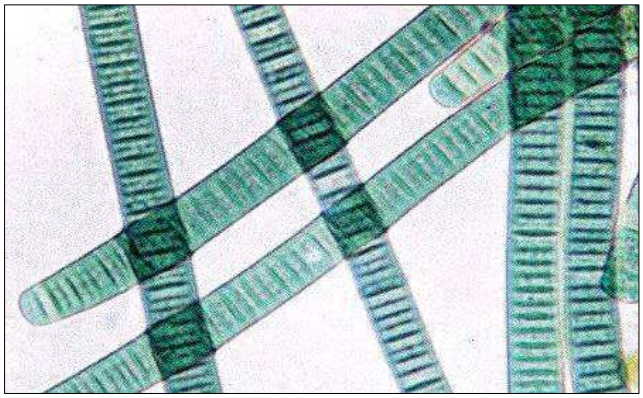
Departamento de Ecología
Instituto del Agua
Universidad de Granada

Physical and Ecological processes in El Gergal Reservoir (Seville): effects on water quality

Procesos físicos y ecológicos en el embalse de El Gergal (Sevilla): consecuencias sobre la calidad del agua



PhD Thesis

Anna Rigosi

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Physical and Ecological processes in El Gergal Reservoir (Seville): effects on water quality

Memoria presentada por Anna Rigosi para optar al titulo de Doctor en la Universidad de Granada

Anna Rigosi
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Dr. Luis José Cruz Pizarro
Universidad de Granada

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Contents

List of Figures

List of Tables

Introducción General y Objetivos

Los cambios en la abundancia y composición de la comunidad fitoplanctónica en lagos y embalses pueden afectar seriamente la calidad del agua y, en el caso de que el recurso que almacenan se destine a abastecimiento, comprometer la eficacia de los procesos de tratamiento aplicados en las plantas de potabilización. Por ejemplo, episodios de proliferación de algas azules en embalses para abastecimiento de agua potable pueden provocar la obstrucción de filtros, generar problemas de sabor y olor del agua e incluso inducir problemas de salud como consecuencia de la producción de substancias toxicas (Guven and Howard, 2006; Margalef, 1983).

La composición de las comunidades fitoplanctonicas y la abundancia relativa de las especies que las componen están sujetas a cambios continuos a diferentes escalas temporales. Estas escalas varían desde frecuentes reorganizaciones de la comunidad existente a escalas diarias o sub-diarias, pasando por cambios estacionales que acompañan a las fluctuaciones cíclicas de insolación y temperatura (sucesión), hasta llegar a cambios a largo plazo donde patrones cíclicos recurrentes se ven remplazados por otros (Reynolds, 1984). Este tipo de patrones, más bien específicos de grupos de especies que de especies particulares, ocurren en diferentes lagos y embalses (Evans, 1988; Margalef, 1983) y sugieren que tiene que existir un mecanismo común en juego.

En el campo de la Ecología se han dedicado considerables esfuerzos a comprender y predecir los mecanismos que subyacen los cambios en la comunicad fitoplanctónica (Morris, 1980; Reynolds, 1984; Sommer, 1988; Reynolds, 19979. Sommer et al., (1986) propusieron que la composición de la comunidad fitoplanctónica depende no solo de la estrategia de las especies o de las adaptaciones fisiológicas de los organismos encaminadas a explotar los recursos del hábitat (factores endógenos), sino también de los cambios en las condiciones ambientales que alternan las ventajas competitivas entre especies (factores exógenos). Si fueran dirigidos sólo por procesos endógenos, los cambios en la comunidad fitoplanctónica terminarían teóricamente en un clímax estable o estado de equilibrio, en el cual la biodiversidad sería mínima y la biomasa total sería máxima (Tansley, 1939). Por lo tanto, cualquier cambio en la comunidad fitoplanctónica, tanto si está caracterizada a nivel de especies como a nivel de grupos de especies con la misma sensibilidad a los cambios ambiéntales (grupos funcionales, Reynolds, 1997) debería ser el resultado de cambios en las condiciones ambientales. En particular, estos cambios están asociados a variaciones en las limitaciones físicas (clima de luz) y químicas (disponibilidad de nutrientes) para el crecimiento algal (Margalef, 1997; Reynolds, 1997; Naselli-Flores & Barone, 2000). Por un lado, el clima lumínico experimentado por las células planctónicas está relacionado con la mezcla turbulenta, que determina el tiempo de residencia de las micro-algas en la capa eufótica (MacIntyre et al., 2000). Por otro lado, la distribución y disponibilidad de nutrientes en la capa eufótica es el resultado de procesos de transporte que interactúan con los procesos biológicos. Estos cambios en las condiciones ambientales experimentados por las algas están estrictamente ligados a las fuerzas físicas (hidráulica y meteorológica) que controlan los procesos de mezcla y transporte en el lago, y tienen la tendencia, dada la variedad de adaptaciones ambientales del fitoplancton, a promover el crecimiento de algunos grupos (o especies), desfavoreciendo otros (Huisman *et al*., 1999; Passarge *et al*., 2006; Litchman and Klausmeier, 2001). Por lo tanto, el conocimiento y la predictabilidad de la composición de las comunidades planctónicas y su evolución se ha de fundar en el conocimiento de los procesos físicos

de transporte y mezcla que determinan la turbulencia, la distribución de nutrientes y la penetración de la luz en la columna de agua.

De acuerdo con esta percepción de sucesión en ecosistemas acuáticos, ampliamente aceptada, los modelos matemáticos empleados para simular la evolución de las comunidades fitoplanctonicas están basados en una descripción apropiada de los procesos físicos y de su relación con el crecimiento algal. Estos modelos matemáticos son un valioso instrumento heurístico de investigación para responder a cuestiones ecológicas, y también han recibido considerable atención en el ámbito de la gestión de la calidad del agua, principalmente en su vertiente predictiva. A pesar del considerable interés que han levantado los modelos de sucesión entre ecólogos e ingenieros, se han realizado pocos análisis focalizados específicamente en estos tipos de modelos. Reynolds (1999) es uno de los pocos autores que han revisado los planteamientos utilizados por los modelos de sucesión del plancton en los lagos. Sin embargo, éste autor se centró en la posibilidad de asistir en la toma de decisiones para la gestión. Su trabajo no discute los problemas singulares de los modelos de sucesión provocados por el hecho de que simulan de forma explícita las interacciones no lineares entre múltiples grupos de fitoplancton.

El primer objetivo de esta tesis es revisar el estado del arte, los éxitos y los problemas encontrados en la modelación de la sucesión de comunidades fitoplanctonicas en lagos y embalses. Primero analizamos los diferentes enfoques utilizados para simular los cambios en los componentes físicos, químicos y biológicos de los modelos de sucesión fitoplanctónica. Examinamos las metodologías de evaluación adoptados por diferentes modelos de sucesión y su habilidad predictiva. El objetivo de este trabajo fue definir un enfoque valido para desarrollar y testar un modelo de sucesión para el embalse de El Gergal, que pueda ser utilizado para (1) propósitos de investigación y (2) perdición de calidad de agua.

Los modelos utilizados para comprender y predecir los cambios en la sucesión de las comunidades fitoplanctonicas (Griffin et al., 2001; Kuo et al., 2006) están basados en un enfoque funcional o mecanicista en el cual un conjunto de ecuaciones diferenciales, derivadas de los principios físicos de conservación de masa, momento y energía, representan la evolución de los diferentes elementos del ecosistema (Hamilton and Schaldow, 1997; Omlin et al., 2001; Reynolds et al., 2001; Arhonditsis and Brett, 2005). Los modelos mecanicistas típicamente contienen un número elevado de parámetros cuyos valores son específicos del sistema y en muchas ocasiones son desconocidos cuando se define por primera vez un problema de predicción del comportamiento de un ecosistema. La combinación especifica de parámetros que mejor describen las tasas de los procesos en un ecosistema puede ser seleccionada a través de un largo y complejo proceso de experimentación en situ (see Gal et al., 2009) o, alternativamente, mediante calibración. Éste último es el método mas comúnmente utilizado en la modelación de la calidad del agua (Markensten & Pierson, 2007; Omlin et al., 2001; Rose et al., 2007; Mieleitner and Reichert, 2008). Es más económico que la experimentación pero puede ser largo dependiendo del coste computacional del modelo y del número de parámetros a calibrar. Por eso, cualquier avance en las estrategias de calibración para modelos de sucesión contribuirá a generalizar su uso para la gestión de la calidad del agua. Las estrategias de calibración automáticas pueden ser una alternativa válida (Eckardt & Arnold, 2001) a las calibraciones tradicionales basadas en el principio de prueba-error, eficientes solamente calibrando modelos con un número limitado de parámetros (Tanentzap et al., 2007; Kuo et al., 2006; Bonnet and Poulin,

2004) o cuando la mayoría de los valores de los parámetros han sido previamente aproximados por vía experimental (Hillmer et al., 2008; Gal et al., 2009). Las calibraciones automáticas están diseñadas para buscar la combinación de parámetros que minimiza una función objetivo, que representa la norma de la diferencia entre variables observadas y modeladas, y se dividen en dos clases: optimizaciones de gradiente y globales. Los métodos de gradiente han sido ampliamente utilizados en la calibración de modelos de distinta complejidad (Omlin et al., 2001; Rose et al., 2007; Mieleitner and Reichert 2008), pero pueden converger en un mínimo local de la función objetivo y no en el mínimo global, comprometiendo la efectividad del método en modelos con un número elevado de parámetros. Las técnicas de optimización global evitan la convergencia en mínimos locales, introduciendo en el proceso de búsqueda un cierto grado de aleatoriedad (Klepper and Hendrix, 1994; Hansen et al., 2003; Duan et al., 1992; Eckardt & Arnold, 2001; Skahill & Doherty, 2006). Estos métodos de optimización global se han utilizado ampliamente en la calibración de modelos hidrológicos complejos (Tonkin and Doherty, 2005; Skahill & Doherty, 2006; Marcé et al., 2008; Gupta et al., 1998), pero pocos ejercicios de calibración global se han aplicado a modelos de calidad de agua (Mulligan et al., 1998; Ostfeld and Salomons, 2005; Goktas el al., 2007). Además, la aplicabilidad de estas técnicas a la calibración de modelos de sucesión del fitoplancton todavía no ha sido indagada en la literatura.

El segundo objetivo general de esta tesis es proponer y testar una estrategia para calibrar un modelo determinista físico-biológico con alto número de parámetros para el embalse de El Gergal, basada en un algoritmo que combina calibración de gradiente y global. Queremos verificar si la integración de estrategias de calibración automáticas es un enfoque de utilidad para modelos ecológicos complejos.

El modelo calibrado de El Gergal se ha empleado para analizar el rol de las salidas de agua sobre el control de la sucesión fitoplanctónica. Hoyer et al. (2009) identificaron cambios bruscos en una sucesión general de grupos funcionales que coincidían con periodos de vientos fuertes o con cambios en tasas de salidas de aguas, y concluyeron que las extracciones de agua eran, probablemente, el factor externo más importante en el control de cambios de composición y abundancia de la comunidad planctónica en embalses mediterráneos. Su conclusión concuerda con la de Naselli Flores (2000), que estudió veintiún embalses de Sicilia que mostraban diferentes estados tróficos y concluyó que la abundancia y composición del fitoplancton está más influenciada por el régimen hidráulico que por la disponibilidad de nutrientes. Los estudios sobre la relación entre sucesión fitoplanctónica y salidas de agua son escasos en la bibliografía. Además, los que se han publicado son, en algunos casos, contradictorios (Barbiero et al., 1997; Hoyer et al. 2009). Ninguno de ellos ha investigado los mecanismos por los cuales las salidas de agua a diferentes niveles pueden afectar a la sucesión.

El tercer objetivo general de esta tesis es comprender los mecanismos por los cuales las salidas de agua a diferentes profundidades pueden inducir cambios en la composición de las comunidades fitoplanctónicas. El puntote parida fue la hipótesis de que cambios en los niveles de salida pueden afectar de forma distinta las condiciones ambientales, y favorecer el desarrollo de algunas especies y perjudicar a otras, como consecuencia de sus diferentes respuestas a las modificaciones ambientales. Se ha utilizado un modelo conceptual y simplificado para evaluar los cambios en el clima de luz y temperatura inducidos por extracciones de agua a diferente nivel, y los

consecuentes cambios en grupos de fitoplancton dependiendo de su respuesta específica. Así mismo, se han utilizado simulaciones obtenidas con un modelo unidimensional hidrodinámico-ecológico (DYRESM-CAEDYM) calibrado para el embalse de El Gergal para valorar los efectos del nivel de salida de agua sobre dos grupos de algas con diferentes adaptaciones a las condiciones ambientales.

Observaciones sobre la adquisición de datos y la estructura de la tesis

Durante el periodo de investigación se desarrolló un estudio preliminar en el embalse de Béznar (Granada). Datos físicos, químicos y biológicos fueron recopilados durante el año 2005 para (1) la elaboración de un modelo del embalse de Béznar utilizando el modelo DYRESM-CAEDYM, y (2) para analizar las fuentes de incertidumbre en la predicción de variables físicas y ecológicas. Los resultados de este estudio se presentaron en 2006 en la discusión del D.E.A. (Diploma de Estudios Avanzados) titulada "A physical-ecological model of lake Beznar ecosystem; Porpagation of uncertainty from physical to population dynamic predictions", y no están incluidos en este documento.

Mi trabajo ha sido financiado por el Ministerio Español de Educación y Ciencia, a través el proyecto: CGL2005-04070/HID *Coupling hydrodynamics and plankton: impact of exogenus perturbations in a mesotrophic reservoir in Southern Spain (El Gergal, Sevilla)*. La Empresa Metropolitana de Abastecimiento y Saneamiento de Aguas de Sevilla (EMASESA) fue uno de los participantes claves en este proyecto y nos proporcionó su base de datos, resultado de su plan rutinario de supervisión de la calidad del agua. Parte de los datos utilizados han sido recopilados por investigadores de las Universidades de Granada, Málaga y Jaén, durante algunos experimentos de campo en El Gergal en 2007 y 2008. El embalse de El Gergal, por sus características hidro-morfológicas, se ha considerado aquí como un ejemplo prototipo de los embalses mediterráneos tipo cañón que ocupan valles estrechos y profundos. El embalse está gestionado para suministrar agua de la mejor calidad posible a una planta de tratamiento para el suministro de agua potable a la ciudad de Sevilla. El desarrollo y la implementación de un modelo ecológico para El Gergal, que pueda ser utilizado de forma rutinaria para predicciones de calidad de agua es el objetivo final de la investigación empezada con el proyecto CGL2005-04070/HID. Este trabajo representa el primer paso en esta dirección.

Un primer periodo de investigación se ha dedicado a la calibración del modelo ecológico y a la simulación de la biomasa total del fitoplancton en El Gergal en los años 2001 a 2005. Durante este periodo no estaban disponibles datos sobre concentración de clorofila-a de distintos grupos de algas, necesarios para la calibración de un modelo de sucesión. Los resultados para estos años no se han incluido en la tesis, que está centrada en la sucesión de fitoplancton, pero se han presentado en una tesis de Master en Hidráulica Ambiental en el 2007, titulada "Modelling thermal structure and phytoplankton dynamics in El Gergal Reservoir (Seville, Spain)".

Este documento está organizado en capítulos independientes. Cada uno es un articulo que ha sido enviado o será enviado próximamente a diferentes revistas científicas para su publicación. El primer capitulo ha sido publicado en "Environmental Reviews", el segundo está siendo revisado para "Environmental Modeling and Software" y el tercero se enviará a "Ecological Modelling".

General Introduction and Aims

The changes in abundance and composition experienced by phytoplankton communities in lakes and reservoirs in the course of a year may severely affect the quality of the water and even compromise the effectiveness of treatment processes undertaken in downstream water treatment plants. For example, the occurrence of blue-green algal blooms in water supply reservoirs may lead to severe clogging problems during the filtering operations; or it may lead to taste, odor and even health problems as a consequence of several species and stocks of blue green-algae producing toxic substances (Guven and Howard, 2006; Margalef, 1983). The composition of phytoplankton communities and the relative abundances of component species undergo continuous changes on varying scales. These scales range from frequent reorganizations of existing community structures, through seasonal compositional changes that accompany cyclical fluctuations in insolation and temperature (succession), to longer-term floristic changes, where one recognizable recurrent cycle is supplanted by another (Reynolds, 1984). Similar temporal patterns, specific to species groups rather than individual species, tend to occur in different lake and reservoir systems (Evans, 1988; Margalef, 1983) and suggest that there must be a common mechanism at play.

Considerable efforts have been devoted in ecology to understand these mechanisms underlying phytoplankton community changes (Morris, 1980; Reynolds, 1984; Sommer, 1988; Reynolds, 1997). Sommer et al. (1986) proposed that the assemblages of species in a given phytoplankton community depends on the species strategies or physiological adaptations to exploit habitat resources (autogenic factors), but, also on changes in the environment conditions that alter the competitive advantages among different species (allogenic factors). If it were only driven by autogenic processes, the changes in the phytoplankton community would theoretically culminate in a stable climax or equilibrium state, in which biodiversity would be minimal and the overall biomass would be maximized (Tansely, 1939). Hence, any changes in abundance and composition experienced by any given phytoplankton community, whether they are characterized at species level or in terms of assemblages of species with similar tolerance to environmental conditions (functional groups, Reynolds, 1997), should be a result of changes in the environmental conditions. In particular, they are associated to changes in the physical (light climate) and the chemical (nutrient availability) constraints for algal growth (Margalef, 1997; Reynolds, 1997; Naselli-Flores & Barone, 2000). The light environment experienced by phytoplankton cells is, on one hand, are related to turbulent mixing, which determines the residence time of micro-algae within the euphotic layer (MacIntyre et al., 2000). On the other hand, the distribution and bioavailability of nutrients in the euphotic layer is the result of transport processes interacting with biological phenomena. These changes in the physical and chemical environment experienced by algal cells are, in turn, tightly linked to the physical (hydraulic and meteorological) forcing driving mixing and transport processes within the lake, and they tend to promote the growth of certain groups or species in detriment of others, given the variety of adaptations of phytoplankton to the environment (Huisman *et al*., 1999; Passarge *et al*., 2006; Litchman and Klausmeier, 2001). Hence, the knowledge and predictability of the composition of phytoplankton communities and its evolution needs to be grounded on the appropriate knowledge and

prediction of the physical processes of transport and mixing, which determine turbulence levels, nutrient distribution and light penetration in the water column.

Consistent with this widely accepted perception of succession in aquatic ecosystems, mathematical models used to simulate the evolution of phytoplankton communities are based on the appropriate description of the physical processes and their relationship with algal growth. Not only these mathematical models are a valuable research tool to answer ecological questions, but they have also received considerable attention in the field of water quality management, mainly for their predictive abilities. In spite of the considerable interest drawn by succession models among ecologists and engineers, few works have been published that specifically focus on the analysis of this type of models. Reynolds (1999) is one of the few authors that have reviewed approaches used to model phytoplankton succession in lakes. However, he focused on the usefulness to assist in management decisions. He did not discuss the unique problems of succession models that arise from the fact that they simulate explicitly the non-linear interactions existing among multiple phytoplankton groups.

The first general aim of this thesis is to review the latest developments, achievements and problems encountered in the modeling succession of phytoplankton communities in lakes and reservoirs. We first reviewed the different approaches used to model and simulate the changes in the physical, chemical, and biological components of phytoplankton succession model. We examined the type of model evaluation adopted by different succession models and their ability of prediction. My goal in this work was to define a valid approach to develop and test a succession model of El Gergal reservoir, which could be used both for (1) research purposes and (2) water quality prediction.

Models used to predict and understand successional changes in the phytoplankton communities (Griffin et al., 2001; Kuo et al., 2006) are based on a functional or mechanistic approach to modeling natural processes, in which differential equations derived from the physical principles of mass, energy and/or momentum conservation are used to represent the evolution of the different components of the ecosystems (Hamilton and Schaldow, 1997; Omlin et al., 2001; Reynolds et al., 2001; Arhonditsis and Brett, 2005). Mechanistic models typically contain a large number of parameters, with values that are site-specific and typically unknown when modelers are first posed with the problem of predicting the behavior of a particular ecosystem. The particular set of parameter values that best describes the process rates in any given ecosystem can be selected either through a time-consuming and resource intensive process involving in-situ experimentation (see Gal et al., 2009) or, alternatively, through calibration. The latter is, by large, the most common method adopted in water quality modeling (Markensten & Pierson, 2007; Omlin et al., 2001; Rose et al., 2007; Mieleitner and Reichert, 2008). It is more economical than experimentation, but it can be very time consuming depending on the computational cost of the model and on the number of parameters to be calibrated. Thus, any progress in calibration strategies of coupled physical-succession models will contribute to generalize their use for water quality management purposes. Automatic calibration approaches may be a valid alternative (Eckardt & Arnold, 2001) to traditional trial and error calibration strategies, only efficient in calibrating models with a small number of parameters (Tanentzap et al., 2007; Kuo et al., 2006; Bonnet and Poulin, 2004) or when most parameter values have been determined through experimentation (Hillmer et al., 2008; Gal et al., 2009). Automatic calibration are designed to search the parameter set that minimize an objective function, representing the norm of the difference between modeled and

observed variables, and can be divided in two classes: gradient and global optimization methods. Gradient methods have been widely applied in the calibration of phytoplankton models of varying complexity (Omlin et al., 2001; Rose et al., 2007; Mieleitner and Reichert 2008), however, they can potentially converge to a local minimum of the objective function, rather than global minimum, compromising its effectiveness in highly parameterized models. Global optimization techniques avoid the convergence to local minima, by introducing a certain degree of randomness in the search process (Klepper and Hendrix, 1994; Hansen et al., 2003; Duan et al., 1992; Eckardt & Arnold, 2001; Skahill & Doherty, 2006). These global optimization methods are extensively used to calibrate complex hydrological models (Tonkin and Doherty, 2005; Skahill & Doherty, 2006; Marcé et al., 2008; Gupta et al., 1998), but few global calibration exercises applied to water quality models have been published (Mulligan et al., 1998; Ostfeld and Salomons, 2005; Goktas el al., 2007). Moreover, the applicability of these approaches to the calibration of phytoplankton succession models has not been explored in the literature.

The second general aim of this thesis is to propose and test a strategy, based on an hybrid gradient-global calibration algorithm, to calibrate a highly parameterized, and deterministic physical-biological model for El Gergal Reservoir. We want to verify if the integration of automatic calibration strategies is a useful approach in complex deterministic ecological models.

A calibrated model of El Gergal is used to analyze the role of withdrawal on the control of phytoplankton succession. Hoyer et al. (2009) identified abrupt changes of a general succession sequence of functional groups coinciding in time either with strong wind events or changes in withdrawal rates, and concluded that water withdrawals were, probably, the most important allogenic factor controlling the changes in composition and abundance of the phytoplankton community in Mediterranean reservoirs. Their conclusion agreed with that of Naselli Flores (2000), who studied twenty-one Sicilian reservoirs of varying trophic states, and argued that the abundance and composition of phytoplankton were more strongly influenced by the hydraulic regime than by nutrient availability. Few studies have been published that focus on the relationship between phytoplankton succession and withdrawals. Furthermore, those few that have been published are, to some extent, contradictory (Barbiero et al., 1997; Hoyer et al. 2009). None of them explore the mechanisms by which withdrawals may affect succession.

The third general aim of this thesis is to understand the mechanisms by which withdrawal could induce changes in the composition of phytoplankton communities. Our working hypothesis is that changes in the withdrawal elevation may impact differently on the environmental conditions, and may favor the development of certain species in detriment of others, as a consequence of their different response to the modified environment. A conceptual and simplified model is used to evaluate the changes in the light and temperature fields induced by selectively withdrawing at different levels, and the subsequent changes in different phytoplankton groups, depending on their response to these changes. Simulations conducted with a one-dimensional hydrodynamic-ecological model (DYRESM-CAEDYM) calibrated for El Gergal reservoir, are then used to evaluate the effects of different withdrawal levels on two algal groups with different adaptations to the environment interacting.

Remarks on data acquisition and thesis structure

During the period of research a preliminary study was conducted in Beznar Reservoir (Granada). Physical, chemical and biological data were collected during year 2005 in order to elaborate a Beznar Reservoir model using Dyresm-Caedym and analyze sources of uncertainty predicting physical and ecological variables. Results of this study were presented in 2006 in the dissertation of D.E.A. ("Diploma de Estudios Avanzados") titled "A physical-ecological model of lake Beznar ecosystem; Porpagation of uncertainty from physical to population dynamic predictions" and were not included here.

My work was funded by Spanish Ministry of Education and Science, through project CGL2005-04070/HID *Coupling hydrodynamics and plankton: impact of exogenus perturbations in a mesotrophic reservoir in Southern Spain (El Gergal, Sevilla)*. The Seville Water Supply Company (EMASESA) was a key participant in that project and made their data set, collected during their routine reservoir water quality monitoring program, available to us. Another part of the data used was collected by personnel from the University of Granada, Málaga and Jaén, in the course of several field experiments conducted in El Gergal, during 2007 and 2008. El Gergal Reservoir, is taken here as a prototypical example of Mediterranean Canyon-type reservoir, occupying deep and narrow valleys. The reservoir is managed to deliver water with the best quality as possible to a Water Treatment Plant (WTP) from which drinking water is supplied to the city of Seville. The development and implementation of an ecological model for El Gergal, which can be routinely used for water quality predictions, is the ultimate goal of the research line initiated with project CGL2005-04070/HID. This work is the first step in that direction.

A first period of research was dedicated to calibrate the ecological model and simulate total phytoplankton concentration in El Gergal from 2001 to 2005. No information of chlorophyll-a concentration separated a per-group basis needed for the calibration of a succession model was available for that period of time. Results for these years were not included in this thesis that is focused on phytoplankton succession, but were presented in the Master's thesis in Environmental Hydraulics in 2007 titled "Modelling thermal structure and phytoplankton dynamics in El Gergal Reservoir (Seville, Spain)".

This document is organized in three independent chapters. Each one is an article which has been submitted or will be submitted for publication in scientific journals. The first chapter has been accepted to be published in "Environmental Reviews", the second is under review in "Environmental Modeling and Software", and the third will be sent to "Ecological Modelling".

Resume

Chapter n. 1

Dynamic phytoplankton succession models are an essential instrument to improve scientific knowledge on the development of algal blooms characterized by a specific composition and to support water quality management decisions. The peculiar structure and formulation of these models generate questions that differ from the ones found in modeling eutrophication and are related to simulation of multiple phytoplankton groups. In this work a classification of phytoplankton models simulating several algal groups is provided. Coupled succession models, explicitly describing non-linear interactions between physical and biological processes and capturing the response of phytoplankton community to environmental changes, are analyzed in detail. Approaches, actual achievements and developments of succession models are examined. In particular we discuss the level of discrimination adopted, number and type of algal groups simulated, biomass unit employed, type of model evaluation used and efficacy of prediction achieved. Simulations of multiple phytoplankton group behavior still produce significant deviations over time or in magnitude compared to the patterns observed. Goodness of fit estimation frequently is only graphical and statistics adopted do not allow a direct comparison between different models. To facilitate comparisons we propose the use of a common statistic that would be applied, separately, to all the phytoplankton groups differentiated in each model. Each model's level of complexity in relation to prediction ability is also analyzed. Through this work we aspire to orientate upcoming works and encourage others to apply mechanistic succession models, including the description of physical and biological relationships, specific phytoplankton behavior and interactions between phytoplankton groups.

Chapter n. 2

A fundamental problem in water quality modelling is adequately representing the changing state of aquatic ecosystems as accurately as possible, but with appropriate mathematical relationships without creating a highly-complex and overly-parameterized model. A model more complex that necessary will require more input and result in unaffordable calibration times. In this work we propose and test a calibration strategy for a one-dimensional dynamic physical-ecological model (DYRESM-CAEDYM) to reproduce the seasonal changes in the functional composition of the phytoplankton community existing in El Gergal Reservoir (Seville, Spain). The community is described as a succession of functional groups with different response to environmental conditions. First, we performed a sensitivity analysis to identify the parameters to include in the calibration process, and then applied a global optimization algorithm to fit the model for each algal group in a sequential fashion. Finally we simulated all the functional groups adopting parameter values established during the group-by-group calibrations. Our results show that the performance of this approach is strictly related with: (1) the level of system description (i.e. the model structure and the number of functional groups simulated); (2) the level of information included in the calibration process (i.e. the observations); and (3) the nonlinear interactions among functional groups. Functional segmentation of the model should be minimized even though groups

with different environmental requirements must be discriminated. Although magnitudes of biomass peaks were not always estimated correctly, the calibrated model was able to predict peak sequence and timing of dominant phytoplankton groups. Thus our study showed that: (1) model structure and nature of observations adopted have to be in agreement with the level of organization in the system; (2) integration of automatic calibration strategies is a useful approach in complex deterministic ecological models.

Chapter n. 3

Phytoplankton composition and abundance in reservoirs are controlled to the greatest extent by a combination of different factors as light-nutrient availability, mixing regimes and biological interactions between species. Few studies, based on the analysis of field observations, showed a correspondence between withdrawals events and changes in phytoplankton community composition. In this work we want to analyse the specific reaction of phytoplankton groups, aggregated depending on their particular response to environmental conditions, to withdrawals level variation. We started from the idea that changes in the environmental conditions generated by withdrawals operations may favor the development of certain species in detriment of others. Our analysis was conducted first with the help of a conceptual model and then with a one-dimensional hydrodynamic-ecological model (DYRESM-CAEDYM) evaluating effects induced by different withdrawal levels in a Mediterranean medium-size reservoir (El Gergal, Seville). Model results showed that shifting extractions from intermediate to surface or bottom levels had effects on phytoplankton group development while shifting from bottom to lower extractions do not produce variation in phytoplankton group concentration at short term. The response of the studied phytoplankton groups (Cyanobacteria group H, Chlorophytes groups J and N) was dependent on the relative position between the level of extraction and the depth of the phytoplankton group development in the water column. Magnitude of variation in phytoplankton group concentration was dependent on the magnitude of outflow rate and on the bathymetry of the reservoir.

Chapter 1

"La variedad de las pretensiones no tiene fin.
Hasta existe quien tiene la pretensión de no tenerlas."
Santiago Rusiñol i Prats

State of the art and recent progresses in phytoplankton succession modeling

1. Introduction

The composition of phytoplankton communities and the relative abundances of component species undergo continuous changes on varying scales. These scales range from frequent reorganizations of existing community structures, through annually recurrent cycles of compositional changes (succession) that accompany the underlying cyclical fluctuations in insolation and temperature, to longer-term floristic changes, where one recognizable recurrent cycle is supplanted by another (Reynolds, 1984). Similar temporal patterns, specific to specie groups rather than individual species, tend to occur in different lake and reservoir systems. For example, the dominant species in phytoplankton communities in early spring and late fall are usually Diatoms; during summer time the phytoplankton communities may often be dominated by flagellates (Evans, 1988; Margalef, 1983). These recurrent patterns suggest that there must be a common mechanism at play. Considerable efforts have been devoted in ecology during the last few years to understand and predict these mechanisms underlying phytoplankton succession changes (Morris, 1980; Reynolds, 1984; Sommer, 1988; Reynolds, 1997). Today, it is widely accepted that the abundance and composition changes experienced by phytoplankton communities in aquatic ecosystems are tightly linked to: (1) the hydrography of the system that affects the permanence of the water body and (2) the variations in the physical-chemical constraints as light climate and nutrient availability (Margalef, 1997; Reynolds, 1997; Naselli-Flores & Barone, 2000). Specie compositional changes over time have been traditionally referred as succession. First this term was used to define the autogenic or internally driven process where pioneer plants establish in a habitat, create conditions for other specie growth and are later replaced by others (Tansley, 1939). However, the assembly of the community depends not only in specie strategies or organism physiology adaptations exploiting habitat resources (autogenic factors) but also on changes in the environment conditions that alter competitive advantages among different species. These allogenic factors are externally imposed and can reverse or retard the community assemblage (Sommer *et al.*, 1986). Observing the effect of changing seasons on phytoplankton composition changes in English lakes, Pearsall (1923; 1932) introduced the concept of seasonal

succession for phytoplankton species. The theoretical culmination of a succession driven by autogenic processes is a stabilized climax maintaining the maximal biomass and interaction among species (Tansely, 1939). Although, considering the potential speed of phytoplankton community assembly, external forces are often frequent or severe enough to ensure that progress toward climax is persistently "disturbed". Frequency of physical environment change is usually greater than time-scales required by species to take advantage and develop a population increase before the selective favour is shifted elsewhere. The idea, that maximum diversity is maintained at intermediate disturbance frequencies, is called intermediate disturbance hypothesis and was developed by Connell (1978).

A large body of literature, still growing, has highlighted the concept of succession being subject to external environmental control, through the analysis of experimental observations either collected in the framework of field monitoring programs or in microcosms and mesocosms. Antenucci *et al*. (2005), for example, report the effects of long-term artificial destratification on the abundance and composition of the phytoplankton community in a subtropical lake. They show a reduction of total biomass (in particular, Diatom and Chlorophyte biomass), and a persistence of solitary filamentous Cyanobacteria dominance (*Cylindrospermopsis raciborskii*), in response to increase mixing levels in the water column. Sommer and Lengfellner (2008), working with mesocosms and analyzing phytoplankton growth at different light and temperature regimes, demonstrated that light intensity may control the timing of spring blooms and that the biomass of Diatoms (*Tabularia* and *Navicula*) tends to decrease with rising water temperatures and increasing insolation, probably due to their photoadaptive abilities that are not as well developed as other phytoplankton species. Cyanobacteria *Oscillatoria*, for example, is extremely efficient in enhancing its light dependent growth efficiency (Reynolds, 1997). Similar experiments by De Senerpont Domis *et al*. (2007) showed that artificially warming the environment may not change the phytoplankton succession sequence, but tends to increase the abundance of Cyanobacteria species (*e.g., Microcystis*) relative to other groups in the community (*e.g.,* Diatoms *Asterionella* and Chlorophytes *Scenedesmus*). Applying a Principal Component Statistical Analysis to a long-term field data set, Moustaka-Gouni *et al*. (2007) showed that Cyanobacteria (*Limnotrix redekei*, *Microcystis aeruginosa* and *Cylindrospermopsis raciborskii*) persistence in steady-state phases can be promoted by warm climate and smooth seasonal changes in irradiance. Hence Cyanobacteria are tolerant to water temperature increases, showing superior performance over other groups under this particular condition. Different responses of phytoplankton competition for the same limited resource were tested through experiments conducted under controlled environmental conditions (Huisman *et al*., 1999c; Passarge *et al*., 2006; Litchman and Klausmeier, 2001). Huisman *et al*. (1999c) showed that a green alga (*Scenedesmus*) was displaced by Cyanobacteria species (*Aphanizomenon* and *Microcystis*) while another green alga (*Chlorella*) was even more competitive at lower light intensities. Passarge *et al*. (2006) showed that under phosphorus limited conditions a Cyanobacteria specie (*Synechocystis*) was able to displace a Chlorophyte specie (*Chlorella*).

The vast and growing research in phytoplankton succession has been integrated in the form of conceptual models, which express our understanding of how the changes in the composition of phytoplankton communities occur. Margalef (1983; 1997) developed the concept that phytoplankton succession is the result of a nutrient-turbulence balance, a description known as Margalef's Mandala. Developing upon this idea, a conceptual model was proposed by Reynolds (1984; 1997; *et al*., 2002) who

stated that the particular phytoplankton community existing in a lake at any given time can be predicted from the environmental conditions prevailing in the water column. Reynolds characterized this in terms of two key variables: the ratio of the euphotic depth to the surface mixed layer depth (z_{eu} / z_{mix}) and phosphorus concentration, representing energy limitation and nutrient availability for phytoplankton growth, respectively. This conceptual model states that, during the annual course of lake conditions, the habitat or environment for phytoplankton growth goes through three main stages: (1) high nutrient availability and intense turbulence, (2) high nutrient availability and low turbulence, and, (3) low nutrient concentrations and low turbulence. The first habitat stage would be colonized by ruderal phytoplankton species (*i.e.*, Diatoms), the second by colonizer microalgae species (*i.e.*, Chlorophytes) and the third by stress-tolerant (or climax) species (*i.e.*, Cyanobacteria followed by Dinoflagellates) (Grime, 1979; Reynolds, 1984; Wetzel, 2001). A more detailed differentiation of phytoplankton response to habitat conditions was proposed by Reynolds (1997; *et al*., 2002), suggesting that species belonging to the same functional group occupy the same region within the two-dimensional (energy and nutrient limitation) habitat matrix. Reynolds' conceptual model has been successfully applied to explain long-term seasonal patterns of phytoplankton succession observed in temperate lakes (Lindenschmidt and Chorus, 1998; Jaworska and Zdanowski, 2009; Tolotti *et al*., 2010), temperate rivers (Descy, 1993), subtropical ecosystems (Hambright and Zohary, 2000; Arfi *et al*., 2003) and tropical ecosystems (Figueredo and Giani, 2001).

