International Congress on Environmental Modelling and Software

8th International Congress on Environmental Modelling and Software - Toulouse, France - July 2016

Jul 12th, 3:10 PM - 3:30 PM

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Slaughter, A. R. and Mantel, S. K., "The validation of algal growth processes in a water quality model using remote sensing data" (2016). *International Congress on Environmental Modelling and Software*. 52.
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International Environmental Modelling and Software Society (iEMSs)
8th International Congress on Environmental Modelling and Software
Toulouse, France, Sabine Sauvage, José-Miguel Sánchez-Pérez, Andrea Rizzoli (Eds.)
http://www.iemss.org/society/index.php/iemss-2016-proceedings

The validation of algal growth processes in a water quality model using remote sensing data

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Abstract: The Water Quality Systems Assessment Model (WQSAM) uses the concept of requisite simplicity within the context of modelling water quality of data scarce South African surface waters. Although WQSAM has successfully simulated the frequency distribution of observed historical nutrient data for various catchments in South Africa, the validation of algal and macrophyte growth processes in the model is a challenge because of a lack of observed data. Remote sensing data can provide an estimate of algal growth within reservoirs. Therefore, this study aimed to validate the WQSAM simulations of algal growth using remote sensing estimations of primary production in reservoirs. Algal growth was simulated for the Loskop and Kwena dams in South Africa. For the same dams, chlorophyll *a* (chl *a*) was evaluated using MEdium Resolution Imaging Spectrometer (MERIS) data. For the validation, modelled algal biomass was converted to a maximum/minimum band of chl *a* using observed relationships from the literature. The WQSAM simulations showed a stronger seasonal trend within algal growth than the MERIS data, with summer peaks and winter lows. However, the MERIS chl *a* data in all cases fell within the band of chl *a* produced by WQSAM. This study broadly verified the simulations of algal growth by WQSAM using remote sensing data. Although a rigorous validation between model simulations and remote sensing data was not possible, this was expected due to the approach of requisite simplicity adopted by WQSAM as well as the uncertainties associated within the relationship between algal biomass and chl *a* and within remote sensing data.

***Keywords**:* WQSAM; remote sensing; water quality; South Africa; algal growth

1 INTRODUCTION

The Water Quality Systems Assessment Model (WQSAM) was designed specifically for use within water quality management of data scarce South African catchments. In this context, WQSAM adheres to the principle of requisite simplicity (Stirzaker et al., 2010), and therefore aims to simulate only the water quality processes that explain the majority of water quality variation. WQSAM has focussed on nutrients as a water quality concern due to eutrophication. Algal and macrophyte growth is known to assimilate nutrients; therefore, these processes are represented within WQSAM. WQSAM has adopted these processes from established models, such as the CE-QUAL-W2 model (Cole and Wells, 2008); however, these processes have been simplified so as to be able to use the available observed data and to avoid over-parameterisation of the model. For example, whereas more complex models may simulate different taxonomic groups of algae separately, WQSAM models all algae as a single group (Slaughter et al., 2015a).

By simulating processes affecting nutrient concentrations, including chemical speciation, decomposition and algal assimilation (Chapra, 1997; Cole and Wells, 2008), WQSAM has successfully simulated the frequency distribution of observed nutrients (nitrates + nitrites, ammonia/ammonium, phosphates) for various catchments in South Africa (Slaughter et al., 2015a). The simulations of algal and macrophyte uptake of nutrients has a dramatic effect on instream nutrient concentrations in the model; therefore, it is important that these processes represented in WQSAM are validated. It is common within hydrological and water quality modelling that multiple sets of parameters will obtain the same outcome, which is termed equifinality (Bevan, 2006). Therefore, under equifinalty, WQSAM may be simulating the correct frequency distribution of nutrients, but for the incorrect reasons. To reduce the prevalence of equifinality within WQSAM, the processes of algal and macrophyte growth simulated in WQSAM require validation. However, this could prove challenging, as *in situ* data of observed algal or hyacinth biomass are not available in most cases.

