal aquatic ecosystems. This report focusses on the capabilities of satellite remote sensing to detect, monitor and assess the quality of inland and coastal waters, and discusses the challenges of transforming the space-based measurements into validated environmental information products essential for water quality management applications. Specific recommendations are directed toward three audiences of this report: end users (Chapters 1–4), the science community (Chapters 5–6), and the space agencies (Chapters 7–8). Many of these recommendations cut across the report's sections indicating that significant interactions are needed between these three audiences. Relevant advancement of satellite remote sensing for water quality therefore relies on collaboration between all three audiences. Priorities for the continued development of an Earth observation-based, global water quality monitoring service, are also included.

9.1 Stakeholders and End User Community

With water-quality applications of remote sensing being relatively new, many management and policy professionals lack a base knowledge in remote sensing since it has not yet been incorporated into professional training curriculums. Moreover, in many countries the legislation for assessing water quality has not been adapted to include Earth observation derived information. However, recognition of the potential use for these Earth observation derived water quality products is building, for example, Swim Drink Fish Canada (https://www.swimdrinkfish.ca/) represents inland and coastal recreation waters for North America. Recommendations for the end user community include:

- Understanding the trade-offs of different satellite sensor platforms and other methodology: satellite-derived geospatial data and traditional discrete sampling provide answers at very different scales. Appropriate consultation with the Group on Earth Observation (GEO) initiatives such as AquaWatch will ensure EO exploitation can be tailored to meet user requirements.
- Strengthening partnerships between aquatic ecosystem managers and the science community through activities such as pilot projects to advance the uptake of satellite-derived

water quality information. This report presents successful end-user relevant case studies. Continued efforts to build on these successes will build trust, confidence and communication across the water quality community.

- ❖ Engaging and participating in water quality community of practices such as the GEO AquaWatch, GEOBON Global Wetlands Observing System, Blue Planet and GEOGLOWS (GEO Global Water Sustainability, a coordination framework for all water initiatives under the GEO programme).
- ❖ Using citizen scientists and crowd sourcing activities to collect and provide water quality data.

9.2 Science Community

Much scientific and methodological progress has been achieved over the past 30 years regarding research in inland and coastal water quality. Priorities, gaps and other considerations that need to be addressed are listed below.

- ❖ Earth observation should be part of an interdisciplinary approach to meeting end user requirements. The scientific community should ensure that the stakeholders and end users are engaged during the project conceptualization phase and are allowed to define the needs and requirements of the project. This will improve communication and utilization of satellite-derived products. Scientists should also advance their training in translational science, knowledge-to-action frameworks, and public communication.
- ❖ Systematically correcting the satellite-measured signal for atmospheric contamination is one of the greatest challenges in operational Earth observation for inland and near-coastal waters.
- ❖ Concentration-specific inherent optical properties (SIOPs) of lakes may vary widely. Methods are available to forward model the water-leaving light field depending on these SIOPs, and to invert the satellite-measured light field if a representative set of SIOPs is known, but currently the generation of a validated global water quality product has not yet been achieved. It is essential to understand the range of possible SIOPs and their geographic distribution.
- ❖ Additional new satellite-derived products beyond the primary products discussed in this report, are required. Examples may include the ratio of organic to mineral matter in total suspended matter (TSM), particle size distribution, proxy indicators for microbial communities as well as hybrid products (e.g., a eutrophication index) that require the linking of EO data with a lake ecosystem model.
- ❖ A rigorous, global, inland waters, *in situ* monitoring programme is required to support the use of satellite data providing both parameterisation and validation data. Uncertainties of *in situ* data measurements should be addressed, and calibration, quality control and quality assessment procedures agreed upon. Harmonised *in situ* data measurement protocols (including inter-calibration of instruments) should be undertaken.
- ❖ Earth observation algorithm evaluation should occur in each of the application settings.

Dedicated R&D studies are important to close algorithmic gaps and to improve quality and robustness of water quality products. Uncertainties of satellite raw data, processing algorithms and *in situ* data should be taken into account rigorously.

- The use of the next generation of high resolution sensors (e.g., Sentinel-2 MSI and Landsat OLI) should be explored, and could yield significantly improved products for small and hydrologically-complex waterbodies. Near future hyperspectral sensors will provide improved detection methods for phytoplankton species and functional types, TSM, CDOM, turbidity, transparency and vertical attenuation of light products, as well as aiding the development of atmospheric correction.