Mathematical models which represent conceptual models of phytoplankton succession and simulate more than one phytoplankton group are used to understand changes in quantity and composition of phytoplankton communities in lakes and reservoirs and the underlying mechanisms at play. Therefore mathematical models are a valuable research tool in answering ecological questions. They have also received considerable attention in the field of water quality management, mainly for their predictive abilities. Predicting succession changes in phytoplankton communities is of interest to water supply managers, given that phytoplankton may severely affect the quality of the water and even compromise the effectiveness of treatment processes undertaken in downstream water treatment plants. The occurrence of blue-green algal blooms in water supply reservoirs, for example, may lead to severe clogging problems during the filtering operations; or it may lead to taste, odor and even health problems as a consequence of several species and stocks of blue green-algae producing toxic substances (Guven and Howard, 2006; Margalef, 1983). Furthermore succession patterns are indicative of the integrity of the ecosystem (Bonnet & Poulin, 2004; Gal *et al*., 2009; Mieleitner & Reichert, 2008) and any changes experienced in the normal succession behavior of phytoplankton can be used as a sensor of the ecological state of water bodies. For example, it is commonly accepted that long-term increases in the supply and availability of nutrients in water bodies (cultural eutrophication) induce changes in the qualitative nature of algal associations, which become dominated by bloom-forming Cyanobacterial species (Harper, 1992, Hutchinson, 1957, 1967).

Independent of the focus of the mathematical modeling, considerable efforts have been devoted in the last few years to develop and test the predictive ability of mathematical succession models applied as management tools in particular water bodies; and these models have been developed and used in ecological research, to understand the underlying mechanisms controlling succession. In spite of the considerable interest drawn by succession models among ecologists and engineers, few reviews have been done that specifically focus on these types of models, and their specific problems and developments. Some authors have attempted to provide general

guidelines in developing ecological models that have then been applied and customized into succession models. Jakeman *et al*. (2006) proposed an iterative approach for the development of environmental models, consisting of ten steps, starting from defining the model scope and contents, and concluding with its evaluation. This iterative approach was critically evaluated by Robson *et al*. (2008), and applied in the development of a model of phytoplankton succession and nutrient concentrations in the Swan-Canning Estuary (Western Australia). Jørgensen (1995) also provided a critical overview of procedures used in ecological research to set up biochemical models of freshwater ecosystems. In his review, Jørgensen (1995) included a brief overview of existing ecological models, their evolution and their ability to generate reliable results once applied to different study sites. Succession models were included as one of the last generation in the large family of ecological models. The rigid structure of the present models that adopt a fixed parameter set to represent ecosystem processes would be replaced by a time-varying parameter set (Jørgensen, 1999). Arhonditsis and Brett (2004) conducted an extensive review of ecological modeling practices and analyzed the predictive ability of biogeochemical models applied to different types of aquatic ecosystems. They constructed frequency histograms of the number of models existing for each ecosystem type (coastal, lagoons, lakes, reservoirs and ocean), and documented the number of variables (*e.g*., temperature, dissolved oxygen, nutrients, phytoplankton, zooplankton, and bacteria) included in each model. It was shown that the ability of ecosystem models to predict changes in nutrient concentration and phytoplankton biomass was low (relative error 40%) when compared with their ability to predict changes in physical variables. Reynolds (1999) is one of the few authors that focuses on succession models, and reviews the types and general approaches used to model the change in composition experienced by phytoplankton communities in lakes. In his work he focused on model contributions to management issues and he differentiated capacity models, rate models, composition and descriptive models, considering their main features and relating their ability to assist in management decisions. Still, he did not discuss the unique problems of succession models and how they discriminate phytoplankton groups or how they evaluate individual group predictions. Guven and Howard (2006) also presented a review of models developed to predict the growth of Cyanobacteria, a particular type of algae whose occurrence is typically associated with problems in water treatment plants. Models that predict one algal group development, though, are not phytoplankton succession models, but can be associated with phytoplankton bloom models. Those models, commonly adopted in oceanography, are not interested in reproducing the temporal evolution of phytoplankton composition simulating multiple groups, but in predicting algal bloom formation, dynamics and diffusion (*e.g*., Franks, 1997).

Our goal is to review developments and achievements in succession modeling of phytoplankton communities in lakes and reservoirs. Our work is structured as follows. First we analyze how the phytoplankton community is classified and grouped, and how the size of each group is defined. Second, we discuss the level of complexity used to describe the physical and the biological components of phytoplankton succession models. Third, we examine the type of model evaluation adopted and ability of model prediction. Our ultimate aim, in reviewing, is to stimulate critical thinking among water utility managers, to orientate modelers' future works and to encourage the water supply industry to apply fundamental principles of ecology and mass transport in stratified water masses. This approach should be adopted in the process of managing water quality and carefully designing strategies to control succession and predict the occurrence of algal blooms.

2. Modeling paradigms

Succession models consider that the phytoplankton community is integrated by N groups, each of them with biomass concentration $\{B_i, i = 1, N\}$. The goal of succession models is to estimate the biomass of group i at time t ($B_{i,t}$), as a function of the biomass of that same group at previous times, $\{B_{i,t-k}, k > 0\}$, the biomass of other groups $\{B_{j,t-k}, j = 1, N, j \neq i\ , k > 0\}$, and the environmental conditions prevailing in the water column, *i.e.*,

$$\frac{\partial B_i}{\partial t} = f_i\left[\left\{B_{i,t-k}, (k \geq 1)\right\}, \left\{B_{j,t-k}, (j = 1, N), (k \geq 1)\right\}, I, T, N, P, C, ...\right] \quad [1]$$

where I and T, refer to light and temperature, and N, P, C, refer to nitrogen, phosphorus and carbon concentrations in the water column. Note that the growth of different algal groups in Eq. [1] is linked and interdependent given that the different groups compete for nutrient and light resources. This makes succession models very different from eutrophication models, where the competitive relationship between algal species and sub-groups is simply ignored. Two alternative approaches (empirical and mechanistic) can be followed to define the relationship expressed in Eq. [1]. In the empirical modeling approach (also referred to as inductive or data-based), the functions f_i are constructed using statistical or other type of tools, from empirical observations (or data). In the mechanistic (deductive or theoretical) approach, the functions f_i are constructed using theoretical relationships, in particular, the principle of conservation of mass. While the empirical approach focuses on the variable predictions, the process-based approach aims at explicitly representing the particular processes through which the state variables become interrelated (Fig. 1. 1). For example, Eq. [2] represents the change of biomass of the phytoplankton group i, as the result of processes such as algal settling (f_i^{SET}), resuspension (f_i^{RES}), growth and mortality (R_i) (*i.e.,* including respiration and zooplankton grazing).

$$\frac{\partial B_i}{\partial t} = f_i^{SET} + f_i^{RES} + \left\{\mu_{\max i} \cdot f_i(I, N, P, C, T)\right\} \cdot B_i - R_i \cdot B_i \quad [2]$$

Note that the growth rate is defined in terms of a group-specific maximum growth rate, multiplied by a limiting function that depends on the environmental conditions. In this case, it is through the influence of other phytoplankton groups on environmental conditions that their growth influences the growth of group i. Growth and mortality are modeled in Eq. [2] using first order kinetic expressions. The empirical approach is preferable in cases where the modeled system is poorly known, while the mechanistic approach is recommended when the system knowledge is good (Jakeman *et al*., 2006).

Empirical models

Empirical models of succession, with a large number of physical and biological variables involved and interacting in a highly non-linear manner, have been constructed using mainly two approaches or techniques: fuzzy logic (Salski, 1992; Chen and Mynett, 2005) and artificial neural networks (Hsu *et al.,* 1995). One of the main differences between these approaches lies in the description of the relationship between inputs and outputs variables. In fuzzy logic models this knowledge is represented in the form of linguistic rules, while in artificial network it assumes a numerical form (weights). Linguistic rules, in fuzzy logic models, are represented by "if-then" sentences that connect the inputs with the outputs variables through a level of influence (*e.g*., low, middle, high) (Salski, 1992; Lilover and Laanemets, 2006). The fuzzy model

build-up includes three steps: (1) fuzzification, in which the input data are translated through membership functions, in qualitative terms (membership sets), (2) inference, in which a set of knowledge rules between classes of aspects are defined, and (3) defuzzification where the qualitative output of the model is translated into quantitative value. The defuzzification step is needed to communicate the results (Fig. 1. 2a). Conventional membership functions usually assume a value of one when an element belongs to a set and zero if not. In the case of fuzzy models a membership function can assume all the values that are included in the interval [0, 1] allowing processing of imprecise information. An example of the fuzzy model structure is to consider surface layer temperature, wind mixing and phosphate condition as model input factors and Cyanobacteria biomass as model output. The selection of level of influences and the tuning of the knowledge rules are performed by trial and error tests.

The architecture of artificial neural networks comprises an input and output layer containing neurons (or nodes) representing model variables. Each neuron is connected to other neurons with an axon and the activity of each neuron is determined by the input received from the other neurons connected to it (Fig. 1. 2b). Connections between variables (neurons) are not explicitly defined but established by a randomized back-propagation algorithm that assigns weights (W) to each connection (Olden, 2000; Recknagel, 1997). The back-propagation algorithm trains the network by iteratively adjusting all the connection weights among neurons, with the goal of finding a set of connection weights that minimizes the error of the network, *i.e*., sum-of-the-squares between the actual and predicted output (least squares error function). Observations are sequentially presented to the network, and weights are adjusted after each output is calculated depending on the magnitude and direction of the error.

Fuzzy models and neural networks models have been mainly applied to predict phytoplankton blooms particularly in the sea (Liliover and Laanemets, 2006; Lilover and Stips, 2008), but also in lakes (Recknagel, 1997; Chen and Mynett, 2003). Recknagel (1997), for example, predicted five different blue-Green algal species (*Anabaena, Oscillatoria, Microcystis, Phormidium* and *Gomphosphaeria*) in Lake Kasumigaura (Japan) for years 1986 and 1993, with contrasting environmental conditions (*e.g*., solar radiation, water temperature, Secchi depth, zooplankton density). He compared the simulated concentration of total Chlorophyll-a (Chla) against observations collected about every 40 days. Total Chla concentration simulated with the model agreed very well with the observations. The timing and magnitude of the observed and simulated Chla peaks agreed well in time and magnitude; in this case evaluation was only graphical. Separate predictions of number of cells showed a maximum error of about 50% in peak predictions of *Anabaena* and *Oscillatoria*, while it showed good agreement for *Microcystis spp*. Neural networks also were applied to study phytoplankton succession, in particular simulating Diatoms and Cyanobacteria (Recknagel *et al*., 2006) or phytoplankton community composition including also Crysophytes, Cryptophytes and Chlorophytes (Olden, 2000). These studies demonstrated good forecasting abilities and attempted to evaluate relationships between algal abundance and chemical water quality conditions (phosphorus, nitrite, nitrate and ammonium concentrations). Recknagel *et al*. (2006) showed that supervised artificial neural networks facilitate the forecasting of water quality changes while non-supervised artificial neural networks are useful in addressing the ecological relationships between seasons and phytoplankton development. Supervised means that the algorithm is guided by known output patterns, while non-supervised means that it learns the patterns from features of the inputs. Non-supervised artificial neural networks can be used to

test hypotheses on algal specific preferences for environment conditions (Recknagel *et al*., 2006).

These empirical techniques enable users to predict rather than to explain the processes of the system or explain variables behavior. The work of Olden (2000) illustrated how neural network models can evaluate associations between variables, for example correlating patterns in phytoplankton community composition with nutrient patterns and zooplankton (Daphnid Cladocera) biomass patterns. Even if neural networks are beneficial in evaluating variable interactions, the mechanisms driving phytoplankton succession cannot be inferred from correlative studies. If external environmental conditions would vary, these models would not be able to capture the response of phytoplankton behavior to these changes. So, if the aim is to predict phytoplankton community response to long terms events, they are not a useful tool for the study of phytoplankton succession and the generation of bloom events. However, it is possible that these models could be applied to analyze the link between physical and biological processes if the meaning of the network connections could be extracted and interpreted (Maier and Dandy, 2000).

Mechanistic models

The mechanistic approach remains, by far, the most frequently used method to modeling phytoplankton succession in aquatic ecosystems. Mechanistic succession models existing in literature vary in complexity according to the discretization level used to describe the biogeochemical elements (kinetic segmentation) and the physical space (physical segmentation) (Fig. 1. 3). The kinetic segmentation defines the level of description used to account for the mass existing in a given compartment into which the lake may have been divided (Fig. 1. 3b). The chemical segmentation depends on the number of elemental cycles modeled (*e.g.* Carbon, Nitrogen, Phosphorus, Silica, and Oxygen), and whether the organic, inorganic and dissolved forms or fractions of the elements are included or not (*e.g*., Arhonditsis and Brett, 2005; Gal *et al*., 2009; Bonnet and Poulin, 2004). Biological segmentation, in turn, refers to the number of phytoplankton groups simulated. This number varies from two (Burger *et al*., 2008; Chen *et al*., 2002; Roué-Le Gall *et al*., 2009) to several phytoplankton groups (Bonnet and Poulin, 2002; Bonnet and Poulin, 2004; Reynolds *et al*., 2001). In some cases, other biological groups are included in the model. Roué-Le Gall *et al*. (2009), Chen *et al*. (2002) and Gal *et al*. (2009), for example, simulate bacteria and respectively one, two and three zooplankton groups.

In food-web models that simulate more than one algal group, the physical space of the ecosystem is typically described as a single well-mixed compartment, with uniform properties (Roelke, 2000; Rose *et al*., 2007). This level of physical segmentation, however, is not appropriate for deep or moderately deep lakes and reservoirs, where stratification develops on seasonal time scales, imposing severe restrictions to water movements in the vertical direction. The simplest approach to account for stratification in succession models consists of considering the lake as formed by two compartments or layers (epilimnion and hypolimnion) separated through an interface (thermocline) (*e.g*., Scavia, 1980). The vertical transport across the thermocline is typically described using diffusion coefficients which are derived from changes in the observed temperature profiles (*e.g*., Scavia, 1980). The two layer discretization of the physical space has been used, for example, by Huisman and Sommeijer (2002), Arhonditsis and Brett (2005), and Mieleitner and Reichert (2008), among others. A large number of succession models use multiple layers to discretize the physical space (Riley and Stefan, 1988; Hipsey *et al*., 2004; Elliott *et al*., 2001;

Elliott and Thackeray, 2004; Markensten and Pierson, 2007; Moreno Ostos *et al*., 2007). Multi-layer models present the advantage that physical, chemical and biological components are modeled with similar order of detail, which reduces the possibility of weak links in the modeling process (Riley and Stefan, 1988). In particular they allow representation of the water column stratification more accurately and hence allow descriptions of the environment that benefits one algal group, favoured by stratified conditions and insolated epilimnia (*e.g.,* Cyanobacteria *Anabaena or Aphanizomenon sp.)* versus others, favoured by mixing conditions that allow them to entrain in suspension (*e.g.,* Diatoms). Some succession models have, consequently, evolved by improving vertical physical resolution. For example, the earlier versions of the generic model described in Reynolds *et al*. (2001) described the environment as if it were unstratified. In later versions the model describes the physical environment using uniform layers (each of 10^{-1}m), and includes a description of vertical motion of phytoplankton in the water column (Reynolds *et al*., 2005b). Physical description is still simplified compared to other models (*e.g.,* Romero *et al.,* 2004) and not all the hydrodynamic and heat exchange processes are solved between layers (Reynolds *et al*., 2001).

Multi-layer models of lakes are based on a one-dimensional (1-D) assumption; that is, the variations in the vertical direction are more important than those in the horizontal direction. The 1-D assumption is based on observations that the density stratification usually encountered in lakes and reservoirs inhibits vertical motions while horizontal variations in density are quickly relaxed by horizontal advection and convection. Horizontal exchanges generated by weak temperature gradients are communicated over several kilometres on time scales of less than a day, suggesting that the 1-D model is, in general, suitable for representing the physical processes of transport at synoptic and larger time scales. In some instances, such as shallow lakes, lakes with sheltered basins or lakes with very irregular morphology the 1-D assumption is not entirely adequate. In those cases, two- or three-dimensional (2-D; 3-D) models need to be applied in order to correctly capture the spatial variability of the environment that results from the physical process of transport and mixing. Few publications exist that apply succession models with a 3-D discretization of the space, given partly to the high computational cost that executing those codes involves, partly to the calibration efforts and the extent of observations required. Some examples include, the work of Alexander and Imberger (2009), who studied the dispersion of Dinoflagellates during wind events in San Roque Reservoir; the work of Robson and Hamilton (2004) who analyze the occurrence of Cyanobacteria blooms in the Swan River estuary; or the work of Romero *et al*. (2004) who studied the changes in the biogeochemical fluxes occurring during flood events in the Lake Burragorang. Common to those studies is the focus on the analysis of short-term changes that occur in the phytoplankton communities in response to major physical perturbations. To the authors' knowledge, 3-D models have not been applied in the study of seasonal changes experienced by the phytoplankton communities in response to seasonal changes or environmental conditions, but instead have been analyzed mainly using lower levels of physical segmentation.

Some of the succession models described in literature require that the physical and chemical environment are provided as an external input (*e.g*., earliest version of PROTECH: Reynolds *et al*., 2001; and CE-QUAL-ICM: Cerco and Cole, 1995). The CE-QUAL-ICM 3-D eutrophication model (Cerco and Cole, 1993; Cerco and Cole, 1995), for example, incorporates multiple forms of algae but does not compute hydrodynamics which must be provided to the model. Other phytoplankton models are grounded on predictions provided by a physical model of transport and mixing in the

water column, which are, algorithmically, coupled to the ecological model. Examples of coupled models are the 1-D DYRESM-CAEDYM (Romero *et al*., 2004), DyLEM (Bonnet and Poulin, 2004) and PROTECH simulating thermal stratification in the vertical dimension (Reynolds et al., 2001); or the 3-D ELCOM-CAEDYM (Laval and Hodges, 2000; Robson and Hamilton, 2004). Coupled models may be required when describing chemical and biological processes that closely interact with physical conditions. For example suspended solids and algal concentration both affect light intensity distribution in the water column with a direct effect on thermal structure (physical environment) (Romero *et al.*, 2004). Thus, connections between hydrodynamics and biology are not always independent and a non-coupled model would not be successful capturing those processes. Coupled models are extremely useful in analysing and understanding the ecological response of the lake to external forces such as meteorological conditions, management strategies, inflow nutrients reduction, *etc.* (Griffin *et al*., 2001; Kuo *et al*., 2006).

Within the large number of models representing succession, our interest is on process-based (or mechanistic), coupled physical-ecological models. Being mechanistic they incorporate ecological knowledge, and being coupled with a physical model they incorporate a widely accepted concept that the environmental conditions largely control succession. With this work we do not pretend to realize an inventory of the existing phytoplankton models, but to analyze distinctive features, level of performance and limitations of coupled succession models. Process-based coupled models that simulate two or more phytoplankton groups are presented in Table 1. 1. Some of the models have a generic structure that can be applied to different sites while others were developed for specific ecosystems. Physical and biological characterizations of the system are described for each model. Most of them discretized the water column as multiple physical layers while a reduced number differentiate only two layers (epilimnion and hypolimnion). The biological description includes from two (Chen *et al*., 2002) to eight different phytoplankton groups (Reynolds *et al*., 2001).

3. Phytoplankton community segmentation and biomass assessment

The criteria used to classify the individual species existing in the phytoplankton community are not unique and will vary from model to model. Most models will consider the phytoplankton community as an ensemble of up to five phytoplankton classes: Diatoms, Dinoflagellates, Cyanobacteria, Cryptophytes, Chlorophytes (*e.g*., Omlin *et al*., 2001; Chen *et al*., 2002; Hipsey *et al*., 2004). Phytoplankton classes are established on phylogenic, physiological, biochemical and structural properties of algae that assume a considerable relevance in relation to nutritional requirements, adaptive behavior, productivity and dynamics. Other criteria adopted to differentiate the phytoplankton community are: (1) morphology, due to the fact that size and shape can determine specific performances (*e.g*., Mieleitner and Reichert, 2008); (2) trophic preferences as autotrophic or mixotrophic grazed or non-grazed organisms (Roué-Le Gall *et al*., 2009), or even (3) dominant genera or functional groups (*e.g*., Markensten and Pierson, 2007; Reynolds *et al*., 2001) as assemblages of species that show the same sensitivity or tolerance to environmental changes (see Reynolds *et al*., 2002). The criteria used to classify phytoplankton cells in groups is part of the model conceptualization step and depends on the purpose of the succession model (Jakeman *et al.,* 2006). For example, phytoplankton functional groups that group algal species depending on their response to environmental conditions is ideal when the objective is an understanding of the control exerted by the environment on succession. Classifying

the community in trophic preference groups (*e.g*., edible or non-edible by zooplankton), in turn, is an excellent choice when the objective is an understanding of phytoplankton relationships with zooplankton and higher trophic levels. The exact number of groups used to describe the phytoplankton community varies with the goals of the effort.

Models also differ from each other depending on how biomass is assessed within each phytoplankton group (Table 1. 1). The biomass of any given group in the community can be evaluated in terms of (1) Chlorophyll-a concentration, (2) carbon concentration (Roué-Le Gall *et al*., 2009 ; Bonnet and Poulin, 2004; Chen *et al*., 2002) (3) wet/dry weight (Mieleitner and Reichert, 2008 or Omlin *et al*., 2001) and, (4) even, in some cases, bio-volumes (Markensten and Pierson, 2007). All these types of assessments are a kind of "analogue" for phytoplankton biomass and are not used to measure it explicitly. Chla concentration is the most frequent variable used to assess biomass. Four of the nine succession models adopted Chla accounting, three of them used carbon, two used wet/dry weight and only one included bio-volumes. This is probably due to historical reasons, given that many succession models have evolved from eutrophication models. In the latter, only the size of the phytoplankton community is of interest, and it was typically quantified in terms of Chla concentration in water; Chla concentration measurements are straightforward, compared to other approaches to quantify algal biomass, can be estimated with *in situ* equipment and were readily available in many instances. The main difficulty of using Chla concentration as a basis to evaluate the biomass of separate phytoplankton groups in succession models lies in the fact that gathering observations of Chla concentration on a per group basis is not straightforward. Recently, *in vivo* spectro-fluorimetric methods (Tolstoy, 1977) have been used to discriminate Chla concentrations of different groups of algae. These methods quantify the intensity of the fluorescence signal in a number of bands of the spectrum. The intensity of each band is correlated with the Chla concentration of different phytoplankton groups. The spectro-fluorometer can discriminate the Chla concentrations of a limited number of groups. Beutler *et al*. (2002) were able to discriminate between Green algae (Chlorophytae), grey algae (including Dinoflagellates and Diatoms), Cyanophyceae and Cryptophyceae. Alternatively, one can assess the biomass of each functional, trophic or phylogenic group by: (1) counting the number of cells *nc* (i) pertaining to each group, i, with an optic inverted microscope, following the Utermohl's method (Utermohl, 1956), and (2) converting the number of cells to biomass, multiplying the nc(i) by a factor which expresses the biomass per cell $B_c(i)$. The Chla content per cell, though, can exhibit large variations depending on the lake, season, phytoplankton species, nutrient availability and light conditions (Tolstoy, 1979; Vörös y Padisák, 1991; Kalchev, 1996). Phytoplankton species vary in size, and this partly accounts for the differences in Chla content per unit cell among species. The bio-volumes of each group can be estimated accurately from the shape and size of the cells and the enumerations. Standardized geometric shapes and mathematical equations have been designed to calculate phytoplankton bio-volumes and minimize efforts of microscopic measurements (Sun and Liu, 2003; Hillebrand *et al*., 1999). But the Chla content per unit cell-volume $Chla_v$ can vary significantly depending on external factors (light and nutrients) or on the cell position in the water column. For example, higher $Chla_v$ levels tend to occur at low light availability with no limitation of nutrients (Chapra, 1997; Laws and Chalup, 1990). Reynolds (1984) reports that $Chla_v$ may range from 1.5 to 19.7 µg Chla mm^{-3}. Even within the same group (*e.g*., Chlorophytes), the differences in $Chla_v$ can be of up to 13 µg Chla mm^{-3} (Reynolds, 1984). Furthermore, the $Chla_v$ also varies with increasing water temperature and in relation to the day-night cycle (Margalef, 1983). In spite of this variability, some authors assume that the $Chla_v$

content of any given phytoplankton class is constant during the year (Reynolds, 1984), or even that the $Chla_v$ content is the same for all groups considered in the model (Bonnet and Poulin, 2004).

Carbon concentration (mg of C per unit volume of the environment) is an alternative approach to assess biomass on a per-group basis, given that carbon content per cell of live biomass still displays a high variability, even if not as strong as Chla (Menden-Deuer and Lessard, 2000). Carbon cell content multiplied by the number of cells per unit volume, obtained by counting, results in carbon concentration per unit volume of water in the environment. Carbon cell content varies according to the photosynthetic production, but a carbon to phytoplankton cell volume relationship can be established as an assumption, in the same way as was done for $Chla_v$ content. For example, Menden-Deuer and Lessard (2000) determined a carbon (pg C $cell^{-1}$) to volume (μm^3) relationship valid for most protist plankton (*e.g.*, Dinoflagellates, Chlorophytes, Chrysophytes and Cryptophytes). Diatoms have a smaller percentage of carbon and their carbon to volume relationship was defined by a separate equation (Menden-Deuer and Lessard, 2000).

In order to compare Chla and C measurements in the environment a relationship between $Chla_v$ and carbon cell content must be defined. The ratio of $Chla_v$ to carbon varies according to environmental conditions: it tends to increase under nutrient rich environments, while it tends to decrease under high levels of radiation. Following this relationship, $C/Chla_v$ ratio variation has been modeled according to light and nutrient conditions (Chapra, 1997; Laws and Chalup, 1990). Even though, field observations, coming from a long term data base of $Chla_v$ and primary production, showed that variability of $C/Chla_v$ ratios at any particular sampling can be higher than the one observed at a seasonal scale (Yacobi and Zohary, 2010).

Mieleitner and Reichert (2008) and Omlin *et al*. (2001) use dry/wet phytoplankton mass to quantify the relative abundance of different phylogenic phytoplankton groups. Biomass on a per-group basis was calculated in those studies from phytoplankton counts and bio-volume data, assuming a constant ratio of dry or wet weight to bio-volume. The results of Quinones *et al*. (2003) and Quintana *et al*. (2002) supported the validity of this assumption. To determine separate phylogenic group biomass, Gal *et al*. (2009) converted phytoplankton wet weight to carbon units using specie specific carbon/wet-weight ratios. These ratios were, in turn, determined experimentally from samples taken during mono-specific blooms (or cultures) using mass spectrometry to determine C content (Zohary, 2004).

4. Evaluation of model performance: approaches and results

To evaluate the performance of succession models, simulated and observed values of algal biomass are compared. Surface (Roué-Le Gall *et al*., 2009) or depth-averaged values of biomass (*e.g*., Chen *et al*., 2002; Bonnet and Poulin, 2004; Mieleitner and Reichert, 2008) are typically compared for model evaluation purposes. Rarely found are comparisons of vertical profiles (Omlin *et al*., 2001). In some instances, simulated and observed values of total biomass are compared (Chen *et al*., 2002; Bonnet and Poulin, 2004). However, this approach is not appropriate given that it does not assess the ability of succession models to perform the task for which they were designed, *i.e*., to represent the alternative dominance of different algal groups. To test that ability, observed and simulated values of biomass should be compared group-by-group, as is done, in other instances (Gal *et al*., 2009; Elliott *et al*., 2000; Mieleitner and Reichert, 2008; to mention some of them).

All works on succession modeling studied (Table 1. 1) compare simulated and observed values of biomass (or biomass related variables) in graphical form. Graphical results are useful, as they provide a fast and intuitive means to assess the difference between simulations and observations. From the graphics one can get rough estimates of model errors and whether the model follows the trends. In particular, one can estimate whether the model is capable of representing accurately the magnitude of the peak concentrations (magnitude error) or its timing (timing error). Only in a few cases is the agreement between observations and simulations also quantified using statistics (Arhonditsis and Brett, 2005; Gal *et al*., 2009; Elliott *et al*., 2000). Statistics used to evaluate the goodness of fit between simulations and observations include (Table 1. 2): (1) mean error, calculated as sum of the difference between observed and simulated values divided by the number of observations (Arhonditsis and Brett, 2005; Elliott *et al*., 2000); (2) mean absolute error relative to observed mean (Elliott *et al*., 2000; Gal *et al*., 2009); (3) coefficient of determination (r^2) (Arhonditsis and Brett, 2005; Gal *et al*., 2009); (4) mean percent or absolute errors, (5) root mean squared error RMSE, (6) general standard deviation, (7) relative error and (8) the Theil's inequality coefficient (Elliott *et al*., 2000). Statistics allow one to compare objectively and accurately the prediction ability of different models. However, one should be careful when comparing the error statistics between any two models, and one should not derive false conclusions on whether any given modeling approach is preferable compared to others based only on the values of the statistics. This caution is required given that the magnitude of the statistics not only depends on the modeling approach itself, but it also depends on (1) the length of time simulated, (2) the number of observations used for comparison, (3) the variables used to evaluate biomass, and (4) the level of aggregation of the observations. For example, r^2 values obtained by Arhonditsis and Brett (2005) were *ca*. 0.90 and r^2 values obtained by Gal *et al.* (2009) ranged between 0.1 and 0.5. But Arhonditsis and Brett (2005), calculated r^2 values from observed and simulated total Chla concentration values during a one-year period, with peak values of 300 μg C L^{-1}. Gal *et al*. (2009), in turn, calculated r^2 values for each algal group over a six-year period, with maximum biomass values that were < 6 μg C L^{-1}. In general, one finds lower error measures when comparing total Chla concentration rather than Chla on a per-group basis. For instance, Elliott *el al*. (2000), simulating the growth of two different algal groups, reported a standard deviation of 0.44 when comparing simulated and observed total Chla. This represents, at most, 20% of the peak values observed. The standard deviations of the error that results from comparing simulations and observations of each algal group separately were at least twice as much (1.05 and 0.81). Also, when comparing algal biomass on a per-group basis, Markensten and Pierson (2007), Gal *et al*. (2009), or Mieleitner and Reichert (2008) report errors of more than 40% in magnitude. They also find that the simulated biomass peaks are often displaced up to one month from the time at which the values were observed.

In evaluating the performance of any given model, one needs to take into consideration that the magnitude of the error depends on a large number of factors, including: the number of groups simulated, the level of parameterization of the biological growth, the variables used to assess the algal biomass or the complexity of the physical sub-model. It also depends on whether the model parameters are either determined experimentally or calibrated, on the particular strategy used to calibrate the model, and on the data used for model error assessment (*i.e.,* the length of time simulated, the number of observations used for comparison and their quality, and the level of aggregation of the observations and simulations compared). In any case, and due to the high level of complexity of biological processes which we are just beginning

to understand, the differences encountered between simulated and observed biomass in succession models are not comparable with level of agreement reached with the physical or hydrological models (Robson *et al*., 2008). For instance the normalized mean error of temperature simulations in Gal *et al*. (2009) was 0.04, while the normalized errors of the biological variables (including phytoplankton and zooplankton groups) ranged between 0.50 and 4.54.

In general, models simulating a lower number of phytoplankton phylogenic, functional or morphological groups will tend to exhibit higher levels of accuracy. The succession model proposed by Chen *et al.* (2002) for Lake Michigan, simulating two algal groups, exhibited errors of up to 1.5 µg Chla L^{-1}, for maximum concentrations of 4 µg Chla L^{-1} during the studied period, *i.e.,* error of nearly 40%. Similar or even larger errors have been reported for succession models simulating an intermediate number of groups (four to five groups). Bonnet and Poulin (2004) compare total biomass and report errors of up to 50% and 60% near the surface at the times of the peaks; the timing of the peaks, though, were well captured by the model. Roué-Le Gall *et al*. (2009), modeling five groups, report errors on a per-group basis. The largest errors reported were close to 50% in magnitude for one of the mixotrophic algal groups. Magnitude errors for two autotrophic groups were lower (about 20%). In this case, the timing error was up to 45 days. Mieleitner and Reichert (2008), studied three different sites, and report magnitude errors of up to 50% for two phytoplankton groups (small algae and Diatoms) of the four groups simulated, when comparing phytoplankton groups separately. Models simulating a high number of functional groups (7-8 groups) show variable prediction behaviour depending on the type of groups simulated. However, in general, they are not yet mature enough to be used for predictions of phytoplankton seasonal succession. Markensten and Pierson (2007), for example, reported maximum differences between simulated and observed biomass values of up to 15µg Chla L^{-1} during a period of time when peak concentrations of 30 µg Chla L^{-1} were observed, and timing errors of about one month. When comparing simulations and observations group-by-group, some of them were not well characterized. Dinoflagellates (*Ceratium*) were over-predicted with peak values of 10-15 µg Chla L^{-1} at times when their concentration should be close to zero (Markensten and Pierson, 2007). When comparing the simulated biomass of five different algal groups against observations, Gal *et al*. (2009) reported timing errors lower than one month for three out of five groups. The maximum magnitude error observed for Dinoflagellates, the group most abundant in the lake, was almost 60% of the maximum concentration.

Due to the range of timing and magnitude errors observed when simulating phytoplankton groups, there are still important limitations with model predictions. Through the continued improvement in application and performance, models will be a fundamental instrument in advising water quality managers on strategies and decisions. Before making any management decisions, the confidence of the succession model results should be established through a strict uncertainty analysis.

5. Model parameterization and developments on calibration

Mechanistic models typically contain a large number of parameters whose values are site-specific and typically unknown when modelers are first posed with the problem of predicting the behaviour of a particular ecosystem. The particular set of parameter values that best describes the process rates in any given ecosystem can be selected either through a time-consuming and resource intensive process involving *in situ* experimentation (see Gal *et al*., 2009) or, alternatively, through calibration. Those

efforts can be reduced if some of the parameters are derived from information previously available or easily accessible. For example, even though highly parameterized to distinguish the elevated number of phytoplankton groups simulated, the model adopted by Reynolds *et al*. (2001) uses parameters where values can be obtained knowing the physical dimensions of a particular phytoplankton group. Replication rate, light dependent growth and temperature sensitivity of each species are calculated from their surface area and volume (Reynolds *et al*., 2001). While determining surface areas and volumes of dominant species for one particular site represents important work, it also would be useful to calculate bio-volumes and obtain an estimate of biomass for phytoplankton groups. In most highly parameterized models (*e.g*., Burger *et al*., 2008; Gal *et al*., 2009) the parameter values have to be defined independently so the information required to complete the parameters set is extensive. Calibration is more commonly used for defining parameters than experimentation in water quality modeling (Markensten and Pierson, 2007; Omlin *et al*., 2001; Rose *et al*., 2007; Mieleitner and Reichert, 2008). Calibration is more economical than experimentation, but it can be very time consuming depending on the computational cost of the model and on the number of parameters requiring calibration. This should not dissuade managers from using these useful tools on a routine basis. The first step in calibrating a set of parameters for a given ecosystem is establishing parameter ranges on the basis of previous works applied over a large variety of ecosystems. Reference values on growth rates, mortality rates, settling velocities, nutrient uptake rates and others parameters can be found in Bowie *et al.* (1985) and in several other works (*e.g.,* Jørgensen and Bendoricchio 2001; Hipsey *et al*.,2004; Hamilton & Schladow, 1997; Schladow & Hamilton,1997; Margalef, 1983). The second step consists in selecting a calibration procedure. Calibration procedures are evolving at the same time as model development to reduce the time required for application, to extend their use to different sites and to improve their predictions. Trial and error calibration strategies, traditionally adopted in water quality modeling, require a lot of expertise with the model being used, and are only efficient in (1) calibrating models with a small number of parameters (Tanentzap *et al*., 2007; Bonnet and Poulin, 2004) or (2) calibrating a small subset of parameters whose values cannot be determined through experimentation (Hillmer *et al*., 2008; Gal *et al*., 2009). The trial and error approach has been used by Kuo *et al*. (2006) to calibrate a 2-D hydrodynamic and water quality model applied to two reservoirs, by Bonnet and Poulin (2004) to calibrate a 1-D Cyanobacteria model of Villerest reservoir and by Lewis *et al*. (2002) to calibrate a succession model of Myponga reservoir with multiple species.