The increasing availability of remote sensing data allows the possibility of furthering our understanding of natural variation in environmental variables, drivers of change, and as inputs to models (Politi et al., 2015). Remote sensing data complements *in situ* water quality data, and can provide some data for ungauged catchments. Remote sensing data are however usually at a coarser spatial scale than *in situ* data, and can be compromised by atmospheric conditions such as cloud cover. Water quality variables measured using remote sensing technology include chlorophyll *a* (chl *a*), for example, the Landsat family of satellites and the MODerate-resolution Imaging Spectroradiometer (MODIS). Due to the coarse spatial scale of the freely available remote sensing data, estimates of water quality are usually only available for reservoirs and lakes.

Remote sensing data therefore offers an opportunity to validate the processes of algal growth represented within WQSAM. Therefore, the aim of the current study was to validate algal growth simulated by WQSAM for selected reservoirs using appropriate remote sensing products.

2 METHODS AND STUDY SITES

2.1 Study sites

Figure 1 shows the study sites for the current study, namely Loskop Dam on the Olifants River and Kwena Dam on the Crocodile River. The Olifants River originates from the east of Johannesburg, with the upper Olifants extending from the catchment divide with the Vaal River to Loskop Dam. The dam has a capacity of 374.31×10^6 m^3 and a surface area of 24.28 km^2. The Olifants River is generally regarded as one of the most modified rivers in South Africa, as it is extensively dammed and highly polluted (Balance et al., 2001; de Villers and Mkwelo, 2009; van Vuuren, 2009). Apart from considerable water extraction, the river suffers pollution originating from coal mining, petrochemical industries, waste water from various large and small urban centres as well as runoff from extensive agriculture (Heath et al., 2010), resulting in acid mine drainage and eutrophication (van Vuuren, 2009). There are high spikes in nutrients, with nitrates + nitrites as high as 3 mg ℓ^{-1}, with concentrations > 0.5 mg ℓ^{-1} approximately 5% of the time, spikes in ammonium of up to 5.5 mg ℓ^{-1}, and spikes in phosphate of up to 0.6 mg ℓ^{-1} (Slaughter et al., 2015a). Much of the pollution is manifested within Loskop Dam, with frequent reports of crocodile and fish deaths within the dam (van Vuuren, 2009).

Kwena Dam is located on the upper Crocodile River Catchment, situated in the province of Mpumalanga. The catchment is economically important, contributing to industry, agriculture and tourism (Deksissa et al., 2004). The dam has a capacity of 158.93×10^6 m^3 and a surface area of 12.50 km^2. The catchment is affected by various human activities, including wheat and maize farming, runoff and return flow from urban areas and mining return flow (Deksissa et al., 2004; Roux et al., 1994). Due to the geology of the area, the salinity is relatively low. However, nutrients within Kwena Dam are moderate, with spikes in nitrates + nitrites as high as 1 mg ℓ^{-1} and > 0.2 mg ℓ^{-1} approximately 40% of the time, ammonium spikes as high as 0.3 mg ℓ^{-1}, and > 0.1 mg ℓ^{-1} approximately 5% of the time, and spikes of phosphate as high as 0.45 mg ℓ^{-1}, and > 0.1 mg ℓ^{-1} approximately 2% of the time (see Slaughter et al., 2015a).

2.2 Water quality modelling of the study catchments

Water quality modelling for the two study reservoirs was performed by modelling the entire upstream catchment for each reservoir, using the Water Quality Systems Assessment Model (WQSAM) (Hughes et al., 2013; Hughes and Slaughter, 2015; Slaughter et al., 2012; Slaughter et al., 2015a, b; Slaughter and Hughes, 2014). The conceptual and technical representation of water quantity and quality processes represented within WQSAM, as well as the modelling of water quality for historical conditions are outlined in detail in Slaughter et al. (2015a). Briefly, WQSAM was designed specifically for water quality management in South Africa, and therefore is designed to be as simple as possible while still representing the processes explaining the majority of water quality variation. WQSAM links with water quantity systems models that are used routinely within management of water quantity in South Africa, such as the Water Resources Modelling Platform (WReMP) (Mallory et al., 2011), as the flow output of these models drive the water quality simulations within WQSAM, and the system representation of the modelled catchment within WQSAM mirrors that of the system model (Figure 2A, Slaughter et al., 2015b).