9.3 Space Agencies

- Agencies are encouraged to establish user-support programmes specifically for inland and near-coastal waters (e.g., no inland water programmes are currently in place). User consultation meetings should be conducted as part of user support programmes for inland waters. Validation should be included in the user programmes.
- Thematic workshops organized by space agencies (CEOS), relevant GEO groups as well as the IOCCG (e.g., the International Ocean Colour Science meetings, https://iocs.ioccg.org/) are essential to foster exchange amongst scientists, end-users and space agencies.
- Requirements for an "ideal" inland and near-coastal water quality sensor include an imaging spectrometer with 5 to 8 nm spectral bands from 340 to 1000 nm, and a minimum of three SWIR bands for atmospheric correction, a preferred spatial resolution of 17 m ground sampling distance (GSD) to at least 33 m GSD, and a noise equivalent radiance difference (NEdL) of at least 0.010 mW m^{-2} sr^{-1} nm^{-1}. Revisit frequency should be as high as is affordable (ideally a mix of polar, equatorial or geostationary orbits). Sun glint must be avoided through overpass timing and pointing the satellite sensor away from the sun.
- Space agencies are encouraged to add operational ground segments dedicated to inland and near-coastal water quality such as the Copernicus Global Land service in Europe.
- New software support tools should be explored specifically for inland and coastal waters including content-based image retrieval (CBIR), data cubes, mobile technology and cloud computing.
- International programmes should be encouraged to organize workshops and training courses to help share successes and "lessons learned" between different end-user communities. Strategies for supporting managers as well as management applications should be encouraged
- Space agencies are encouraged to expand their ability to work together and leverage both mission and funding opportunities as mentioned in the proceedings of the IOCS-2017 meeting (IOCS 2017) and the NAS 2017 Decadal Survey (National Academies of Sciences and Medicine 2018).

Acronyms and Abbreviations

ALI	Advanced Land Imager
AOPs	Apparent Optical Properties
AOT	Aerosol Optical Thickness
ARPH	Adaptive Reflectance Peak Height
AUV	Autonomous Underwater Vehicle
BRR	Bottom of Rayleigh Reflectance
CBIR	Content-Based Image Retrieval
CBTR	Content-Based Time-series Retrieval
CCI	Climate Change Initiative
CDOM	Coloured Dissolved Organic Matter
CEMS	Climate, Environment and Monitoring from Space (UK)
CEOS	Committee on Earth Observation Satellites
Chl	Chlorophyll-*a*
CI	Cyanobacteria Index
CMEMS	Copernicus Marine Environment Monitoring Service
CPC	Cyanophycocyanin
CPE	Cyanophycoerythrin
CZCS	Coastal Zone Color Scanner
DIAS	Data and Information Access Services
DOC	Dissolved Organic Carbon
DOM	Dissolved Organic Matter
DUE	Data User Element
EEA	European Environment Agency
EO	Earth Observation
EONEMP	Earth Observation National Eutrophication Monitoring Programme (South Africa)
EPA	Environmental Protection Agency (USA)
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FAI	Floating Algae Index
FAV	Floating Aquatic Vegetation
FLH	Fluorescence Line Height
FR	Full Resolution
FTP	File Transfer Protocol
FWHM	Full Width at Half Maximum
GEMS	Global Environment Monitoring System