To calibrate models with a large number of parameters, automatic calibration approaches may be a viable alternative (Eckardt and Arnold, 2001). They are designed to search the parameter set that minimizes a given objective function, representing the norm of the difference between modeled and observed variables. Automatic calibration approaches can be divided into two classes: gradient and global optimization methods. Gradient methods search the parameter space using information of the local gradient of the objective function and, starting from an initial guess, to find the parameter set that minimizes the model error. Due to their low computational cost, they have been widely applied to the calibration of phytoplankton models of varying complexity: a model with two phytoplankton groups and one zooplankton group (Omlin *et al*., 2001); a model with two phytoplankton groups and three zooplankton groups (Rose *et al*., 2007); and a model with four phytoplankton groups (Mieleitner and Reichert, 2008). In all of these studies, though, the magnitude and timing error is significant, when comparing observed and simulated biomass on a group-by-group basis. Gradient methods, in spite

of their low computational cost, can potentially converge to a local minimum of the objective function, compromising its effectiveness in highly parameterized models. Global optimization techniques avoid the convergence to local minima, by introducing a certain degree of randomness in the search process (Klepper and Hendrix, 1994; Hansen *et al*., 2003; Duan *et al*., 1992; Eckardt and Arnold, 2001; Skahill and Doherty, 2006). Global optimization methods have been intensively used to calibrate complex hydrological models (Tonkin and Doherty, 2005; Skahill and Doherty, 2006; Marcé *et al*., 2008). However, few publications exist that apply global calibration algorithms to phytoplankton models (Ostfield and Salomons, 2005; Goktas and Aksoy, 2007). Applying global calibration algorithms to multi-parameterized phytoplankton models would be a way of increasing calibration efficiency and reducing efforts in determining site-specific parameters. We also suggest the creation of a common data base, easily accessible to all ecological modelers, which would aggregate the parameter values from model calibrations in different ecosystems.

6. Modeling stressors on phytoplankton community

To analyze effects of stressors on the phytoplankton community, models typically make explicit assumptions (*e.g*., fixing a water temperature condition or an environment with low nutrient availability). These models differ from ones of higher complexity that describe particular ecosystems and were previously presented. In this case the interest is not the prediction of a particular environment but the understanding of main concepts. These theoretical models, starting from previous notions on phytoplankton photosynthetic and buoyancy characteristics (see for example Talling, 1957 and Morris, 1980), show the effects of external factors such as light climate, temperature stratification and nutrient availability on bloom development and specie composition.

An early experimental approach and theoretical model was used by Tilman (1977) to analyze effects of limiting silicate or phosphate to different diatom species (*Asterionella* and *Cyclotella*). A similar approach was also adopted to relate the nutrient concentration available in the environment with phytoplankton growth rate (Auer *et al*., 1986). Sommer (1988) performed several experiments to describe algal competition between diatom and non-diatom algae, under nutrient limitation and zooplankton grazing.

Effects of stratification and turbulence on phytoplankton blooms and specie composition were studied with a theoretical, simplified model that simulated phytoplankton growth and diffusion, neglecting buoyancy, sinking, nutrient limitation and photo-inhibition (Huisman *et al*., 1999a). In a completely mixed system, species with lowest critical light intensity are favored; while in non-uniformly mixed systems, species that are able to move and best maintain an optimum position in the water column are most competitive. For one phytoplankton specie, critical light intensity was a good predictor for the outcome of competition in completely mixed waters, but not in non-uniformly mixed waters where position in the light gradient becomes the dominant factor (Huisman *et al*., 1999b). Consequently, changes in turbulence mixing rates induced shifts in specie composition. These results also indicated that buoyancy and motility, which also influence algal position in the water column, are central in determining light, temperature and nutrient availabilities. Thus, the potential advantages or disadvantages for phytoplankton cells in nutrient uptake and light absorption are the results of a combination of those factors. Model results of competition for light between buoyant and sinking species showed that more buoyant

Cyanobacteria is likely to dominate at low turbulence diffusivity while sinking Diatoms and Green algae are likely to dominate at high turbulent diffusivity. These results were supported by a lake experiment using artificial mixing. In a year where artificial mixing was applied the phytoplankton composition was dominated by Diatoms, while in another year without mixing by Cyanobacteria (Huisman *et al*., 2004).

Including both nutrient and light limitations (Huisman and Weissing, 1994), if two species were limited by light, the one with lowest light requirement will dominate. In the same way, if two species were limited by nutrients, the one with lowest nutrient requirement will dominate. When two species competed for light and nutrients either competitive exclusion, stable coexistence or alternative dominance can theoretically occur. Experimental and modeling results showed that competitive exclusion occurred when species that were strong competitors in phosphorus were also strong competitors in light. Alternative dominance occurred when there was a tradeoff between competitive abilities for light and nutrients with results also dependent on initial conditions (Passarge *et al*., 2006).

Other experimental and modeling studies analyzed phytoplankton growth and competition under the effects of: temperature variation between different diatom species (Van Donk and Kilham, 1990); nutrient limitation between Chlorophyte and Cyanobacterium (Ducobu *et al*., 1998); and different mixing regimes between diatom and dinoflagellate species (Diehl *et al*., 2002). Van Donk and Kilham (1990) showed how increasing temperature resulted in higher growth rates for three different diatom species (*Asterionella, Stephanodiscus, Fragilaria*) and that *Asterionella* was the superior competitor for phosphorus.

The presence of some phytoplankton species can be a stress factor for other phytoplankton classes and influence the sequence of algal composition changes. Hulot and Huisman (2004) simulated the interactions between toxin-producing phytoplankton species (*e.g*., Cyanobacteria) and toxin-sensitive phytoplankton species (*e.g*., Chlorophytes), in the presence of bacteria and under two different environmental conditions: completely mixed and stratified. The prevalence of the toxin-producing or the toxin-sensitive phytoplankton groups may depend on the species that dominates first. In presence of bacteria that degrade toxins, toxin-sensitive phytoplankton specie dominance was favored; however, under weak mixing conditions, toxin-producing species became dominant (Hulot and Huisman, 2004).

7. State of art- discussion

Our knowledge of quantitative relationships in ecosystems and of the link between ecological properties and the environment has increased significantly through adopting mathematical models (Jørgensen and Bendoricchio, 2001). On one hand, simplified mathematical models, studying relationships between phytoplankton growth and external factors in a theoretical way, allowed exploration of general phytoplankton group behavior. On the other hand, complex multifunctional models allowed the description of specific ecosystems. From analyzing simulation results of several complex multifunctional models it emerged that these models often do not reproduced the observed phytoplankton succession pattern correctly, or do not capture, in some periods, the same magnitude of variation as detected by observation. Most of the succession models analyzed can be adopted to reproduce the succession in time of different phylogenic, morphological or functional phytoplankton groups and to analyze their peculiar behaviour. However, succession models should be used with great caution for predicting bloom episodes of specific groups because the magnitude of the

blooms can be underestimated and the timing error can be, in some cases, close to one month.

Model Complexity

Modeling strategies that examine shifts in phytoplankton communities are not based on elementary approaches that frequently neglect some aspects of system dynamics, but include complex mathematical representations (Zhao *et al.*, 2008). Dialogue between hydrodynamic modelers and biologists is needed in order to ensure a good representation of the biological behavior in the construction of dynamic models and avoid oversimplification of their structure (Flynn, 2005). The principal strength and, at the same time, the weakness of mechanistic, multi-group dynamic models is their high level of complexity. Their strength is that the relation between multiple physical and biological variables is clearly defined through mathematical equations and not by probabilistic connections. Their weakness is that mathematical equations include a large number of parameters whose values, that characterize a particular system, are frequently not well-known or even unknown. Parameter values must be determined by experiment or by model calibration. Moreover, a higher number of parameters correspond to increased calibration complexity. Thus, the model detail of a system description should be in accordance with the system complexity and reduced to this minimum in order to optimize its utility. The success of the modeling and calibration process critically depends on the consistency between the functional structure of the community and the description made in the model and achieved through observations of that structure. Each group included in the model should represent a specific response to environmental conditions.

Another approach in optimizing complex phytoplankton model applicability would be to apply advanced calibration strategies to coupled, physical-succession models that will move toward generalized use in water quality management.

Model applications in water quality evaluation require both simplicity to obtain rapid and consistent predictions of the algal blooms, and elaboration to describe relationships between a bloom occurrence and the external factors responsible for its generation. On one hand administrators are concerned with acquiring high probability in predictions and on the other hand are interested in understanding the causes that underlie water quality problems in order to remove or at least reduce them. The actual trend suggests that future phytoplankton models will be even more closely related to the selection and the evaluation of management strategies.

Contrasting theories

Coupled multifunctional, mechanistic models are usually based on the theory that phytoplankton groups develop at different time periods, depending on environmental conditions and on presence-absence of other algal groups. Under these assumptions, phytoplankton group development can be simulated and predicted. Huisman and Wessing (1999) used a well-known resource competition model to demonstrate that phytoplankton specie dynamics are driven, not just by external factors such as temperature variability, caused by fluctuating weather conditions, or spatial heterogeneity, but also by intrinsic dynamics of specie competition that produce chaotic responses. The competition dynamics of a system with more than two limiting resources are different from those with only two. Specie oscillations create an opportunity to increase specie diversity and allow the persistence of a great number of competitors, even under constant resource supply and constant physical conditions (Sommer, 1999). Seasonal variation in weather conditions led to a seasonal succession

of species, yet specie composition varied from year to year in an irregular fashion. Recurrent environmental patterns generated by the seasonal cycle would interfere with intrinsic specie interactions and would have both stabilizing and destabilizing effects on the specie interannual variability (Dakos *et al*., 2009).

The idea that interaction between multiple species may give rise to oscillation and chaos implies that phytoplankton dynamics are unpredictable in annual or longer time scales when viewed in detail (*e.g*., weekly or daily time scales). However, on a higher aggregation level, as total algal biomass, phytoplankton dynamics may show quite regular seasonal patterns (Scheffer *et al*., 2003). This concept is in accordance with the fact that models show greater success in predicting total algal concentration than concentrations of a single functional group. As we show, model predictions of multiple phytoplankton groups are frequently presented in aggregated form, improving their results.

8. Conclusions

Succession models that simulate the changes of composition experienced by the phytoplankton community existing in lakes and reservoirs during a given period of time have received considerable attention in the last few years. This interest arises both among ecologists and among water resource managers, given the application of succession models both to answer ecological questions and as tools to analyze water quality management strategies. The succession of phytoplankton species (or groups of species aggregated on dimension, trophic preference or tolerance to environmental changes) is at least partly driven by changes in environmental conditions which are, in turn, determined or modified by the presence of algal species resulting in complex non-linear interactions. To model these interactions, researchers have used either sophisticated empirical approaches (mainly fuzzy logic and neural networks) or have constructed mechanistic models based on the mathematical statement of conservation of mass and explicit first-order differential equations describing the physical and biological processes occurring in the water column.

The mechanistic succession models are the focus of this work and differ from the well-known and widely used eutrophication models in several aspects. First, succession models need to represent the different responses among phytoplankton species trying to use the same pool of nutrient and light resources. Hence, these models include in their formulation wildly non-linear interactions. Second, the number of variables and parameters involved in the model may be very large, given that the number of sub-models simulating the behavior of specific phytoplankton functional or morphological groups is typically large. Being different from eutrophication models, the problems faced by modelers working with succession models are also necessarily different. For example, they are related to the limitations inherent in assessing biomass concentration on a group basis or establishing the level of description of the biological features of the model (biological segmentation).

Several approaches have been followed to assess the biomass of different phylogenic, functional or morphological groups in which the phytoplankton community is structured. Chla concentration is probably the most commonly used. Other approaches include Carbon concentration, wet/dry weight and, in some cases, bio-volumes; all represent an alternative proxy for phytoplankton biomass adopted by modelers when differentiating per group assemblages. Obtaining observations of Chla concentration on a per group basis is not as straightforward as determining Chla total concentration that was historically used as unit in eutrophication models.

Concentrations can be assessed *in vivo* with spectro-fluorometry that only discriminates a limited number of groups, or counting numbers of cells of each group and multiplying them by a factor to convert them into biomass. Adopting Chla or Carbon content per cell as a metric also results in approximated values due to the fact that they exhibit variations depending on site, light availability, nutrient and temperature conditions. The use of conversion factors does not allow nor intend to calculate Chla or Carbon concentration in the water column, but is a deliberate procedure to estimate phytoplankton biomass per group.

In this work we described and compared different types of evaluations used for phytoplankton succession models. Evaluation is mostly done by graphically displaying simulations and observations on the same plot. The variable represented, in most cases, is the total algal biomass and less frequently, one finds comparisons of biomass on a per-group basis. Furthermore, the length of time simulated and the quality of the observational data set used to assess the model performance varies considerably among model applications. Hence, any inter-comparison exercise between models should be done with care. In order to facilitate these inter-comparisons among modeling approaches it would be necessary (1) to apply the models to a common set of sites, (2) to use a common data set collected with the same temporal and group resolution during a sufficiently long period of time; and (3) to use a complete data set in which the biomass of different genera and groups has been discriminated and expressed in different units. A one year period has been suggested (Dahl and Wilson, 2006) as the ideal length of time for model evaluation, given the fact that a longer term would require a very extensive data collection. In our opinion, for an adequate model evaluation, considering the variability that one system experiences from one year to another, a one year period should be used for model calibration and a second year for model validation. A shorter term period would not be enough to evaluate model ability in capturing phytoplankton succession on a seasonal basis.

In general we conclude that succession models are not yet mature enough to confidently forecast the behavior of separate specific phytoplankton groups. Errors in the predictions can be either in magnitude or in the timing of the peak abundance of the groups modeled. Even in well-applied models, errors of up to 50% in magnitude and one month in timing have been reported when comparing observed and simulated phytoplankton biomass of separate groups. Lower errors, of up to 20% in magnitude and about fifteen days in timing, are reported when comparing observed and simulated biomass of all algal groups existing in the community. The predictive ability of succession models is still far from that of physical models, mostly due to the high level of complexity and non-linearity of biological processes. To improve the current level of confidence in succession models, more efforts should be directed towards: (1) the evaluation of the model complexity required to correctly describe the dynamic processes of an ecosystem; (2) the development of new strategies of biomass measurements or assessment methodologies on a per group basis; (3) the applicability of model parameters at different sites, through elaboration of rapid and efficient calibration methods; (4) the increase of physiological research to ascertain parameter coefficients explaining the large variation in reported parameter values; and (5) the integration between model development and field sampling design. Frequently, larger errors have been reported for models with a larger number of phytoplankton groups. Increasing the subdivision of the phytoplankton groups also involves increasing the number of parameters whose values need to be known, and hence, it will increase the cost of calibration. Therefore, in deciding the level of group detail of a succession model, the simplest possible option should be preferred, as long as the complexity of the

ecosystem studied is adequately represented. Also, any advances in the field of automated calibration of multi-parameterized models will facilitate the task of finding site-specific parameters for succession models, and should favor the application and routine use of phytoplankton succession models.

Another advance in predicting separate phytoplankton group behaviours should be obtained by taking into account that intrinsic competition dynamics between multiple species can lead to chaotic oscillation of phytoplankton composition that interfere with seasonal succession patterns. The effects of chaotic oscillations influencing model results should be tested at different time scales in order to develop a methodology that would allow including them in the modeling process.

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TABLES

Phytoplankton multifunctional groups process-based coupled models						
MODEL	**Number of groups**	**Type of groups**	**Phytoplankton biomass**	**Physical Layers**	**Evaluation**	**References**
Physical-microbial food web model	5	Autotrophic grazed; autotrophic no-grazed; mixotrophic-osmotrophic; mixotrophic pahotrophic grazed; mixotrophic pahotrophic no-grazed;	Carbon concentration (µg C L^{-1})	Multiple layers	Graphical: temporal biomass evolution at 1m depth	Roué-Le Gall et al., 2009
Lake Michigan model	2	Diatoms; non-Diatoms	Carbon concentration (g C L^{-1})	Multiple layers	Graphical: biomass vertical distribution; average depth time evolution	Chen et al., 2002
Protech	8	Dominant species (from a library of 18 species)	Chlorophyll-a concentration (µ Chla L^{-1})	10 cm multiple layers	Graphical: biomass temporal evolution (often aggregated into Stress-tolerant, Ruderals, Competitors) & Goodness of fit statistics (Modelling efficiency; Mean Absolute Error MAE, Root mean square error RMSE)	Reynolds et al., 2001; Elliott & Thackeray, 2004; Lewis et al., 2003 ; Elliott et al., 2000; Elliott *et al*., 2001; Moreno Ostos *et al*., 2007
Protbas	8	Dominant species (Aulacoseira; Stephanodiscus; Aphanizomenon; Anabaena; Rhodomonas; Cryptomonas; Microcystis; Ceratium)	Chlorophyll-a concentration (µ Chla L^{-1}) and Biovolume (mm^3 L^{-1})	10 cm multiple layers	Graphical: biomass temporal evolution	Markensten and Pierson, 2007

Table 1. 1 Phytoplankton process-based coupled models that simulates more than one algal group. Resume of the characteristics of the models and type of evaluation adopted.

Phytoplankton multifunctional groups process-based coupled models						
MODEL	**Number of groups**	**Type of groups**	**Phytoplankton biomass**	**Physical Layers**	**Evaluation**	**References**
Dyresm-Caedym	7	Dinoflagellates; Cyanobacteria; Nodularia; Chlorophytes; Cryptophytes; Marine Diatoms; Freshwater Diatoms	Chlorophyll-a concentration (µChla L^{-1}) Carbon concentration (g C L^{-1})	Multiple layers; Sediments	Graphical & Goodness of fit statistics (Root mean square error RMSE, Spearman Correlation coefficients)	Hamilton and Schladow, 1997; Romero et al., 2004; Trolle et al., 2008; Burger et al., 2008; Gal et al., 2009
DyLEM	5	Dominant species (Microcystis; Cyclotella; Asterionella; Pediastrum; Staurastrum)	Carbon (g C m^{-3})	Multiple layers	Graphical: biomass temporal evolution; relative abundance	Bonnet and Poulin, 2004; Bonnet and Poulin, 2002
Lake Zurich model	2	Cyanobacteria*;* other algae	dry mass or wet mass (g DM/L; g WM L^{-1})	Multiple layers; Sediments	Graphical: monthly vertical profiles	Omlin et al., 2001
BELAMO	4	Small algae; large Diatoms; large algae; Cyanobacteria	weight (g WW m^{-3})	Epilimnion; Hypolimnion; Sediments	Graphical: biomass temporal evolution	Mieleitner & Reichert, 2008
Lake Washington	3	Diatoms; Chlrophytes; Cyanobacteria	Chlorophyll-a concentration (µChla L^{-1}); Carbon concentration (µg C L^{-1}); proportion of Cyanobacteria (%)	Epilimnion; Hypolimnion	Graphical & Goodness of fit statistics (mean error, relative error; coefficient of determination)	Arhonditsis & Brett, 2005a; Arhonditsis & Brett, 2005b;

Table 1.1 cont. Phytoplankton process-based coupled models that simulate more than one algal group. Resume of the characteristics of the models and type of evaluation adopted.

STATISTICS Symbol	Name	Formula	References
ME	mean error	$\left(\sum (o - s)\right)/ n$	Elliott et al., 2000; Arhonditsis and Brett, 2005b
M%E	mean percent error	$100\left(\sum (o - s)/ s)/ n\right)$	Elliott et al., 2000
MSE	mean square error	$\left[\sum (o - s)^2\right]/ n$	Elliott et al., 2000
MAE	mean absolute error	$\left(\sum \lvert o - s \rvert\right)/ n$	Elliott et al., 2000
MA%E	mean absolute percent error	$100\left(\sum \lvert o - s \rvert / o\right)/ n$	Elliott et al., 2000
U	Theil's inequality coefficient	$\left\{\left[\sum (o - s)^2\right]/ s^2\right\}^{0.5}$	Elliott et al., 2000
RMSE	root mean square error	$\left\{\left[\sum (o - s)^2\right]/ n\right\}^{0.5}$	Elliott et al., 2000
MAE/ō or NMAE	mean absolute error relative to observed mean	$\left[\left(\sum \lvert o - s \rvert\right)/ n\right]/\left[\left(\sum o\right)/ n\right]$	Elliott et al., 2000; Gal et al., 2009
RMSE/ō	general standard deviation	$\left\{\left[\sum (o-s)^2\right]/n\right\}^{0.5}/\left[\left(\sum o\right)/n\right]$	Elliott et al., 2000
EF	model efficiency	$1 - \sum (o - s)^2 / \sum \left(o - \left[\left(\sum o\right)/ n\right]\right)^2$	Elliott et al., 2000
RE	relative error	$\sum \lvert o - s \rvert / \sum o$	Arhonditsis and Brett, 2005b
r^2	coefficient of determination	$1 - (SS_{BF})/\left(\sum (o - s)^2\right)$	Arhonditsis and Brett, 2005b; Gal et al., 2009

where o is observed data, s is simulated data, SSBF is sum of squares about line of best fit and ō = $\left(\sum \text{o}\right)/ n$

Table 1. 2 Statistics used to evaluate the goodness of fit between simulations and observations.

FIGURES

FIGURE 1.1

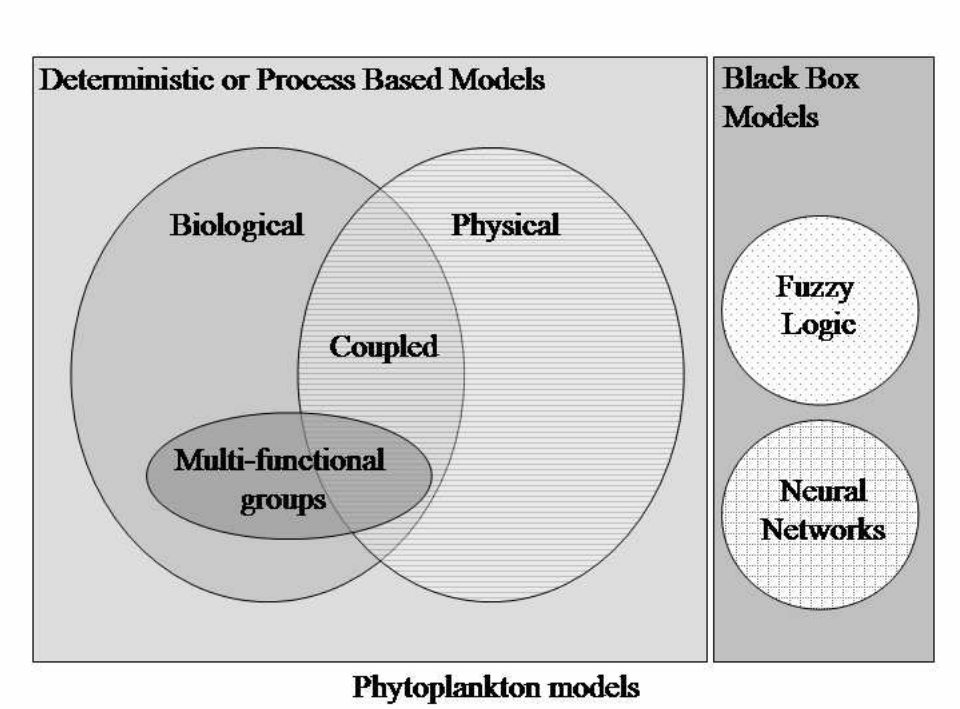

Figure 1.1 Scheme representing types of phytoplankton models.

FIGURE 1.2

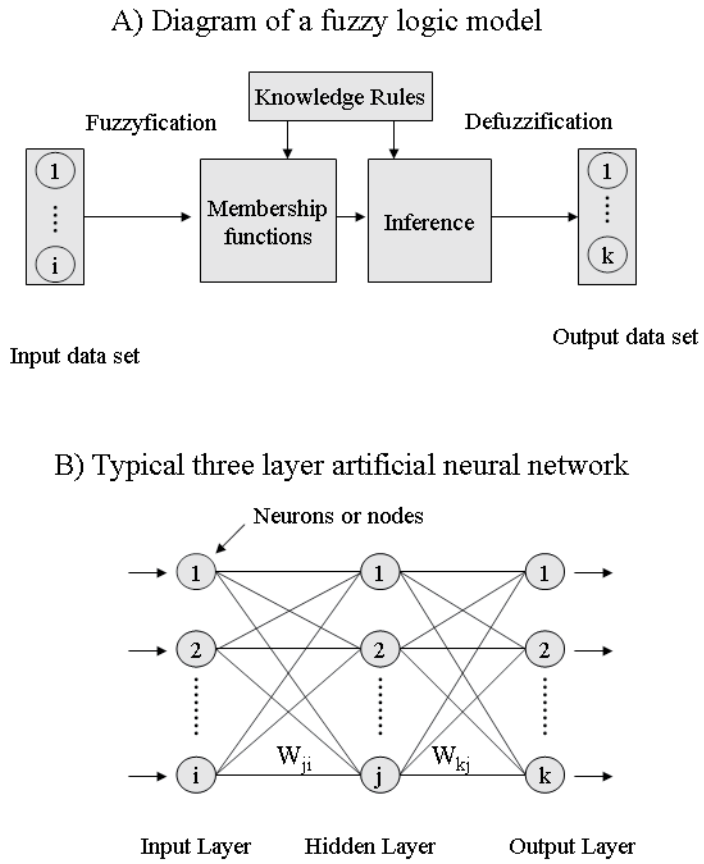

Figure 1. 2. Empirical model approaches: fuzzy logic and artificial neural network structures.

FIGURE 1.3

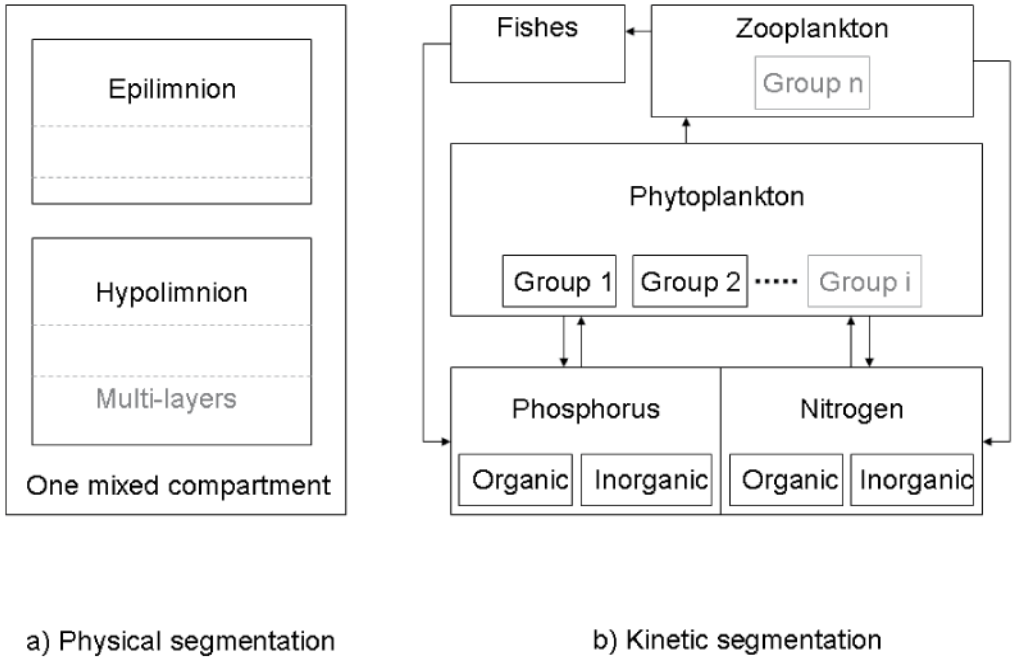

Figure 1. 3. Typical physical and kinetic segmentations of mechanistic phytoplankton succession models.

Chapter 2

"No entiendes realmente algo a menos que seas capaz de explicárselo a tu abuela."
Albert Einstein

A calibration strategy for dynamic succession models including several phytoplankton groups

1. Introduction

The changes in abundance and composition experienced by phytoplankton communities in lakes and reservoirs in the course of a year may severely affect the quality of the water and even compromise the effectiveness of treatment processes undertaken in downstream water treatment plants. For example, the occurrence of blue-green algal blooms in water supply reservoirs may lead to severe clogging problems during the filtering operations; or it may lead to taste, odor and even health problems as a consequence of several species and stocks of blue green-algae producing toxic substances (Guven and Howard, 2006; Margalef, 1983). Recently, considerable effort has been devoted to modeling algal communities with the aim of predicting and understanding changes in phytoplankton abundance (Di Toro et al., 1975; Kuo &Thomann, 1983; Cole & Buchak, 1995; Gurkan et al., 2006; among others) and composition (Hamilton & Schladow, 1997; Eliott et al., 1999; Omlin et al., 2001; Markensten & Pierson, 2007; among others).

It is widely accepted that the changes in phytoplankton communities, whether they are characterized at species level or in terms of the functional structure or size/biomass distribution (e.g. Lindenschmidt & Chorus, 1998; Reynolds et al., 2002; Padisák et al., 2003), are associated with variations in the physical (light climate) and the chemical (nutrient availability) constraints for algal growth (Margalef, 1997; Reynolds, 1997). On one hand, the light environment experienced by phytoplankton cells is related to turbulent mixing, which determines the residence time of microalgae within the euphotic layer (MacIntyre et al., 2000). On the other hand, distribution and bioavailability of nutrients in the euphotic layer is the result of transport processes interacting with biological phenomena. Consequently, the knowledge and predictability of the composition of phytoplankton communities and its evolution needs to be grounded on the knowledge of the physical processes of transport and mixing, which determine turbulence levels, nutrient distribution and light penetration in the water column. Consistent with this widely accepted perception of succession in aquatic ecosystems, most mathematical models used to predict the evolution of phytoplankton communities are based on the appropriate description of the relationship between the physical environment (in particular, thermal stratification and mixing energy) and algal growth. Two general approaches have been used to model the link between the physico-

chemical environment and the abundance and composition of phytoplankton communities. The first is a black-box modeling approach, in which expert knowledge systems are used to represent the relationship existing between the ecosystem components. The processes in this method are not explicitly represented (Liliover & Laanemets, 2006; Olden, 2000; Recknagel, 1997). The second approach is functional or mechanistic, which is also called deterministic or process-based modeling approach. In this procedure differential equations are derived from the physical principles of mass, energy and/or momentum conservation to represent the evolution of the different components of the ecosystems (Hamilton and Schaldow, 1997; Omlin et al., 2001; Reynolds et al., 2001; Arhonditsis and Brett, 2005). This latter approach is preferable when the goal is not only to predict phytoplankton community changes but also to understand the interactions between the physical and the ecological variables (Griffin et al., 2001; Kuo et al., 2006).

Mechanistic models typically contain a large number of parameters, with values that are site-specific and typically unknown when modellers are first posed with the problem of predicting the behaviour of a particular ecosystem. The particular set of parameter values that best describes the process rates in any given ecosystem can be selected either through a time-consuming and resource intensive process involving in-situ experimentation (see Gal et al., 2009) or, alternatively, through calibration. The latter is, by large, the most common method adopted in water quality modelling (Markensten & Pierson, 2007; Omlin et al., 2001; Rose et al., 2007; Mieleitner and Reichert, 2008). It is more economical than experimentation, but it can be very time consuming depending on the computational cost of the model and on the number of parameters to be calibrated. This may dissuade researchers from using these tools on a routine basis. Thus any progress in calibration strategies of coupled physical-succession models will contribute to generalize their use for water quality management purposes. Trial and error calibration strategies, traditionally adopted in water quality modelling, require a lot of expertise with the model at play, and, are only efficient in calibrating models with a small number of parameters (Tanentzap et al., 2007; Kuo et al., 2006; Bonnet and Poulin, 2004) or when most parameter values have been determined through experimentation (Hillmer et al., 2008; Gal et al., 2009). To calibrate models with a large number of parameters, automatic calibration approaches may be a valid alternative (Eckardt & Arnold, 2001). They are designed to search the parameter set that minimize an objective function, representing the norm of the difference between modeled and observed variables. Automatic calibration approaches can be divided in two classes: gradient and global optimization methods. Gradient methods search the parameter space using information of the local gradient of the objective function and, starting from an initial guess, find the parameter set that minimizes the model error. Due to their low computational cost, they have been widely applied in the calibration of phytoplankton models of varying complexity (Omlin et al., 2001; Rose et al., 2007; Mieleitner and Reichert 2008). However, gradient methods can potentially converge to a local minimum of the objective function, rather than global minimum, compromising its effectiveness in highly parameterized models. Global optimization techniques avoid the convergence to local minima, by introducing a certain degree of randomness in the search process (Klepper and Hendrix, 1994; Hansen et al., 2003; Duan et al., 1992; Eckardt & Arnold, 2001; Skahill & Doherty, 2006). Some of these global sampling methods evolved from the implementation of Markov Chain Monte Carlo methods (MCMC) (Hastings, 1970) and include the CMA-ES (Hansen et al., 2003) the shuffled complex evolution algorithm (SCE-UA) (Duan et al., 1992), its modification SCEM-UA (Vrugt et al., 2003), the multiobjective complex evolution algorithm (MOCOM-

UA) (Gupta et al., 1998) and the multialgorithm genetically adaptive multiobjective method (AMALGAM) (Vrugt and Robinson, 2007). These global optimization methods are extensively used to calibrate complex hydrological models (Tonkin and Doherty, 2005; Skahill & Doherty, 2006; Marcé et al., 2008; Gupta et al., 1998), but few global calibration exercises applied to water quality models have been published (Mulligan et al., 1998; Ostfeld and Salomons, 2005; Goktas el al., 2007). Moreover, and to the extent of the authors' knowledge, the applicability of these approaches to the calibration of phytoplankton succession models has not been explored in the literature. In this work we propose and test a strategy, based on an hybrid gradient-global calibration algorithm, to calibrate a highly parameterized, and deterministic physical-biological model.

2. Materials and Method

Study site

El Gergal (37º 34´ 13´´ N, 6° 02´ 57´´ W) is a small, canyon-shaped and eutrophic reservoir, and one of the four input-output reservoirs (Aracena, Zufre, La Minilla and El Gergal) existing along the Rivera de Huelva river that supply water to the city of Seville. The reservoir receives water from two regulated rivers (Rivera de Huelva and Rivera de Cala) and from two non-regulated streams (Cantalobos and Encinilla). Inflows from Rivera de Huelva enter the reservoir through a small stilling pond (Guillena). The annual inflow volume is ca. 7000 m^3 with extreme oscillation on seasonal scales. Outflows occur from either a spillway located at 50 m.a.s.l.or from a deep outlet at 17 m.a.s.l. directly into the river, or from four other withdrawal structures located at 41.2, 39.8, 38 and 26 m.a.s.l. flowing into a water treatment plant to be distributed to the city of Seville. When full, the volume of water stored in the reservoir is 3500 m^3, its surface area is 250 ha, and the maximum length is 7750 m. The maximum depth is 37 m, close to the dam, and the mean depth is 15.7 m (Figure 2. 1).

El Gergal reservoir is warm and monomictic. Water never reaches temperatures below 4ºC (Cruz Pizarro et al., 2005). The lake stratifies in summer from the beginning of March to the middle of October, and de-stratifies towards the end of the year. Algal blooms may develop under stratified conditions and nutrients availability posing serious challenges to water quality managers. The concentration of soluble phosphorous at the surface during the study period was on average 0.0733 mg PO_4L^{-1} during the studied period with peaks of up to 0.3 mg PO_4L^{-1} in winter. The algal community of the reservoir is mainly composed by Cyanobacteria (*Aphanizomenon sp., Microcystis sp., Anabaena sp., Oscillatoria sp.*), Chlorophytes (*Scenedesmus sp., Pediastrum sp., Coleastrum sp., Cosmarium sp.*), Cryptophytes (*Rhodomonas sp., Cryptomonas sp.*), Dinoflagellates (*Ceratium hirundinella*) and Diatoms (*Cyclotella sp.*, *Synedra sp.*). The size, shape, type of aggregation, composition, mechanisms of suspension and resistance to reduced light-nutrient conditions vary from group to group (even among the species) resulting in different behaviours in the water column.