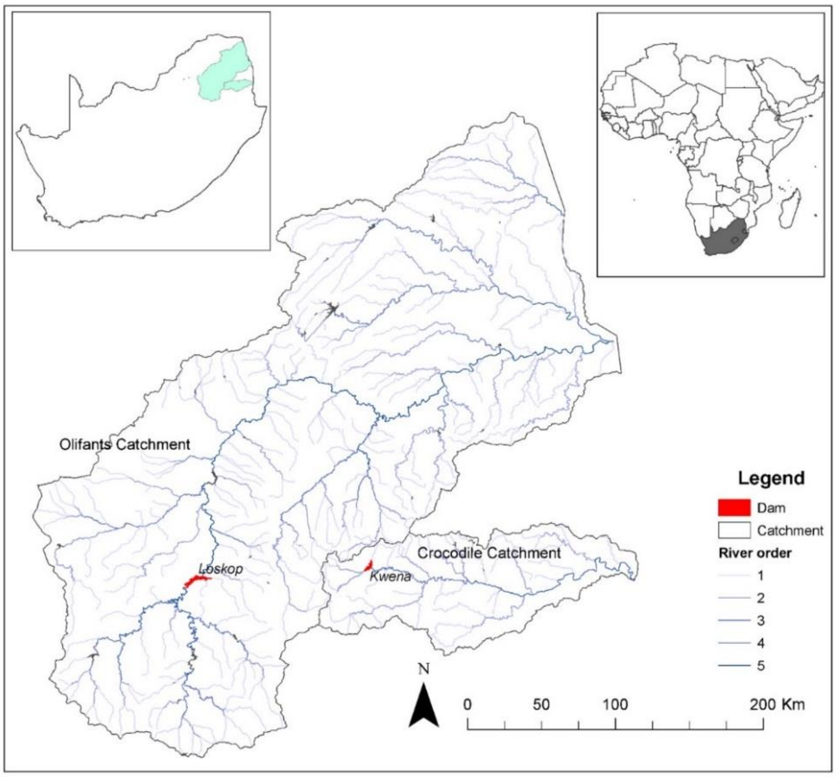

Figure 1. Map showing the Crocodile and Olifants river catchments, with the positions of the Kwena and Loskop dams shown.

Since the flows generated by the systems models typically are at a monthly time step, and daily flows are required for the daily time step WQSAM, incremental and cumulative flows from the systems model are disaggregated from monthly to daily flows (Figure 2B and Figure 2D, respectively in Slaughter et al., 2015b). Incremental flow (natural flow runoff from tributaries) is broken down into surface flow, interflow and groundwater flow according to the method by Hughes et al. (2003). The separation into flow fractions is to facilitate the simulation of diffuse source inputs of water quality loads within the model. The actual water quality simulations are facilitated within the last tier of the model (Figure 2E). These are broken down into various modules. Water temperature is simulated in WQSAM as temperature drives many of the processes affecting water quality, such as chemical speciation, algal growth and decomposition (Chapra, 1997), and the simulation within WQSAM is driven by air temperature using a method by Rivers-Moore et al. (2008). The inputs driving nutrient simulations include catchment runoff contributions (through the assigning of water quality concentrations to incremental flow fractions) and point source inputs. Instream processes affecting nutrients were adapted from more complex models, such as CE-QUAL-W2 (Cole and Wells, 2008), and include decomposition, uptake by algal and macrophyte growth and chemical speciation. These instream processes as well as their links are represented within Figure 3.