GEO	Group on Earth Observations
GEOSS	Global Earth Observation System of Systems
GIS	Geographic Information System
GLOS	Great Lakes Observing System
GLWQA	Great Lakes Water Quality Agreement
GS	Ground Segment
GSD	Ground Sampling Distance
HAB	Harmful Algal Bloom
HICO	Hyperspectral Imager for the Coastal Ocean
HNAB	Harmful or Nuisance Algal Bloom
HPLC	High Performance Liquid Chromatography
IaaS	Infrastructure as a Service
IOPs	Inherent Optical Properties
IR	Infrared
L1	Level-1 data
L2	Level-2 data
L3	Level-3 data
LSWT	Lake Surface Water Temperature
MCI	Maximum Chlorophyll Index
MERIS	Medium Resolution Imaging Spectrometer
MESA	Monitoring of Environment and Security in Africa
MODIS	Moderate resolution Imaging Spectroradiometer
MPH	Maximum Peak Height
MSI	Multispectral Imager
NAP	Non-Algal Particles
NDFD	National Digital Forecast Database
NEdL	Noise Equivalent Radiance Difference
NEdR	Noise Equivalent Reflectance Difference
NERC	Natural Environment Research Council (UK)
NIR	Near Infra-Red
NOAA	National Oceanic and Atmospheric Administration (USA)
NWQMC	National Water Quality Monitoring Council
OAC	Optically Active Constituent
OBPG	Ocean Biology Processing Group (NASA)
OCR	Ocean Colour Radiometry
OCTAC	Ocean Colour Thematic Assembly Centre
OGC	Open Geospatial Consortium
OLCI	Ocean and Land Colour Imager
PaaS	Platform as a Service
PB	Petabytes
PML	Plymouth Marine Laboratory

QC	Quality Control
SaaS	Software as a Service
SAR	Synthetic Aperture Radar
SAV	Submerged Aquatic Vegetation
SeaDAS	SeaWiFS Data Analysis System
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
SEOM	Scientific Exploitation of Operational Missions
SIOP	Specific Inherent Optical Property
SNAP	Sentinel Application Platform
SNR	Signal-to-Noise Ratio
SPM	Suspended Particulate Matter
STAR	Satellite Applications and Research
STSE	Support to Science Element
SVC	System Vicarious Calibration
SWIR	Shortwave Infra-Red
TB	Terabytes
TEP	Thematic Exploitation Platform
TOA	Top of Atmosphere
TSM	Total Suspended Matter
TSS	Total Suspended Solids
UAV	Unmanned Aerial Vehicle
UCT	University of Cape Town
UNEP	United Nations Environment Programme
USGS	United States Geological Survey
VIIRS	Visible Infrared Imaging Radiometer Suite
VIS	Visible
WCS	Web Coverage Services
WFS	Web Feature Service
WMO	World Meteorological Organization
WMS	Web Mapping Service
WQP	Water Quality Portal

Mathematical Notation

Symbol	Description	Typical Units
$a(\lambda)$	Total absorption coefficient $a_p(\lambda) + a_{NAP}(\lambda) + a_{CDOM}(\lambda) + a_w(\lambda)$	m^{-1}
$a_{CDOM}(\lambda)$	Absorption coefficient of coloured dissolved organic matter (CDOM)	m^{-1}
$a^*_{CDOM}(\lambda)$	Specific absorption coefficient of CDOM	m^2 mg^{-1}
$a_{NAP}(\lambda)$	Absorption coefficient of non-algal suspended particles	m^{-1}
$a^*_{NAP}(\lambda)$	Specific absorption coefficient of non-algal particulate material	m^2 mg^{-1}
$a_p(\lambda)$	Absorption coefficient of phytoplankton	m^{-1}
$a^*_p(\lambda)$	Specific absorption coefficient of phytoplankton	m^2 mg Chl-a^{-1}
$a_w(\lambda)$	Absorption coefficient of pure water	m^{-1}
b	Scattering coefficient	m^{-1}
b_b	Backscattering coefficient	m^{-1}
β	Volume scattering function	m^{-1} sr^{-1}
$c(\lambda)$	Total volume attenuation coefficient	m^{-1}
$E_d(\lambda)$	Downwelling irradiance	W m^{-2} μm^{-1}
$E_u(\lambda)$	Upwelling irradiance	W m^{-2} μm^{-1}
K_d	Diffuse attenuation coefficient for downwelling irradiance	m^{-1}
L_{sat}	Radiance measured by the satellite sensor	W m^{-2} μm^{-1} sr^{-1}
$L_u(\lambda)$	Spectral upwelling radiance	W m^{-2} μm^{-1} sr^{-1}
L_w	Water-leaving Radiance	W m^{-2} μm^{-1} sr^{-1}
ϕ	Azimuth angle	degree
R	Reflectance	
R_{rs}	Remote sensing reflectance	sr^{-1}
S_y	Spectral slope for CDOM absorption coefficient	nm^{-1}
τ_a	Aerosol optical thickness	
θ	Zenith angle	degree
z	Depth	m
Z_{SD}	Secchi disk depth	m

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