Succession model

A process based one-dimensional hydrodynamic and ecological model (DYRESM-CAEDYM, Imberger and Patterson, 1981; Hamilton and Schladow, 1997; Schladow and Hamilton, 1997) is applied to simulate phytoplankton succession in El Gergal reservoir. DYRESM (DYnamic REservoir Simulation Model) provides predictions of the physical environment which are used to drive water quality simulations in CAEDYM (Computational Aquatic Ecosystem DYnamics Model). Our choice of model is justified in that (1) it has been widely used as a management tool and

(2) it explicitly represents the links between physical and biogeochemical processs, which allow one to analyze and understand the control exerted by the physics on water quality. The choice of a 1-D model, instead of 2- or 3-D model is justified because the simulation and calibration of a succession model with several algal groups, with a 2-D or 3-D model would have substantially increased model run time and, consequently, the calibration efforts. The 1D assumption was also supported by calculations based on Lake and Wedderburn numbers (not shown) and the observations collected during field data collection campaigns in El Gergal, which demonstrate that the spatial heterogeneity of algal concentrations existed at the time when data was collected but it was weak (Vidal et al., 2010). DYRESM includes descriptions of mixing and transport processes associated with river inflow, natural or man-made outflows, diffusion in the hypolimnion and mixed-layer dynamics, and it is used to predict the variation of water temperature and salinity with depth and time. These physics of the model are free of calibration, which implies that the level of process description, including temporal and spatial scales in the model, is fundamentally correct (Hamilton and Schladow, 1997). It has been used extensively in the existing reviewed literature to predict the vertical distribution of temperature, salinity and water quality parameters in a wide range of applications for small to medium-size reservoirs. For example, it has been successfully applied to Lake Burragorang - Australia (Romero et al., 2004), Lake Constance - Europe's Alps (Hornung, 2002), San Roque reservoir - Argentina (Antenucci et al., 2003) and Lake Kinneret - Israel (Gal et al., 2003). CAEDYM consists of a series of coupled first-order differential equations representing the major biogeochemical processes influencing water quality including primary and secondary production, nutrient and metal cycling, oxygen dynamics and the movement of sediment. It is a flexible model so that it can be configured with different degrees of complexity to focus on particular processes. In the most complex configuration, it can simulate up to seven phytoplankton groups, five zooplankton groups, fish and submerged macrophytes (Copetti et al., 2006; Trolle et al., 2008; Gal et al., 2009).

Experimental data set

The model was setup to simulate the succession of algal populations in El Gergal from January to September in 2007 (study period), when detailed experimental data were available. Water samples were collected during the morning, between 11 and 12 am, on a weekly or bi-weekly basis at 0, 2, 5, 10, 15, 20, 25 and 30 m depths at a fixed location near the dam using a 5 L Van-Dorn sampler. Sub-samples for phytoplankton were fixed *in situ* using lugol. Once in the laboratory, the water samples were immediately filtered and analyzed for nutrient concentrations following standard procedures. Total phosphorus (TP), total nitrogen (TN), total carbon (TC), soluble reative phosphorus (PO_4), nitrate (NO_3), ammonium (NH_4), dissolved inorganic and organic carbon (DIC, DOC), silica (SiO_2) and suspended solids were measured following APHA-EPA-ISO procedures (APHA, 1992). Water pH and dissolved oxygen (DO) were measured using a TURO Quality Analyser Sensor (TURO T 611). Biological oxygen demand (BOD) was estimated from the BOD-TC correlation rate tables of Wilson (1997). Secchi disk depths were measured at the same location and at the time interval of water samples. Phytoplankton species were identified and counted under inverted microscope following the Utermöhl method (1958). The genera were then classified into functional groups, following Reynolds (1997, 2000). Abundances of the different Reynold's functional groups were estimated by adding the abundances corresponding to the member species at each depth. The bio-volumes of each group were estimated from the shape and size of the cells and from the counting data. We

followed the standardized geometric shapes and mathematical equations that have been designed by Hillebrand *et al*. (1999) to calculate phytoplankton bio-volumes and minimize efforts of microscopic measurements.

An alternative and coarser functional description of the phytoplankton community was constructed with a submersible four-channel spectro-fluorometer (bbe Moldaenke). The spectro-fluorometer is able to discriminate the chlorophyll-a (from here on, Chla) concentration of four different functional groups: green algae (chlorophitae), grey algae (including dinoflagellates and diatoms), cyanophyceae and cryptophyceae. It has a resolution of 0.05 μg $L^{-1}$and a measuring range of 0-200 μg L^{-1}. A more detailed description of the spectro-fluorometer can be found in Beutler et al. (2002) and Gregor et al. (2005). Chlorophyll-a profiles were collected with the spectro-fluorometer every 1-2 weeks, at the same point and time that water samples were taken. Each profile consisted of four different values Chlorophyll-a concentration (one for each functional group), every ca. 50 cm from near the surface to a depth of 20-25 m.

Hydrological data (rainfall, water levels, inflow volumes and outflow volumes and withdrawal depth) were provided on a daily basis by the Seville water supply company (EMASESA). Water levels in the reservoir ranged from 29 to 39 m a.s.l. during the study period, with the largest variations occurring during summer time (Figure 2. 2a). Inflows were mostly from Cala in winter and fall. In summer only two inflow events occurred, entering through non-regulated streams (Figure 2. 2b). Water was withdrawn mainly from the lower outlet in summer, from the intermediate outlet in fall, and from the upper outlets in winter and spring (Fig. 2. 2c). The reservoir was well mixed with a temperature of approximately 9ºC at the start of the study period. Maximum top-bottom temperature differences of 16ºC developed in summer.

Meteorological information include hourly records of incoming/outgoing shortwave/longwave radiation, relative humidity, wind speed and direction, air temperature and atmospheric pressure collected on a floating device located near the dam (Fig. 2. 1). Water temperature profiles were recorded near the deepest point of the reservoir (see Fig. 2. 1) at 1-m depth intervals using a multiparameter probe (YSI-8000UPG Environmental Monitoring System).

A similar experimental data set, including meteorological, hydrological, chemical and spectro-fluorimetric data, was available from 10th March 2008 to the end of October 2008. Those data were used for model validation, after calibrating the model with year 2007 data set.

Model setup

The biogeochemical model was set up to simulate the growth of five different phytoplankton groups (Chlorophytes, Cyanobacteria, Cryptophytes, Diatoms and Dinoflagellates), with the physical environment (temperature, radiation and mixing energy) determining the vertical distribution and the growth of algal cells. Chemical conditions were, in turn, set to follow our observations. First order differential equations, of the form,

$$\frac{\partial Chla_i}{\partial t} = \left\{ \mu_{\max,i} \cdot f_i(I,N,P,C,Si,T) - R_i \right\} \cdot Chla_i \qquad (1)$$

are used to model the growth of phytoplankton cells. In Eq. 1, $Chla_i$ represents chlorophyll-a concentration (μg/L) of algal group *i,* μ_{max} is the maximum growth rate that phytoplankton exhibits under optimal conditions, and *f* is a function representing the limiting effect due to non-optimal light levels *I*, nitrogen *N*, phosphorus *P*, carbon *C* and silica *Si* concentrations and temperature *T* in the water column. Finally, the term *R* represents the effects of all sinks of phytoplankton biomass. Functions and parameters

in Eq. 1 are different for each algal group *i*, representing in this manner, the specific response of different species to environmental conditions. The limiting function associated with Silica concentration is used to simulate specifically the growth of diatoms. The concentrations of phytoplankton from the inflows were considered negligible because no significant variations of phytoplankton composition were detected after the main inflow events. Zooplankton populations were not modeled. The grazing of zooplankton on phytoplankton was represented through a constant algal loss term, which also accounts for the effects of respiration and mortality. Nutrients, suspended solids, dissolved oxygen and pH were not simulated. Instead, time-varying profiles of those variables were constructed from field data, and provided to the model to force the ecological model simulations. The light conditions in the water column were estimated, according to Romero et al. (2004b), from incoming solar radiation values, and by the concentration of suspended solids and the algae abundance, determining the attenuation of light in water. Light extinction coefficients in the water were estimated from Secchi disk depths observations following Martin and McCutcheon (1999). The water temperature conditions are calculated in the physical model (DYRESM). The particular environmental conditions experienced by the algal cells depend not only on the spatial distribution of the environmental variables, but also on the position of the algae in the water column. This, in turn, is the result of a subtle interplay between mixing processes and the ability of cells to regulate their vertical position, which varies by group. The vertical movements of the algal cells are modeled through a constant settling and migration velocity. Further details of the model can be found in Romero et al. (2004b). A complete list of state variables (both modeled or supplied as field data) used in our model of El Gergal is presented in Table 2. 1. Model parameters are listed in Table 2. 2.

The simulations were forced using observed hydrological and meteorological data. Inflow temperatures (no observed) were presumed equal to the surface temperature of the reservoir. This assumption was justified in that the inflows during the study period were mainly from the surface of the stilling pond existing upstream of El Gergal on the Rivera de Huelva river (see Fig. 2.1). Field data collected in Guillena and El Gergal during a short period of time in 2008, suggest that this assumption indeed is valid at least in summer time. Simulations were conducted with a 1 hour time step, and the state variables were output every 24 hours at 11:00 am. The minimum layer thickness was set to 0.5 m, and the maximum layer thickness was 4m. The base extinction coefficient was estimated as the minimum extinction coefficient observed during the studied period (1.188 m^{-1}). The results of the physical model were checked by comparing simulated water levels and temperature profiles against observations. The results of the ecological model, in turn, were checked by comparing Chla concentrations for each of groups simulated by the model, against the spectro-fluorometric observations. Comparisons were depth and date specific for both physical and ecological models in order to include all the information available.

Sensitivity analysis

A screening was first conducted to isolate a small set of parameters to which the phytoplankton simulations were most sensitive. The first-order variance analysis (FOVA), as outlined by Blumberg and Georgas (2008) was adopted to quantify model sensitivity. The sensitivity of any model output variable F to perturbations in any given parameter p in FOVA, is quantified through a dimensionless sensitivity coefficient S_p constructed as follows

$$S_p(p_0) = \frac{\Delta F / F(p = p_0)}{\Delta p / p_0} \quad (2)$$

In Eq. 2, ΔF is the change in the output variable that results from a sufficiently small (<10%) change or perturbation in the parameter Δp, from a reference or baseline value p_0. This approach can be repeated one at a time for each parameter of any given set, providing a relatively simple and straightforward alternative to other techniques that have been proposed in the literature (Spear and Hornberger, 1980; Stow et al., 2007). The output variable F was set equal to the Root Mean Squared Error RMSE (as in Beven, 2001) of the difference between the Chla concentrations simulated by the model and observed in the field. The S coefficients were calculated running the model perturbing each parameter of the complete data set following Eq.2, first considering differences in Chla concentration of one algal group (Chlorophytes) and then considering the effect of each parameter over the total Chla concentration in the water column. An arbitrary threshold S value has to be defined at the end of the calculations in order to select the most sensitive parameters.

Calibration strategy

The values of those parameters to which the model was most sensitive were calibrated to minimize the RMSE of the difference between observed and simulated Chla concentrations. We first proceeded on a group-by-group basis. To calibrate the growth model of a particular functional group *i*, we fixed the Chla concentration of the other four groups to the observed values, leaving only the Chla of group *i* as the state variable. The interactions among groups in the phytoplankton community are explicitly accounted in this manner. After the group-by-group calibration, all groups were simulated simultaneously, and minor changes in the parameter values were introduced manually. A global and iterative optimization algorithm, referred to as the Covariance Matrix Adaptation Evolutionary Strategy (CMAES), implemented in the parameter estimation and optimization modeling software PEST (Doherty, 2004), was used in the calibration process. An important component of this methodology is the combination of a random search in the parameter space with the capacity to adapt the same search on the basis of knowledge gained by previous iterations (Doherty, 2004; Hansen and Ostermeier, 2001; Hansen et al., 2003).

In this way the chances of being trapped in a local minimum of the objective function are greatly reduced. Hansen and Ostermeier (2001) showed that the local adaptation mechanism of CMAES improves global search properties and it was able to reach final parameter values in a reduced number of function evaluations. In this work the search of parameter combinations was iteratively repeated within the established parameter ranges, until the algorithm did not detected any reduction in the objective function or any relative change of the parameters in the last 40 iterations. Usually the number of iterations for each group-by-group calibration was less than 50.000. Model executions were done in parallel mode as implemented in PEST, in order to reduce time of calibration. Previous to calibration using real data, we assessed the performance of our calibration strategy using a synthetic algal concentration trace obtained with known model parameters.

3. Results

Biological observations

The succession patterns observed in El Gergal in the study period, obtained by the spectro-fluorometer (Figure 2. 3) agrees, in general, with those proposed previously

for systems with limited energy and resources availability (Reynolds, 1984), and are largely driven by environmental changes in the water column (Hoyer et al. 2009). A more detailed functional description was obtained through algal abundances: in January, algae of group B (Diatoms, mainly *Cyclotella sp.*) were the most abundant and typically develop in well-mixed environments and tolerate low light intensities. By the end of that month group B was replaced by Cryptophytes (group Y) that, being tolerant to low nutrient concentrations, develop under a wide range of habitats (Figure 2. 4a; Table 2. 3a and 3b). In May, under weakly stratified conditions and high nutrient availability, the community is characterized by the Chlorophytes of group J (mainly *Coleastrum spp.*), and after that, by Diatoms of group B (*Cyclotella sp*.). *Aphanizomenon flos-aque* (Cyanobacteria of group H) was the most abundant species during summer, under strongly stratified conditions. In September, group H was replaced by Diatoms of group B (*Cyclotella sp*.), and Dinoflagellates of group L (*Ceratium hirundinella*) (Fig. 2. 4a). The species *Ceratium hirundinella* (Dinoflagellates, group L) appeared at the same time as the Diatoms of group B. Their response to environmental factors is such that some authors (Pasadik et al., 2009) have proposed to include them in one unique group B. Note that the two maxima in the time series of Chla concentration for Chlorophytes (on day 150 and around day 220) correspond to two different species, which are classified as two different functional groups in the Reynolds classification scheme. Note also that two peaks of in the time series of Chla concentration of Diatoms and Dinoflagellates (days 170 and 230) include different combinations of species from both groups. This is indicative that the functional description of the phytoplankton community obtained from spectro-fluorometric sensors is not equivalent to that arrived at through counting (and later classification) (Figs. 3 and 4a). Both, in turn, are also different from that arrived at by converting the counting information in bio-volumes (Fig. 2. 4b). For example Chlorophytes (Reynolds group J) are not visible when shifting to bio-volumes, due to the fact that cells belonging to this group often have a smaller dimensions compared to cells belonging to Cyanobacteria (Reynolds group H, *Aphanizomenon* and group M, *Mycrocistis*). In general dominant phytoplankton groups in term of bio-volumes will not correspond with the most abundant group in term of cell numbers. The fact that use of bio-volume could mask apparition of small-sized cells, observed when considering counting data, was reported also by Hoyer et al. (2009). To avoid confusion, in the text we have used the term maximum abundance when referring to counting and dominance when referring to biomass concentration.

Hydrodynamic model results

Both the water balance and the thermal structure were reasonably well simulated (Figs. 2 and 5). For example, simulations and observations of water levels differed at most in 0.30 m during the study period. The root mean squared error RMSE quantifying the differences between observed and simulated temperatures during the study period was 0.48ºC. Our model, though, tended to overestimate surface water temperatures in summer. The level of agreement in our simulations is comparable to other studies conducted with 1D models. For example, Trolle (2008) report RMSE values of 1.44ºC and 0.87 ºC for their temperature simulations in the epilimnion and hypolimnion respectively; Gal (2003), reported absolute differences of up to 0.6 ºC when comparing simulated and observed surface temperatures in Lake Kinneret.

Sensitivity analysis

The parameters to which the model exhibited the larger sensitivity in the First Order Variance Analysis were settling velocity (v_s) and the half saturation constant for

phytoplankton phosphorus uptake (K_P) (Figure 2. 6). A threshold *S* value of 1 was chosen in order to select a reduced set of parameters to be included in the calibration process. Seven parameters had $S > 1$, which were: maximum growth rate of phytoplankton (μ_{max}), half saturation constant for phytoplankton phosphorus uptake (K_P), half saturation constant for phytoplankton nitrogen uptake (K_N), phytoplankton temperature multiplier for growth (θ), settling velocity (v_s), specific extinction coefficient (k_e) and temperature multiplier for respiration (θ_L). Each of these parameters is specific to the five functional groups. Hence, a total of 35 parameters were selected for the calibration process.

Cross-check of the calibration strategy

A synthetic time-series of Chla was constructed with a known set of parameter values, that was used as pseudo-observations in a test calibration exercise. Different calibration strategies were explored. First, we conducted a group-by-group calibration. Then, we attempted to calibrate several groups (up to four) at the same time. The algorithm was able to find a set of parameters which were close to the target set, when we calibrated group by group (see Table 2. 4, synthetic series). However, when we tried to calibrate several groups at a time, the algorithm was not able to find the target set of parameters for every algal group. Furthermore, the computational time increased considerably as we increased the number of groups being calibrated. For example, simulation time increased from one to four days working in a parallel mode using two 3.19 GHz processors, each one with three threads (Processor Intel Xeon T7400, RAM 3Gb, Operative System Windows Vista 32bits). The largest deviations from the synthetic trace occurred for those groups with lower Chla concentrations while the dominant group was correctly calibrated. We tried, unsuccessfully, to use different weighting schemes to guarantee the same success for all groups. These results confirmed the need for a group-by-group calibration strategy, since the high irregularity of the multidimensional objective function and the presence of many local minima rendered the joint calibration of several phytoplankton groups numerically intractable. When simulating several groups at a time, using the set of parameters obtained from the group-by-group calibration process, it was found that the agreement between simulations and the synthetic series decreased as the number of phytoplankton group simulated increased (Table 2. 4). This result suggests that there are strong, non-linear interactions among sub-models representing the growth of individual groups. The sensitivity coefficient (*S*), defined as in Eq. 2, was used to quantify the level of interaction among sub-models (Table 2. 5). Changing the values of parameters of group 1 by 1%, for example, the settling velocity (v_s) and the specific extinction coefficient (k_e) induced important changes in the results of group 3 simulation. The results of this exercise indicate a high interaction between group 1 and group3.

Group-by-group calibration against field observations

All sensitive parameters were included in the group-by-group calibration process. The range of possible values assigned to each parameter was taken from the literature (Table 2. 2). The parameters values arrived at with automatic calibration are consistent with those reported in other studies. For example, Cyanobacteria maximum growth rate (0.56 d^{-1}) is within in the range used for Cyanobacteria *Microcystis sp.* and *Aphanizomenon sp.* (0.41- 0.70 d^{-1}) by Gal (2009). Temperature multipliers for growth for all algal groups have ranges of variation very similar to the study by Gal et al. (2009): respectively 1.08 to 1.11 (no unit) and 1.07 to 1.10. Settling velocity parameter values also respect ranges employed in several applications of other models (Reynolds

et al., 2001; Elliott et al., 1999). The Chla concentrations simulated by the model after the sequential calibration are, in general, consistent with the observations, and comparable with previous modeling performances (Markensten and Pierson, 2007; Gal et al., 2009).The model did not reproduce accurately the magnitude of the peak of Cyanobacteria (close to 30µg Chla/L) towards the end of July, but it captured correctly the timing of this bloom (Figure 2. 7a). The RMSE for the simulations of Cyanobacteria was 3.62 µg Chla/L. Cryptophytes, which appeared with lower concentrations than Cyanobacteria, were also well represented by the model (Figure 2. 7b). For example, the abrupt decrease of Chla concentration that occurred at the beginning of May (ca. day 120) was captured in the simulations. The RMSE of the model results for Cryptophytes was 0.55 µg Chla/L. The succession model was also able to replicate the first peak of Chla concentration of Chlorophytes (on days 150 and 180) but did not capture the second peak that occurred around day 230 (Figure 2. 7c). The RMSE of the simulations of Chlorophytes was 1.9 µg Chla/L. The model was not able to reproduce the observed values of Chla concentration of Diatoms and Dinoflagellates, which are lumped in the information provided by the spectro-fluorometer (Fig. 2. 7d). The RMSE in this case was 6.91 µg Chla/L.

4. Discussion

Approach

In constructing a succession model that provides a reasonable description of the behavior of several phytoplankton groups it is necessary to go beyond several limitations, such as over-parameterization, excessive calibration times, strong interaction between parameters or the high non-linearity of the model leading to the possibility of reaching local minima during the calibration process (Beck and Halfon, 1991). Through the calibration method used here, these problems were, in great part, overcome. First, through the sensitivity analysis and the group-by-group calibration strategy the number of parameters requiring calibration at a time was reduced considerably. In this manner, taking into account that the computing time of the present model was about 10 minutes, calibration time was reduced from several months to several weeks. Moreover the problems arising in the calibration process from the interactions among parameters that describe the behavior of different algal groups were, in a first term, avoided. Second of all, a global automated calibration procedure, that includes randomness and the ability to learn during the search process, was used which guarantees that the multi-dimensional parameter space was thoroughly explored and local minima were, to a large extent, avoided (Doherty, 2004; Hansen et al., 2003).

Effect of community segmentation on model calibration

One of the major problems faced during the calibration process was the fact that the experimental spectro-fluorometric values of Chla do not differentiate between groups that respond differently to environmental conditions. *Coelastrum spp.* and *Cosmarium spp.*, for example, are two green algae (or Chlorophytes) that grow under different nutrient conditions: *Coelastrum spp.* grows preferably in nutrient-rich environments, while *Cosmarium spp.* is tolerant to nutrient limitation (Padisák et al., 2009). As a consequence, they appear in different groups in the Reynolds (2002) functional classification: group J (*Coelastrum spp.*) and group N (*Cosmarium spp.*). Each one of these green algae appeared as the most abundant during two separate periods of time in the data set: *Coelastrum spp.* was present from day 22 to 190, while *Cosmarium spp.* developed after that. The average PO_4 values near the surface were 0.1

mg/l before day 190, and decreased to 0.05 mg/L after that time. The concentration of NO_3 changed also from 6.10 mg/L before day 190 to 1.7 mg/L towards the end of the study period (days 210-240). The model was only able to reproduce both peaks in the abundance of green algae if two different functional groups, representing *Cosmarium spp*. and *Coelastrum spp.*, were simulated and calibrated separately (Fig. 2. 8). The RMSE of the first group (*Cosmarium spp*.) was 1.55 µg Chla/L and for the second group (*Coelastrum spp.*), the RMSE was 0.79 µg Chla/L. The parameter sets arrived at through calibration of each group independently were (K_P, K_N, θ, θ_L) = (0.0025, 0.0546, 1.0812, 1.1) for *Cosmarium spp*. and (0.032, 0.0998, 1.135, 1.057) for *Coelastrum spp.* The larger nutrient half-saturation constants of the latter indicate that it is less tolerant than the former to nutrient limitation, which agrees with previous observations (Padisák et al., 2009). *Cosmarium spp.* was calibrated as neutrally buoyant (10^{-5} m s^{-1}) while *Coleastrum spp.*was calibrated as negatively buoyant (-2.6×10^{-5}m s^{-1}) (see Table 2. 6). This is consistent with previous reports that indicate that *Cosmarium spp*. commonly appears as individual cells, while *Coelastrum spp.* tend to form spherical colonies of more than 30 cells with lower buoyancy (John et al., 2002). The volume of the individual cells is also different. In El Gergal, it was found that the cells' volume of *Coelastrum spp.* were ca. 18600 μm^3, while the volume of *Cosmarium spp*. was 5800 μm^3 (J. Blanco, personal communication).

When including two Chlorophytes groups (representing groups J and N, in Reynolds notation), Cyanobacteria and Cryptophytes in the simulation (Fig. 2. 8), the model produced results similar to that of the sequential calibration runs, only if the parameters arrived at by the automatic calibration runs were manually adjusted (Table 2. 4). Starting from the parameter set obtained by the automatic calibration, parameter values of each algal group were lightly increased or decreased in order to improve the model results. The need for the final fine-tuning when simulating all the algal groups probably reflects the need to account for the non-linear interactions among sub-models representing the growth of individual groups. Note that Diatoms and Dinoflagellates were not modeled in these simulations, but forced. The parameter values used in this simulation are shown in Table 2. 6. Only five parameters ($\mu_{max\ Cyano}$, $K_{P\ Crypt}$, $\theta_{\ Crypt}$, $\mu_{max\ Chlor2}$, $K_{e\ Crypt}$) out of a total of 35 parameters being calibrated were manually adjusted (Table 2. 6). It should be stressed that this final manual calibration was a straightfoward and fast procedure thanks to the previous automatic calibration. The simulations including all four groups captured the relevant aspects of the phytoplankton succession. In particular, the model always reproduces the dominant group of the community at each time. The timing of the peaks was also captured correctly by the model. The magnitudes of the peaks, however, are not captured with the same precision. The largest differences between simulations and observations occurred in the Cyanobacterial prediction (up to 53% difference at the time of the second peak). The calibrated model provides an accurate description of the changes in abundance and composition of the phytoplankton community which is comparable to the results of previous studies that include fewer (Chen et al., 2002; Kuo et al., 2006; Elliott et al., 2000) or similar numbers of functional groups (Markensten and Pierson, 2007; Gal et al., 2009). Moreover the physical bases of the current ecological model describe processes more in detail when compared to other phytoplankton models where not all the hydrodynamic and heat exchange processes are solved (Reynolds et al., 2001).

Diatoms (mainly *Cyclotella sp*.) and Dinoflagellates (mainly *Ceratium hirundinella*) are also two functional groups with very different adaptations to environmental conditions that are not differentiated in the spectro-fluorimetric data. Diatoms have lower reprodution rates, ranging from 0.2 to 2.16 d^{-1}, while

Dinoflagellates reprodution varies from 1.6 to 3.3 d^{-1} (Bowie et al., 1985). Diatoms are also negatively-buoyant micro algae with higher settling velocities (-2.1×10^{-4} m s^{-1}) due to their heavy silica walls (Margalef, 1984). Consequently, Diatom growth is favored by strong mixing in the water column. Dinoflagellates, in turn, can actively swim in the water column exhibiting upward and downward velocities of up to 1.16×10^{-5} m s^{-1} (Reynolds et al., 2001). As a result *Cyclotella sp*. and *Ceratium hirundinella* appear in different groups (B and L, respectively) in the functional classification of Reynolds (2002). The calibration process, in which the Chla content of both groups are lumped into a single value that is compared with spectro-fluorometric data, was not successful. Generating separate estimates of Chla concentration for Diatoms and Dinoflagellates from the observations, to calibrate each group individually, was not possible for several reasons. First, Diatoms and Dinoflagellates co-existed at all times. Dinoflagellates of the genera *Ceratium* only appeared among the dominant group (in number of individuals per unit volume) towards the end of the study period (Table 2. 3a and 3b), but co-existed with the diatoms of genera *Cyclotella* at all times. Even though the number of *Ceratium* cells was less than the number of individuals of *Cyclotella*, its contribution to the total Chla concentration in the water column could be similar or even larger, given the strong differences in volume between them (e.g. *Cyclotella sp.* 1.593 μm^3 and *Ceratium Hidrundinella* 49.152 μm^3, J. Blanco, personal communication). Second, the content of Chla per cell changes in time during the course of a year. Depending on the phytoplankton group, Chla concentration per volume in phytoplankton cells vary from 1.5 to 19.7 µg Chl-a mm^{-3} and within the same group (e.g. Chlorophytes) the difference is up to 13µg Chl-a mm^{-3} (Reynolds, 1984). Moreover, Chloropyll-a concentration por cell in phytoplankton varies with increasing water temperature and in relation to the day-night cycle (Margalef, 1983). The Chla content per cell exhibits large variations depending on the season, phytoplankton species, nutrient availability and light conditions (Tolstoy, 1979; Vörös and Padisák, 1991; Kalchev, 1996). In consequence, we could not use the phytoplankton counts or bio-volume information to separate the lumped spectro-fluorometric information. These results suggested that both the complexity (or functional segmentation) of the phytoplankton model and the resolution of the experimental data should all be consistent with the functional structure and complexity of the phytoplankton community in the lake that is being simulated.

The validity of calibrated parameters for simulations of separate years

The model was used to simulate phytoplankton succession in 2008, using the parameter set calibrated with data from 2007. The period simulated in 2008 started on day 70 (March 10th) and it was 232 days long, when the necessary observational data was available for model setup and validation. Maximum phytoplankton concentrations in 2008 were low (ca. 10 µg Chla/l) compared to 2007 (ca. 30 µg Chla/l) and all groups (Diatoms, Cryptophytes and Chlorophytes) coexisted at different concentrations at all times. Diatoms and Dinoflagellates were forced, as they were in 2007. The results in 2008 indicate that phytoplankton succession was not well captured (Fig. 2. 10). A peak of Chlorophytes was simulated around day 130 while Chlorophytes growth was observed starting from day 200 (RMSE of 1.7 µg Chla/l). Cryptophytes simulated developed close to day 120, as observed, but two peaks of about 3 µg Chla/l (at day 90 and 270) were not reproduced by the model (RMSE of 0.73 µg Chla/l). The model simulates an increase in the concentration of Cyanobacteria but the predicted timing of the proliferation was not correct (on day 180 instead of day 150), resulting in a RMSE of 3.5 µg Chla/l. The failure of the 2007-calibrated model to simulated correctly

succession in 2008 was something expected, given the different functional composition of the phytoplankton community in 2008 and in 2007. In 2008, for example, a large number of Reynolds groups coexisted and were classified as Chlorophytes. Until middle of May Chlorophytes were composed mostly by group X1 (*Anykra sp*.) and J (*Oocystis sp*.); in June by group J (*Coleastrum sp*.); and from the end of June by a combination of group J (*Oocystis sp*.), group X1 (*Chlorella sp*.) and group F (*Sphaerocystis sp*.). In 2007, only two groups of Chlorophytes (J and N) were encountered, and they occurred at separate times (see section above). New groups should have been included in the model and, their parameters, should have been calibrated in order to simulate accurately the phytoplankton succession in 2008. The presence of new phytoplankton groups in this year invalidates the parameter set calibrated with data from 2007. The information available, though, was not sufficient to separate the total Chla among functional groups, each with a different response to environmental conditions.

Uncertainty generated from the physical sub-model

The differences between observed and simulated values of Chla can be explained, first, in terms of errors in the physical sub-model that propagate into the ecological sub-model. Any errors in the prediction of the mixing environment, or equivalently, the thermal structure, can potentially alter the abundance and composition of the phytoplankton community given that different groups respond differently to the environmental conditions. The growth of Cyanobacteria, for example, is favored under stable stratified conditions, while the Diatoms will likely become the dominant groups in the community in a well-mixed water column (Reynolds, 1984). From day 134 to 246 the simulated surface mixed-layer was deeper than observed (see Figure 2. 5), and consequently model results reduced Diatoms potential to develop while it favored Cyanobacteria growth. Given that the level of process description in the physical model is fundamentally correct (Hipsey et al., 2004), the errors in the description of the physical variables (stratification and mixing) are the results of errors in the boundary condition assumptions. For instance, inflow temperatures were assumed to be equal to the surface temperatures during the simulations. This is a good assumption for inflows entering from Rivera de Huelva through the stilling pond of Guillena, as the field data suggest; but it may not be good for inflows entering through non-regulated streams Cantalobo and Encinilla or inflows from Cala Reservoir, immediately upstream of El Gergal. The stronger stratification predicted by the model after day 127 was likely due to the inflow event entering the reservoir from the non-regulated streams, for which we do not have temperatures data, and for which we assumed a temperature equal to that of the surface in El Gergal.

Uncertainty generated by initial or boundary conditions

Uncertainty in the results of the succession model can also be the result of uncertainty in model boundary or initial conditions. Moreno Ostos et al. (2007) demonstrated that some changes in the phytoplankton community in El Gergal occur as a consequence of inflows introducing species from upstream reservoirs. In the present study phytoplankton inoculums were considered insignificant because no changes in algal composition were detected after the three main inflow events (days 120, 150 and 240). For example, the dominant Chlorophytes specie developing at day 120 was already observed in the reservoir one week, and even two weeks, before the inflow event. On the other hand, to evaluate uncertainty generated by initial conditions two experiments were conducted testing the sensitivity of model results when modifying initial phytoplankton concentration in the reservoir. In the first, the initial concentration

of Cyanobacteria was increased 50%, while in the second, it was the initial concentration of the green algae that was increased 50% (Figure 2. 10 A and B). In the first case, peak concentrations of Cyanobacteria decreased as well as Chlorophytes group N and J. In the second case, the peak concentrations of the green algae increased, while the concentration of Cyanobacteria decreased. In both cases, the timing of the peaks was not modified and temporal succession was respected.

Effects of increasing number of algal groups

Given that different groups compete among themselves for nutrient resources and light, any errors in the simulation of any specific phytoplankton groups may lead to significant errors in the simulation of other groups. Consequently, the error of the sub-model of any functional group increased as the number of groups simulated increased. For example the RMSE of the Cyanobacteria sub-model increased from 3.62 μg Chla/l, to 4.8 μg Chla/l when simulating four groups (see Table 2. 4, field series). A similar effect was observed also when using synthetic series.

5. Conclusions

[1] A one-dimensional, process-based and coupled physical-ecological model is used to simulate the phytoplankton succession in a reservoir. The phytoplankton community is represented in the model as a series of functional groups, each one developing at different times, which respond differently to environmental conditions. These types of models typically contain a large number of parameters, with values that are site-specific and typically unknown. A global, hybrid and automated optimization algorithm, applied in a sequential manner, is proposed for the calibration of this succession model. The most sensitive parameters are first identified through First Order Variance Analysis. The optimization algorithm is then applied to calibrate each algal group separately. In these partial calibration runs, the model is set to simulate one only functional group while specifying the abundance of the remaining groups at observed values. The model is finally run, with all groups simulated, using the parameter values found in the group-by-group calibration.

[2] The group by group calibration approach is shown to yield satisfactory results when applied to calibrate separate phytoplankton group models against synthetic time series of Chla. The goodness of the fit between simulations with calibrated parameters and synthetic runs depends, though, on the number of functional groups being simulated. The larger the number of groups included the larger are the differences between the calibrated model and the synthetic series used as a reference, which suggests that there exist strong and non-linear interactions among group sub-models. These results, altogether, suggest that the level of functional segmentation in the model should be minimized.

[3] The success of the calibration process critically depends on the consistency between the functional structure of the community, and the description made in the model and achieved through observations of that structure. Each group included in the model should represent a specific response to environmental conditions. The observations should also discriminate between groups with different environmental requirements.

[4] When applied to calibrate the model against the available field data in the reservoir, however, the sequential calibration approach did not produce the expected results. This is partly due to lack of resolution in the spectro-fluorometric data, used as a

reference in the calibration process, that did not discriminate among groups that exhibit different responses to environmental conditions. Non-linear interactions among individual group models or between ecological and physical sub-models might also be responsible for the lack of success. In any case, the model was capable to predict relevant aspects of the succession, such as the timing of the peaks, and the sequence in which the different groups appear as dominant in the phytoplankton community.

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Tables

Notation	Description	Units
	Modelled state variables	
I	Light intensity	μEm^{-2}
T	Temperature	ºC
K_d	Light exctintion coefficient	m^{-1}
Chla (CHLOR)	Chlorophyll-a concentration Chlorophytes	mg Chla L^{-1}
Chla (CRYPT)	Chlorophyll-a concentration Cryptophytes	mg Chla L^{-1}
Chla (CYANO)	Chlorophyll-a concentration Cyanobacteria	mg Chla L^{-1}
Chla (FDIAT)	Chlorophyll-a concentration Freshwater diatoms	mg Chla L^{-1}
Chla (DINOF)	Chlorophyll-a concentration Dinoflagellates	mg Chla L^{-1}
	Field data	
SSOL	Suspended Solids	mg L^{-1}
pH	pH	
DIC	Dissolved inorganic carbon	mg C L^{-1}
DOC	Dissolved organic carbon	mg C L^{-1}
TN	Total Nitrogen	mg N L^{-1}
NH_4	Ammonium concentration	mg N L^{-1}
NO_3	Nitrate concentration	mg N L^{-1}
TP	Total Phosphorus	mg P L^{-1}
PO_4	Soluble reactive phosphorus	mg P L^{-1}
BOD	Biochemical Oxygen Demand	mg O m^{-3}
DO	Dissolved Oxygen concentration	mg O L^{-1}
SiO_2	Silica	mg Si L^{-1}

Table 2. 1 List and short description of variables modelled during Dyresm-Caedym simulations.