Water quality for the Olifants and Crocodile river catchments were modelled for historical conditions (1920–2003 and 1954–2003, respectively) down to Loskop Dam and Kwena Dam, respectively. The model simulations of nutrients were calibrated against historical monitoring data collected by the South African Department of Water and Sanitation (DWS). Algal growth within the dams was simulated within WQSAM so as to achieve frequency distributions of nutrient concentrations that were representative of the DWS monitoring data. Unfortunately, the DWS does not routinely measure algal biomass, and therefore there are typically no *in situ* data for algal biomass or growth; hence, the current study was necessary to validate WQSAM estimations of algal growth in the model.

2.3 Quantitative analysis of reservoir chl *a* using remote sensed imagery from MERIS data

The open-source visualising and processing package Basic ERS and Envisat (A) ATSR and MERIS Toolbox (BEAM) version 5.0 was used to quantitatively assess chl *a* using the MERIS lakes processor for eutrophic waters (Doerffer and Schiller, 2008).

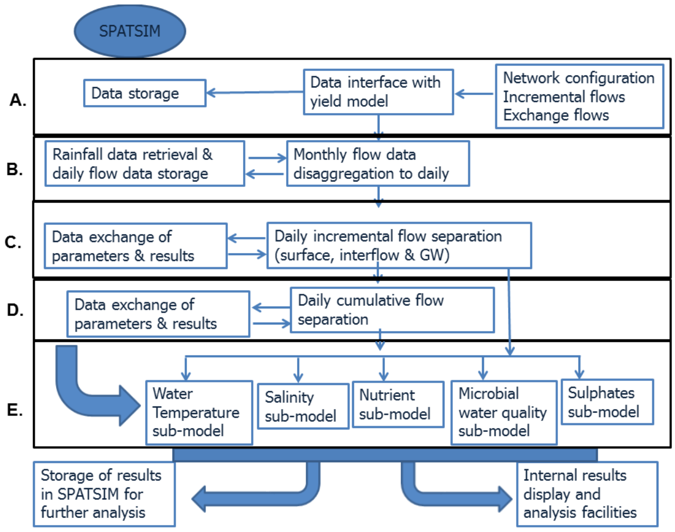

Figure 2. Conceptual representation of the model components in the Water Quality Systems Assessment Model (WQSAM).

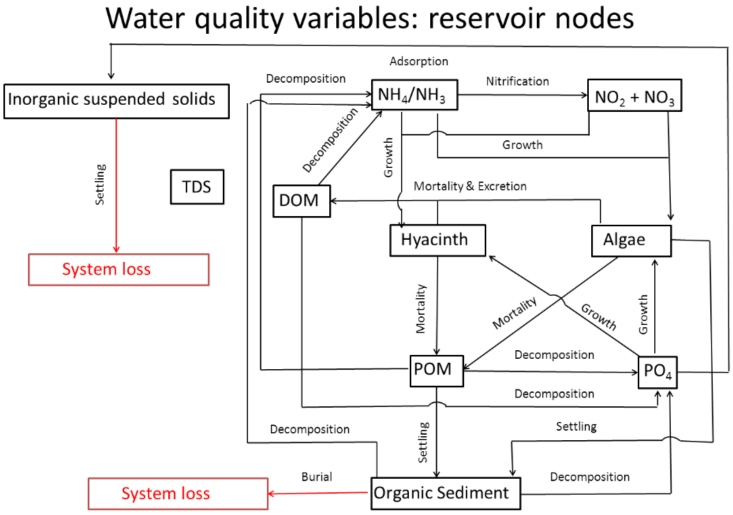

Figure 3. Conceptual modelling framework for simulation of water quality variables for reservoir nodes within WQSAM.