Number	Symbol	Group	Name	Unit	Range	Calibrated value
1	μ_{max}	CHLOR	Max Growth Rate	day^{-1}	0.2 - 3.6	3.600
		CYANO			0.2 - 1.5	5.69 E-1
		CRYPT			0.2 - 1.5	1.480
		DINOF			0.2 - 3.6	4.73 E-1
		FDIAT			0.2 - 3.6	1.850
2	k_r	(five groups)	Respiration rate	day^{-1}		
3	K_P	CHLOR	Half Saturation Constant for Phytoplankton P uptake	$mg\ L^{-1}$	0.0001 - 0.04	2.54 E-3
		CYANO			0.0003 - 0.04	3.0 E-4
		CRYPT			0.001 - 0.04	3.99 E-2
		DINOF			0.0001 - 0.04	1.55 E-2
		FDIAT			0.0001 - 0.04	1.0 E-4
4	K_N	CHLOR	Half Saturation Constant for Phytoplankton N uptake	$mg\ L^{-1}$	0.02 - 0.2	5.47 E-2
		CYANO			0.02 - 0.2	8.46 E-2
		CRYPT			0.02 - 0.2	2.0 E-2
		DINOF			0.02 - 0.2	1.21 E-1
		FDIAT			0.02 - 0.2	2.0 E-2
5	K_C	(five groups)	Half saturation constant for Carbon	$mg\ L^{-1}$		
6	K_{Si}	(five groups)	Light saturation for maximum production	$mg\ L^{-1}$		
7	ϑ	CHLOR	phytoplankton temperature multiplier for growth	(no units)	1.06 - 1.14	1.081
		CYANO			1.06 - 1.14	1.092
		CRYPT			1.06 - 1.14	1.062
		DINOF			1.06 - 1.14	1.105
		FDIAT			1.06 - 1.14	1.111

Table 2. 2 List of parameters included in the ecological model relative to the different phytoplankton groups. Parameters' ranges adopted for the calibration process, using the global optimization algorithm, were indicated only for the sensitive parameters included in the calibration. Final calibrated parameter values obtained during group-by-group calibration are included.

Number	Symbol	Group	Name	Unit	Range	Calibrated value
8	v_s	CHLOR	Constant settling velocity	ms^{-1}	-5.83 E-4 - 1 E-5	-2.57 E-5
		CYANO			-5.83 E-4 - 0.5 E-5	-1.12 E-6
		CRYPT			-5.83 E-4 - 0.5 E-5	4.97 E-6
		DINOF			-5.83 E-4 - 1 E-4	1.001 E-4
		FDIAT			-5.83 E-4 - 1 E-4	-6.72 E-5
9	k_e	CHLOR	Specific extintion coefficient	m^2 $mgChla^{-1}$	0.014 - 0.20	1.140 E-1
		CYANO			0.014 - 0.15	1.264 E-1
		CRYPT			0.014 - 0.15	1.497 E-1
		DINOF			0.014 - 0.15	3.413 E-2
		FDIAT			0.014 - 0.15	3.306 E-2
10	ϑ_L	CHLOR	temperature multiplier respiration, loss term	(no units)	1.05 -1.10	1.095
		CYANO			1.05 -1.10	1.069
		CRYPT			1.05 -1.10	1.095
		DINOF			1.05 -1.10	1.056
		FDIAT			1.05 -1.10	1.050
11	I_k	(five groups)	initial slope Phyto-irradiance curve	$\mu E\ m^{-2}\ s^{-1}$		
12	τ_{cs}	(five groups)	typical shear stress	$N\ m^{-2}$		
13	α	unique	resuspension rate constant	$mgChla\ m^{-2}\ s^{-1}$		
14	K_{res}	(five groups)	control rate of resuspension	$mgChla\ m^{-2}\ s^{-1}$		
15	k_p	unique	photo respiration phytoplankton DO loss	(no units)		
16	f_{res}	(five groups)	fraction of phytoplankton respiration relative to total loss rate	(no units)		
TOT: 72	References:	Hipsey et al.,2004; Hamilton & Schladow, 1997; Schladow & Hamilton,1997; Bowie et al., 1985; Reynolds, 1984; Margalef, 1983				

Table 2.2 cont.

Day of year	1st Abundant Genera	Cells/ml	2nd Abundant Genera	Cells/ml	3rd Abundant Genera	Cells/ml
3	*Cyclotella*	7.7	*Cryptomonas*	5.0	*Aulacoseira*	3.7
8	*Cyclotella*	7.9	*Aulacoseira*	5.2	*Cryptomonas*	2.3
15	*Cyclotella*	10.4	*Cryptomonas*	6.8	*Aulacoseira*	5.8
22	*Cyclotella*	11.7	*Aulacoseira*	9.0	*Rhodomonas*	8.3
36	*Rhodomonas*	198.2	*Cyclotella*	22.3	*Aulacoseira*	10.8
43	*Rhodomonas*	107.8	*Cyclotella*	18.3	*Aulacoseira*	10.3
50	*Rhodomonas*	144.5	*Cyclotella*	31.3	*Cryptomonas*	6.0
57	*Rhodomonas*	167.9	*Cyclotella*	33.5	*Cryptomonas*	23.8
64	*Cryptomonas*	128.8	*Rhodomonas*	68.5	*Cyclotella*	53.4
78	*Cryptomonas*	202.2	*Rhodomonas*	27.8	*Cyclotella*	9.0
85	*Cryptomonas*	19.6	*Cyclotella*	6.7	*Sphaerocystis*	6.2
99	*Cryptomonas*	509.7	*Rhodomonas*	112.9	*Cyclotella*	25.6
106	*Cryptomonas*	253.5	*Cyclotella*	84.4	*Rhodomonas*	72.3
113	*Aphanizomenon*	39.8	*Cyclotella*	32.0	*Cryptomonas*	11.8
127	*Cyclotella*	95.5	*Aphanizomenon*	72.9	*Rhodomonas*	13.1
134	*Coelastrum*	380.5	*Cyclotella*	251.9	*Aphanizomenon*	62.8
141	*Coelastrum*	396.8	*Cyclotella*	270.2	*Scenedesmus*	68.8
148	*Coelastrum*	224.9	*Cyclotella*	129.1	*Scenedesmus*	59.7
155	*Cyclotella*	182.7	*Sphaerocystis*	151.5	*Coelastrum*	147.5
162	*Cyclotella*	665.5	*Fragilaria*	279.6	*Rhodomonas*	114.5
169	*Cyclotella*	730.8	*Fragilaria*	692.1	*Sphaerocystis*	240.9
176	*Cyclotella*	929.5	*Fragilaria*	215.1	*Cosmarium*	48.3
183	*Cyclotella*	923.8	*Rhodomonas*	55.4	*Scenedesmus*	46.7
190	*Cyclotella*	197	*Aphanizomenon*	146.6	*Scenedesmus*	21.3
197	*Aphanizomenon*	905.7	*Anabaena*	307.8	*Cyclotella*	12.5
204	*Aphanizomenon*	1627.1	*Cyclotella*	327.1	*Anabaena*	198.7
211	*Cyclotella*	665.7	*Aphanizomenon*	378.7	*Ceratium*	179.6
218	*Cyclotella*	415.7	*Ceratium*	346.6	*Aulacoseira*	111.0
233	*Ceratium*	443.2	*Cyclotella*	345.9	*Aphanizomenon*	129.5
246	*Cyclotella*	371.6	*Ceratium*	294.8	*Aphanizomenon*	217.2
253	*Cyclotella*	439.5	*Ceratium*	148.6	*Rhodomonas*	46.0

Table 2. 3a. Most abundant phytoplankton Genera observed and number of organisms counted for each Genera, during the sampling dates.

Phytoplankton list			
Algae class	Genera	Reynolds group	Characteristics
Chlorophytes	*Closteriopsis*	P	Tolerant to moderate light, sensitive to stratification, eutrophic habitat
	Scenedesmus	J	Prominent in highly enriched systems
	Sphaerocystis	F	Neutrally buoyant, tolerant to low nutrients availability
	Coelastrum	J	
	Pediastrum	J	
	Staurastrum	P	
	Schroederia		
	Tetraedron	J	
	Tetrachlorella		
	Cosmarium	N	Tolerant to nutrient deficiency, sensitive to stratification
	Ankyra	X1	Tolerant to stratification, sensitive to nutrient deficiency
	Chlamydomonas		
	Crucigeniella		
	Tetraedron	J	
	Volvox	G	Tolerant to high light, sensitive to nutrient deficiency
	Ankistrodesmus	X1	
	Closteriopsis	P	
	Oocystis	J	
Diatoms	*Aulacoseira*	B	Tolerant to light deficiency, sensitive to Si deficiency
	Cyclotella	B	
	Synedra	B	
	Nitzschia		
	Fragilaria	P	
	Cymatopleura		
	Navicula	MP	Tolerant to turbidity and high light
	Asterionella	C	Tolerant to light deficiency, sensitive to stratification
Cyanobacteria	*Aphanizomenon*	H	Tolerant to low nitrogen, sensitive to mixing
	Microcystis	M	Sensitive to low light and mixing
	Anabaena	H	
	Merismopedia		
	Gomphosphaeria	L	Tolerant to low nutrients, sensitive to mixing
Cryptophytes	*Cryptomonas*	Y	Tolerant to low light
	Rhodomonas	Y	
Dinoflagellates	*Ceratium*	L	
Euglenophyta	*Phacus*	W1	Tolerant to high organic matter,
	Trachelomonas	W1	
	Euglena	W1	
References: Reynolds et al., 2002; Padisak et al. 2009			

Table 2. 3b. Phytoplankton Genera observed in El Gergal in 2007 classified in algae classes and related to the corresponding Reynolds group.

a) Synthetic series	**RMSE (µg Chla L^{-1})**				
	Separate Runs	*2 Groups*	*2 Groups*	*3 Groups*	*4 Groups*
GROUP 1	0.6597	1.2365	-	1.8792	2.5052
GROUP 2	0.4725	0.4784	-	0.6096	0.6747
GROUP 3	0.1696	-	0.1838	0.5564	0.5652
GROUP 4	0.3185	-	1.2130	-	1.2391

b) Field series	**RMSE (µgr Chla L^{-1})**							
	Separate Runs automatic calibration	*2 Groups Cyano & Crypt*	*2 Groups Chlor J Chlor N*	*3 Groups*	*4 Groups*	*4 Groups manual calibration*	*4 Groups initial condition Cyano*	*4 Groups initial condition Chlor J*
CHLOR J	1.55	forced	2.4496	2.3495	3.0764	1.517	2.19	1.5
CYANO	3.62	3.9088	forced	3.924	4.8365	3.6277	3.94	3.68
CHLOR N	0.79	forced	1.1157	1.0582*	2.071	1.041	1	1.28
CRYPT	0.55	0.6365	forced	forced	13.25	0.6773	0.73	0.68
FDIAT+DINOF	forced	forced	forced	forced	forced	forced	forced	forced

**not reproducing chlor_2 peak as in 2 groups simulations*

Table 2. 4 Root mean squared errors (RMSE), calculated between (A) synthetic series and simulations and (B) field observations and simulations. Results for different calibration strategies involving variable number of phytoplankton groups are included. *Forced* means that the group was set to observed values during simulations.

Analysis of one group's parameters sensitivity to the others algal groups					
		Group 1	Group 2	Group 3	Group 4
Parameter (Group 1)	$\Delta p/p_0$	S	S	S	S
μ_{max}	0.0317	1.3571	1.9478	77.7532	0.7025
K_P	0.1000	3.0197	1.3066	3.1068	0.0694
K_N	0.0236	0.0000	0.0000	0.0479	0.0000
ϑ	0.0220	1.5573	0.9105	0.0000	0.1358
v_s	0.0101	14.6632	13.6545	99.0674	11.3930
k_e	0.0118	31.8033	10.7382	283.8327	0.4701
ϑ_L	0.0202	6.1487	2.3640	76.8057	0.1560

Table 2. 5 Sensitivity coefficients (S), showing the effect of changes parameter values of one functional group on the simulations of other algal groups. The parameters that are changed in this exercise are those of the sub-model representing the growth of Group 1. S values are calculated following Eq. 2.

Symbol	Group	Unit	Automatic calibration	Manual calibration
μ_{max}	CHLOR_J	day^{-1}	3.6	3.600
	CYANO	day^{-1}	0.59	0.55
	CHLOR_N		3.6	2.130
K_P	CHLOR_J	mg L^{-1}	2.54 E-3	2.54 E-3
	CHLOR_N		3.17 E-2	3.17 E-2
	CRYPT		3.991 E-2	3.999 E-2
K_N	CHLOR_J	mg L^{-1}	5.47 E-2	5.47 E-2
	CHLOR_N		9.98 E-2	9.98 E-2
ϑ	CHLOR_J	(no units)	1.081	1.081
	CHLOR_N		1.135	1.135
	CRYPT		1.062	1.080
v_s	CHLOR_J	ms^{-1}	-2.57 E-5	-2.57 E-5
	CHLOR_N		0.101 E-4	0.101 E-4
k_e	CHLOR_J	m^2 $mgChla^{-1}$	1.140 E-1	1.140 E-1
	CHLOR_N		1.876 E-1	1.876 E-1
	CRYPT		1.49 E-1	0.89 E-1
ϑ_L	CHLOR_J	(no units)	1.095	1.095
	CHLOR_N		1.056	1.056

Table 2. 6 Final parameter set considering two Chlorophytes subgroups (N and J). The parameters' ranges adopted for calibration processes were the same reported in Table 2. 2 (Chlorophytes range was adopted for both group N and J). The final calibrated parameter values obtained during the group-by-group automatic calibration for the two Chlorophytes subgroups were included, the rest of the values were the same of Table 2. 2. Cyanobacteria and Cryptophytes parameters were included only if their values were adjusted during the final manual calibration, simulating all the algal groups (bold values).

Figures

FIGURE 2.1

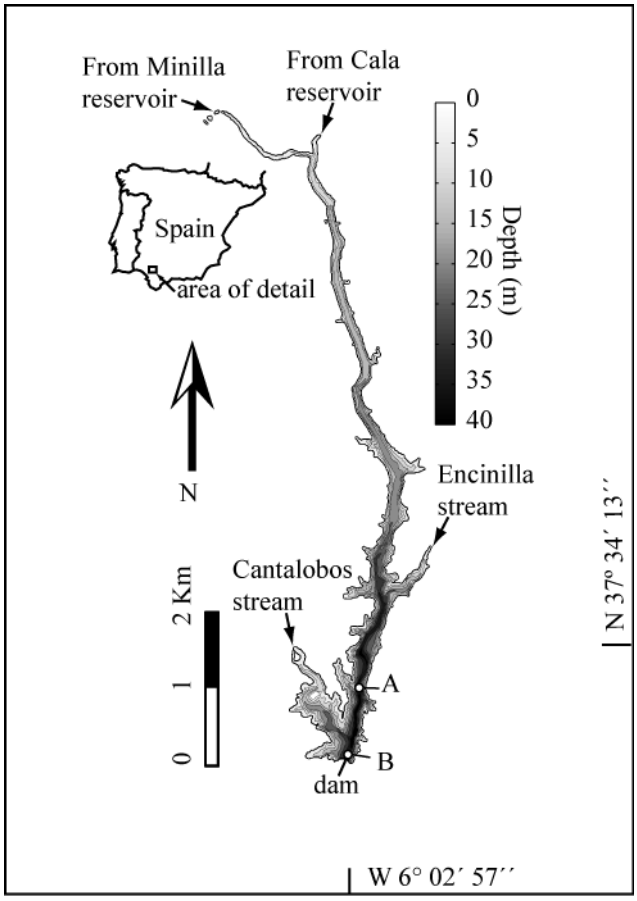

Figure 2. 1. El Gergal Reservoir bathymetry and main inflows. Location of the meteorological station (A) and sampling and data recording point (B) is also indicated.

FIGURE 2.2

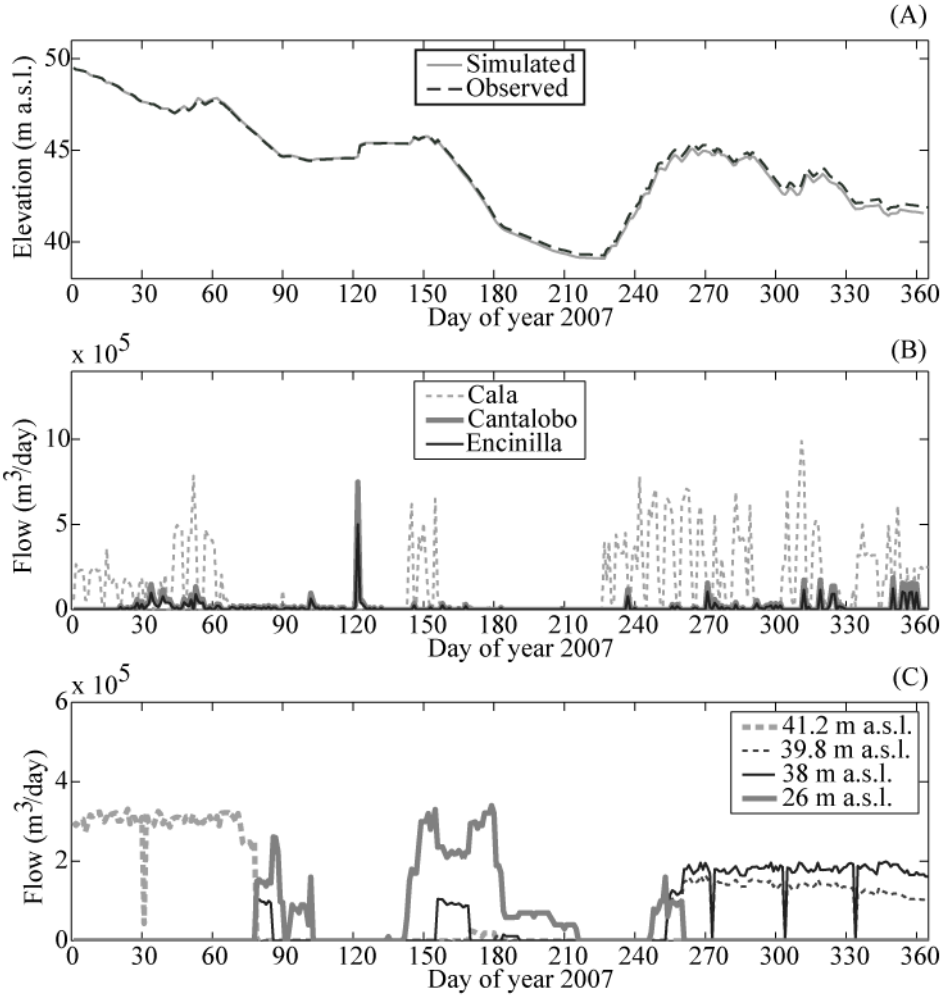

Figure 2. 2. Comparison of simulated and observed free surface elevation (m a.s.l.) in El Gergal during 2007 (A). For reference, time series of inflows (Cala, Cantalobos, Encinilla) (B) and outflows distribution between the four operational outlets (C) are also plotted.

FIGURE 2.3

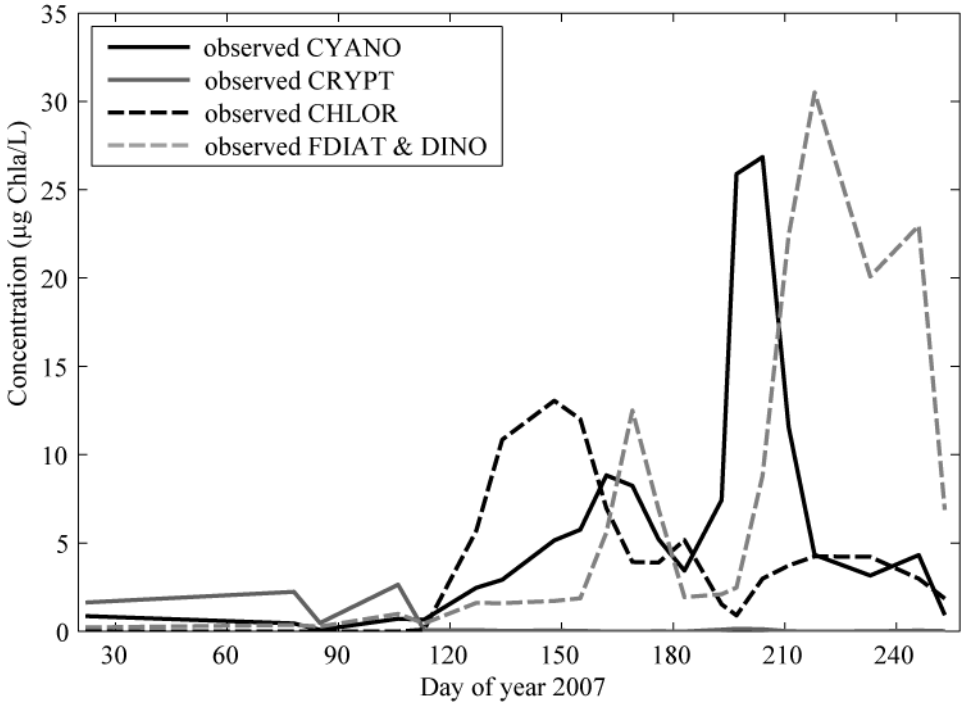

Figure 2. 3. Evolution of Chlorophyll-a concentration as measured by the spectro-fluorometer. Four groups were identified: Cyanobacteria (CYANO), Cryptophytes (CRYPT), Chlorophytes (CHLOR), sum of freshwater Diatoms and Dinoflagellates (FDIAT & DINO).

FIGURE 2.4

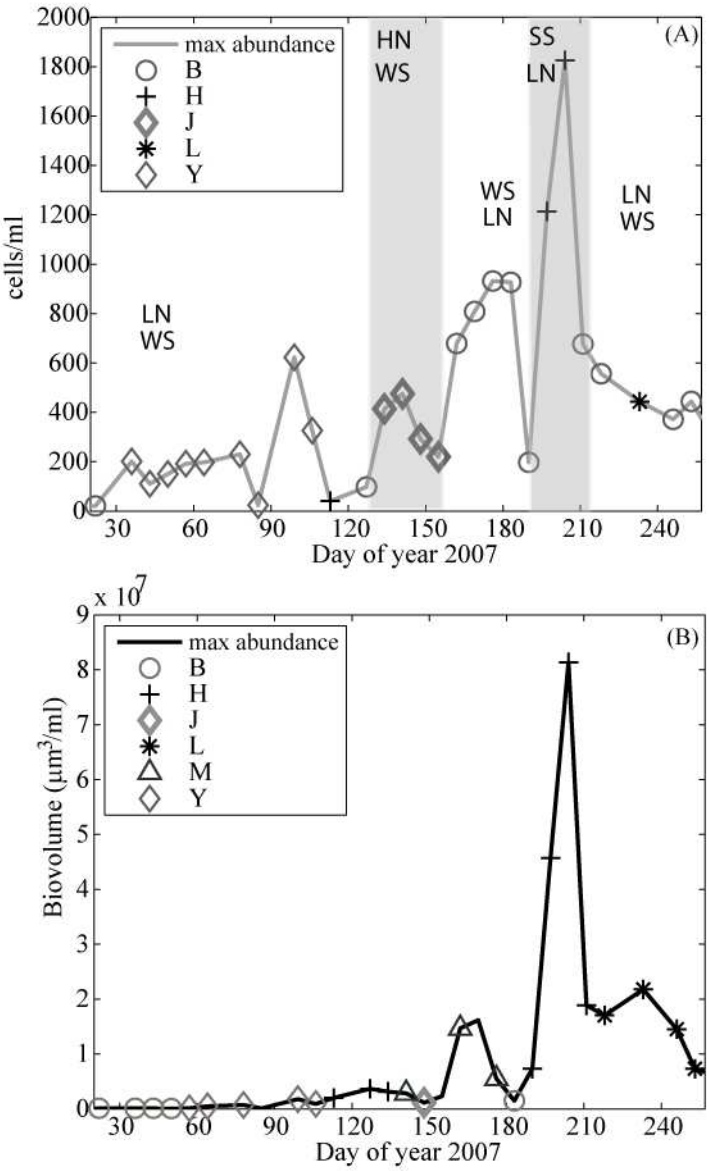

Figure 2. 4. Time trace of total phytoplankton abundance (panel A) and of total phytoplankton biomass in terms of bio-volumes (panel B). The most abundant Reynolds' groups associated to the different sampling occasions are identified by a symbol. Shadings represent relevant environment conditions: weak stratification (WS), strong stratification (SS), low nutrient availability (LN) and high nutrient availability (HN). Reynolds groups B, H, J, L, M, Y were identified, dominated by Diatoms, Cyanobacteria (*Aphanizomenon*), Chlorophytes, Dinoflagellates, Cyanobacteria (*Mycrocistis*) and Cryptophytes respectively.

FIGURE 2.5

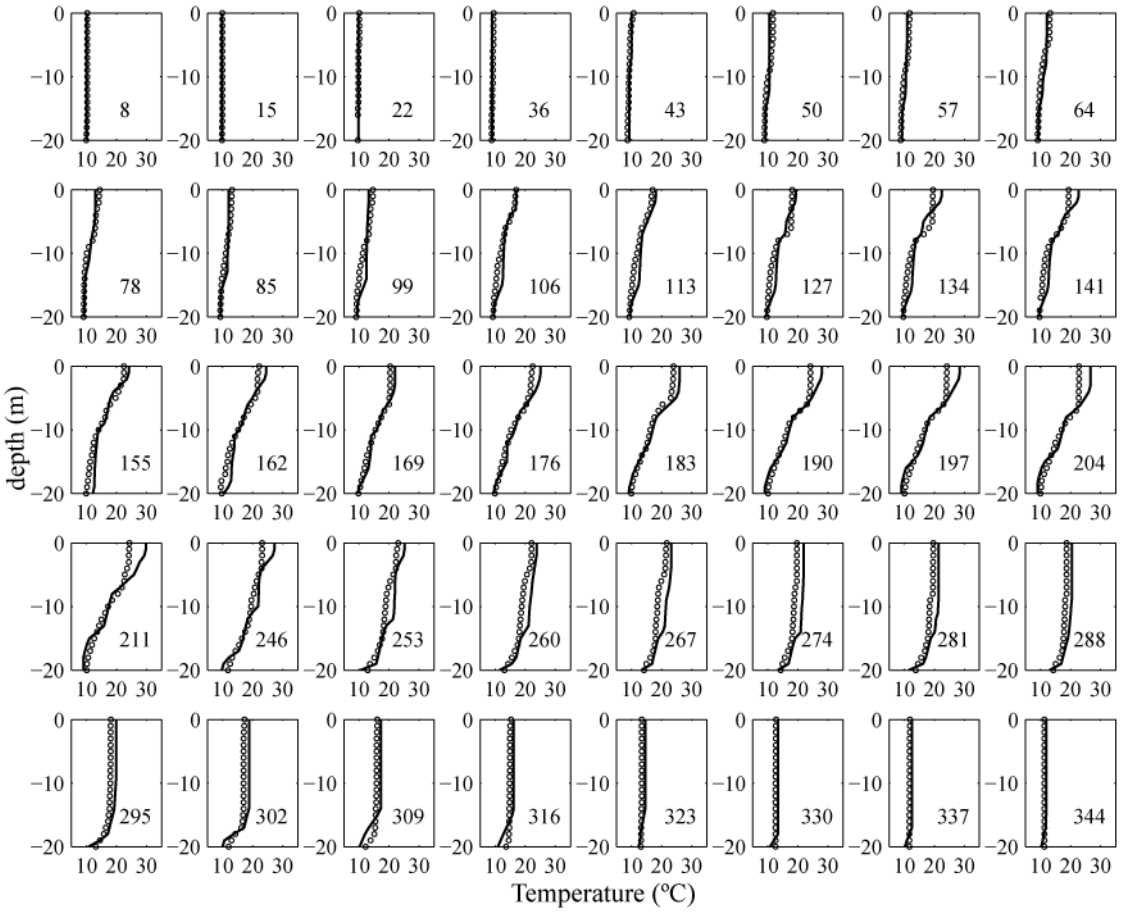

Figure 2. 5. Simulated water temperature profiles (solid black lines) against observations (black dotted lines). The number inside subplots indicates the day of year.

FIGURE 2.6

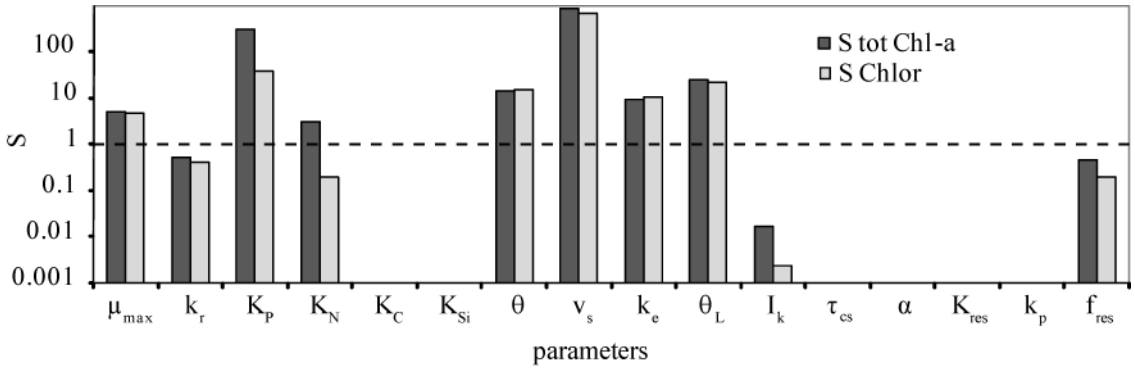

Figure 2. 6. Results of the sensitivity analysis, expressed as *S* coefficient values. Low *S* values indicates low model sensitivity to the changes of that particular parameter. Sensitivity was evaluated on two outputs: Chloropytes Chla concentration (S Chlor) and total Chla concentration in the water column (S tot Chla). The value used in this paper as a threshold to include a parameter in the calibration process (*S*=1) is indicated as a dashed line. Parameter acronyms are defined in Table 2.

FIGURE 2.7

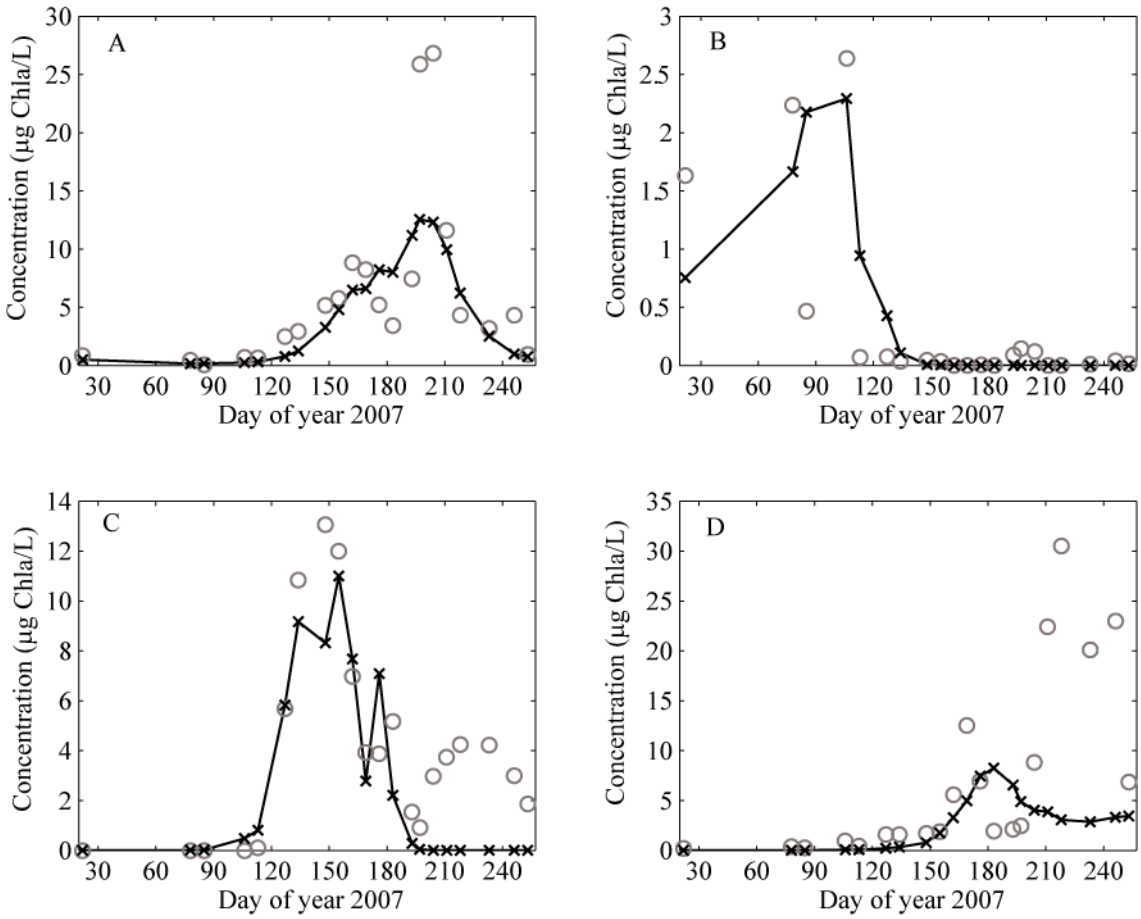

Figure 2. 7. Observed and simulated chlorophyll-a concentration after group-by-group calibration. Panel A is for Cyanobacteria, panel B for Cryptophytes, panel C for Chlorophytes, and panel D for the sum of Diatoms and Dinoflagellates. Concentrations are averaged over volume in the first 20 m of the water column.

FIGURE 2.8

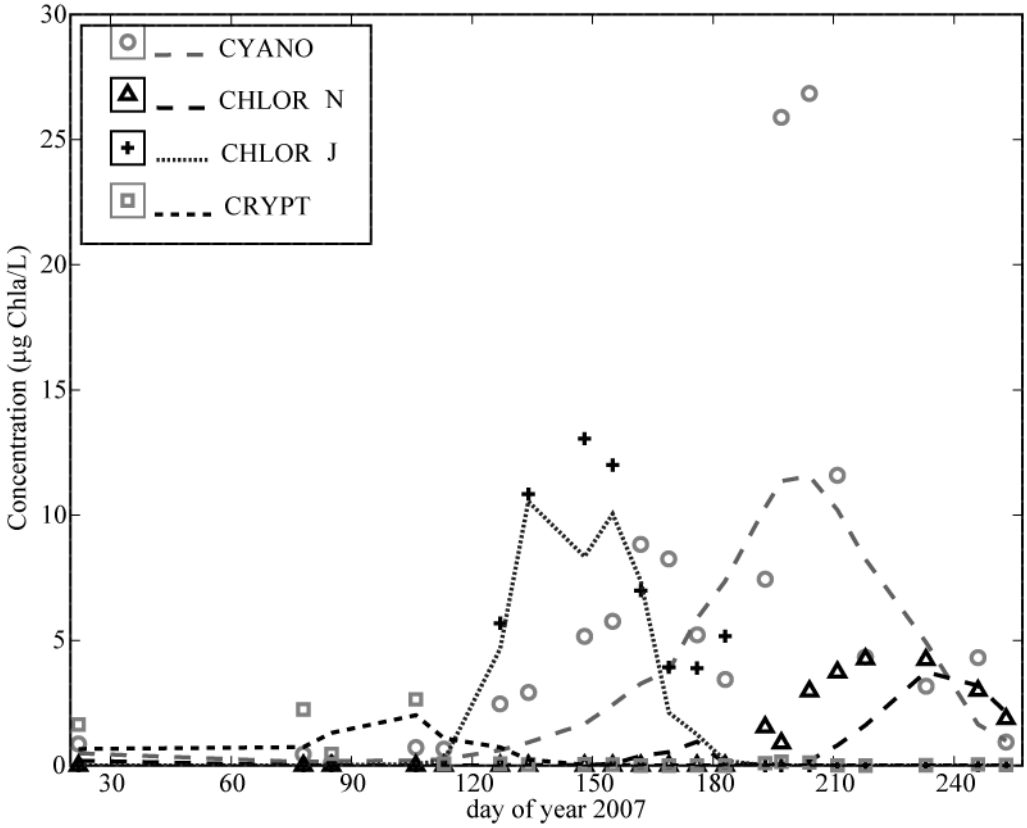

Figure 2. 8. Phytoplankton succession observed (symbols) and modeled (lines), adopting four phytoplankton groups: Cyanobacteria, Cryptophytes, Chlorophytes group J, Chlorophytes group N. In this exercice, Diatoms and Dinoflagellates were set to observed values. Therefore, they were not included in the calibration process. Concentrations are averaged over volume in the first 20m of the water column.