The data used were atmospherically corrected MERIS radiance data for the period 2002–2005. The processor used has been validated for lakes in Europe and Africa, although challenges were experienced in validating the data for the African lakes.
The chl *a* results of the lakes processor were compared to DWS monitoring data of chl *a*. Since the lakes processor provides data over the total reservoir surface whereas the DWS monitoring data are restricted to the gauging location, this comparison has limitations.

2.4 Validation of the WQSAM estimates of algal growth using MERIS measures of chl *a*

WQSAM produces simulations of algal biomass; therefore, validation of WQSAM simulations using chl *a* data would require some way of converting algal biomass to chl *a*. The relationship between algal biomass and chl *a* has in fact been of interest in past limnology and oceanography studies. These studies have however found that this relationship is not constant or easy to determine, and varies according to the trophic status of the reservoir, the taxonomic composition of algae within the community and the size frequency distribution of algal cells (Felip and Catalan, 2000; Kasprzak et al., 2008). Using past studies, Kasprzak et al. (2008) found that within a wet weight biomass range of 0.1–50 g m^{-3}, chl *a* content ranges from 0.18% to 2.5%. Therefore, in the current study, this range was used as an uncertainty range, with WQSAM simulations of algal biomass converted to a minimum and maximum chl *a* range of 0.18% and 2.5%, respectively. This minimum-maximum range of ch *a* derived from WQSAM estimates of algal biomass was then compared to MERIS quantifications of chl *a*. The comparison was done as an average monthly (seasonal) comparison, as the WQSAM simulations only go as far as 2003 due to constraints to observed rainfall data, whereas MERIS estimates of chl *a* only begin in May 2002, although data for the scenes relevant for this study are only available from November 2002. Therefore, the comparison was for average long-term seasonal patterns in chl *a*, rather than for specific years that may be influenced by extreme hydrological events.

3 RESULTS

3.1 Model simulations of algal growth

For both the Olifants and the Crocodile river catchments, the subcatchments upstream of the study reservoirs (Loskop and Kwena dams) were progressively calibrated from upstream to downstream, following the process outlined in Slaughter et al. (2015b). For the study reservoirs, processes such as algal growth, respiration, mortality and settling rate, as well as algal minimum, maximum and optimal water temperature were set so as to obtain a time series of algal biomass within each reservoir that resulted in simulated nutrient concentrations (algae assimilate nutrients during growth) with a frequency distribution relatively representative of that of the observed data. Figure 4 shows the monthly average (seasonal) algal biomass as simulated by WQSAM for the Loskop and Kwena dams for the period 1920–2003 and 1954–2003, respectively. It is evident that there is a seasonal signature within the algal biomass within Loskop Dam which is less pronounced for Kwena Dam, with a summer maximum and winter minimum.

3.2 MERIS measures of chl *a*

Figure 5 shows the time series of chl *a* concentration for Loskop and Kwena dams for the period 2002–2005 derived from the MERIS data using the Lake processor in BEAM. It is immediately evident that chl *a* concentration in Loskop Dam shows higher peaks and more variation than in Kwena Dam.

3.3 Validation of WQSAM simulations of algal biomass using MERIS data

The simulations of algal biomass were converted to the uncertainty band of chl *a* by using the relationships between algal wet biomass and chl *a* determined by Kasprzak et al. (2008), with the lower bounds equating to 0.18% chl *a*: algal biomass and the upper bounds equating to 2.5% chl *a*: algal biomass. Figure 6a represents the results of the analyses for Loskop Dam. The results show that the BEAM measures of chl *a* (average of values estimated for 2002–2005) fall within the uncertainty band of chl *a* produced by WQSAM using the conversion range by Kasprzak et al. (2008), although the simulations of algal growth by WQSAM show a much more pronounced and slightly different seasonal signature as compared to the BEAM measures, as a relatively slight maximum chl a is indicated by the BEAM measures during March/April, whereas the simulations by WQSAM show a much more pronounced summer (December–January) maximum and winter (July–August) minimum.