FIGURE 2.9

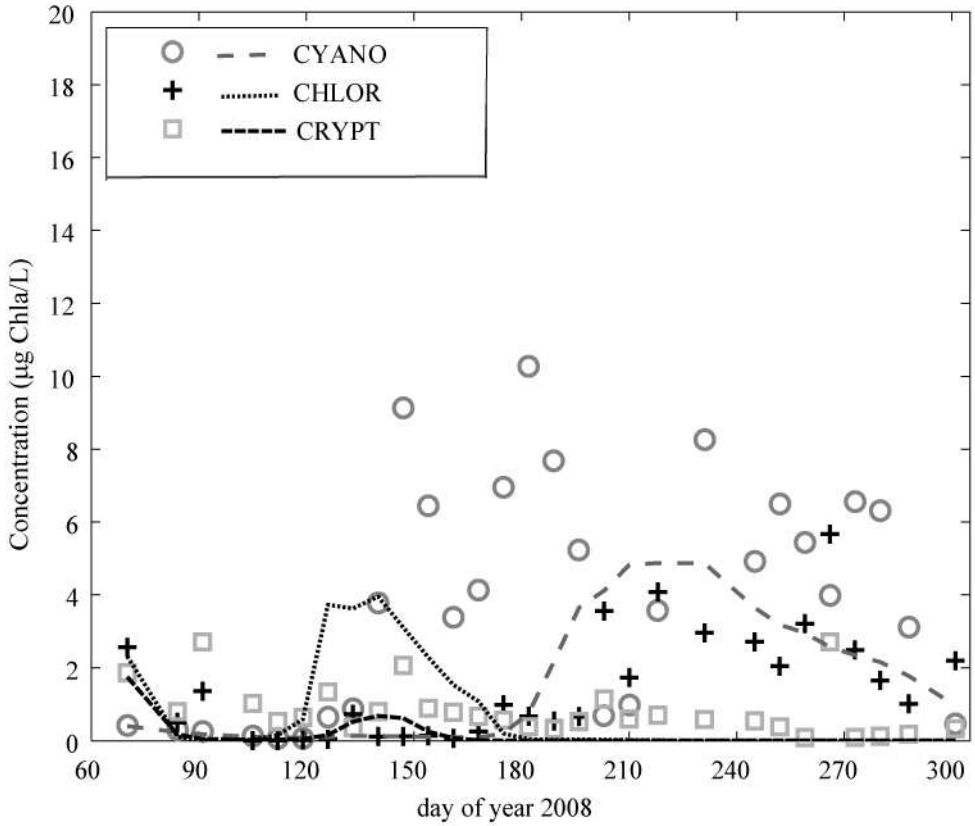

Figure 2. 9. Phytoplankton succession observed (symbols) and modelled (lines) during 2008 adopting three phytoplankton groups: Cyanobacteria, Cryptophytes and Chlorophytes. Simulation was conducted adopting the parameter set found after 2007 calibration. Chlorophytes were simulated using parameter set of Chlorophytes group J. Diatoms and Dinoflagellates were set to observed values. Concentrations are averaged over volume in the first 20m of the water column.

FIGURE 2.10

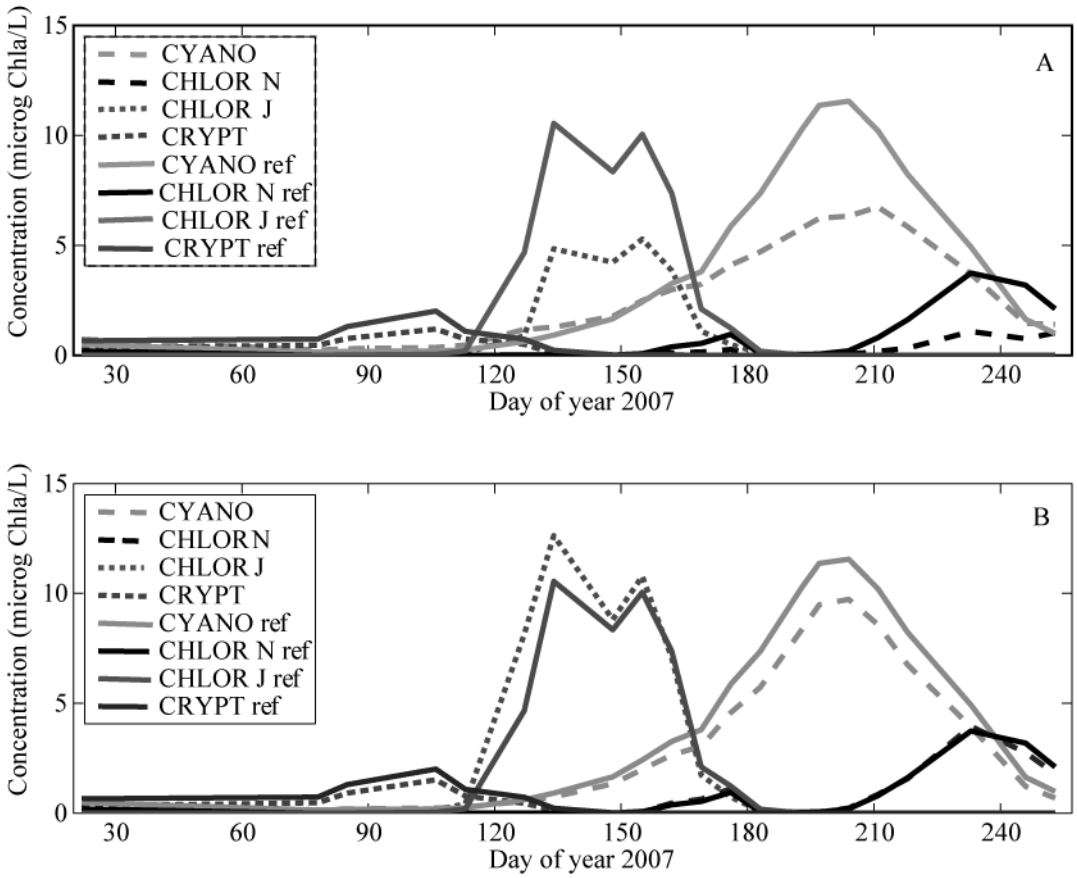

Figure 2. 10. Two examples of the effect of initial conditions on the modelled phytoplankton seasonal succession including four algal groups. (A) Initial concentration of Cyanobacteria increased by 50%. (B) Initial concentration of Chlorophytes group J increased by 50%. Concentrations are averaged over volume in the first 20m of the water column. Solid lines represent the reference simulation obtained without modifying initial conditions.

Chapter 3

"Sorprenderse, extrañarse, es comenzar a entender"
José Ortega y Gasset

Is the composition of the phytoplankton community of reservoirs modified on the short-term by withdrawal operations?

1. Introduction

The changes in abundance and composition experienced by phytoplankton communities in lakes and reservoirs are the result of variations in the physical (light climate) and the chemical (nutrient availability) constraints for algal growth (Margalef, 1983; Reynolds, 1984; Margalef, 1997; Reynolds, 1997). Light climate experienced by phytoplankton cells is tightly related to turbulent mixing, which determines the residence time of microalgae within the well-illuminated upper layers of the water column (MacIntyre, 1998). On the other hand, nutrients distribution and their bioavailability in the upper layers where light levels are adequate for phytoplankton growth, is the result of transport processes interacting with biological phenomena. These changes in the environmental conditions experienced by algal cells are tightly linked to the physical forcing driving mixing and transport processes within the lake, and they tend to promote the growth of certain groups or species in detriment of others, given the variety of adaptations of phytoplankton to the environment (Huisman *et al*., 1999; Passarge *et al*., 2006; Litchman and Klausmeier, 2001).

The concept of succession being subject to external environmental control has been extensively supported through the analysis of experimental observations either collected in the framework of field monitoring programs or in microcosms and mesocosms, through theoretical arguments, and, also, by means of numerical simulations and experiments. Huisman *et al*. (2004), for example, demonstrated that Cyanobacteria tend to dominate at low turbulence diffusivity while sinking diatoms and green algae are favored at high turbulent diffusivity. Huisman *et al*. (1999), also, demonstrated that a green alga (Scenedesmus) was competitively displaced by Cyanobacteria species (Aphanizomenon and Microcystis) while another green alga (Chlorella) was even more competitive at lower light intensities. Passarge *et al*. (2006) showed that under phosphorous limited conditions Synechocystis spp (a Cyanobacteria) was able to displace Chlorella sp. (a Chlorophytes). Sommer and Lengfellner (2008), working with mesocosms and analyzing phytoplankton growth at different light and temperature conditions, demonstrated that light intensity may control the timing of spring blooms. They also demonstrated that the biomass of Diatoms tends to decrease with rising water temperatures. Similar experiments by De Senerpont Domis *et al*. (2007) showed that artificially warming the environment may not change the

phytoplankton succession sequence, but tends to increase the abundance of Cyanobacterial species relative to other groups in the community. More recently, Hoyer et al. (2009) analyzed the seasonal changes experience by the phytoplankton community in a water supply reservoir in Southern Spain during a period of time of 8 years. To characterize the composition of the community they used the functional classification proposed by Reynolds (2002). In this classification, the predominant genera of algae are grouped according to their responses or adaptation to particular environmental conditions, characterized in terms of two key variables: the ratio of the euphotic depth to the surface mixed layer depth (z_{eu} / z_{mix}) and phosphorus concentration, representing energy limitation and nutrient availability for phytoplankton growth, respectively. Hoyer et al. (2009) were able to identify a general succession sequence of functional groups which was frequently disrupted during events in which the phytoplankton assemblage experienced sudden and abrupt changes (i.e shifts and reversions). These changes coincided in time either strong wind events or changes in withdrawal rates. Hoyer et al. (2009) concluded that water withdrawals were, probably, the most important allogenic factor controlling the changes in composition and abundance of the phytoplankton community in Mediterranean reservoirs. Their conclusion agreed with that of Naselli Flores (2000), who studied twenty-one Sicilian reservoirs of varying trophic states, and concluded that the abundance and composition of phytoplankton are more strongly influenced by the hydraulic regime than by nutrient availability.

Few studies have been published in the literature that explore in detail the role of hydraulic forcing in particular, withdrawals, on the seasonal or short term evolution of the functional structure of phytoplankton communities in stratified reservoirs. Moreover, the few studies that exist are, to some extent, contradictory. Barbiero et al. (1997), for example, pointed out that long term surface withdrawals in reservoirs could induce a decline in the population of Cyanobacteria. Hoyer *et al*. (2009), instead, suggested that deep withdrawals could favor development of Chlorophytes or Diatoms, while surface extractions could favor the growth of Cyanobacteria. These conclusions regarding the effects of water withdrawal on the phytoplankton community, however, were based on the analysis of observations. Our goal in this manuscript is to understand the mechanisms by which withdrawal could induce changes in the composition of phytoplankton communities. Two mechanisms are likely at play. The first is purely physical, and consists of the selective removal of species developing at or near withdrawal level, favoring the growth of others which could be occupying other layers. The second is associated with the environmental conditions (light, temperature and nutrients) experienced by phytoplankton communities, at a given layer, which can be different depending on the withdrawal level. Casamitjana et al. (2003), for example, showed that the evolution of the thermal structure in reservoirs can be significantly different, depending on the withdrawal levels. Of course, the sensitivity of the thermal structure to withdrawals will depend on the size of the basin and the magnitude of the outflow rates. These changes in the environmental conditions, in turn, may favor the development of certain species in detriment of others, depending on their response to particular environmental conditions. Here we will focus on this second mechanism. First, we will propose a conceptual model through which we will evaluate the changes in the light and temperature fields induced by selectively withdrawing at different levels. We will then assess the effects of those changes in the growth of two functional groups characterized by different sensitivity to light and temperature. Second, we analyze the results of simulations conducted with a one-dimensional hydrodynamic-ecological model (DYRESM-CAEDYM) to evaluate the effects of different withdrawal levels on the environmental conditions experienced by two algal groups with different

adaptations to the environment, coexisting either at the same layer or at different layers. Our arguments and simulations are particularized for the conditions observed in El Gergal, a small to medium-sized reservoir in southern Spain, previously studied by Hoyer et al (2009). DYRESM-CAEDYM was successfully calibrated and applied to El Gergal by Rigosi et al. (2010) to simulate phytoplankton succession in 2007. The initial and boundary conditions in these simulation experiments are constructed from observations existing in the data set used in that work.

2. Methods

Study site

El Gergal (37º 34´ 13´´ N, 6° 02´ 57´´ W) is a small, canyon-shaped and eutrophic reservoir, supplying water to the city of Seville. The annual inflow volume, coming from regulated rivers and not regulated streams is ca. 70 hm^3 with extreme oscillation on seasonal scales. Outflows occur from either a spillway located at 50 m.a.s.l. or from a deep draining outlet at 17 m.a.s.l. directly into the river, or from 4 other withdrawal structures located at 41.2, 39.8, 38 and 26 m.a.s.l. flowing into a water treatment plant to be distributed. When full, the volume of water stored in the reservoir is 35 hm^3, its surface area is 250 ha, and the maximum length is 7750 m. The maximum depth is 37 m, close to the dam, and the mean depth is 15.7 m (Fig. 3.1). El Gergal reservoir is warm and monomictic. Water never reaches temperatures below 4ºC (Cruz Pizarro *et al*., 2005). The lake stratifies in summer from the beginning of March to the middle of October, and de-stratifies towards the end of the year.

Approach

Our working hypothesis is that different withdrawal levels may induce different changes in the environmental conditions, which, in turn, will favor the development of certain algal groups in detriment of others. The effect of environmental conditions is assessed through a first order model of phytoplankton growth, in which the chlorophyll-a concentration (μg L^{-1}) of an algal group *i*, $Chla_i$, is represented as

$$\frac{\partial Chla_i}{\partial t} = \left\{\mu_{\max,i} \cdot \min\left[f_i^I(I), f_i^{II}(N), f_i^{III}(P)\right]\right\} \cdot f_i(T) - R_i \cdot Chla_i \qquad (1)$$

Here, $\mu_{\max,i}$ is the maximum growth rate that phytoplankton exhibits under optimal conditions, R_i represents the effects of all sinks of phytoplankton biomass (including mortality, respiration and grazing), and the functions f_i (f^I, f^{II}, f^{III}, and f), represent the limiting effects on growth of light levels *I*, nitrogen *N* and phosphorus *P* concentrations and temperature *T* in the water column. The limiting function for temperature is represented as:

$$f_i(T) = \vartheta_i^{T-20} - \vartheta_i^{k_i(T-a_i)} + b_i \text{ and } f(\mathrm{T}) \text{ is equal 1 at } T = T_{standard} \qquad (2)$$

where θ is a temperature multiplier ($\theta > 1$), *T* is the observed temperature, *k*, *a* and *b* are parameters of the model. The limitation function for light, in turn, is given by:

$$f_i^I(I) = 1 - \exp\left(\frac{-I}{I_{ki}}\right) \qquad (3)$$

where I is the average photo-synthetically active radiation in one layer and I_{ki} is the initial slope of the irradiance curve. Nutrient limiting functions are defined as follows:

$$f_i^{II}(P) = \frac{PO_4}{PO_4 + K_{Pi}} \tag{4}$$

$$f_i^{III}(N) = \frac{NH_4 + NO_3}{NH_4 + NO_3 + K_{Ni}} \tag{5}$$

where K_{Pi} and K_{Ni} are the half saturation constants for phosphorus and nitrogen. All parameters in Eqs. (1)-(5) are specific of each algal group (indicated by the subscript i), representing the different adaptations to environmental conditions. The growth model given by Eqs (1)-(5) is included in the ecological model CAEDYM, and, is used in this work as a valid representation of phytoplankton growth.

Experimental data set

The changes experienced by the phytoplankton community in El Gergal occurring during two periods of time in 2007 were carefully analyzed. At those times, the reservoir was stratified, the only hydraulic forcing was due to withdrawal and the composition of the phytoplankton community was subject to significant changes. In this work, we were interested in analyzing independently the withdrawals' effects so we excluded period with inflows. The significance of the changes was determined as follows. Phytoplankton species existing in the reservoir were identified and counted under inverted microscope following the Utermöhl method (1958), on a weekly basis during 2007. The genera were then classified into functional groups, following Reynolds (1997, 2000). Abundances of the different Reynold's functional groups were estimated by adding the abundances corresponding to the member species at each depth. Most abundant functional groups were B, H, J, L, Y, mainly by Diatoms, Cyanobacteria, Chlorophytes, Dinoflagellates, and Cryptophytes, respectively. Time series in phytoplankton abundance and the dominant functional group at each time is depicted in Figure 3.2 (A).The changes in the composition of the phytoplankton community were described using the Index of Community Change σ (or ICC), as proposed by Reynolds (1984). The time series of ICC (Fig. 3.2B) was calculated as:

$$\sigma = \frac{\sum \left[\{ b_i(t_1) / \beta(t_1) \} - \{ b_i(t_2) / \beta(t_2) \} \right]}{t_1 - t_2} \tag{6}$$

where $b_i(t)$ is the abundance of group i at time t and $\beta(t)$ is the total abundance of the phytoplankton community. ICC was computed using phytoplankton countings (individuals ml^{-1}), rather than biomass so that the development of small-cells could be taken into account (Hoyer *et al*., 2009). We used an arbitrary threshold value of ICC (σ = 0.12) to separate small from significant changes in the composition of phytoplankton community. Only two periods of time satisfied the necessary conditions established at the onset of this work to be analyzed. Period one (P1) started on day 162, and, period two (P2) on day 190. The length of the periods analyzed were in both cases 15 days, which, according to our observations, is sufficient for the phytoplankton community to exhibit large and significant changes both in size and composition.

Most of the outflows (82%) during P1 were withdrawn from the lower intake (26 m a.s.l.). Of the remaining 28%, 15% were withdrawn the intermediate intake (38 m a.s.l) and only 3% from the upper intake (41.2 m a.s.l.). The average volume withdrawn per day during this period was ca. $3x10^5$ m^3. During period P2, a large fraction of the total outflows (99%) were withdrawn from the lower intake, and the remaining 1% were extracted from the intermediate intake. The average outflow rate in this case was $7x10^4 m^3$ day^{-1}, almost one order magnitude less than in P1. Thermal conditions also differed between the study periods. Surface temperatures were about 20ºC in P1 and 24ºC in P2. During the first period the population of Cyanobacteria (group H) and Chlorophytes (group J) declined. Diatoms (group B) became dominant at that time (Fig. 3.2). On the second period, the population of Cyanobacteria (group H) increased, while the number of Chlorophytes (group N) declined. Specific light, phosphorus and temperature functions for Cyanobacteria-H, Chlorophytes–N and -J, are represented in Figure 3.3. Cyanobacteria-H were more sensitive to light limitation than Chlorophytes-N and –J. Chlorophytes-N was the less tolerant group to phosphorus limitation followed by Chlorophytes-J and by Cyanobacteria-H. Temperatures higher than 20ºC favor Cyanobacteria-H rather than Chlorophytes-J and –N.

Succession model

A process based one-dimensional hydrodynamic and ecological model (DYRESM-CAEDYM, Imberger and Patterson, 1981; Hamilton and Schladow, 1997; Schladow and Hamilton, 1997) is applied to simulate phytoplankton succession in El Gergal reservoir. DYRESM (DYnamic REservoir Simulation Model) provides predictions of the physical environment which are used to drive water quality simulations in CAEDYM (Computational Aquatic Ecosystem DYnamics Model). Our choice of model is justified in that (1) it has been widely used as a management tool and (2) it represents explicitly the two-way links existing between physical and biogeochemical processes. DYRESM includes descriptions of mixing and transport processes associated with river inflow, outflows, diffusion in the hypolimnion and mixed-layer dynamics, and it is used to predict the variation of water temperature and salinity with depth and time. For example, it has been successfully applied to Lake Burragorang - Australia (Romero *et al*., 2004), Lake Constance - Europe's Alps (Hornung, 2002), San Roque reservoir - Argentina (Antenucci *et al*., 2003) or Lake Kinneret - Israel (Antenucci *et al*., 2000). CAEDYM consists of a series of coupled first-order differential equations representing the major biogeochemical processes influencing water quality including primary and secondary production, nutrient and metal cycling, oxygen dynamics and the movement of sediment. It is a flexible model so that it can be configured with different degrees of complexity to focus on particular processes (Copetti *et al*., 2006; Trolle *et al*., 2008; Gal *et al*., 2009).

Model setup and calibration

The biogeochemical model was set up to simulate the growth of four different phytoplankton groups (Chlorophytes-J, Chlorophytes-N, Cyanobacteria, and Cryptophytes). The biomass of each algal group was assessed in terms of chlorophyll-a (from here on, Chla). Phytoplankton growth is represented as in Eqs. (1)-(5). Algae are allowed to describe vertical movements, modeled in our implementation, with a constant settling velocity. The changes in the physical (temperature and solar radiation) and the chemical (nutrient) environment experienced by the algal cells is the result of the calculations made by the physical sub-model (DYRESM) coupled with the biological sub-model (CAEDYM). Further details of the model can be found in Romero

et al. (2004b). A complete list of state variables (both modeled or supplied as field data) used in our model of El Gergal is presented in Table 3.1.

The model was calibrated manually to minimize the difference between observations and simulations (evaluated as the Root Mean Squared Error) considering data at all the depths observed during the two study periods. The Chla concentration in the field was assessed with a submersible four-channel spectro-fluorometer (bbe Moldaenke). The spectro-fluorometer is able to discriminate the Chla concentration of four different functional groups: green algae (chlorophitae), grey algae (including dinoflagellates and diatoms), cyanophyceae and cryptophyceae. Our calibration exercise started from a parameter set for algal growth, which was proposed in Rigosi *et al.* (2010), when calibrating the successional model for El Gergal, with nutrient concentrations forced (i.e. not simulated). Here, we include nutrients as state variables, to account for the effects of withdrawal on the nutrient fields, hence, the need to re-calibrate the model parameters. A first-order variance analysis (Blumberg and Georgas, 2008) was used to isolate the sensitive parameters to be adjusted in the manual calibration (Table 3.2). Trial and error calibration strategy is traditionally applied in water quality modelling (Lewis *et al*. 2002; Tanentzap *et al*., 2007; Bonnet and Poulin, 2004; Hillmer *et al*., 2008).

A list of sensitive parameters and corresponding calibrated values are shown in Table 3.2 (a complete list of the model parameters can be found in Hipsey *et al*., 2004). Simulations were conducted with a 1 hour time step, and the state variables were output every 24 hours at 11:00 am. The results of the physical-chemical model were checked by comparing simulated water levels, temperature and nutrients profiles against observations (depth and date specific) (Figure 3.4). The results of the ecological model, in turn, were checked by comparing Chla concentrations for each of groups simulated by the model, against the spectro-fluorometric observations. Figure 3.5 depicts variation of simulated and observed phytoplankton group concentration averaged in the first 20m of the water column (see Appendix A for details on calibration).

Model simulations

Several experiments were initially conducted with DYRESM-CAEDYM, under simplified scenarios, to understand the effect of withdrawal levels on the growth of phytoplankton groups with different sensitivities to light and temperature changes. Only one algal group was simulated at a time in El Gergal. Algae were assumed to be neutrally buoyant and maximum growth rates and mortalities were set to constant values. Initial water surface elevation, temperature and Chla profiles were set equal to the observations. Nutrients concentrations, in turn, were forced and set equal to a high and constant value, to avoid nutrient limitation on growth. Water was extracted alternatively from upper, intermediate and lower intake or from the draining outlet (deeper than the lower intake).

The model was then used to simulate the changes in the phytoplankton community in El Gergal during the two study periods, under more realistic conditions. All groups existing in the lake during the study periods were simulated with specific growth rates, mortalities and settling velocities, as calibrated (see Appendix A). Nutrients were also state variables and simulated by the model. Three different scenarios were simulated for each study period (see Table 3.3). In all scenarios, withdrawal rates were as observed. The base case scenario corresponds to a realistic simulation, in which water was withdrawn as indicated above (Experimental data set). For period 1, the first scenario (P1S1) consists of withdrawing water only from the drainage outlet (17 m a.s.l.); in the second scenario (P1S2) water was only withdrawn

from the upper intake. The first scenario during two (P2S1) consists of shifting the outflow level from 26 m a.s.l. level to 24.5 m a.s.l. (closer to bottom). The second scenario in this period (P2S2) the withdrawal levels is shifted to 38 m a.s.l. (intermediate intake) (see Table 3.3), the highest operative intake at that time (about 3 m from surface).

3. Results

Conceptual model

The reservoir will be conceived as a stack of three horizontal layers which are free to move vertically (advection) and to contract and expand in response to outflows (Fig. 3.6A). Each layer remains homogeneous at all times and property differences between layers represent the vertical distribution of those properties. Vertical transport across layers will be assumed negligible. Water released at any given level is withdrawn from a narrow layer approximately centred at the off-take level. All layers were considered to have the same volume V_l, and their thickness was calculated from the depth-area curve for El Gergal. Note that the thickness of the layer increases with depth as a consequence of the decreasing form of the depth-area curve of natural basins. In a period of 15 days it will be assumed that the volume of water withdrawn is equal to V_l. In our idealized model of a reservoir, if the volume of the bottom layer is withdrawn, all layers above it will descend, their average areas will decrease, and, consequently, their thickness will increase, to keep their volume constant. The average light conditions within the different layers will consequently decrease. Three scenarios are considered, depending on the location of the outlet: (A) surface intake; (B) intermediate intake; (C) lower intake. Assuming no limitation for growth due to temperature or nutrients concentrations, any changes in the growth rate of phytoplankton should be result of changes in light levels occurring as a result of water withdrawal. These levels, in turn, are determined by the distance of algal cells to the free surface (Fig. 3.6). Light limitation factors (Eq. 3) for Cyanobacteria-H and Chlorophytes-J (with different sensitivities to light, Fig. 3.3A) were calculated for the initial and final conditions in each withdrawal scenario.

Consider first the case of algae occupying the first layer. In scenario (B) or (C), Cyanobacteria-H will grow more slowly (0.012%), while Chlorophytes-J should not vary significantly (Table 3.4). The differences in growth are associated to differences light sensitivity. As layer 1 descends, its thickness increases, and the average light levels within it will decrease. The light limiting factor for Cyanobacteria-H will decrease too, due its higher sensitivity (Fig. 3.3A). The light limiting factor for Chlorophytes-J, in turn, will remain constant (Fig. 3.3A). If water is withdrawn from the first layer, the population of both group H and J will decline, as a consequence of the outflow. Consider now the case when algae occupy the intermediate layer. The growth of Cyanobacteria-H, in this case, is favored in scenario A (withdrawal from upper intake), but disfavored in scenario C. The same effect was observed for Chlorophytes-J, but the changes of the growth factors were lower than for Cyanobacteria-H (Table 3.4), given that it is less sensitive to light variations.The abundance of both groups will decline in response to outflows from the intermediate layer.

Layer temperatures will also change in response to changes in layer thickness. When extracting at bottom level layer temperature decreased due to a decrease of surface layer area, exposed to radiation. Radiation absorbed by the layer increased due to the increase of layer thickness, while depth of illuminated layers would be reduced. Instead, when extracting at surface, the intermediate layer temperature increased, being

exposed to surface radiation. Algal groups had a different growth rate response depending on the observed temperature, following Eq.2, Cyanobacteria-H growth are favored at warmer temperatures (higher than 20ºC) while Chlorophytes performance is superior at temperature lower than 20ºC (Fig. 3.3C). Thus, when algae were located at intermediate layer, surface extraction will favor the development of Cyanobacteria-H and bottom extraction favored Chlorophytes-J development.

Synthetic experiments with a 1D hydrodynamic-ecological model

Our conceptual model, being based on a simplified model of the physical behavior of the reservoir, indicates plausible tendencies in the evolution of algal populations, depending on their sensitivity to light and temperature. The actual magnitudes of the effects on growth will depend on factors such as mixing and stratification in the water column, or realistic outflow rates, light attenuation, etc. We test whether the tendencies suggested in the analysis of the conceptual model are confirmed by conducting synthetic experiments with DYRESM-CAEDYM. Figure 3.7 (A and B) depicts the results of the synthetic experiments during the study period P1 for Cyanobacteria-H and Chlorophytes-J. Both groups were equally distributed with depth, at the start of the simulation, with a ca. 7 m thick layer (from 3 to 10 m depth) with maximum Chla concentrations at 5 m. Their distribution, though, changed differently as a consequence of their different light and temperature fields. Cyanobacteria-H grew near the surface independently of the withdrawal level, hence, shading the algae below. The final concentrations varied linearly from a maximum of 20 µg Chla/L at the surface to zero at 2 m. When extracting from the drainage outlet (Fig. 3.7A, black line, or case D), the subsurface peak after 15 days had decreased from 20 µg Chla/L to about 8 µg Chla/L, and the layer hosting the algae had moved away from the free surface: the top of this layers was at 5 m at the end of the simulations. When extracting from the upper intake (Fig. 3.7A, grey line, or case U) the sub-surface peak also decreased shaded by surface algal development, but, the hosting layer approached the surface, extending from a depth of 1.5 m to 6 m. When extracting from intermediate intake (Fig. 3.7A, discontinuous line, or case I) the subsurface peak approached the free surface, but part of the population were flushed out; hence, its magnitude was 35% lower than in case U. Chlorophytes-J also grew near the surface in all cases, but responded (Fig. 3.7B) differently, due to its lower sensitivity to light. When extracting from below the surface (Fig. 3.7B, black solid and discontinuous lines), the final Chla concentration decreased linear from a maximum value at the surface to zero at 5 m. Cyanobacteria-H instead only developed until 2 m in the same scenario, thus, final concentration averaged from zero to 5 m was higher for Chlorophytes-J. Synthetic experiments, when algae were located at intermediate layer, indicated that surface extraction will favor the development of Cyanobacteria-H and bottom extraction favored Chlorophytes-J development as pointed out in the conceptual model. However the response was less evident in synthetic experiments where algae were free to develop at surface.

Synthetic experiments conducted with the stratification and hydraulic forcing prevailing during period P2, and, assuming that algae were initially concentrated near the surface as observed during that period of time, suggest that no significant changes were experienced by any groups when extracting at different levels below the hosting layers (Fig. 3.7C, D).The algal populations only declined when withdrawing water from the intermediate intake (4 m depth), directly from the hosting layer. Cyanobacteria-H were shifted towards the surface, in response to surface withdrawals, and their biomass was flushed out of the reservoir. After 15 days, the concentration of Cyanobacteria-H above 4 m was reduced, in 12% compared to the cases with bottom withdrawals (Fig.

3.7C, discontinued grey line). The population of Chlorophytes-N also shifted towards the surface and declined as a result of surface withdrawals. Their final concentrations at the surface, though, were lower than those reached by the Cyanobacteria-H, as these were favored by the higher temperatures reached by water.

Withdrawal scenarios under realistic conditions

The simulations conducted with calibrated parameters, and realistic withdrawal levels during the two study periods, will be used as a reference and compared with simulations conducted varying the intake levels. The final distribution of group J (Fig. 3.8) did not change between the reference scenario and scenario P1S1, with all water being withdrawn from the drainage outlet. A low increase of Cyanobacteria at about 10 m depth was observed but the vertical distribution was not altered. The increase was due to a shift in layer position: when extracting water from the draining outlet the relative position of algae from surface increased because in the reference simulation water was extracted not only from lower intake but also from intermediate intake. Nutrient concentrations below 15 m were lower than in the reference scenario even if no changes were detected at the layers of algal development (Fig. 3.8). To understand phytoplankton groups' mechanism of response to environmental condition we calculated growth factors (F_i), indicating the relative rate of change of biomass in Eq. (1). Water temperature in the first few m below the surface was 20ºC, and, hence, it did not favor any group in particular (Eq. 2 and Fig. 3.3C). The growth of Chlorophytes-J was limited by phosphorus at about 5 m depth (PO_4< 50 µg L^{-1}; F_{ChlorJ}=0.14), but not below (PO_4>50 µg L^{-1} and F_{ChlorJ}=1.8, at a depth of 10 m). Hence, Chlorophytes-J developed at about 10 m depth. Cyanobacteria-H growth factor calculated at 5 m (F_{Cyano}=0.5), was higher than Chlorophytes-J, explaining Cyanobacteria-H better performance at this layer.

By extracting from the upper intake (scenario P1S2) the subsurface peak of group H shifted towards the free surface: at the end of the period it was developing from surface to about 7 m depth (Fig. 3.9). The Chla concentration of Cyanobacteria-H did not decrease at the surface even if part of its biomass was flushed out. Chlorophytes-J did not develop the last day of the study period. Surface extraction moved the all layers below the intake, with higher nutrients concentrations and lower temperatures than the surface layers, closer to the surface. Nevertheless, resulting nutrients concentrations at surface were still limiting algal growth (Fig. 3.9).

Lowering the intake level (P2S1) did not affect the growth of any of the groups simulated, since in both cases (reference and scenario P2S1) the outflow level was below the algae. Nutrients and temperature distributions were not affected at the level of algal development (Fig. 3.10). The growth of Cyanobacteria–H was favored at the surface as a result of the increase in temperature from 25ºC to 28ºC. Chlorophytes-N, in turn, were limited by nutrients (mainly Phosphorus). Growth factors calculated at 2 m below the free surface following Eq.1 were:

$$F_{Cianobacteria-H} = \{0.6 \cdot \min[1,1,1] \cdot 2.88 - 0.105\} = 1.63$$

$$F_{Chlorophytes-N} = \{2.43 \cdot \min[1,0.4,0.2] \cdot 2.4 - 0.3656\} = 0.801$$

The growth factor for Cyanobacteria-H 10 m below the surface was lower (0.348), hence,their lower development.

Shifting the intake level to the surface (P2S2), where algae were developing, caused a decrease in the population of both groups, Cyanobacteria-H and Chlorophytes-

N. Final concentration of Cyanobacteria-H, the most abundant group, was about 4% less than the reference simulation while concentration of Chlorophytes-N was reduced about 9%. Nutrient and temperature fields remained unchanged (Fig. 3.11).

4. Discussion

Surface withdrawals

Conceptual model indicated that upper intake favored the development of the Cyanobateria-H located at intermediate layers. In synthetic experiments the deep chlorophyll maximum of Cyanobacteria-H was shifted towards the surface, where, if not shaded by other algae developing near the surface and according to our conceptual model, should have experienced higher light levels, hence, increasing its growth rate. However, this effect was masked by Cyanobacteria-H cells developing at surface and shading algae at lower levels. In our realistic simulations, the subsurface population of Cyanobacteria-H was also shifted towards surface (P1S2, Fig. 3.9), and did not decline, even if part of the biomass was flushed. These results together suggest that Cyanobacteria-H is, in fact, favored by surface withdrawals. Surface withdrawals, in turn, caused the surface population of Chlorophytes–J to decrease. This was due to the fact that the concentration of Cyanobacteria-H had increased above 4 m limiting their development. This, in turn, was the result of Chlorophytes-J moving away from the surface layers due to their high settling velocities, compared to Cyanobacteria (Table 3.2) . Simulations conducted with the settling of Chlorophytes-J set to zero, indicate that, in that case they were able to develop in the first 2 m, limiting the surface growth of Cyanobacteria-H (Fig. 3.12 A and B).

Deep withdrawals

Water withdrawals from below layers hosting phytoplankton will favor the growth of species tolerant to low light conditions, in detriment of species more sensitive to light. In synthetic experiments the development of Cyanobacteria-H was not favored when extracting from lower intake or draining outlet: Cyanobacteria-H chlorpyll maximum was moved towards bottom at lower level of light availability limiting growth. . In synthetic experiments when extracting from lower intake or draining outlet, Chlorophytes-J were able to develop from surface to 5 m. Cyanobacteria-H, instead, only from surface to 2 m (Fig. 3.7 A and B, black lines). This was mainly due to Chlorophytes-J tolerance to low light environment and partially to the fact that Chlorophytes-J had a lower specific attenuation coefficient compared to Cyanobacteria (respectively 0.114 and 0.126 μg Chla L^{-1} m^{-1}) that allowed higher light penetration at the same concentration. This would result in Chlorophytes-J concentration at surface higher than Cyanobacteria-H at these conditions.

Withdrawals from the lower intake had the same effect as withdrawals from outlets closer to reservoir bottom. In synthetic experiments modifying extraction from lower intake to draining outlet did not induce changes in the algal distribution both in the first and in the second periods. All layers hosting algae were equally shifted towards the bottom, and the light, nutrient and temperature limiting functions were the same (Fig. 3.8 and 3.10).