Figure 6b represents the results of the analyses for Kwena Dam. It is immediately evident that algal growth, as indicated by both the simulations by WQSAM and the BEAM measures, is lower in Kwena Dam than in the Loskop Dam. The BEAM measures of chl *a* fall within the uncertainty band of chl *a* produced by applying the conversion range by Kasprzak et al. (2008) to simulations of algal biomass by WQSAM. Once again, the seasonal signature in algal growth is much more pronounced within the simulations by WQSAM as compared to the BEAM measures, with a distinct winter (June–August) minimum, whereas the measures of chl *a* by BEAM remain relatively consistent throughout the year.

4 DISCUSSION

The range of chl *a* produced by applying the conversion range of Kasprzak et al. (2008) to the simulations of algal biomass by WQSAM generally encompassed the BEAM measures of chl *a*. It is evident that the simulations of algal growth by WQSAM show a much more pronounced and slightly different seasonal signature as compared to the BEAM measures for both reservoirs.

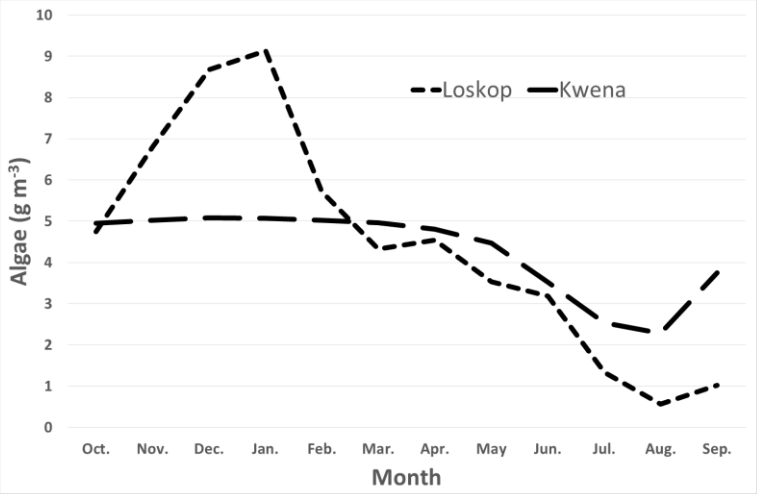

Figure 4. Monthly average (seasonal) algae simulation for Loskop Dam on the Olifants River from 1920 to 2003 and for Kwena Dam on the Crocodile River from 1954 to 2003.

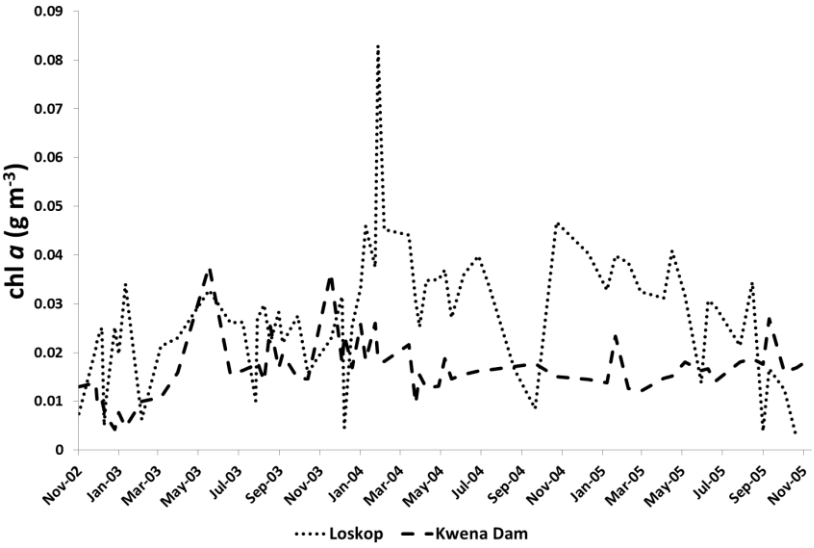

Figure 5 Temporal variation in average chlorophyll a concentration of Loskop and Kwena dams derived from MEdium Resolution Imaging Spectrometer (MERIS) data using the Lakes processor in Basic ERS & Envisat (A) ATSR and MERIS Toolbox (BEAM) for the years 2002–2005.

WQSAM was designed to simulate a limited number of important water quality variables (i.e. salinity and nutrients), represented by a limited number of and simplified water quality processes that explain the majority of water quality variation. This can be described as a ‘requisite simplicity’ approach (Stirzaker et al., 2010). WQSAM therefore includes a simplified algal growth simulation process that places all possible algal groups (that could be distinguished by size or taxonomy for example in more complex models) into a single category, in which algal related rates such as growth, mortality, respiration and settling, as well as water temperature related rates, are used to drive algal growth dynamics as a single group. In addition, the model does not consider stratification, and reservoirs/lakes are modelled as completely stirred tank reactors (CSTRs) (Chapra, 1997), which additionally avoids certain more complex algal dynamics, such as size related algal settling and blooms associated with reservoir overturn and nutrient upwelling. This ‘requisite simplicity’ approach is adopted within WQSAM to reduce the complexity, parameter set and observed data required to successfully run the model. In particular, a reduced parameter set is desirable to avoid equifinality in the model (Bevan, 2006).

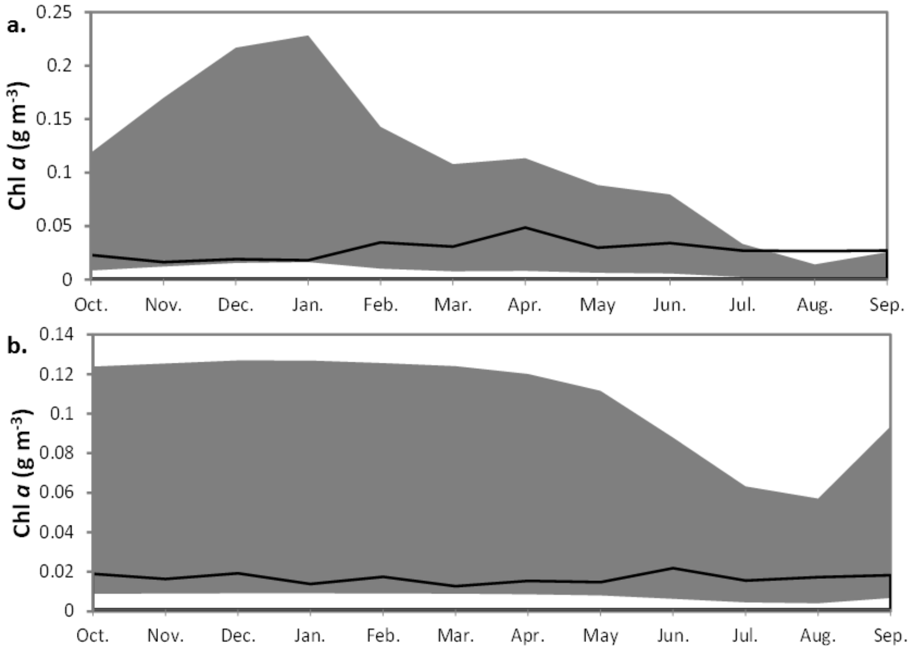

Figure 6 Seasonal distribution of chlorophyll *a* (chl *a*) within Loskop Dam (a) and Kwena Dam (b). Solid line – average chl *a* for the period 2002–2005 as measured by the Basic ERS & Envisat (A) ATSR and MERIS Toolbox (BEAM) remote sensing technology; grey band - estimates of chl *a* by converting simulations of the seasonal distribution of algal biomass by the Water Quality Systems Assessment Model (WQSAM) for the years 1920–2003 and 1954–2003 for Loskop Dam and Kwena Dam, respectively to estimates of chl *a* concentration using the relationships by Kasprzak et al. (2008), with the lower bounds equating to 0.18% chl *a*: algal biomass and the upper bounds equating to 2.5% chl *a*: algal biomass.