Flushing

Withdrawing from the layer hosting the algae will flush out phytoplankton cells causing the population in the reservoir to decline. When extracting from intermediate

intake and both phytoplankton groups were located from surface to intermediate level, the effect was a decrease in both algal concentration, as showed by scenario P2S2 (Fig. 3.11), with no change of the dominant group. The magnitude of the reduction in concentration is due to the low outflow rate in P2. When simulating an increase of outflow rate, the effect observed in P2S2 was enhanced: at the end of the studied period Cyanobacteria-H and Chlorophytes-N concentrations were lower than when withdrawing a smaller amount of water (Fig. 3.12, C and D).

Environmental conditions

Nutrients and temperature conditions can intensify or reduce the effects of withdrawals extractions depending on the particular sensitivity of each phytoplankton group. Considering the simplest case when nutrients were not affected by withdrawals as in P2S1, Chlorophytes-N were limited by phosphorus and their concentration was one order magnitude lower than Cyanobacteria-H. Cyanobacteria-H are usually phosphorous limited when PO_4 concentration starts to be lower than about 30 $\mu g\ L^{-1}$ (Morris, 1980) and have the ability to uptake nitrogen instead of phosphorus in case of PO_4 limitation (Margalef, 1983). Thus, nutrients reductions would primarily compromise Chlorophytes-N development rather than Cyanobacteria-H.

On the other hand, temperature conditions are able to enhance withdrawals effects. For example, extracting from the upper intake at warmer temperature will favor the growth of Cyanobacteria-H both by light and temperature functions, when the growth rate is higher than the rate of biomass extraction from the outlet. Small differences in temperature functions, that are multiplied by the maximum growth rate (see Eq.1), can results in different final growth rates. For example, in synthetic experiments (see Fig. 3.7,C and D) at surface $f(T)_{cyanoH}$=1.5893 and $f(T)_{chlorJ}$=1.5842) with final growth rates of respectively 0.8455 for Cyanobacteria-H and 0.486 day^{-1} for Chlorophytes-J.

Withdrawals operations as an instrument to control phytoplankton abundance and composition

We showed by model simulation experiments, that phytoplankton groups were influenced by the modification of the outflow level from surface to intermediate or bottom layers, but they were not influenced moving the outflow level from the layer below phytoplankton peak, closer to the bottom of the reservoir. The effect was dependent on the position of extraction with respect to the vertical position of the phytoplankton peak in the water column. Each phytoplankton group showed a different response to the alteration of the environment due to its buoyancy and its peculiar tolerance (or sensitivity) to light limitation. Phytoplankton groups' response was also enhanced or reduced depending on their specific nutrients and temperature limitation functions. In particular, the growth of deep chlorophyll maxima dominated by species with low sensitivity to nutrient depletion, high sensitivity to light reduction and with low settling velocity (as Cyanobacteria-H) were favored when extracting from the upper layer, because light availability for these algae, whose relative position from surface decrease, was increased. Phytoplankton groups sensitive to nutrients limitation and with high settling velocities (as Chlorophytes-J) are not favored under those conditions. Settling velocities for this group are such that, even if the intermediate layers are shifted closer to the surface as a result of surface withdrawals, the algae will move downwards away from the surface at a higer speed.

Hoyer *et al*. (2009) suggested the hypothesis that lower withdrawals could favor development of Chlorophytes and Diatoms while surface withdrawals would enhance the growth of Cyanobacteria. Our results, in turn, suggest that the short-term phytoplankton response depend not only on the level of extraction but also on the vertical distribution of the phytoplankton groups. The effects of withdrawals on the vertical distribution of light, temperature and nutrient fields in the water column depend on the magnitude of the outflow rates and the reservoir bathymetry. Bottom withdrawals in the second period, with low outflow rates, caused negligible effects on the vertical distribution of algae, compared to the effects during the first period. Our results, hence, can be generalized to other reservoirs, as long as the differences in morphologic features and hydrologic regimes are taken into account. Our findings indicated that Cyanobacteria was favored at short-term by surface withdrawals, instead Barbiero et al. (1997) observed a decline of Cyanobacteria with long-term surface extractions. This suggests that the phytoplankton response is also dependent on the duration of the extraction.

5. Conclusions

1. Specific responses of phytoplankton groups to withdrawals level were investigated simulating different scenarios through a 1D coupled ecological model for El Gergal Reservoir (Seville). Model results showed that the composition of the phytoplankton community was modified on the short-term by withdrawals operations. The magnitude of variation of algal concentration was related to the magnitude of the outflow rate and was also dependent to the reservoir bathymetry. An outflow rate generating a free surface decrease of about 1.5 m in 15 days, in a reservoir with the size of El Gergal, was able to induce a significant physical displacement of the vertical layers with consequences on the environmental conditions of phytoplankton development.

2. The phytoplankton group response was dependent on the relative position between the level of extraction and the depth of the maximum phytoplankton concentration in the water column. Variations in phytoplankton groups abundance were observed together with modifications of water column physical and chemical structures when shifting extraction from intermediate to surface or bottom layers, but they were not observed increasing outflow depths once below the zone of phytoplankton development.

3. When extracting from surface level and phytoplankton groups were developing at surface, the effect was a reduction in concentration of all the groups independently from their sensitivity or tolerance to environmental conditions, due to exportation of biomass through the outflow. When extracting from surface level and phytoplankton groups were developing at intermediate level the species that were tolerant to nutrient depletion, sensitive to light limitation and had low settling velocities (e.g. Cyanobacteria Reynolds group H), were favored because their position was shifted toward the surface.

4. When extracting from deep layers and phytoplankton groups were developing at intermediate levels, the relative position of the algae from surface increase, so the species that were tolerant to low light conditions (e.g. Chlorophytes) and whose settling

velocities did not avoid growth, were favored. When extracting from deep layers and phytoplankton groups were developing at surface, surface algal development was not affected and the dominant phytoplankton group depended on the environmental conditions at time of extraction, rather than on the effect of the withdrawal.

Appendix A

Calibrated models for the selected periods

The comparisons between observed and simulated physical and chemical profiles for P1 and P2 were showed in Figures 3.4. The model was able to reproduce well the distribution of most physical and chemical variables in both calibrated periods. However, the NH_4 concentration in P1 was overestimated and the NO_3 concentration in P2 was underestimated. Simulated oxygenated layers in both periods were thinner than observed. Figure 3.5 depicts the evolution in time of different phytoplankton groups' concentrations simulated and observed in the two studied periods. Concentration was averaged over volume for the first 20m of the water column. In P1 the model was able to reproduce very well the Chlorophytes-J group concentration and also the decrease of Cyanobacteria-H group at the end of the 15 days. In P2 the patterns of both Chlorophytes-N and Cyanobacteria-H were well represented. However, the magnitude of Cyanobacteria-H concentration at the end of the simulation was underestimated (12 µg Chla/l vs of 17 µg Chla/l). The Root Mean Squared Errors (RMSEs) calculated between observed and modeled physical, chemical and biological variables are included in Table 3.5. Highest RMSEs values, both in period 1 and 2, were relative to PO_4, although these errors have to be referred to their corresponding range of variation. RMSEs founded for biological variables were higher than the ones obtained for physical and chemical variables.

Calibrated functional phytoplankton groups

During the two short-term selected periods we analyze the response of three different phytoplankton groups (Cyanobacteria-H, Chlorophytes-J, Chlorphytes-N) characterized, through parameter calibration, by different behaviors. Cyanobacteria-H were characterized by lower maximum growth rates compared to Chlorophytes-J and Chlorophytes-N that can be defined as colonizer groups. Moreover, Cyanobacteria-H were more sensitive than Chlorophytes-N and -J to light limitation and were favored by high water temperatures. At temperatures lower than 20ºC, Chlorophytes-J and -N performed better than Cyanobacteria-H. Lower K_P values indicate that one is more tolerant to nutrient depletion. Cyanobacteria-H, whose K_P value is $3.0E^{-4}$ mg L^{-1}, are more tolerant to PO_4 limitation than Chlorophytes-N, whose K_P value is $3.17E^{-2}$ mg L^{-1}. Each group was also characterized by different settling rates: Chlorophytes-N were classified as neutrally buoyant, Cyanobacteria-H as low negatively buoyant and Chlorophytes-J as high negatively buoyant (Table 3.2).

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TABLES

Notation	Description	Units
	Modelled state variables	
I	Light intensity	μEm^{-2}
T	Temperature	ºC
K_d	Light exctintion coefficient	m^{-1}
Chla (CHLOR J)	Chlorophyll-a concentration Chlorophytes group J	mg Chla L^{-1}
Chla (CHLOR N)	Chlorophyll-a concentration Chlorophytes group N	mg Chla L^{-1}
Chla (CRYPT)	Chlorophyll-a concentration Cryptophytes	mg Chla L^{-1}
Chla (CYANO)	Chlorophyll-a concentration Cyanobacteria	mg Chla L^{-1}
SSOL	Suspended Solids	mg L^{-1}
pH	pH	
DIC	Dissolved inorganic carbon	mg C L^{-1}
DOC	Dissolved organic carbon	mg C L^{-1}
TN	Total Nitrogen	mg N L^{-1}
NH_4	Ammonium concentration	mg N L^{-1}
NO_3	Nitrate concentration	mg N L^{-1}
TP	Total Phosphorus	mg P L^{-1}
PO_4	Soluble reactive phosphorus	mg P L^{-1}
BOD	Biochemical Oxygen Demand	mg O m^{-3}
DO	Dissolved Oxygen concentration	mg O L^{-1}
SiO_2	Silica	mg Si L^{-1}
	Field data	
Chla (FDIAT)	Chlorophyll-a concentration Freshwater diatoms	mg Chla L^{-1}
Chla (DINOF)	Chlorophyll-a concentration Dinoflagellates	mg Chla L^{-1}

Table 3. 1 List and short description of variables modelled during Dyresm-Caedym simulations.

PARAMETERS							
Symbol	Group	Name	Unit	Range	Reference values	Manual calibrated values (period 1, initial day 162)	Manual calibrated values (period 2, initial day 190)
μ_{max}	CHLOR_J	Max Growth Rate	day^{-1}	0.2 - 3.6	3.600	3.600	3.6000
	CYANO			0.2 - 1.5	0.550	**0.600**	**0.7543**
	CHLOR_N			0.2 - 3.6	2.130	2.130	**2.4267**
	CRYPT			0.2 - 1.5	1.480	1.480	1.480
K_P	CHLOR_J	Half Saturation Constant for Phytoplankton P uptake	$mg\ L^{-1}$	0.0001 - 0.04	2.54 E-3	2.54 E-3	2.54 E-3
	CYANO			0.0003 - 0.04	3.0 E-4	3.0 E-4	3.0 E-4
	CHLOR_N			0.0001 - 0.04	3.17 E-2	3.17 E-2	3.17 E-2
	CRYPT			0.001 - 0.04	3.999 E-2	3.999 E-2	3.999 E-2
K_N	CHLOR_J	Half Saturation Constant for Phytoplankton N uptake	$mg\ L^{-1}$	0.02 - 0.2	5.47 E-2	5.47 E-2	5.47 E-2
	CYANO			0.02 - 0.2	8.46 E-2	8.46 E-2	8.46 E-2
	CHLOR_N			0.02 - 0.2	9.98 E-2	9.98 E-2	9.98 E-2
	CRYPT			0.02 - 0.2	2.0 E-2	2.0 E-2	2.0 E-2
ϑ	CHLOR_J	phytoplankton temperature multiplier for growth	(no units)	1.06 - 1.14	1.081	1.081	1.081
	CYANO			1.06 - 1.14	1.092	1.092	1.092
	CHLOR_N			1.06 - 1.14	1.135	1.135	1.135
	CRYPT			1.06 - 1.14	1.080	1.080	1.080
v_s	CHLOR_J	Constant settling velocity	ms^{-1}	-5.83 E-4 - 1 E-5	-2.57 E-5	-2.57 E-5	-2.57 E-5
	CYANO			-5.83 E-4 - 0.5 E-5	-1.12 E-6	-1.12 E-6	-1.12 E-6
	CHLOR_N			-5.83 E-4 - 1 E-5	0.101 E-4	0.101 E-4	0.101 E-4
	CRYPT			-5.83 E-4 - 0.5 E-5	4.97 E-6	4.97 E-6	4.97 E-6
k_e	CHLOR_J	Specific extintion coefficient	$m^2mgChla^{-1}$	0.014 - 0.20	1.140 E-1	1.140 E-1	1.140 E-1
	CYANO			0.014 - 0.15	1.264 E-1	1.264 E-1	1.264 E-1
	CHLOR_N			0.014 - 0.20	1.876 E-1	1.876 E-1	1.876 E-1
	CRYPT			0.014 - 0.15	0.89 E-1	0.89 E-1	0.89 E-1
ϑ_L	CHLOR_J	temperature multiplier respiration, loss term	(no units)	1.05 -1.10	1.095	1.095	1.095
	CYANO			1.05 -1.10	1.068	1.068	1.068
	CHLOR_N			1.05 -1.10	1.056	1.056	1.056
	CRYPT			1.05 -1.10	1.095	1.095	1.095
vN2		Temperature multiplier for denitrification	(no unit)	1.02-1.14	1.080	**1.100**	**1.1000**
KMAN		Nitrogen Anaerobic organic mineralization rate	day^{-1}	0.002-0.05	0.005	0.005	0.005
KMN		Nitrogen Aerobic organic mineralization rate	day^{-1}	0.002-0.05	0.017	0.017	0.017
vM		temperature multiplier for mineralization	(no unit)	1.02-1.14	1.08	**0.800**	**0.8000**
Nset		Settling velocity for particulate N	ms^{-1}	1.157E-07 - 3.0E-5*	2.50E-05	2.50E-05	2.50E-05
alpN		Resuspension rate constant N	$g\ m^2\ s^{-1}$	1.73E-08 - 5.0E-5	5.00E-05	5.00E-05	5.00E-05
KOAP		Phosphorous Anaerobic organic mineralization rate	day^{-1}	0.001-0.07	0.005	0.005	0.005
KOP		Phosphorous Aerobic organic mineralization rate	day^{-1}	0.01-0.80	0.01	**0.020**	0.0100
Pset		Settling velocity for particulate P	(m/s)	8.1E-07 - 3.5E-5*	3.00E-05	3.00E-05	3.00E-05
alpP		Resuspension rate constants P	$g\ m^2\ s^{-1}$	0-5.6E-07	0	0	0
Smpp		Maximum potential sediment flux	$g\ m^2\ day^{-1}$	0-0.005	0.003	0.003	0.003

References: Hipsey et al.,2004; Hamilton & Schladow, 1997;Schladow & Hamilton,1997;Bowie et al., 1985;Reynolds, 1984;Margalef, 1983;Jorgensen and Bendoricchio, 2001;Di Toro et al., 1975; Rosa, 1985;*DeVicente Immaculada, personal comm.
Forcing nutrients (year 2007 Automatic and Manual calibration); * Simulating nutrients 15 days of simulation

Table 3. 2 Parameters values of sensitive model parameters (values of parameters that are not listed here are the default used in Dyresm Caedym version 2.1, see Hipsey et al., 2004)

P1		P1S1		P1S2	
outlet hight	extraction	outlet hight	extraction	outlet hight	extraction
26 m a.s.l.	81.80%	17 m a.s.l.	100%	41.2 m a.s.l.	100%
38 m a.s.l.	15.40%				
41.2 m a.s.l.	2.80%				
P2		P2S1		P2S2	
outlet hight	extraction	outlet hight	extraction	outlet hight	extraction
26 m a.s.l.	98.90%	24.5 m a.s.l	100%	38 m a.s.l.	100%
38 m a.s.l.	1.10%				

Table 3. 3 Outlet heights of extraction and percentage of outflow volume extracted at each height during periods 1 and 2 (P1, P2) and in scenarios 1 and 2 applied during both time periods (P1S1, P1S2, P2S1, P2S2).

			Change in growth rate		
Algae group	Initial Layer		Bottom extraction	Surface extraction	Intermediate Extraction
Cyanobacteria		1	-0.012%	none	-0.012%
		2	-0.87%	0.80%	none
Chlorophytes J		1	0%	none	0%
		2	-0.090%	0.045%	none
Chlorophytes N		1	0%	none	0%
		2	-0.094%	0.047%	none
			Relative population change		
Algae group	Initial Layer		Bottom extraction	Surface extraction	Intermediate Extraction
Cyanobacteria		1	-0.1%	none	-0.1%
		2	-6.20%	6.02%	none
Chlorophytes J		1	0%	none	0%
		2	-4.23%	2.18%	none
Chlorophytes N		1	0%	none	0%
		2	-2.85%	1.47%	none

Table 3. 4 Conceptual model results: relative growth factor variation and population increase/decrease, in 15 days, of different phytoplankton groups at different light conditions.

Period 1 (day 162-176)			Period 2 (190-204)	
Variables	**RMSE**	Range of variation	**RMSE**	Range of variation
Temperature (ºC)	1.011	10 - 27	2.362	10 - 29
pH	0.439	5 - 10	0.200	6 - 10
DO (mg O2/L^{-1})	2.849	0 - 14	2.240	0 - 10
PO4 (µg /L^{-1})	21.139	0 - 200	42.524	0 - 250
NH4 (mg L^{-1})	0.579	0 - 1.9	0.161	0 - 1.2
NO3 (mg L^{-1})	1.766	0 - 7	0.658	0 - 3
CYANO (Chla L^{-1})	2.859	0 - 8	5.517	0 - 17
CHLOR (Chla L^{-1})	1.487	0 - 6	2.783	0 - 3
CRYPT (Chla L^{-1})	0.010	0 - 1	0.094	0 - 1

Table 3. 5 Root Mean Squared error calculated between observed and simulated physical, chemical and biological variables, modeling two periods of the year 2007. Variables' ranges are also indicated.

FIGURES

FIGURE 3.1

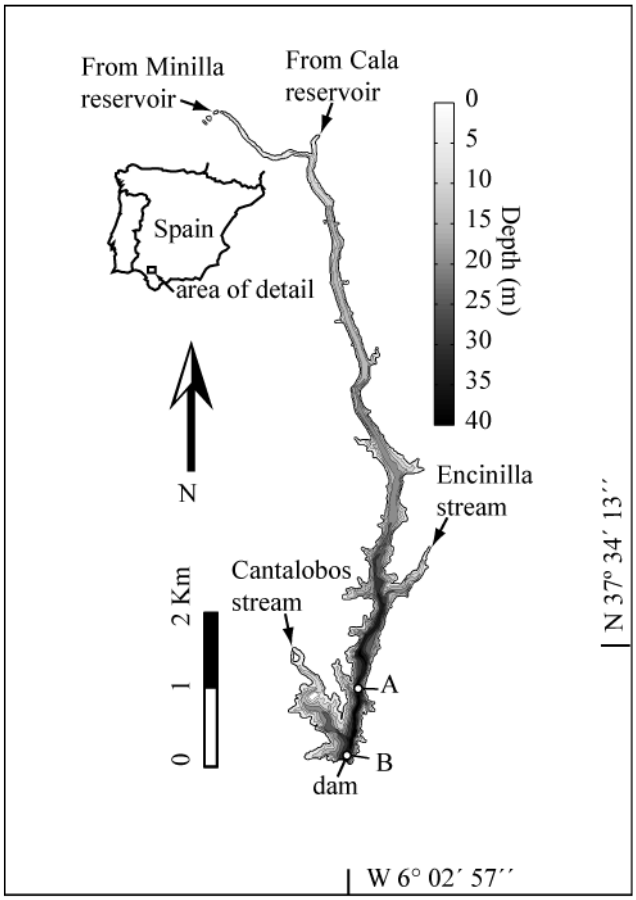

Figure 3. 1. El Gergal Reservoir bathymetry and main inflows. Location of the meteorological station (A) and sampling/data-recording point (B) is also indicated.

FIGURE 3.2

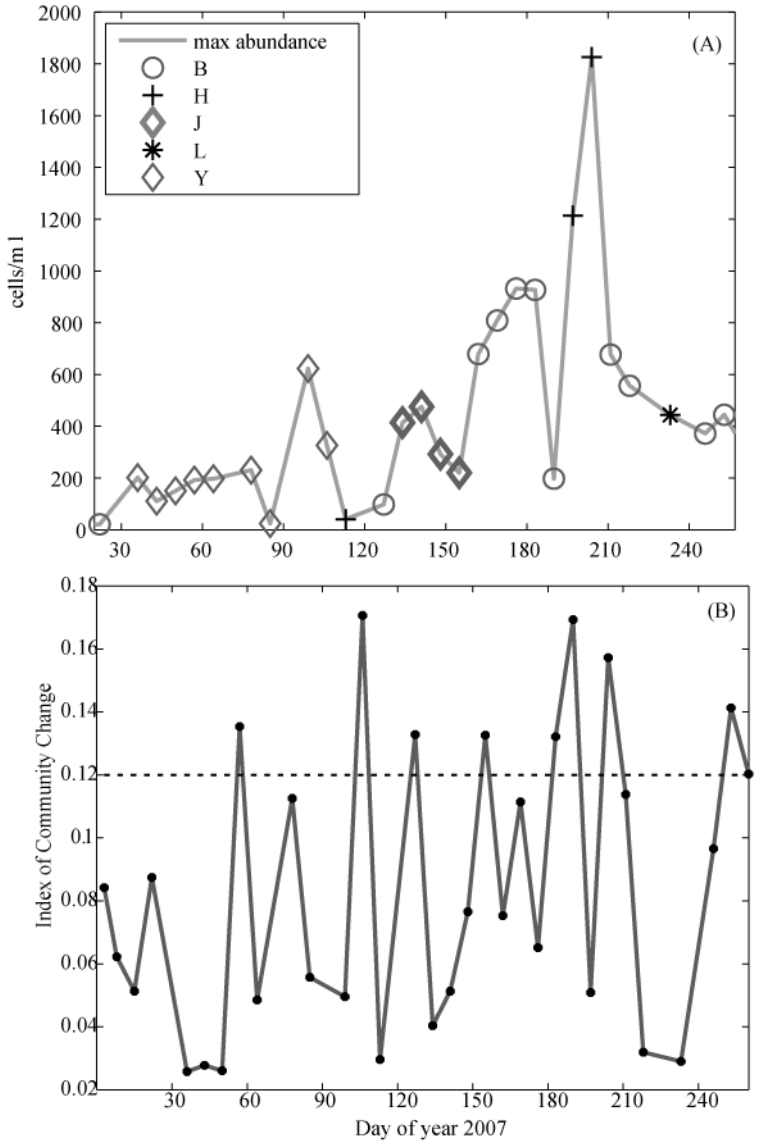

Figure 3. 2. (A): Time trace of total phytoplankton abundance. The most abundant Reynolds' groups associated to the different sampling occasions are identified by a symbol. Reynolds' groups B, H, J, L, Y were identified, dominated by Diatoms, Cyanobacteria, Chlorophytes, Dinoflagellates and Cryptophytes respectively. (B): Index of Community Change variation during year 2007. Dashed line show the arbitrary threshold value 0.12.

FIGURE 3.3

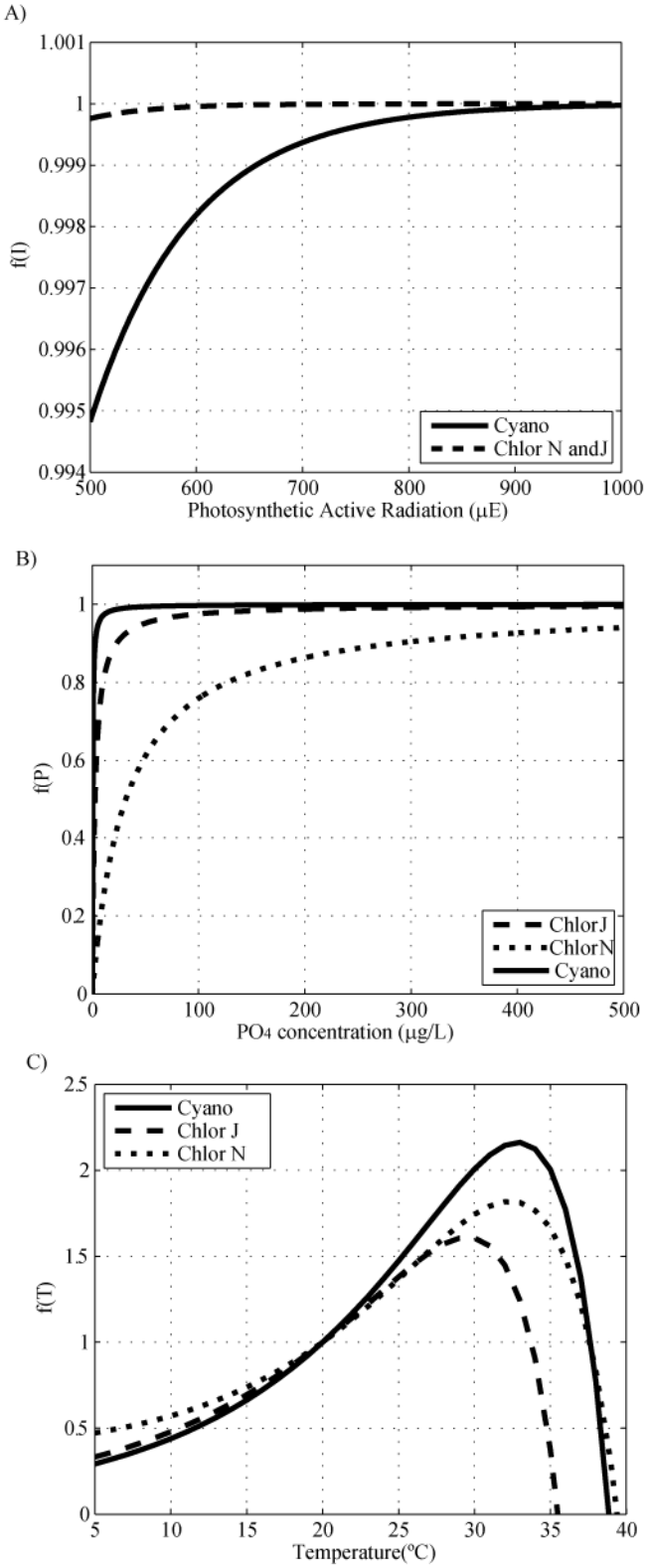

Figure 3. 3. Representation of phytoplankton specific limitation function for growth: light (A), phosphorus (B) and temperature function (C). Each function was represented for Cyanobacteria (Cyano), Chlorophytes group J (ChlorJ) and Chlorophytes group N (ChlorN).

FIGURE 3.4

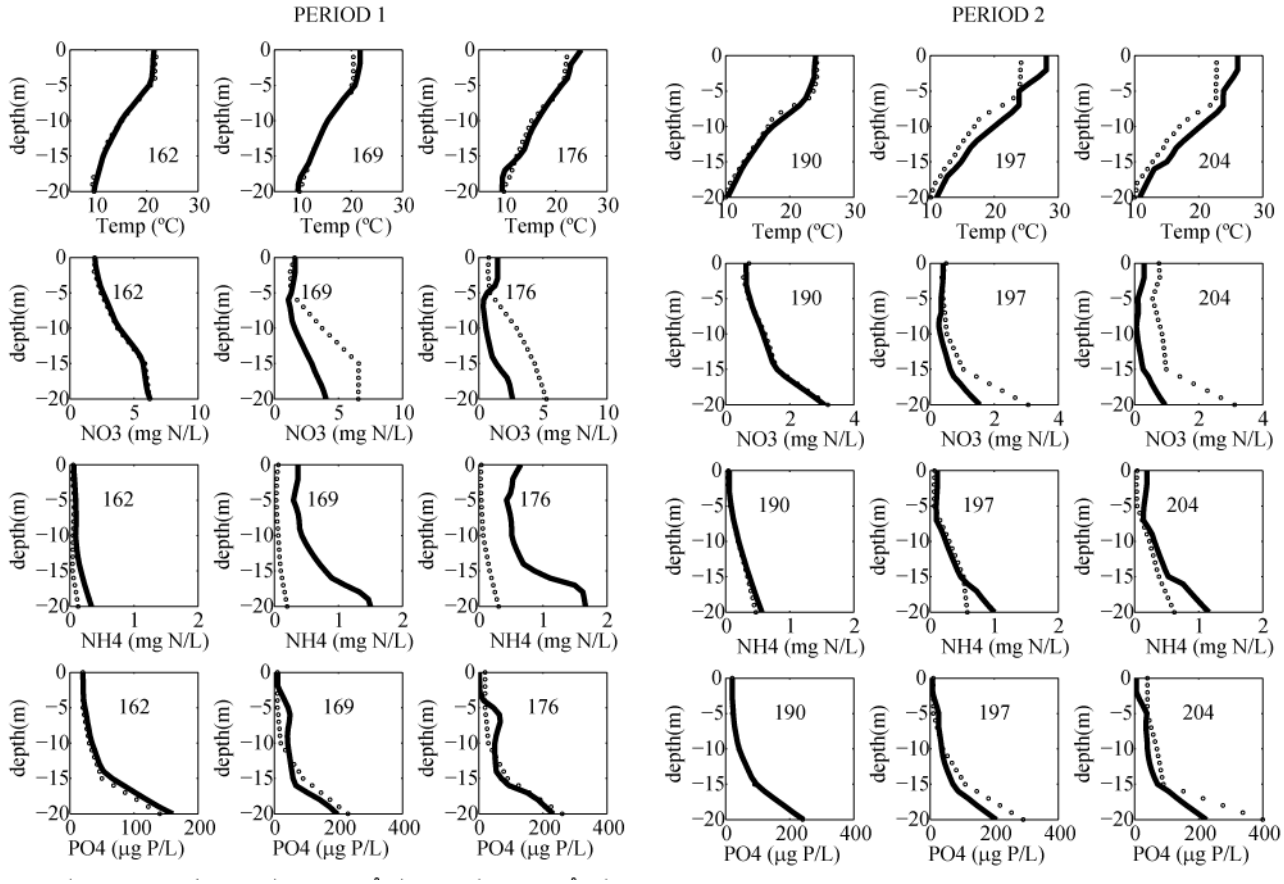

Figure 3. 4. Simulated water temperature and nutrients profiles (solid black lines) against observations (black dotted lines). The number inside subplots indicates the day of year of the first and the second period of simulation.

FIGURE 3.5

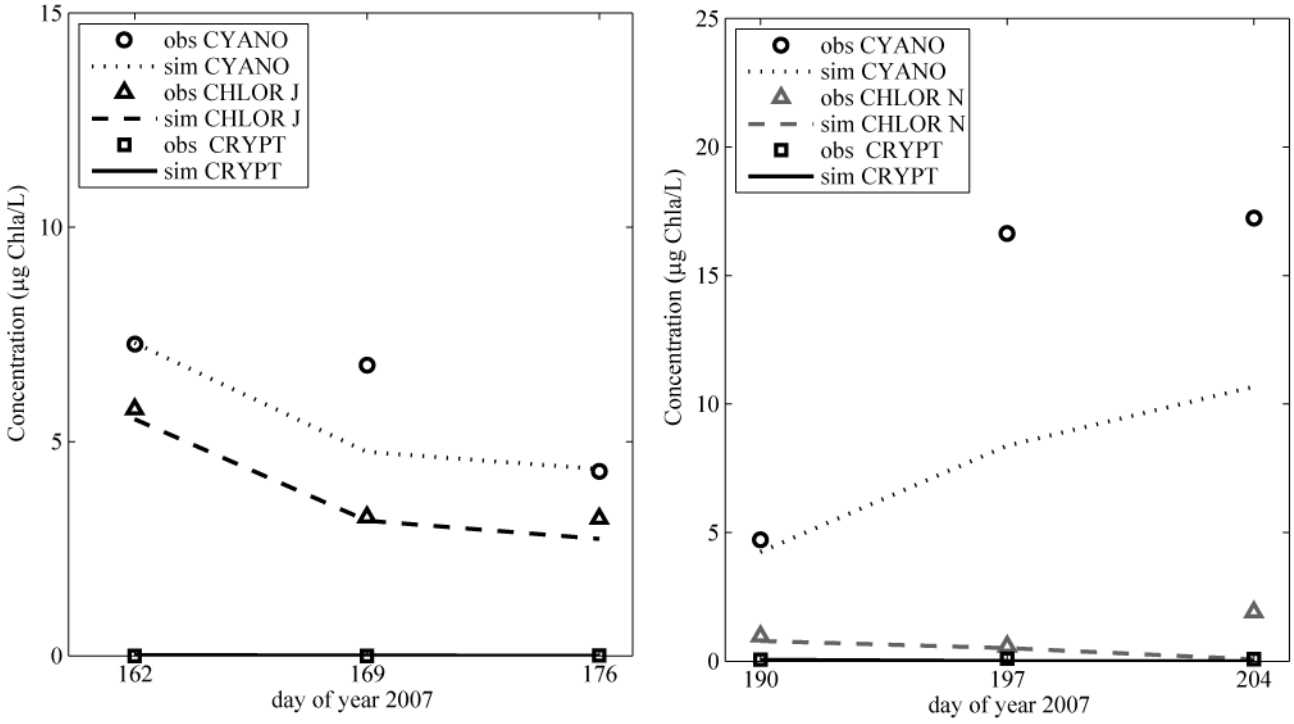

Figure 3. 5. Phytoplankton concentration simulated (sim) and observed (obs) during the first and second period of simulation. Different groups were differentiated: Cyanobacteria (CYANO), Chlorophytes Reynolds group J (CHLOR J), Cryptophytes (CRYPT), Chlorophytes Reynolds group N (CHLOR N). Concentrations are averaged over volume in the first 20m of the water column.

FIGURE 3.6

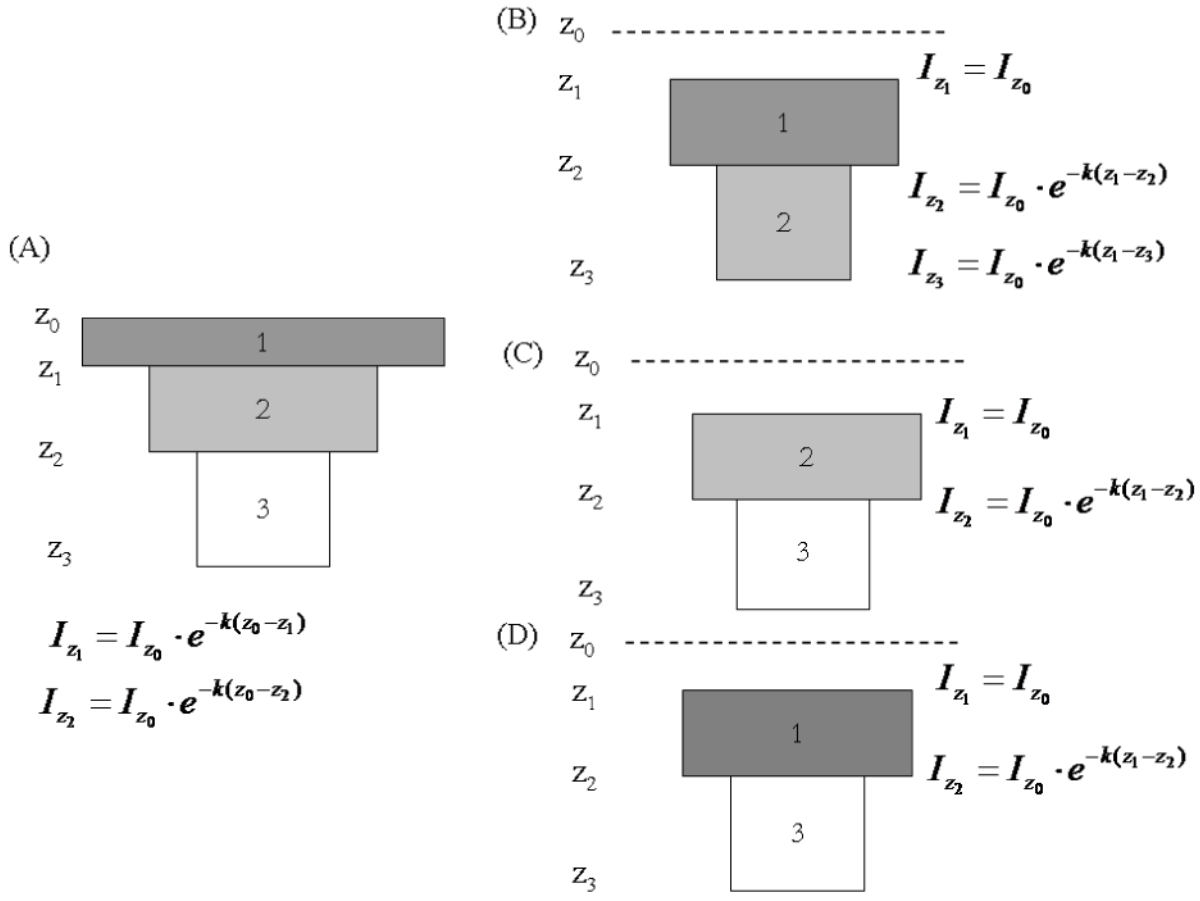

Figure 3. 6. Conceptual model representation: (A) initial conditions, (B) bottom extraction, (C) surface extraction, (D) intermediate extraction. Light dependence with water column depth is stated.