Given the aforementioned approach, it can be argued that WQSAM was never expected to produce accurate simulations of algal growth. However, it is vital that WQSAM produce algal growth simulations that are within the correct range and show the correct seasonal signature as compared to observed data, as this would strengthen the argument that WQSAM is producing accurate simulations of nutrients (the main focus of water quality simulations) due to the broadly correct representation of water quality processes, and not due to equifinality, as this has important ramifications for the application of WQSAM to modelling future scenarios. Therefore, given the overall strategy of requisite simplicity within WQSAM, the uncertainties associated with the relationship between algal wet biomass and chl *a* as given by Kasprzak et al. (2008) and the uncertainties associated with the BEAM measures of chl *a*, it can be argued that the present study achieved an adequate validation of WQSAM measures of algal biomass using the BEAM measures of chl *a* for two reservoirs, the Loskop and Kwena dams, in South Africa. However, the seasonality shown in algal growth appears to be different between the WQSAM simulations of algal biomass and the BEAM measures of chl *a*, with the simulations by WQSAM showing a much more pronounced seasonal and slightly differently timed seasonal signature as compared to the BEAM measures. Within WQSAM, the rate of algal growth is predominantly driven by water temperature, which is in turn driven by air temperature in WQSAM (see Slaughter et al., 2015b). Therefore, the simulations of algal biomass in WQSAM show a strong summer maximum and winter minimum. It has been shown that the method of deriving water temperature in WQSAM: a simple multiple regression driven by air temperature (Rivers-Moore et al., 2008), is not entirely appropriate for deep reservoirs, as stratification is not considered. The results of water temperature simulations for the Loskop and Kwena dam simulations do in fact show that as compared to observed water temperature measures, the simulations are slightly out of step with the observed data by one to two months in regards to the summer maximum and winter minimum, and additionally do not represent certain variability in the observed seasonal water temperature, probably related to the winter reservoir overturn associated with the breakdown of stratification. For this reason, the seasonal variation in algal growth as given by WQSAM may not always be representative of reality, particularly for deeper reservoirs. The stratification of reservoirs has not been included within WQSAM, as the inclusion would greatly increase the complexity, parameter set and observed data requirements of the model.

In addition, Kasprzak et al. (2008) mentions that the relationship between algal biomass and chl *a* for a particular algal taxonomic group may not always be consistent, as it has been shown that the proportion of chl *a* within algal biomass may change with increases and decreases in the algal biomass, and depends on the trophic status of the lake/impoundment, the season, the taxonomic composition of the algal community and the size frequency distribution of the algal cells (Felip and Catalan, 2000; Kasprzak et al., 2008). In particular, it has been noted that the chl *a* content per unit biomass of algae decreases as algal biomass increases. This phenomenon may explain some of the mismatch in seasonal signatures between the WQSAM produced simulations of algal biomass and BEAM measures of chl a, as shown in Figure 6.

5 CONCLUSION

Although a limited validation of algal growth simulations by WQSAM using remote sensing measures of chl *a* was achieved within the present study, it can be argued that given the uncertainties within WQSAM, which are largely due to the unavoidable requisite simplicity approach taken, the uncertainties within the relationship between algal wet biomass and chl a, as well as the uncertainties within remote sensing measures of chl *a*, the validation results obtained in the present study can be argued to be reasonable. Therefore, WQSAM has achieved simulations of algal growth that are adequate for routine water quality management where nutrients are the focus. A more complex model should be used where an accurate simulation of algal growth dynamics or taxonomic composition is required.

ACKNOWLEDGMENTS

MERIS Level 1 data was provided by the European Space Agency. The MERIS Lakes processor for eutrophic waters by Doerffer and Schiller (2008) in BEAM version 5.0 is acknowledged for quantifying chl *a* concentration in dams. The Water Research Commission (WRC) is acknowledged for funding this research.

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