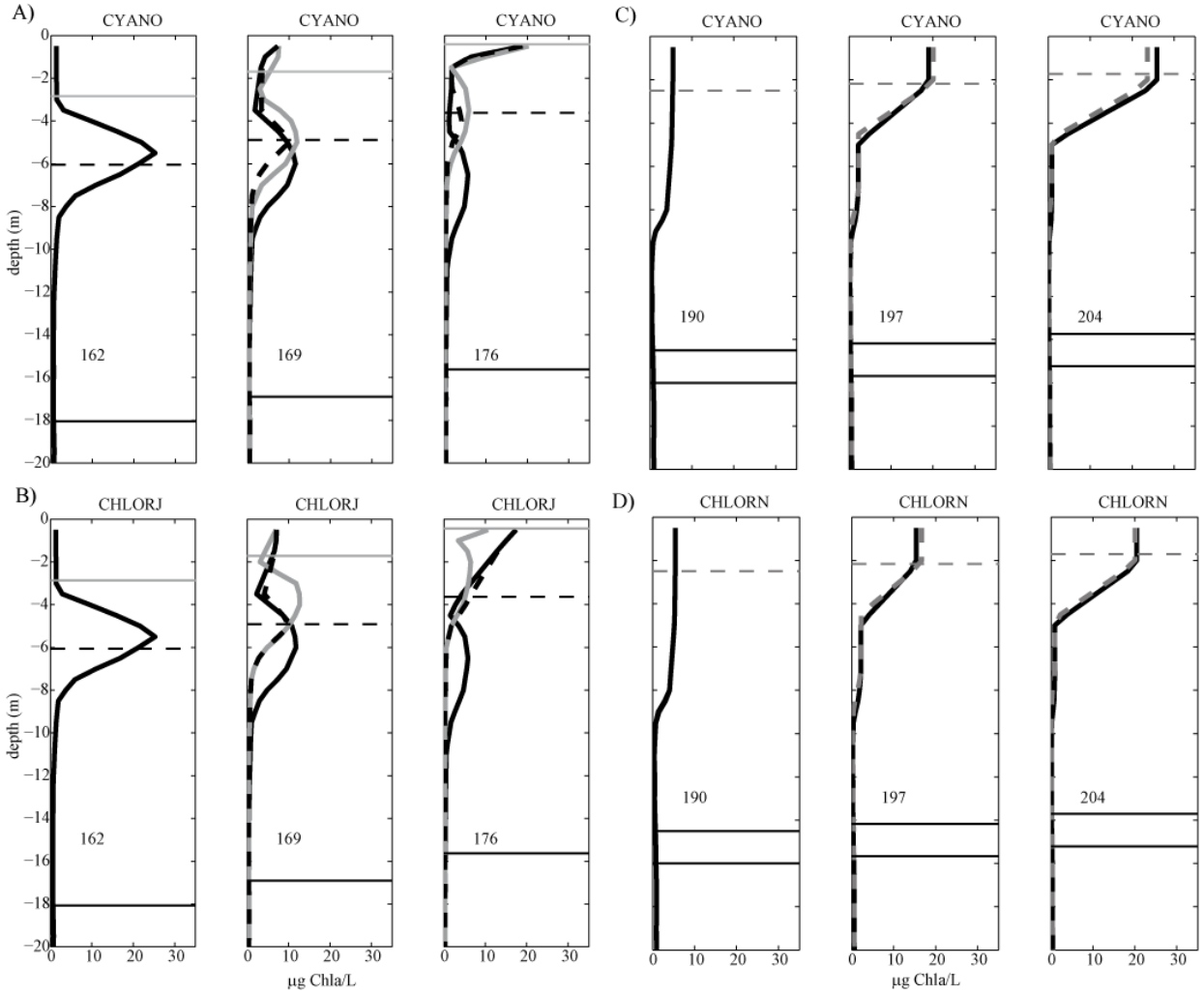

FIGURE 3.7

Figure 3. 7. Synthetic experiments results for P1, Cyanobacteria (A) and Chlorophytes J (B) and P2 Cyanobacteria (C) and Chlorophytes N (D). Algal concentration profiles correspond to extraction at different levels: black line corresponds to low and bottom extraction (same results); gray line corresponds to surface extraction in P1; discontinued black line corresponds to intermediate extraction in P1; discontinued grey line correspond to surface extraction in P2.

FIGURE 3.8

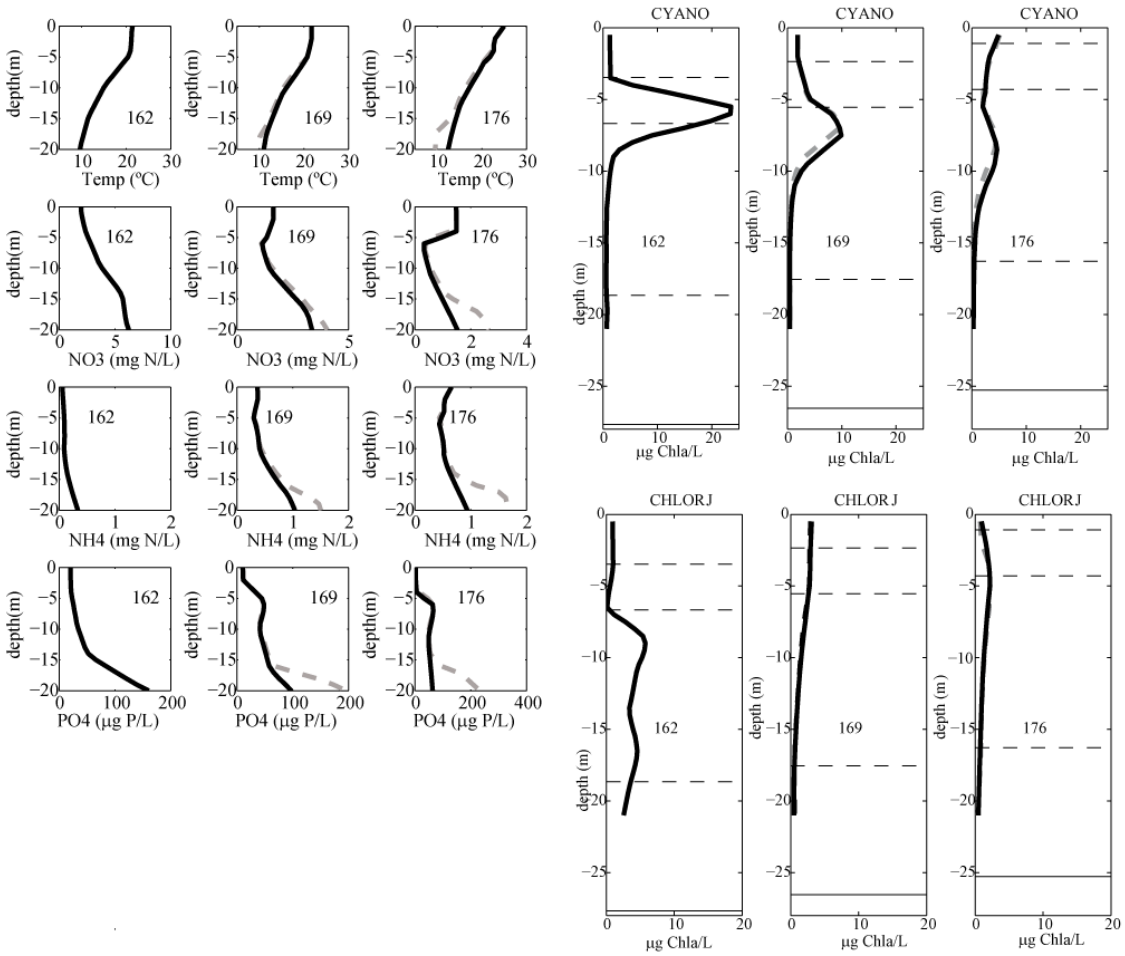

Figure 3. 8. Left: Physical and chemical reference profiles (discontinued grey lines) against simulated profiles (solid black lines) during period 1 and scenario 1 (P1S1). Right: Reference phytoplankton concentration profiles (discontinued gray lines) against simulated profiles (solid black lines) during P1S1. Outflow levels before (discontinued gray line) and after (solid black line) the scenario are showed.

FIGURE 3.9

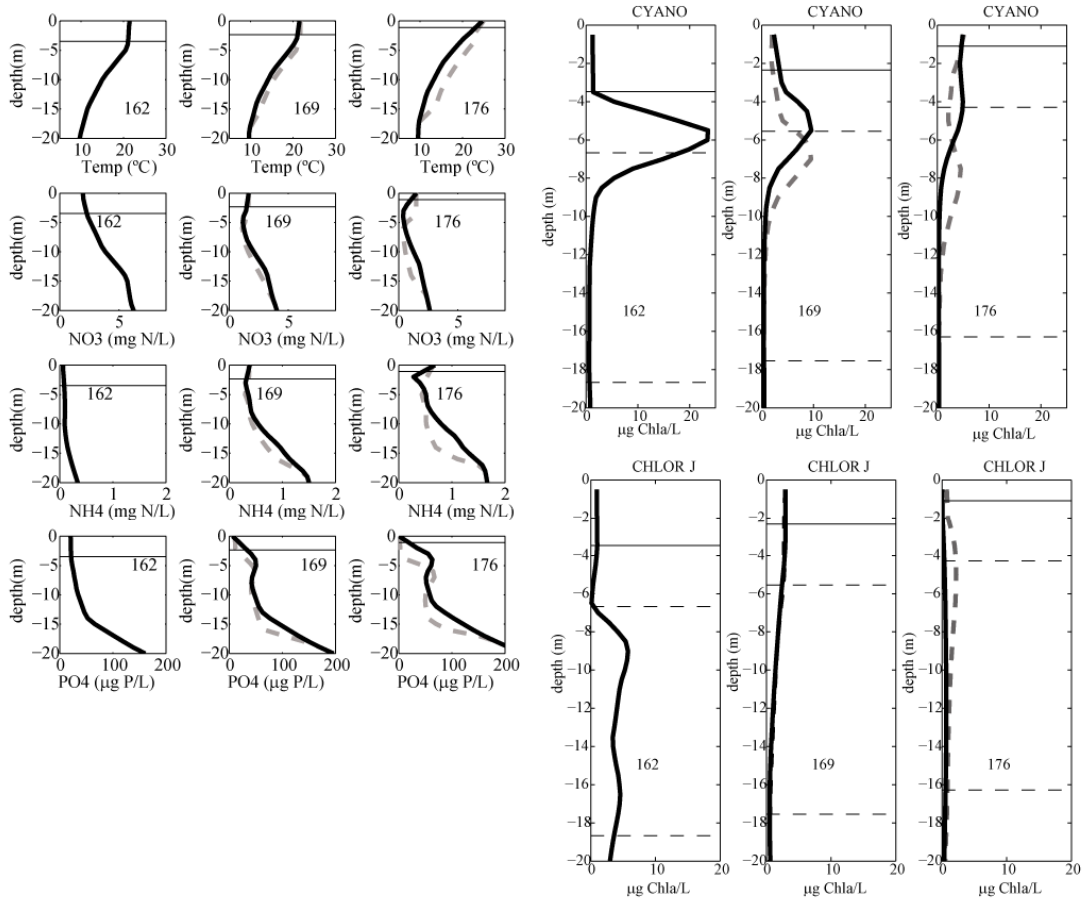

Figure 3. 9. Left: Physical and chemical reference profiles (discontinued grey lines) against simulated profiles (solid black line) during period 1 and scenario 2 (P1S2). Right: Reference phytoplankton concentration profiles (discontinued gray lines) against simulated profiles (solid black lines) during P1S2. Outflow levels before (discontinued gray line) and after (solid black line) the scenario are showed.

FIGURE 3.10

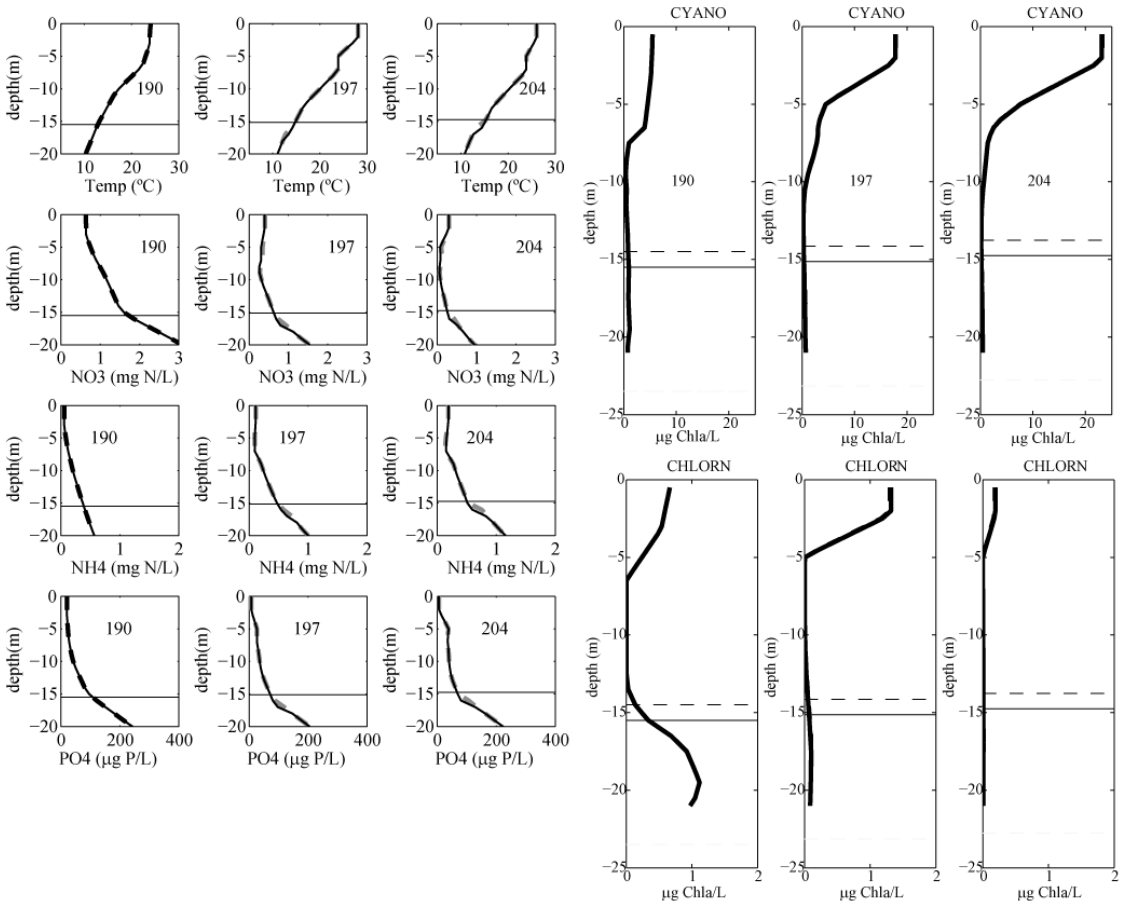

Figure 3. 10. Left: Physical and chemical reference profiles (discontinued grey lines) against simulated profiles (solid black lines) during period 2 scenario 1 (P2S1). Right: Reference phytoplankton concentration profiles were the same as simulated profiles (solid black lines) during P2S1. Outflow levels before (discontinued gray line) and after (solid black line) the scenario are showed.

FIGURE 3.11

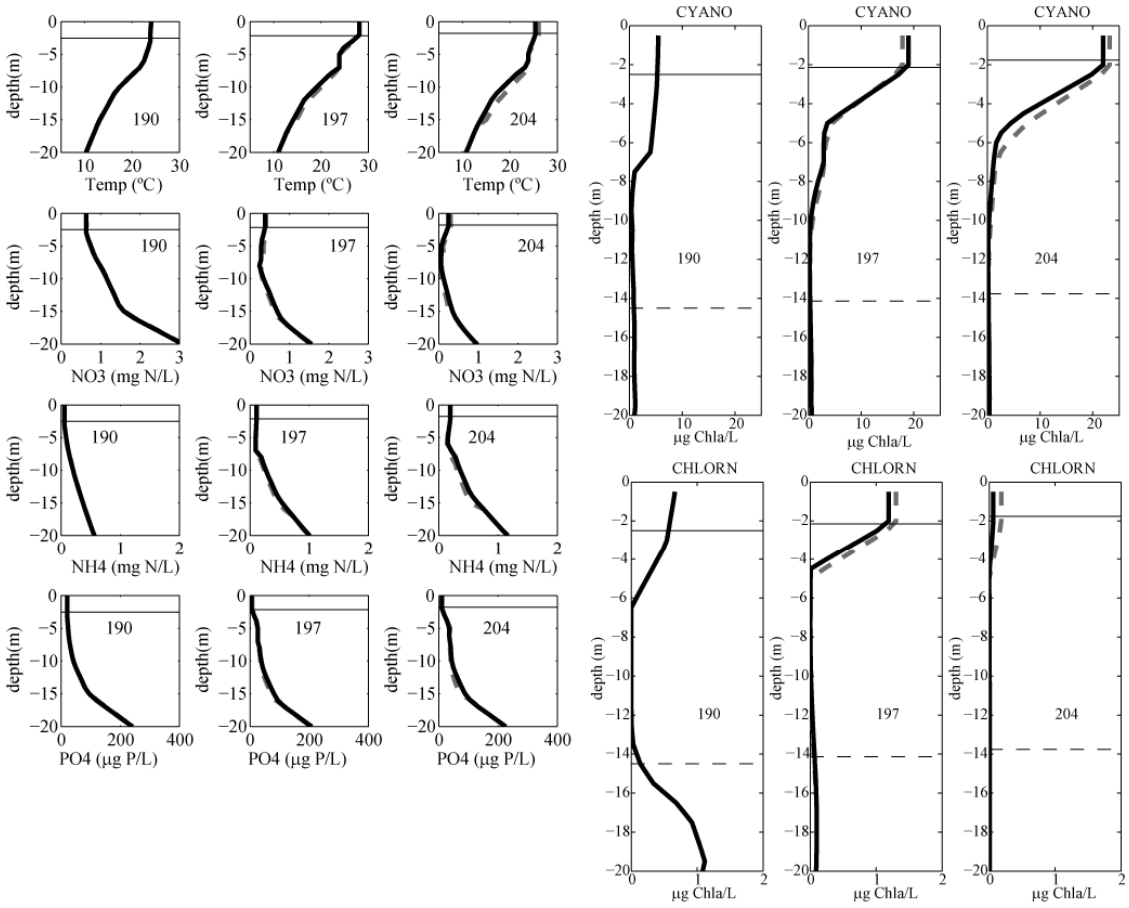

Figure 3. 11. Left: Physical and chemical reference profiles (discontinued grey lines) against simulated profiles (solid black lines) during period 2 scenario 2 (P2S2). Right: Reference phytoplankton concentration profiles (discontinued gray lines) against simulated profiles (solid black lines) during P2S2. Outflow levels before (discontinued gray line) and after (solid black line) the scenario are showed.

FIGURE 3.12

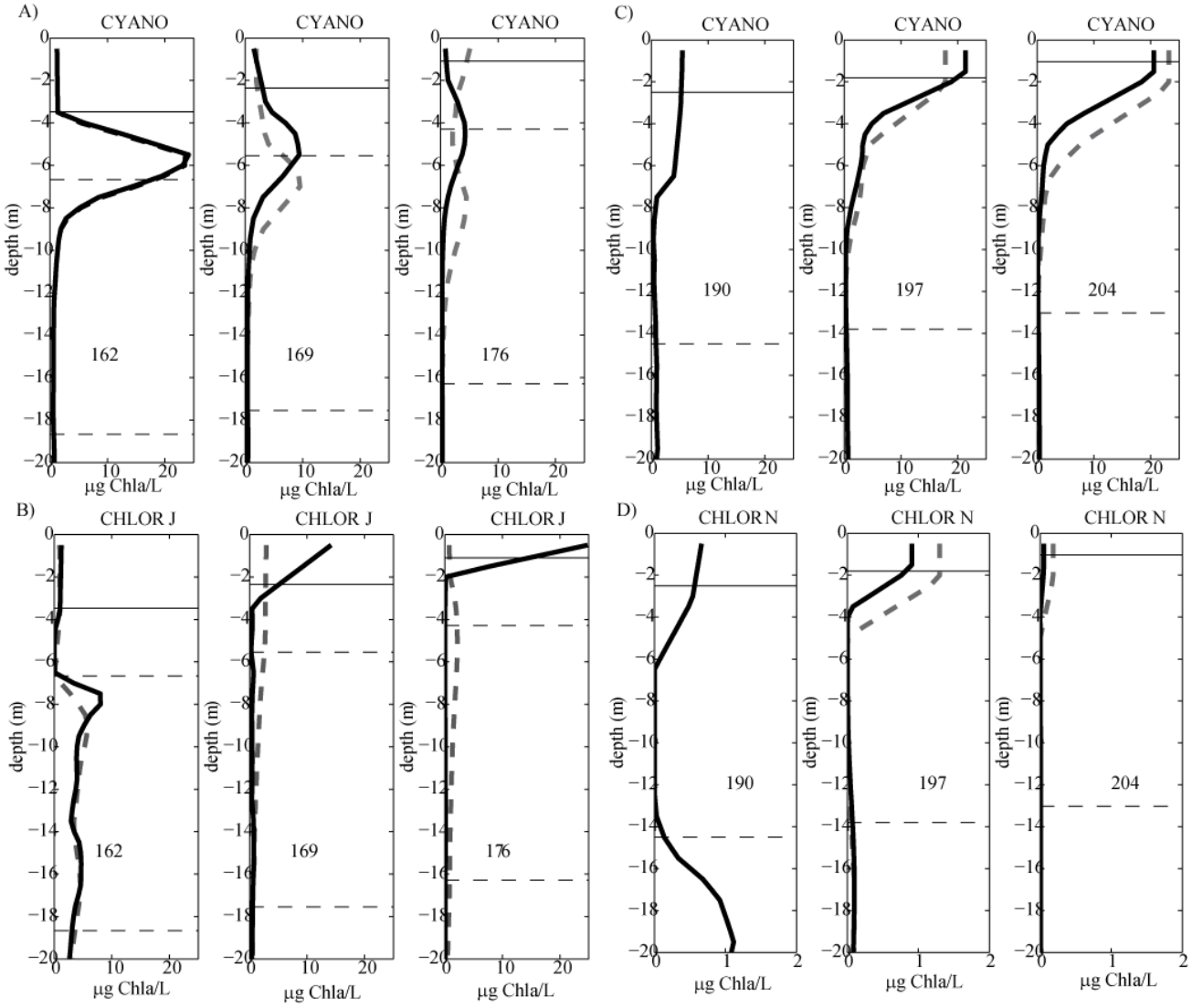

Figure 3. 12. Reference phytoplankton concentration profiles (discontinued gray lines) against simulated profiles (solid black lines) during P1S2 (A and B), simulating Chlorophytes J with settling velocity equal to zero and during P2S2 (C and D) increasing outflow rate. Outflow levels before (gray line) and after (black line) the scenario are showed.

Conclusiones Generales

[1] El mayor problema encontrado por los investigadores que trabajan con modelos de sucesión consiste en (1) cómo establecer el nivel de detalle utilizado en la descripción de las características biológicas del modelo (compartimentación biológica), y (2) cómo determinar y evaluar la biomasa de cada grupo de fitoplancton por separado. La compartimentación biológica de un modelo de sucesión debería estar reducida al mínimo para limitar su complejidad, a condición de que los grupos principales de fitoplancton y sus relaciones con el ambiente físico-químico estén adecuadamente representados. La determinación de biomasa para cada grupo de la comunidad se evalúa en términos de concentración de clorofila-a, concentración de carbono, peso seco y biovolúmenes. Todos ellos son un análogo de la biomasa y no la miden explícitamente. La concentración de clorofila-a es la variable mas usada para determinar la biomasa, aunque obtener observaciones de concentración de clorofila-a por grupo no es fácil. La determinación de biomasa para grupos separados debería basarse en el conteo de células de fitoplancton pertenecientes a cada grupo y en la conversión del número de células a biomasa. Los factores de conversión, que expresan biomasa por célula, deberían ser obtenidos mediante observaciones específicas en el lugar de estudio.

[2] Se han propuesto y aplicado muchos enfoques para simular la sucesión del fitoplancton en lagos y embalses. Los modelos mecanicistas son preferidos debido a su habilidad para representar de forma explícita los procesos de interacció entre los diferentes componentes de un ecosistema acuático. Esta habilidad determina que sean un instrumento útil para la investigación y para la toma de decisiones en la gestión de lagos y embalses. Sin embargo, comparar el rendimiento de los diferentes modelos mecanicistas propuestos es extremadamente difícil utilizando exclusivamente la información contenida en la literatura debido a que: (1) la longitud del intervalo de simulación, (2) la calidad de los datos observados para establecer el rendimiento de un modelo y (3) el tipo de cuantificación del error (grafico vs. matemático, o si se compara la biomasa total de la comunidad o de los grupos de fitoplancton por separado) varían considerablemente entre aplicaciones. Es necesario un ejercicio adecuado de comparación entre modelos para definir un modelo de sucesión que incorpore los aspectos más interesantes de los modelos actuales. Para facilitar esta comparación se sugiere: (a) la aplicación de todos los modelos a un grupo de localidades comunes; (b) utilizar una base de datos común adquirida con la misma resolución temporal y durante un periodo de tiempo suficientemente largo; y (c) utilizar una base de datos completa en la cual la biomasa de diferentes grupos de fitoplancton haya sido calculada y expresada en diferentes unidades. Este tipo de comparación entre modelos no se ha realizado todavía en la literatura.

[3] Debido a su extraordinaria complejidad, asociada a la no-linealidad de las relaciones consideradas y al elevado número de parámetros empleados, los modelos mecanicistas de sucesión existentes son difíciles de implementar y están todavía lejos de poder predecir con exactitud el comportamiento de grupos específicos de fitoplancton. Los errores en la predicción, comparando la evolución de la biomasa observada y simulada de grupos de fitoplancton, llegan al 50% en magnitud y a un mes de intervalo entre máximos de biomasa simulados y observados. Si funcionaran correctamente, estos modelos serian extremadamente útiles como instrumento de investigación y para la gestión de la calidad del agua. Se han sugerido algunas propuestas para facilitar la

aplicabilidad de estos modelos, entre las cuales: (a) le evaluación de la complejidad de un modelo para describir correctamente los procesos dinámicos de un ecosistema; (b) el desarrollo de nuevas estrategias de medición de biomasa o de metodologías para valorar la biomasa por grupo; (c) la aplicación de modelos con los mismos parámetros en diferentes sistemas mediante técnicas de calibración automáticos eficientes; (d) la investigación de la fisiología del fitoplancton para determinar coeficientes que expliquen la elevada variabilidad en los valores de los parámetros; y (e) la integración entre el desarrollo del modelo y el diseño de adquisición de datos experimentales en el campo. Frecuentemente, se han observado errores más elevados para modelos con un número de parámetros elevados. Por lo tanto, al decidir el número de grupos de un modelo de sucesión se debería preferir la opción más simple, a condición de que la complejidad del ecosistema estudiado sea adecuadamente representada.

[4] Se ha propuesto un algoritmo automático de optimización global, aplicado de forma secuencial, para la calibración de un modelo unidimensional, mecanicista, ecológico y acoplado para el embalse de El Gergal. Primero se ha realizado un análisis de sensibilidad para identificar los parámetros a incluir en el proceso de calibración. En segundo lugar, se ha aplicado el algoritmo de optimización global para calibrar el modelo para cada grupo de fitoplancton de forma secuencial. Finalmente, se han simulado todos los grupos funcionales utilizando los valores de los parámetros obtenidos en las calibraciones grupo a grupo. El modelo calibrado fue capaz de predecir los aspectos relevantes de la sucesión, como los periodos de máxima concentración y la secuencia en la que los diferentes grupos aparecen como dominantes en la comunidad fitoplanctónica. Los errores encontrados fueron de un orden de magnitud parecido a otros obtenidos mediante otros modelos de sucesión.

[5] Cuantos más grupos de fitoplancton se incluyen en el modelo, más aumenta la diferencia entre el modelo calibrado y las observaciones, lo que sugiere que existen fuertes interacciones no lineales entre los sub-modelos que describen cada grupo, e indica que el nivel de compartimentación funcional en el modelo único debería ser mínimo. El éxito del proceso de calibración depende de forma crítica en la coherencia entre la estructura funcional de la comunidad y la descripción utilizada en el modelo (obtenida mediante observaciones). Cada grupo incluido en el modelo presenta una respuesta específica a las condiciones ambientales. A su vez, las observaciones deberían diferenciar entre grupos con distintas necesidades ambientales.

[6] Las simulaciones realizadas mediante el modelo calibrado de El Gergal sugieren que la composición de la comunidad fitoplanctónica puede ser modificada considerablemente a corto plazo por cambios en las salidas de agua. Los mecanismos por los cuales las salidas de agua afectan a la comunidad de fitoplancton son múltiples. Uno es puramente físico, y consiste en la remoción selectiva de las especies que se desarrollan al mismo nivel o cerca de la extracción. Las salidas de agua pueden también inducir cambios en las condiciones ambientales experimentadas por las algas y pueden promover el desarrollo de algunos grupos de fitoplancton en vez de otros, dependiendo de su respuesta específica a luz, disponibilidad de nutrientes y temperatura. La magnitud del cambio en las condiciones ambientales experimentada por las células del plancton y generadas por las salidas de agua depende de la tasa de extracción de agua y de la batimetría del embalse.

[7] Se observan cambios en las poblaciones fitoplantónicas cuando se modifica la salida de agua de tal forma que se varía la situación relativa de la salida respecto a la

profundidad donde se sitúan las algas. No se observan cambios cuando las extracciones se desplazan desde una zona más profunda de la que ocupa el fitoplancton, hacia niveles aún más profundos.

[8] Las especies que son tolerantes a poca disponibilidad de nutrientes, sensibles a limitación de luz y que tienen baja velocidad de sedimentación (Cianobacterias, grupo H), están favorecidas por la extracción superficial porque su posición se traslada hacia la superficie. Las especies que son tolerantes a baja luminosidad y que tienen baja velocidad de sedimentación (algunos grupos de Clorófitas) están favorecidas por salidas de agua profundas, porque su posición se traslada hacia el fondo. Para especies con alta velocidad de sedimentación el movimiento hacia las capas no iluminadas ocurre más rápidamente que en el caso anterior, evitando el crecimiento. El cambio de nivel de extracción desde la zona profunda hacia el fondo del embalse no afecta al desarrollo de las algas en superficie, y el grupo de fitoplancton dominante en este caso depende de las condiciones ambientales en el momento de la extracción, y no de los efectos derivados por el cambio de nivel de salida del agua.

General Conclusions

[1] The major problem faced by modelers working with succession models consists of (1) how to establish the level of detail used in the description of the biological features of the model (biological segmentation), and (2) how to assess and evaluate the biomass of each phytoplankton group separately. The biological segmentation of a succession model should be reduced to a minimum to limit its complexity, as long as the main phytoplankton groups of the ecosystem studied and their relationships with the physical-chemical environment are adequately represented. Biomass assessment of any given group in the community is evaluated in terms of Chlorophyll-a concentration, carbon concentration, wet/dry weight, and bio-volumes, being all a king of analogue of the biomass and not measuring it explicitly. Chlorophyll-a concentration is the most frequent variable used to assess biomass even if gathering observations of Chlorophyll-a concentration on a per group basis is not straightforward. Biomass assessment of separate groups should be based on counting phytoplankton cells pertaining to each group and later converting the number of cells to biomass. Conversion factors, expressing the biomass per cell, should be obtained from site-specific observations.

[2] Many approaches have been proposed and applied to simulate phytoplankton succession in lakes and reservoirs. Mechanistic models are preferred due to their ability to represent explicitly the processes by which the different components of an aquatic ecosystem interact, which makes them a very useful tool both for research and management purposes. Comparing the performances of the many mechanistic models proposed, though, is extremely difficult if one uses only literature sources and results, due to the fact that (1) the length of time simulated, (2) the quality of the observational data set used to assess the model performance, and (3) the approaches used to quantify the model error (graphical vs. mathematical, or whether the total biomass of the community or the biomass expressed on a group basis are compared) varies considerably among model applications. Adequate inter-comparison exercises, though, are needed in order to define a successful strategy to model succession that brings together the best aspects of existing modeling approaches. To facilitate these inter-comparison exercises it is suggested: (a) to apply all models to a common set of sites, (b) to use a common data set collected with the same temporal and group resolution during a sufficiently long period of time; and (c) to use a complete data set in which the biomass of different genera and groups has been discriminated and expressed in different units. This type of inter-comparison exercises has not been done, yet, in the literature.

[3] Due to its extraordinary complexity, associated to the non-linearity of the relationships that are accounted for and the large number of parameters used, existing mechanistic succession models are difficult to use, and still far from being able to predict accurately the behavior of separate specific phytoplankton groups. Errors in model predictions are of up to 50% in magnitude and one month in timing, when comparing observed and simulated phytoplankton biomass of separate groups. If they worked properly, these models can be extremely useful as a research tool and also for water quality management. Several tasks are suggested that should be followed to increase the applicability of these modes, which include: (a) the evaluation of the model complexity required to correctly describe the dynamic processes of an ecosystem; (b)

the development of new strategies of biomass measurements or assessment methodologies on a per-group basis; (c) the applicability of model parameters at different sites, through elaboration of rapid and efficient automated calibration methods; (d) the increase of physiological research to ascertain parameter coefficients explaining the large variation in reported parameter values; and (e) the integration between model development and field sampling design. Frequently, larger errors have been reported for models with a larger number of phytoplankton groups, so, in deciding the level of group detail of a succession model, the simplest possible option should be preferred, as long as the complexity of the ecosystem studied is adequately represented.

[4] A global, hybrid and automated optimization algorithm, applied in a sequential manner, is proposed for the calibration of a one-dimensional, process-based (or mechanistic) and coupled physical-ecological model for El Gergal Reservoir. First, we performed a sensitivity analysis to identify the parameters to include in the calibration process, and then applied a global optimization algorithm to fit the model for each algal group one by one in a sequential fashion. Finally we simulated all the functional groups adopting parameter values established during the group-by-group calibrations. The calibrated model was capable to predict relevant aspects of the succession, such as the timing of the peaks, and the sequence in which the different groups appear as dominant in the phytoplankton community. The errors encountered were similar to those reported in other succession modeling exercises.

[5] The larger the number of groups included in the model, the larger were the differences between the calibrated model and observations, which suggests that exist strong and non-linear interactions among group sub-models and that the level of functional segmentation in the model should be minimized. The success of the calibration process critically depends on the consistency between the functional structure of the community, and the description made in the model and achieved through observations of that structure. Each group included in the model should represent a specific response to environmental conditions. The observations should also discriminate between groups with different environmental requirements.

[6] Simulations conducted with the calibrated model of El Gergal suggest that the composition of the phytoplankton community can be significantly modified on the short-term by withdrawals operations. The mechanisms by which withdrawals affect the phytoplankton community are multiple. One of them is purely physical and consists of the selective removal of all the species developing at or near withdrawal level. Water withdrawals can also induce changes in the environmental conditions experienced by algae, and may promote the development of certain phytoplankton groups in detriment of others, according to their specific responses to light, nutrients and temperature. The magnitude of the changes in environmental conditions experienced by phytoplankton cells and induced by withdrawal depends on the outflow rates and on the reservoir bathymetry.

[7] Changes in the size of the population of phytoplankton groups are observed when shifting withdrawal above, below or directly from layers containing algae. They were not observed when intake levels were shifted from below the layers hosting the phytoplankton community to lower levels.

[8] Species that are tolerant to nutrient depletion, sensitive to light limitation and low settling velocities (e.g. Cyanobacteria Reynolds group H), are favored by surface withdrawals because their position is shifted toward the surface. Species that are tolerant to low light conditions and have low settling velocities (e.g. Chlorophytes) are favored when extracting from deep withdrawals because they can develop even if their position is shifted towards the bottom. For species with high settling velocities the shift towards not illuminated layer would occur more rapidly than the previous case, preventing growth. A withdrawal change from deep to bottom layers do not affect the algal development at surface and the dominant phytoplankton group depends on the environmental conditions at time of extraction, rather than on the effect of the withdrawal change.